Thermal diffusion and energy transport for system with more conserved quantities.

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Collaborators: Tomasz Komorowski, Marielle Simon, Alessandra Iacobucci, Gabriel Stoltz

Coupled transport of conserved quantities

One dimensional systems with multiple conserved quantities (*energy, momentum, volume stretch...*).
Easy to simulate dynamically, and (sometime) to be treated mathematically.

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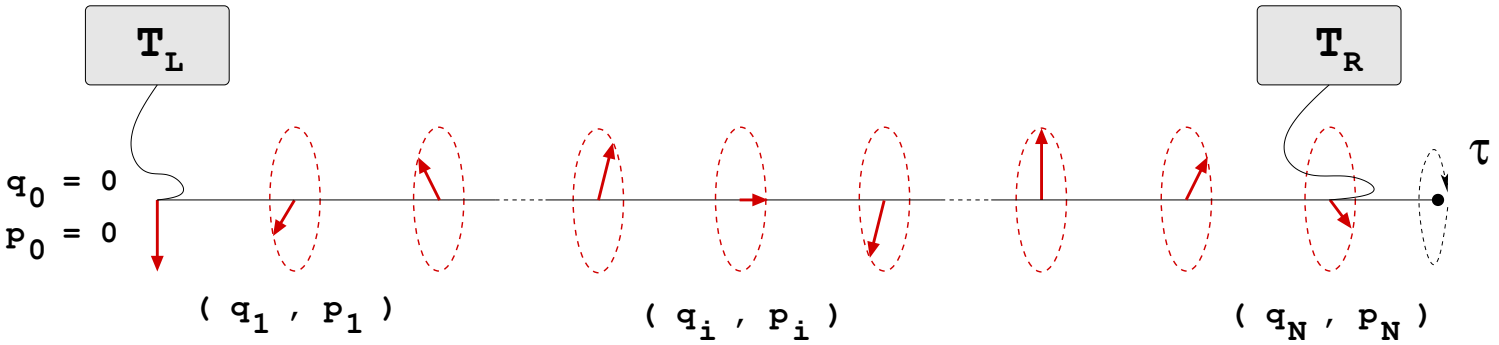
- **Non stationary behaviour**:
  - there could be evolution at different time scales (hyperbolic, superdiffusive) like for the FPUT.
  - or they may evolve all in the same *diffusive time scale*
- **Stationary non-equilibrium states**: induced by boundary forces and thermostats. Interesting phenomena: *uphill diffusion, non monotonous temperature profiles, negative linear response*.

Examples: rotors chain, oscillators chains with conservative noise, non-acoustic chains, discrete non-linear Schrodinger.

Rotors Chain



$$r_i = q_i - q_{i-1} \in \mathbb{S}^1, \qquad V(r) = 1 - \cos(2\pi r)$$

$$\mathcal{H} = \sum^{i} \left(\frac{p_i^2}{2} + V(r_i) \right) = \sum_i e_i$$

$$\dot{r}_i(t) = p_i(t) - p_{i-1}(t), \qquad 1, \ldots, N,$$

$$\dot{p}_i(t) = V'(r_{i+1}(t)) - V'(r_i(t)), \quad i = 2, \ldots, N-1,$$

$$dp_0(t) = \left(\tau_L + V'(r_1(t)) - \gamma p_0(t) \right) dt + \sqrt{2\gamma T_L}\, dw_L(t),$$

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

Conserved quantities, currents, equilibrium states

Two conserved quantities

$$\sum_i p_i \qquad \sum_i e_i = \sum \left(\frac{p_i^2}{2} + V(r_i) \right),$$

microscopic currents

$$\dot{p}_i = j^p_{i-1,i} - j^p_{i,i+1}, \quad j^p = -V'(r_i), \qquad \dot{e}_i = j^e_{i-1,i} - j^e_{i,i+1}, \quad j^e = -p_i V'(r_{i+1}),$$

For $T_R = T_L = \beta^{-1}$ and $\tau_R = \tau_L = \tau$, there is a unique *equilibrium* stationary measure:

$$d\mu_{\beta,\bar{p}} = \prod_i \frac{e^{-\beta e_i + \beta \bar{p} p_i}}{Z_{\beta,p}} \, dr_i \, dp_i$$

with $\bar{p} = \tau \gamma^{-1}$.

