

Diffusive behavior of conserved quantities in systems with thermal and mechanical boundary forcing: hydrodynamic limits and non-equilibrium stationary states.

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Coupled transport of conserved quantities

In many systems energy is not the only *macroscopic* conserved quantity and the interplay between extra conserved quantities and energy has a deep impact on the thermal properties of the system, in particular when all these conserved quantities evolve in the macroscopic diffusive scale.

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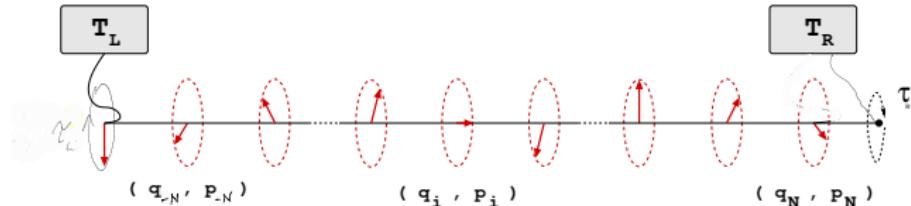
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Examples

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- **Non stationary behaviour:**
- **Stationary non-equilibrium states:** induced by boundary forces and thermostats. Interesting phenomena: *uphill diffusion, non monotonous temperature profiles, negative linear response.*

Rotors Chain



$$r_i = q_i - q_{i-1} \in \mathbb{S}^1, \quad U(r) = 1 - \cos(2\pi r), \quad \mathcal{H} = \sum_{i=-N+1}^N \left(\frac{p_i^2}{2} + U(r_i) \right) + \frac{p_{-N}^2}{2} = \sum_{i=-N}^N e_i$$

$$dr_i = (p_i - p_{i-1}) dt, \quad i = -N+1, \dots, N$$

$$dp_i = (U'(r_{i+1}) - U'(r_i)) dt \quad i = -N, \dots, N-1$$

$$dp_{-N} = (\tau_L + U'(r_{-N})) dt - \gamma p_{-N} dt + \sqrt{2\gamma T_L} dw_L(t)$$

$$dp_N = (\tau_R - U'(r_N)) dt - \gamma p_N dt + \sqrt{2\gamma T_R} dw_R(t)$$

Conserved quantities, currents, equilibrium states

Two conserved quantities

$$p_i, \quad e_i = \left(\frac{p_i^2}{2} + U(r_i) \right),$$

microscopic currents

$$\dot{p}_i = j_{i-1}^p - j_i^p, \quad j_i^p = -U'(r_i), \quad j_N^p = -\tau_R + \gamma p_N - \sqrt{2\gamma T_R} \dot{w}_R, \quad j_{-N-1}^p = \tau_L + \dots$$

$$\dot{e}_i = j_{i-1}^e - j_i^e, \quad j_i^e = -p_i U'(r_{i+1}), \quad j_N^e = \gamma(p_N^2 - T_R) - \sqrt{2\gamma T_R} p_N \dot{w}_R, \quad j_{-N-1}^e = \dots$$

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Equilibrium distribution for $T_R = T_L = T = \beta^{-1}$ and $\tau_R = \tau_L = \gamma \bar{p}$

$$d\mu_{\beta, \bar{p}} = \prod_{i=-N}^N \frac{e^{-\beta e_i + \beta \bar{p} p_i}}{Z_{\beta, \bar{p}}} \prod_{i=-N+1}^N dr_i \, dp_i \, dp_{-N}$$

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For $T_R \neq T_L$ or $\tau_R \neq \tau_L$, even the existence of the *non-equilibrium stationary state* is an open problem.

($N = 2, 3, 4$: Cuneo, Eckmann, Poquet).