Linear Response: Onsager Matrix

A formal linear response argument gives

$$< j^p_{[Nx],[Nx]+1} >\sim J^p\left(\partial_x\beta, \partial_x(p\beta)\right) = K^{p,p}(\beta)\partial_x(\beta p) + K^{p,\beta}(\beta, p)\partial_x\beta$$

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i.e. the macroscopic equation system, after diffusive rescaling of space time:

$$\partial_t p = -\partial_x J^p \qquad \partial_t e = -\partial_x J^e$$

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$$K^{\beta,\beta}(\beta,\bar{p}) = \int_0^\infty \sum_k \langle j^e_{0,1}(0) j^e_{k,k+1}(t)\rangle_{\beta,\bar{p}} dt\,,$$

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Properties of the Onsager coefficients

$$j^p_{i,i+1} = -V'(r_i), \quad j^e_{i,i+1} = -p_i V'(r_{i+1}),$$

$$K^{\beta,\beta}(\beta,\bar{p}) = \int_0^\infty \sum_i \langle j^e_{0,1}(0) j^e_{i,i+1}(t)\rangle_{\beta,\bar{p}} dt = K^{\beta,\beta}(\beta,0) - \bar{p}^2 K^{p,p}(\beta),$$

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$$K^{p,p}(\beta) = -\int_0^\infty \sum_i \langle j^p_{0,1}(0) j^p_{i,i+1}(t)\rangle_{\beta,\bar{p}} dt \ (\leq 0)\,.$$

– S. Iubini, S. Lepri, R. Livi, A. Politi, New J. Phys. 18 (2016)
– F. Huveneers, W. De Roeck, ...

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Recall $T = \beta^{-1}$, there are only two transport coefficient left:

$$D^p(\beta^{-1}) = -\beta K^{p,p}(\beta) \ge 0, \qquad \text{momentum diffusivity}$$

$$\kappa(\beta^{-1}) = \beta^2 K^{\beta,\beta}(\beta,0) \ge 0 \qquad \text{thermal conductivity}$$

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

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

$$\partial_t e = \partial_x \left[D^p(T) \partial_x \left(\frac{p^2}{2} \right) + \kappa(T) \partial_x T \right]$$

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In equilibrium at temperature T and momentum $\bar{p}$

$$e(T, \bar{p}) = u(T) + \frac{\bar{p}^2}{2}, \qquad u \text{ is the internal energy}$$

$c_v(T) = u'(T) > 0$ is the heat capacity of the chain.

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

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

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

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

Taking account of the boundary conditions:

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

$$\partial_t u = c_v(T) \partial_t T = \partial_x \left[\kappa(T) \partial_x T \right] + D^p(T) \left[\partial_x p \right]^2$$

$$T(t,0) = T_L, \quad T(t,1) = T_R, \qquad p(t,0) = \tau_L \gamma^{-1}, \quad p(t,1) = \tau_R \gamma^{-1}$$

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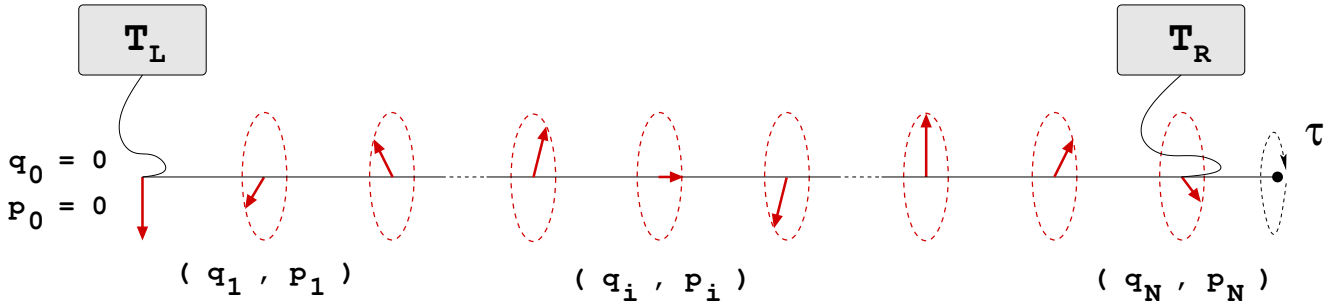
The thermodynamic entropy is $S(u) = \inf_{\beta > 0} \left\{ T^{-1} u + \log Z_{T,0} \right\}$, and $T(u)^{-1} = \beta(u) = S'(u)$ provides the inverse function of $u(\beta)$.