Linear Response: Onsager Matrix (formal argument)

Start with small gradients in temperature and momentum:

$$\begin{aligned}\beta_i &= \frac{1}{2}(\tau_R^{-1} - \tau_L^{-1})\frac{i}{N} + \frac{1}{2}(\tau_R^{-1} + \tau_L^{-1}) \\ \beta_i \bar{p}_i &= \frac{1}{2\gamma}(\tau_R^{-1}\tau_R - \tau_L^{-1}\tau_L)\frac{i}{N} + \frac{1}{2\gamma}(\tau_R^{-1}\tau_R + \tau_L^{-1}\tau_L) \\ \delta(\beta) &= \frac{1}{2}(\tau_R^{-1} - \tau_L^{-1}), \quad \delta(\beta \bar{p}) = \frac{1}{2\gamma}(\tau_R^{-1}\tau_R - \tau_L^{-1}\tau_L),\end{aligned}$$

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$$\begin{aligned}N\langle j_{0,1}^p(t) \rangle_{\tilde{\nu}_N} &= K_N^{p,p}(t)\delta(\beta \bar{p}) + K_N^{p,e}(t)\delta(\beta) + o(|\delta(\beta)|, |\delta(\beta \bar{p})|), \\ N\langle j_{0,1}^e(t) \rangle_{\tilde{\nu}_N} &= K_N^{e,p}(t)\delta(\beta \bar{p}) + K_N^{e,e}(t)\delta(\beta) + o(|\delta(\beta)|, |\delta(\beta \bar{p})|),\end{aligned}$$

Onsager Matrix and symmetries

$$\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} K_N^{a,b}(t) = K^{a,b}(\beta, \bar{p})$$

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Transport coefficients as function of $T = \beta^{-1}$

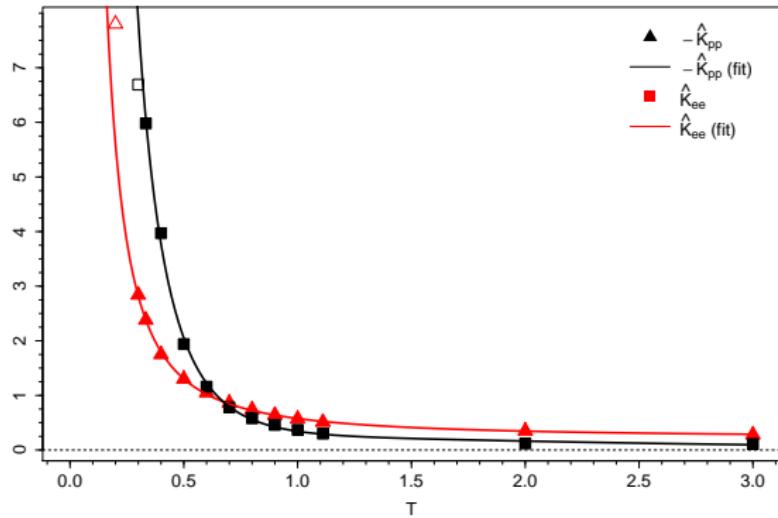


Figure: Onsager coefficients $-\hat{K}^{p,p}$ and $\hat{K}^{e,e}$ as functions of the temperature T .

Macroscopic conservation laws

$$\partial_t p(t, x) = -\partial_x J^p(t, x) \quad \partial_t e(t, x) = -\partial_x J^e(t, x)$$

$$J^p(t, x) = K^{p,p}(\beta, p) \partial_x (\beta(t, x) p(t, x)) + K^{p,e}(\beta, p) \partial_x \beta(t, x)$$

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In order to close the equations, use the thermodynamic relations:

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

$$T = \beta^{-1}, \quad u(T) = -\frac{d}{d\beta} \log \iint e^{-\beta[U(r) + p^2/2]} dr dp, \quad C_v(T) = u'(T),$$

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Momentum diffusivity and thermal conductivity

$$D^p(T) = -\frac{1}{T} K^{p,p}\left(\frac{1}{T}\right), \quad \kappa(T) = \frac{1}{T^2} K^{e,e}\left(\frac{1}{T}\right)$$

Non-stationary macroscopic evolution of $p - T$ profiles

After taking into account all these relation we obtain the closed equations:

$$\partial_t p = \partial_x [D^p(T) \partial_x p]$$

$$C_v(T) \partial_t T = \partial_x [\kappa(T) \partial_x T] + D^p(T) [\partial_x p]^2.$$

$$T(t, -1) = T_L, \quad T(t, 1) = T_R, \quad p(t, -1) = \tau_L/\gamma, \quad p(t, 1) = \tau_R/\gamma$$

Gradients of p rise the temperature locally. This is the transfer of *mechanical energy* into *thermal energy*.

Thermodynamic Entropy dissipation (non-stationary)

$$S(u) = \inf_{\beta} \left\{ \beta u + \log \iint e^{-\beta[U(r)+p^2/2]} dr dp \right\}, \quad S'(u) = \beta(u),$$

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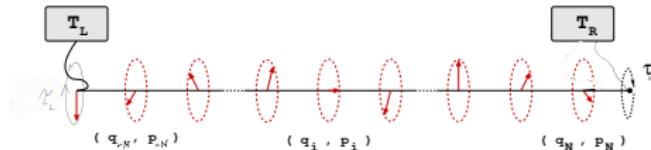
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$$\begin{aligned} \frac{d}{dt} \int_{-1}^1 S(u(t, x)) dx &= \int_{-1}^1 \left[\frac{D^p(T)}{T} (\partial_x p)^2 + \frac{\kappa(T)}{T^2} (\partial_x T)^2 \right] dx \\ &\quad + \frac{J^Q(t, 1)}{T_R} - \frac{J^Q(t, -1)}{T_L} \end{aligned}$$

$$J^Q(t, x) = \kappa(T(t, x)) \partial_x T(t, x) \quad \text{heat flux}$$

Rotors: Non-equilibrium Stationary State



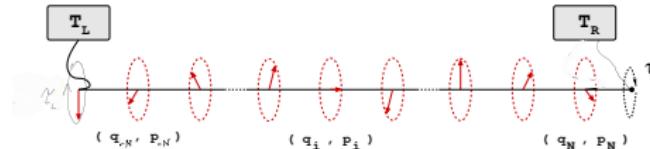
Currents of conserved quantities are constant in space, and we expect that:

$$\lim_{N \rightarrow \infty} N \langle j_{i,i+1}^a \rangle_{N,ss} = J^a(T_L, T_R, \tau_L, \tau_R), \quad a \in \{p, e\},$$

$$\lim_{N \rightarrow \infty} \langle p_{[Nx]} \rangle_{N,ss} = p_{ss}(x), \quad \lim_{N \rightarrow \infty} \langle e_{[Nx]} \rangle_{N,ss} = e_{ss}(x)$$

$$\lim_{N \rightarrow \infty} \langle p_{[Nx]}^2 \rangle_{N,ss} - \langle p_{[Nx]} \rangle_{N,ss}^2 = T_{ss}(x)$$

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$$-J^p = D^p[T_{ss}(x)] \partial_x p_{ss}(x)$$

$$-J^e = D^p[T_{ss}(x)] \partial_x \left(\frac{p_{ss}(x)^2}{2} \right) + \kappa[T_{ss}(x)] \partial_x T_{ss}(x)$$

$$T_{ss}(-1) = T_L, \quad T_{ss}(1) = T_R, \quad p_{ss}(-1) = \frac{\tau_R}{\gamma}, \quad p_{ss}(1) = \frac{\tau_R}{\gamma},$$

Rotors: stationary profiles

$$-J^P = D^P[T_{ss}] \partial_x p_{ss}$$

$$-J^e = D^P[T_{ss}] \partial_x \left(\frac{p_{ss}^2}{2} \right) + \kappa[T_{ss}] \partial_x T_{ss} = -J^M(x) - J^Q(x)$$

= **-mechanical energy current** – **thermal energy current**

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$$p_{ss}(x) J^P - J^e = \kappa[T_{ss}(x)] \partial_x T_{ss}(x) := -J^Q(x)$$

$$\underset{N \rightarrow \infty}{\sim} -N \left((p_{[Nx]} - p_{ss}(x)) U'(r_{[Nx]}) \right)_{N,ss}$$

the *heat current* $J^Q(x)$ is a linear function of $p_{ss}(x)$.