$$\frac{d}{dt} \int_0^1 S(u(t,x)) dx = \int_0^1 \left[\frac{D^p(T)}{T} (\partial_x p)^2 + \frac{\kappa(T)}{T^2} (\partial_x T)^2 \right] dx + \frac{\kappa(T_R)}{T_R} \left[\partial_x T \right]_{T=T_R} - \frac{\kappa(T_L)}{T_L} \left[\partial_x T \right]_{T=T_L}$$

i.e. increase of entropy in the bulk + flux of entropy at the boundary.

Rotors: Non-equilibrium Stationary State



Currents of conserved quantities are constant in space:

$$-J^p = D^p\,(\partial_x p)$$

$$-J^e = D^p \partial_x \left(\frac{p^2}{2}\right) + \kappa \partial_x T$$

$$T(0) = T_L, \quad T(1) = T_R, \quad p(0) = 0, \quad p(1) = \frac{\tau}{\gamma}$$

Rotors: stationary profiles

$$-J^p = D^p \partial_x p$$

$$-J^e = D^p \partial_x \left(\frac{p^2}{2} \right) + \kappa \partial_x T = -J^M - J^Q$$

$$= -\text{mechanical energy current} - \text{thermal energy current}$$

$$T(0) = T_L, \quad T(1) = T_R, \quad p(0) = 0, \quad p(1) = \frac{\tau}{\gamma}$$

$$p(x) J^p - J^e = \kappa \partial_x T := -J^Q(x) \sim -\left\langle \left(p_{[Nx]} - p(x) \right) V'(r_{[Nx]}) \right\rangle_{ss}$$

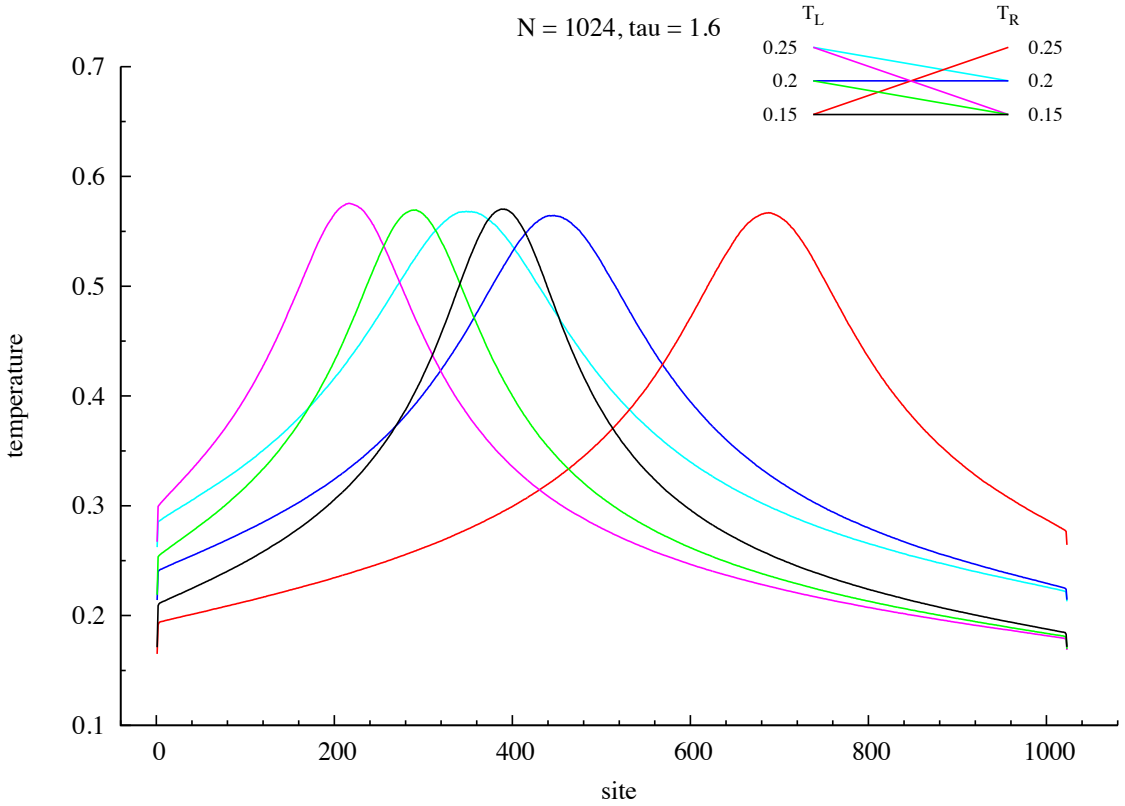
the *heat current* J^Q is a linear function of p.