NESS: Entropy production

$$\sigma_N := (T_L^{-1} - T_R^{-1}) \langle j_i^e \rangle_{N,ss} - \gamma^{-1} (T_L^{-1} \tau_R - T_R^{-1} \tau_L) \langle j_i^p \rangle_{N,ss} > 0.$$

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NESS : uphill diffusion

it can happen that

$$\text{sign} J^e = \text{sign}(T_R - T_L)$$

This is a obvious phenomena, since

$$-J^e = D^P[T_{ss}] \partial_x \left(\frac{p_{ss}^2}{2} \right) + \kappa[T_{ss}] \partial_x T_{ss} = -J^M(x) - J^Q(x)$$

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But a bound follows from the positivity of the entropy production:

$$(T_L - T_R) J^e \geq -|T_L p_R - T_R p_L|$$

NESS: Stationary profiles

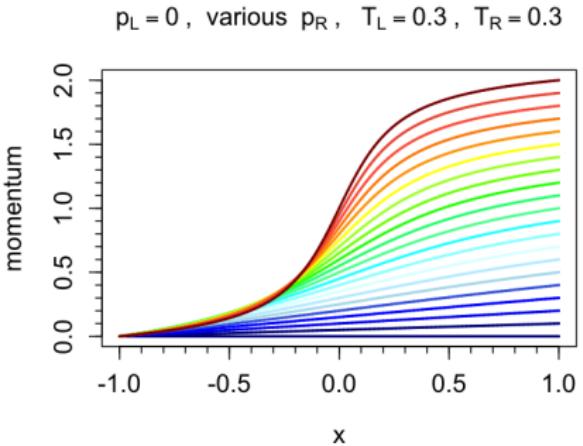
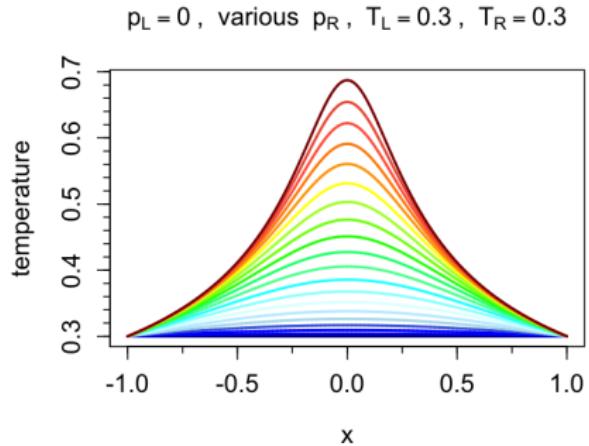


Figure: $T_L = T_R = 0.3$ (no thermal forcing), $p_L = 0$ and values of p_R varying from 0 to 2

NESS: Stationary profiles

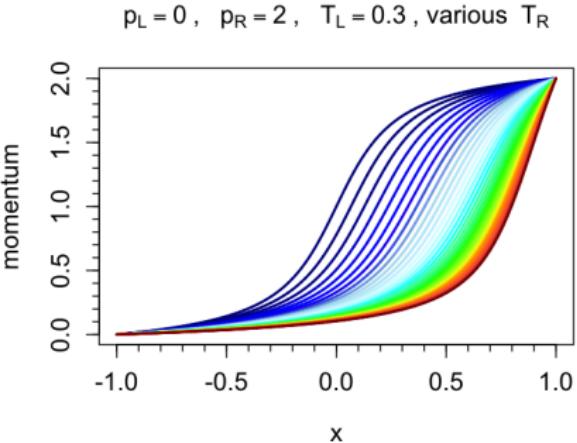
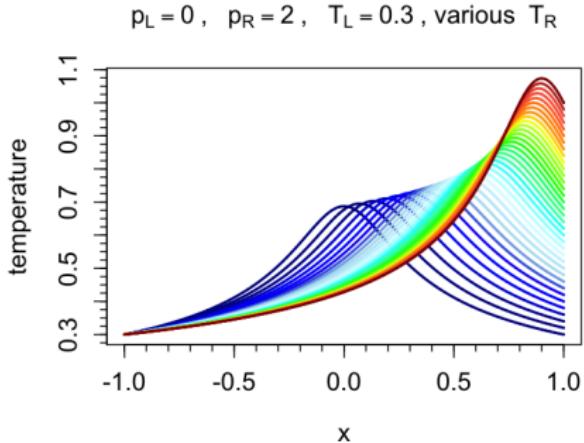
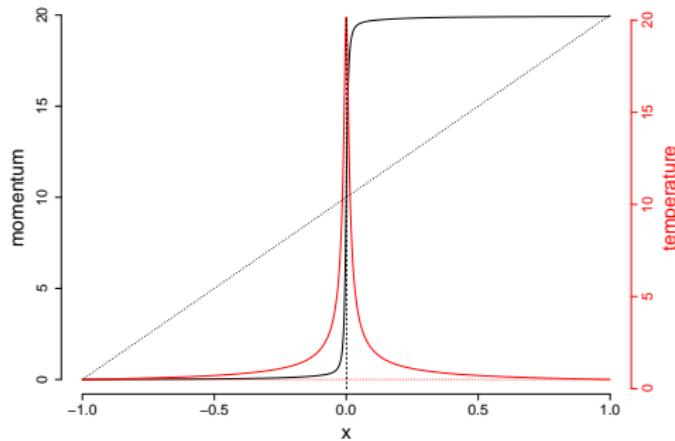