Rotors: stationary state very far from equilibrium

Dynamical simulations:

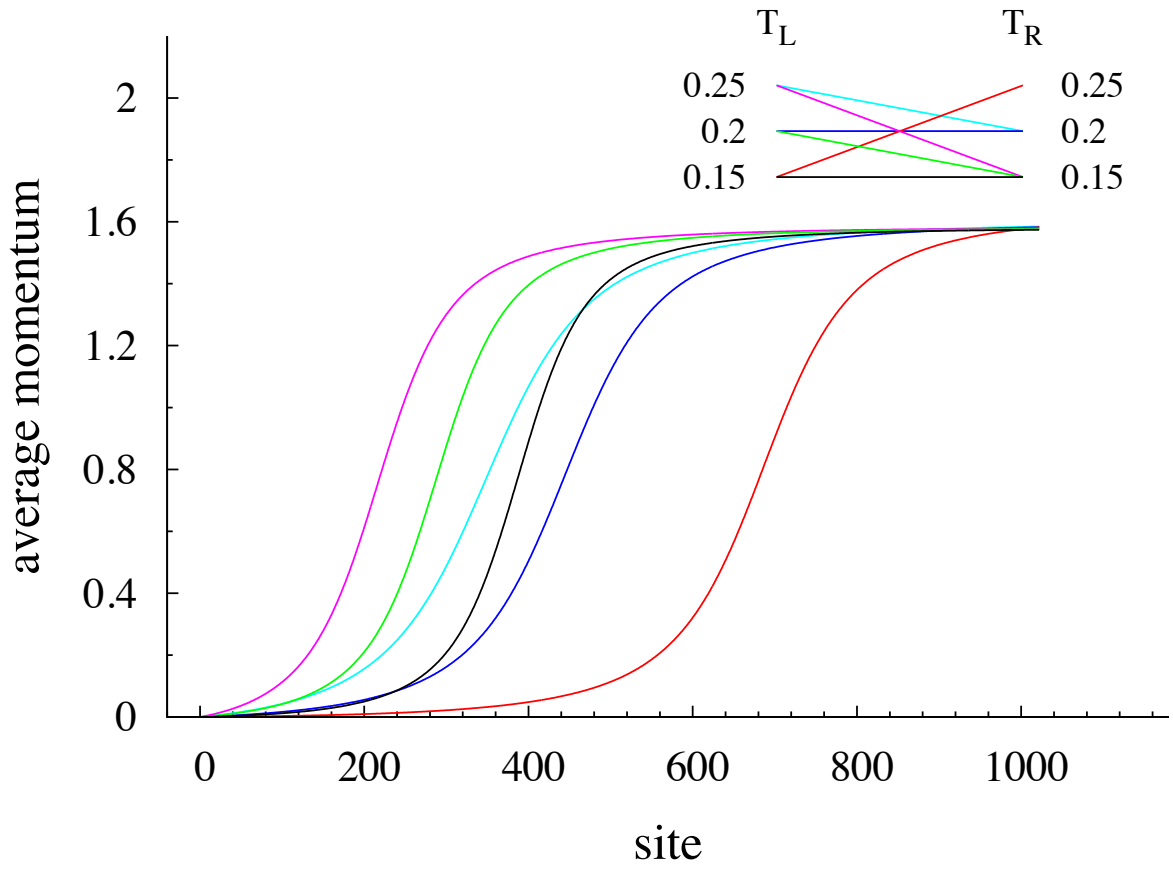
A. Iacobucci, F. Legoll, S. Olla, G. Stoltz, *Negative Thermal Conductivity in Rotor model*, **Phys. Rev. E** 2011.