Figure: Note the different behaviors of $\partial_x T_{ss}|_{x=-1}$ as T_R increases: this derivative is decreasing for large values of p_R .

NESS: low boundary temperatures

For $T_R, T_L \rightarrow 0$, the temperature profile spikes:



This behaviour can be proven analitically and it is due to the non-linear decrease behaviour of $\kappa(T)$ and $D^P(T)$.

Negative linear response (negative thermal conductivity)

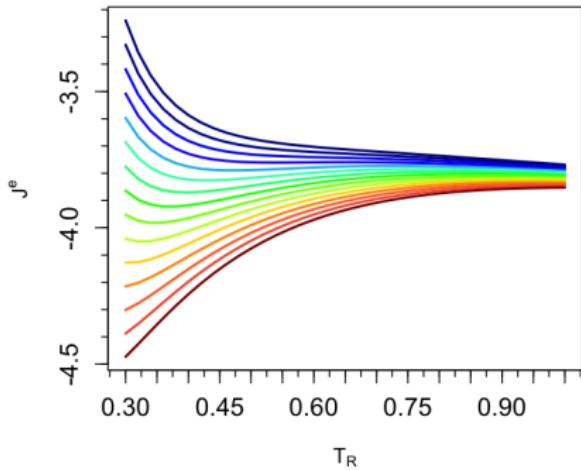
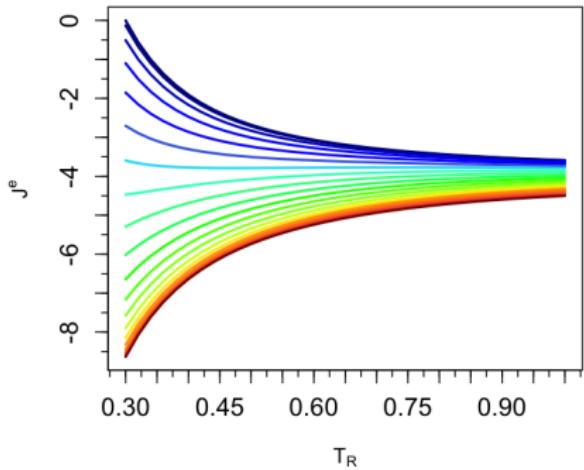


Figure: Energy current J^e as a function of T_R at $T_L = 0.3$. Left: $J^e(T_R)$ for different values of p_R , from $p_R = 0$ (dark-blue line) to $p_R = 2$ (dark-red line), for values of p_R incremented by 0.1. Right: zoom on the range of values $p_R \in [0.56, 0.7]$, increments of 0.01. These plots show how the response of the system to an increase of $\Delta T = T_R - T_L \geq 0$ depends on the value of p_R . In the right panel, we clearly see the emergence of a minimum in J^e for values of $p_R \in (0.6, 0.66)$. Thermal conductivity is as normal up to a temperature T_R corresponding to the minimum of J^e , and becomes negative at larger T_R .