S. Iubini, S. Lepri, R. Livi, A. Politi, *Boundary induced instabilities in coupled oscillators*, **Phys. Rev. Lett.** 2014.



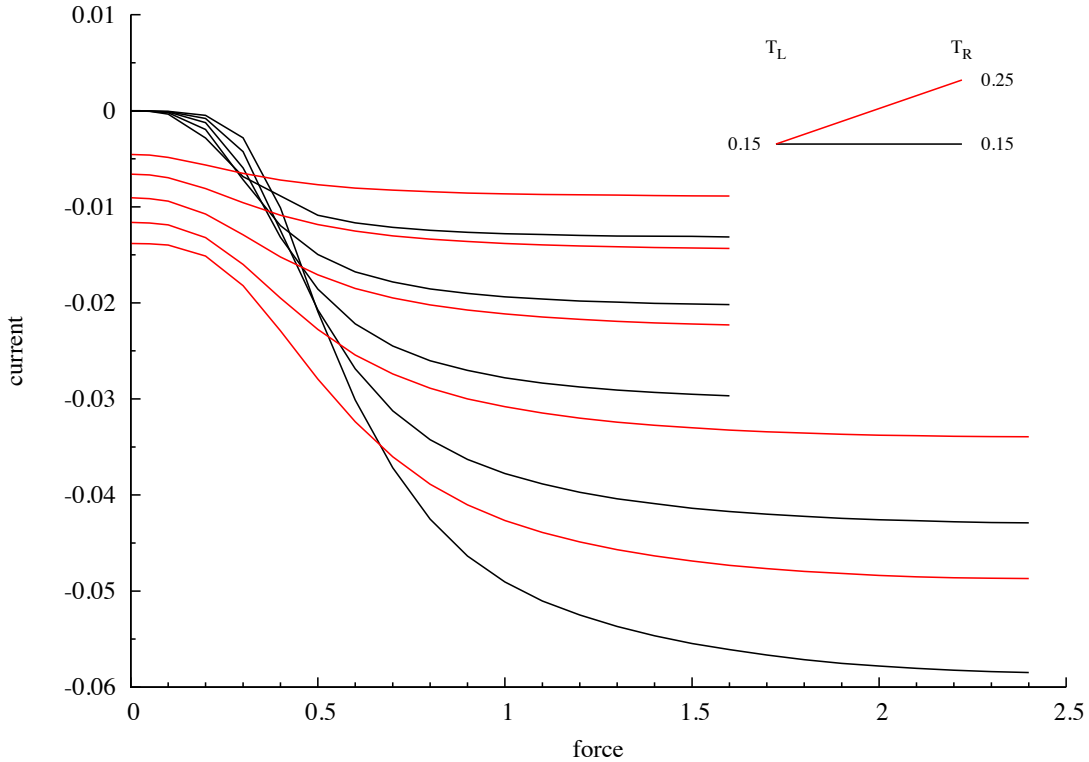
Local equilibrium is verified to high accuracy.

Rotors: average momentum profile



Rotors: negative linear response

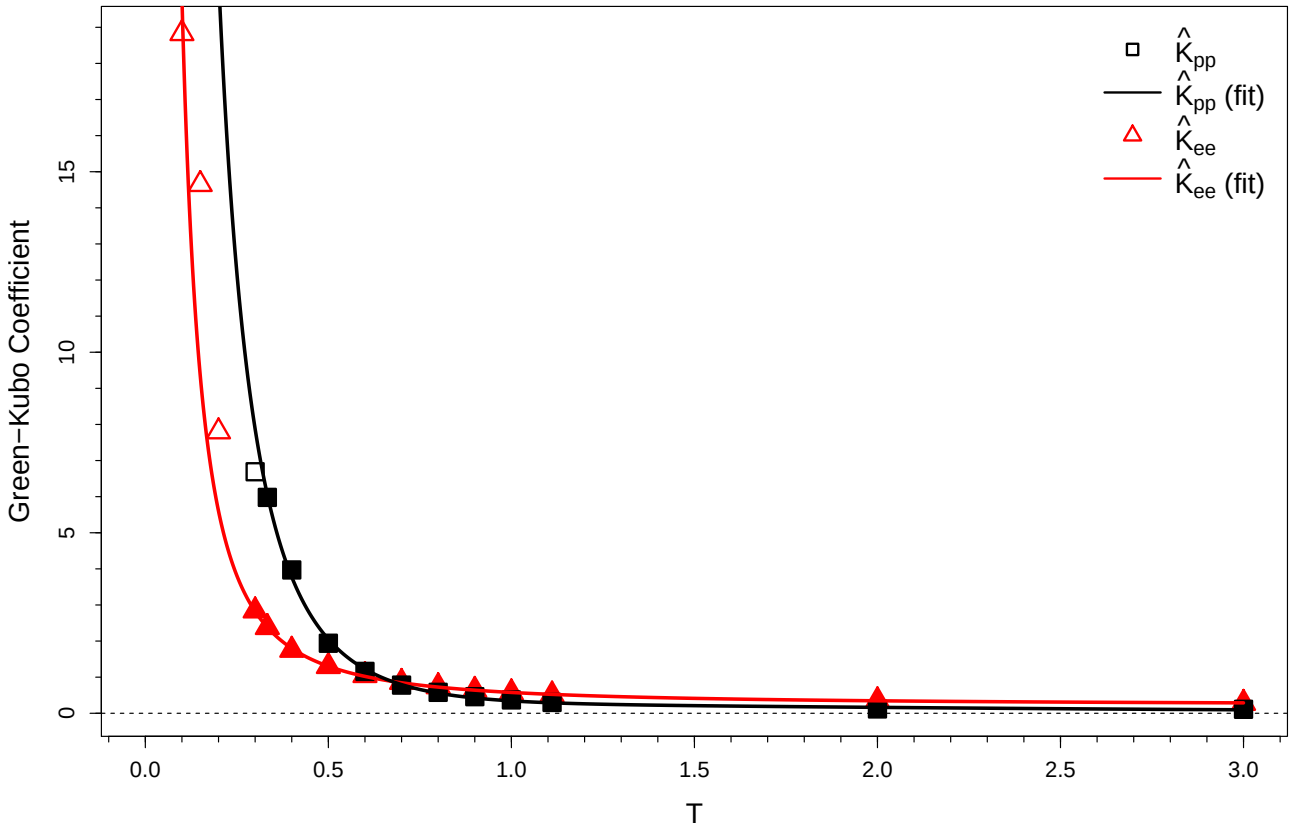
A gradient of temperature at the thermostat can create opposite effect than in equilibrium:



decreasing system sizes N = 2048, 1024, 512, 256, 128

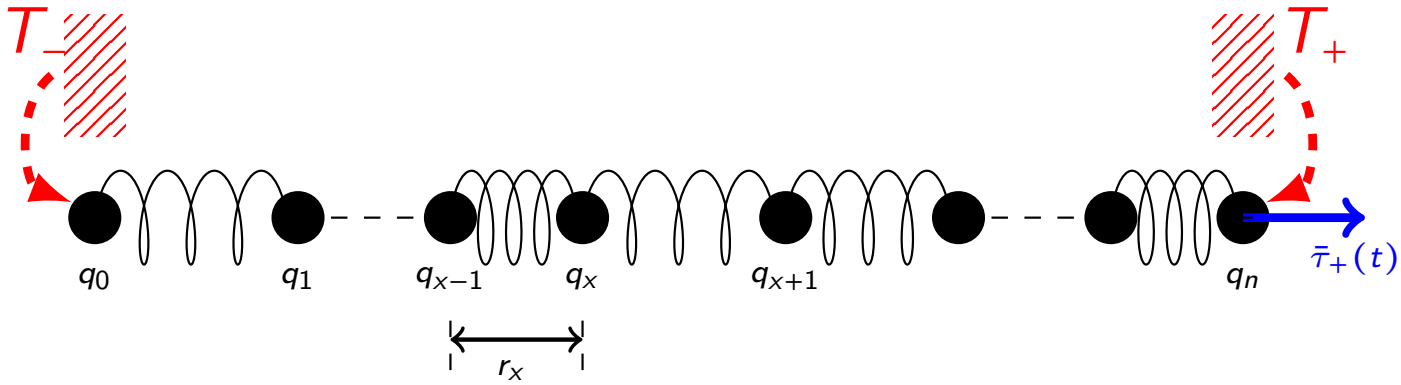
$$-J^e = D^p \partial_x \left(\frac{p^2}{2} \right) + K^e \partial_x T$$