References for the Rotors chain

- O. V. Gendelman and A. V. Savin. *Normal heat conductivity of the one-dimensional lattice with periodic potential of nearest-neighbor interaction.* Phys. Rev. Lett., 84:23812384, 2000.
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 $\kappa(T) \rightarrow +\infty$ for $T \downarrow 0$, $T_0 = 0$.
- Spohn, H.: *Fluctuating hydrodynamics for a chain of nonlinearly coupled rotators* (2014) arXiv:1411.3907
Das, S.G., Dhar, A.: *Role of conserved quantities in normal heat transport in one dimension* (2014) arXiv:1411.5247
Metastable superdiffusive behavior at low temperatures, by *fluctuating hydrodynamics* approximation

References for the Rotors chain

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Other models and rigorous results

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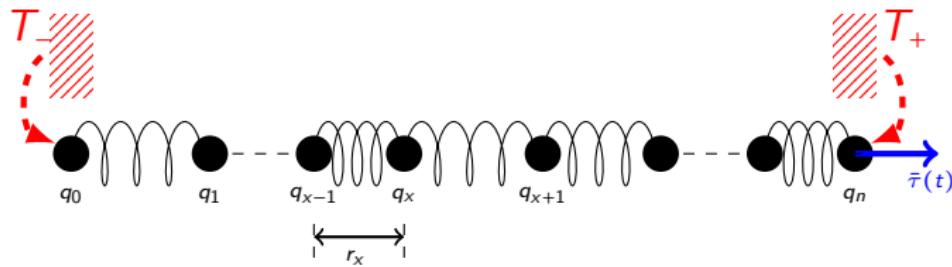
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contrexexample

The *Garrido-Lebowitz* model of hard discs with energy conserving velocity randomization. The presence of *mechanical energy* is important for such behaviour.

Harmonic chain with velocity random flip

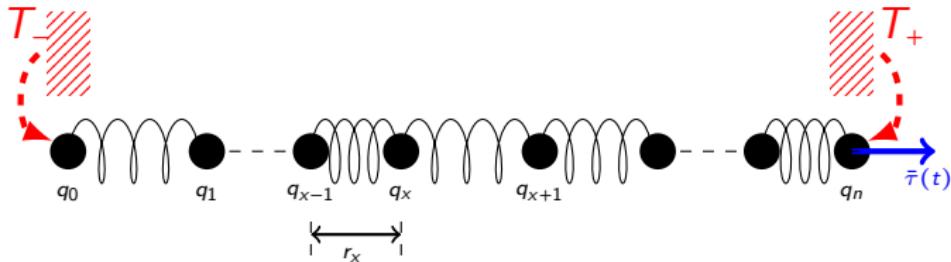
- T. Komorowski, S. Olla, M. Simon, *Hydrodynamic limit for a chain with thermal and mechanical boundary forces*, arXiv:2004.08623, 2020
- T. Komorowski, S. Olla, M. Simon, *An open microscopic model of heat conduction: evolution and non-equilibrium stationary states*, Comm. Math. Sci., 18, 3, 2020



Chain of n harmonic springs,

- with random velocity sign flip: each particle wait an independent exponential time of rate $\tilde{\gamma}$ and then change sign of its velocity
- in contact with two Langevin thermostats at the boundaries,
- pulled on one side by a force $\bar{\tau}$.