Temperature affecting transport coefficient in rotors chain



With these fit we get a good agreement with the solution of the macroscopic diffusive PDE.

FPU chain with velocity random flip



Chain of n an-harmonic springs,

- with random velocity sign flip,
- in contact with two Langevin thermostats,
- pulled on one side by a force $\bar{\tau}$.

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

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

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

FPU chain with velocity random flip

$$\hat{r}_\epsilon(t,x) = \epsilon \sum_i r_i(\epsilon^{-2}t)\delta_{\epsilon i}(x), \qquad \hat{T}_\epsilon(t,x) = \epsilon \sum_i \frac{1}{2} p_i^2(\epsilon^{-2}t)\delta_{\epsilon i}(x). \tag{1}$$

converge to the solution $r(t,x), T(t,x)$ of

$$\partial_t r = \frac{1}{2\gamma}\partial_x^2 \tau(r,T)$$

$$c_v(r,T)\partial_t T = \partial_x\left(\kappa(r,T)\partial_x T\right) + \frac{1}{2\gamma}\left(\partial_x \tau(r,T)\right)^2,$$

$\tau(r,T)$ is the equilibrium tension at length r and temperature T.

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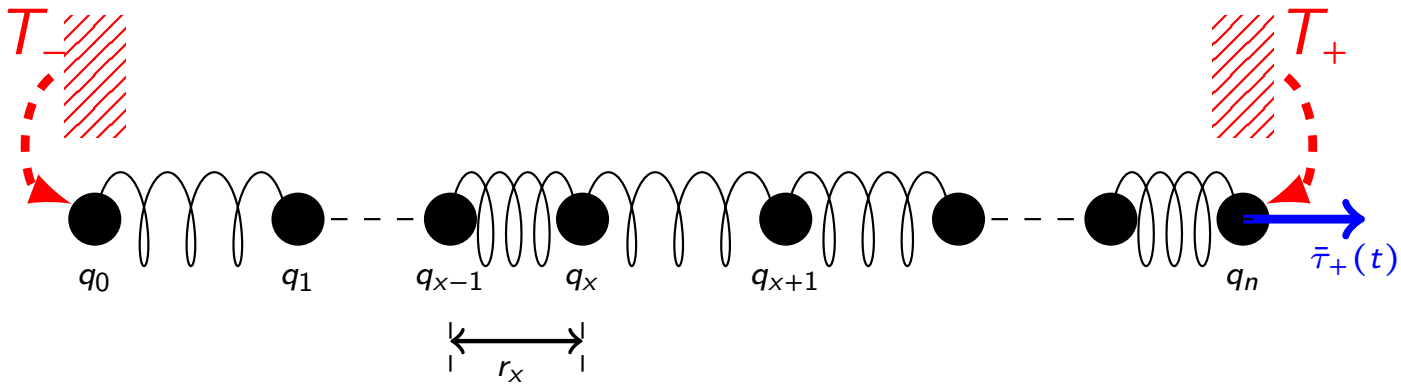
$\tau(r,T)$ is the equilibrium tension at length r and temperature T.
This is still a difficult open problem, but *easier* than the rotors.

Harmonic chain with velocity random flip

Joint work with *Tomasz Komorowski* and *Marielle Simon*, arXiv:1903.11374, 2019.