Harmonic chain with velocity random flip

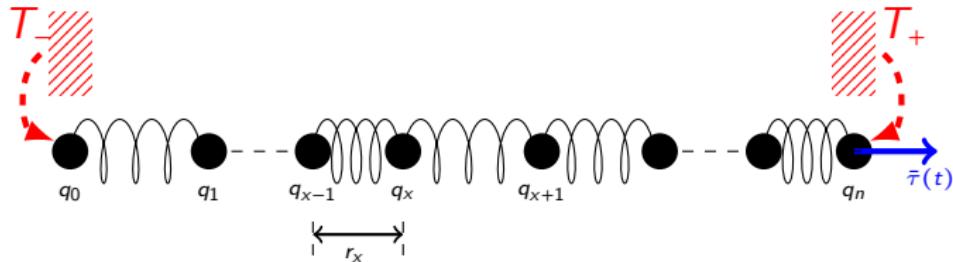


$$r_i = q_i - q_{i-1}, i = 1, \dots, N.$$

$$(\mathbf{r}, \mathbf{p}) = (r_1, \dots, r_N, p_0, \dots, p_N) \in \mathbb{R}^N \times \mathbb{R}^{N+1}.$$

$$\mathcal{H}_n := \sum_i \left\{ \frac{p_i^2}{2} + \frac{r_i^2}{2} \right\} + \frac{p_0^2}{2}.$$

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Two (locally) conserved quantities:

$$r_i \quad \text{volume,} \quad e_i = \left(\frac{p_i^2}{2} + \frac{r_i^2}{2} \right)$$

Conserved quantities and currents

Theorem

$$r_{[Nx]}(N^2 t) \longrightarrow r(t, x), \quad e_{[Nx]}(N^2 t) \longrightarrow e(t, x) \quad \text{weakly in } [0, 1],$$

solution of

$$\partial_t r(t, x) = \frac{1}{2\tilde{\gamma}} \partial_x^2 r(t, x)$$

$$\partial_t e(t, x) = \frac{1}{4\tilde{\gamma}} \partial_x^2 \left(e(t, x) + \frac{r(t, x)^2}{2} \right)$$

$$r(t, 0) = 0, \quad r(t, 1) = \bar{\tau}(t), \quad e(t, 0) = \frac{T_-}{2}, \quad e(t, 1) = \frac{T_+ + \bar{\tau}(t)^2}{2},$$

Evolution of temperature profile

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$$e(t, x) = \frac{T(t, x)}{2} + \frac{r(t, x)^2}{2} = \text{Thermal energy} + \text{Mechanical energy}$$

$$\partial_t T(t, x) = \frac{1}{4\tilde{\gamma}} \partial_x^2 T(t, x) + \frac{1}{2\tilde{\gamma}} (\partial_x r(t, x))^2$$

$$T(t, 0) = T_-, \quad T(t, 1) = T_+.$$

NESS: stationary profiles

$$0 = \partial_x^2 r_{ss}(x),$$

$$0 = \partial_x^2 T_{ss}(x) + 2(\partial_x r_{ss}(x))^2$$

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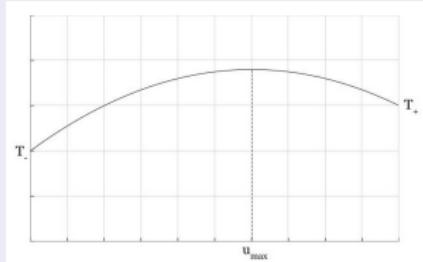
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$$r_{ss}(x) = \bar{\tau}x \quad x \in [0, 1].$$

$$T_{ss}(x) = 2\bar{\tau}^2 x(1-x) + (T_+ - T_-)x + T_-, \quad x \in [0, 1].$$



NESS: Stationary current

stationary energy current is given by

$$J_{ss}^e = -\frac{1}{4\tilde{\gamma}}(T_+ - T_-) - \frac{\bar{\tau}^2}{\tilde{\gamma}}.$$

If $\bar{\tau}^2$ is large enough we can have (*uphill diffusion*).

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No negative linear response, no spiking of temperature profile. These depends on the non-linear decrease of $\kappa(T)$ in the rotors chain.

Non-Acoustic Chains: Beam Dynamics

T. Komorowski, S. Olla, *Diffusive propagation of energy in a non-acoustic chain*,
Arch. Ration. Mech. Appl. 223 (1) (2017)..

$$\mathcal{H} := \sum_i \left(\frac{p_i^2}{2} + \frac{(q_{i+1} + q_{i-1} - 2q_i)^2}{2} \right).$$

Hamiltonian dynamics plus random exchanges of velocities of n.n. particles.