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

Conserved quantities and currents

Two (locally) conserved quantities:

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

Theorem

The empirical volume stretch and kinetic energy (temperature)

$$\frac{1}{N} \sum_i r_i(N^2 t) \delta_{i/N}(dx), \qquad \frac{1}{N} \sum_i p_i^2(N^2 t) \delta_{i/N}(dx)$$

converge pour $N \to \infty$ *to the solution of*

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

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

$$r(t,0) = 0, \quad r(t,1) = \bar{\tau}_+(t), \quad T(t,0) = T_-, \quad T(t,1) = T_+,$$

Conserved quantities and currents

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These are the same equations as in the rotors case, but with constant $K^e = \frac{1}{2}\left(\frac{1}{\gamma}+\gamma\right)$ and $D^r = \frac{1}{\gamma}$.

Stationary Non-equilibrium state

$$r_{\mathrm{ss}}(x) = \bar{\tau}_+ x$$

$$\left(\gamma^{-1} + \gamma\right)\partial_x^2 T(x) + 2\gamma^{-1}\,\bar{\tau}_+^2 = 0,$$

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

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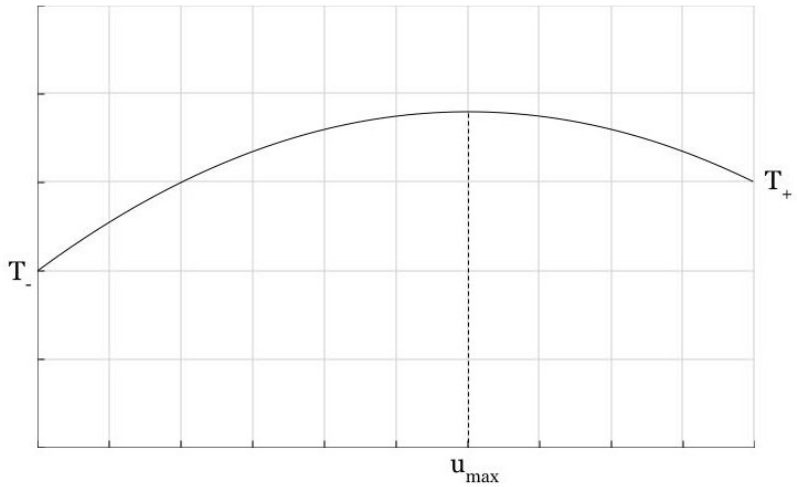
Explicit solution

$$T(x) = \frac{\bar{\tau}_+^2}{1+\gamma^2}\, x(1-x) + (T_+ - T_-)x + T_-, \qquad x \in [0,1].$$



Stationary current

stationary energy current is given by

$$J^e_{\rm ss} = -\frac{1}{2}(\gamma^{-1}+\gamma)(T_+ - T_-) - \frac{\bar\tau_+^2}{2\gamma}.$$

Observe that current can flow against the temperature gradient if $T_- > T_+$ and $|\bar\tau_+|$ is large enough (*uphill diffusion*).

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$$J^Q = -\frac{1}{2}(\gamma^{-1}+\gamma)\partial_x T(x) = -\frac{\bar\tau_+^2}{2\gamma}\,(1-2x) - \frac{1}{2}(\gamma^{-1}+\gamma)(T_+ - T_-)$$

$$J^M = \frac{\bar\tau_+^2}{\gamma}x$$

Non-Acoustic Chains: Beam Dynamics

Tomasz Komorowski, S.O. ARMA, 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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Hamiltonian dynamics plus random exchanges of velocities of n.n. particles.

3 conserved quantities that evolve in diffusive time scale.

$$\sum_i k_i, \qquad k_i = q_{i+1} + q_{i-1} - 2q_i$$

$$\sum_i p_i,$$

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

Non-Acoustic chain: macroscopic equations

Hydrodynamic limit (diffusive scaling):
Bernoulli beam equation + heat equation:

$$\partial_t k = -\partial_x^2 p$$
$$\partial_t p = \partial_x^2 k + \gamma \partial_x^2 p$$
$$\partial_t T = \kappa_\gamma \partial_x^2 T + \gamma \left(\partial_x p\right)^2$$

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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?