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3 conserved quantities that evolve in diffusive time scale.

$$\sum_i k_i, \quad k_i = q_{i+1} + q_{i-1} - 2q_i \quad \textit{bending or curvature}$$

$$\sum_i p_i,$$

$$\sum_i e_i, \quad e_i = \frac{(q_{i+1} + q_{i-1} - 2q_i)^2}{2}$$

Non-Acoustic chain: macroscopic equations

Hydrodynamic limit (diffusive scaling):

Bernoulli beam equation + heat equation:

$$\partial_t k = -\partial_x^2 p$$

$$\partial_t p = \partial_x^2 k + \gamma \partial_x^2 p$$

$$\partial_t T = \frac{1}{\gamma} \partial_x^2 T + \color{red}{\gamma (\partial_x p)^2}$$

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Open question: What about non-linear interaction with potential

$$V(q_{i+1} + q_{i-1} - 2q_i)$$

and deterministic hamiltonian dynamics?

A different class of models: one dimensional point particles with random flip of velocities sign, no mechanical energy

This is a one dimensional version of the Garrido-Lebowitz model. Particles move on the segment $[-N, N]$, with random change of sign of their velocities. We can ignore the deterministic collisions, but add some other random interaction to destroy all other conservation laws, except energy and density.

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At the boundaries particles reflects or are destroyed and recreated with given densities ρ_L, ρ_R and temperatures T_L, T_R .

$$\frac{1}{N} \sum_i G\left(\frac{q_i(N^2 t)}{N}\right) \rightarrow \int_{-1}^1 G(y) \rho(t, y) dy$$
$$\frac{1}{N} \sum_i G\left(\frac{q_i(N^2 t)}{N}\right) p_i(N^2 t)^2 \rightarrow \int_{-1}^1 G(y) \rho(t, y) T(t, y) dy$$

$$\partial_t \rho = \frac{1}{2} \partial_{yy} (\rho T), \quad \partial_t (\rho T) = \frac{3}{2} \partial_{yy} (\rho T^2),$$

$$\rho(t, -1) = \rho_L, \quad \rho(t, 1) = \rho_R, \quad T(t, -1) = T_L, \quad T(t, 1) = T_R$$

Garrido-Lebowitz model

- Garrido, P.L. and Lebowitz J.L. , *Diffusion equations from kinetic models with non-conserved momentum*, Nonlinearity 31 54 (2018).
- Esposito, R., Garrido, P.L., Lebowitz, J.L. and Marra, R., *Diffusive limit for a Boltzmann-like equation with non-conserved momentum*, Nonlinearity in press (2019).
- Garrido, P.L., Lebowitz, *Heat Conduction in a hard disc system with non-conserved momentum*, arXiv:1911.03178, 2019.

Hydrodynamic limit from the Boltzmann equation

$$\partial_t F + v \cdot \nabla F = Q_B(F, F) + \alpha Q_d(F)$$

$$Q_d(F) = \int_{S^2} d\omega [F(v - 2(v \cdot \omega)\omega) - F(v)] |v \cdot \omega|$$

$$F^\epsilon(y, v, t) = F(\epsilon^{-1}y, v, \epsilon^{-2}t)$$

On the mathematical proof of the macroscopic equation

- Usual *relative entropy* techniques are not sufficient with energy conserving models.

On the mathematical proof of the macroscopic equation

- Usual *relative entropy* techniques are not sufficient with energy conserving models.
- *Wigner distributions*

$$\hat{\psi}(t, k) = \hat{r}(t, k) + i\hat{p}(t, k)$$

$$\widehat{W}_N(t, \eta, k) = \frac{1}{2N} \left\langle \hat{\psi} \left(N^2 t, k + \frac{\eta}{N} \right)^* \hat{\psi}(N^2 t, k) \right\rangle$$

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$$W_N(t, x, k) \xrightarrow[N \rightarrow \infty]{} \frac{1}{2} T(t, x) dk + \frac{1}{2} r(t, x)^2 \delta_0(k)$$

= thermal energy + mechanical energy

$T(t, x), r(t, x)$ solution of the macroscopic equations with boundary conditions.