Hydrodynamics and non-equilibrium stationary states for diffusive systems of conservation laws

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Coupled transport of conserved quantities

One dimensional systems with multiple conserved quantities (*energy, momentum, volume stretch...*).

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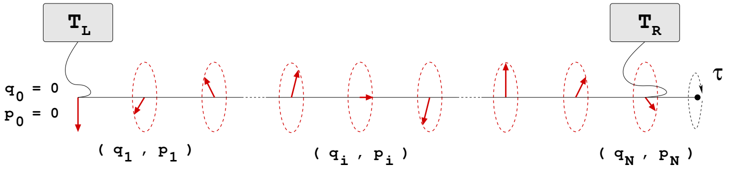
- **Non stationary behaviour**:
  - there could be evolution at different time scales (hyperbolic, superdiffusive) like for the FPUT.
  - they may evolve all in the same *diffusive time scale*
- **Stationary non-equilibrium states**: induced by boundary forces and thermostats. Interesting phenomena: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

Examples: rotors chain, oscillators chains with conservative noise, non-acoustic chains, discrete non-linear Schrodinger (see Livi talk).

Rotors Chain



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

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

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

$$dp_i = \left(U'(r_{i+1}) - U'(r_i) \right) dt \qquad i = 2, \dots, N-1$$

$$dp_1 = \left(U'(r_2) - U'(r_1) \right) dt - \tilde{\gamma} p_1 dt + \sqrt{2\tilde{\gamma} T_L} dw_1(t)$$

$$dp_N = \left(\tau - U'(r_N) \right) dt - \tilde{\gamma} p_N dt + \sqrt{2\tilde{\gamma} T_R} dw_N(t)$$

Two conserved quantities

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

microscopic currents

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

Equilibrium measures for the infinite dynamics are parametrized by $\beta = T^{-1}$ and $\bar{p}$:

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

Linear Response: Onsager Matrix

A formal linear response argument gives

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

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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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$$\begin{aligned}
K^{e,e}(\beta,\bar{p}) &= \int_0^\infty \sum_k \langle j^e_{0,1}(0) j^e_{k,k+1}(t)\rangle_{\beta,\bar{p}} dt\,, \\
K^{e,p}(\beta,\bar{p}) &= -\int_0^\infty \sum_k \langle j^e_{0,1}(0) j^p_{k,k+1}(t)\rangle_{\beta,\bar{p}} dt\,, \\
K^{p,e}(\beta,\bar{p}) &= \int_0^\infty \sum_k \langle j^p_{0,1}(0) j^e_{k,k+1}(t)\rangle_{\beta,\bar{p}} dt \ = K^{e,p}(\beta,-\bar{p})\,, \\
K^{p,p}(\beta,\bar{p}) &= -\int_0^\infty \sum_k \langle j^p_{0,1}(0) j^p_{k,k+1}(t)\rangle_{\beta,\bar{p}} dt\,.
\end{aligned}$$

Properties of the Onsager coefficients

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

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

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

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

Recall $T = \beta^{-1}$

$$D^p(\beta) = -\beta K^{p,p}(\beta) \geq 0, \quad K^e(\beta) = \beta^2 K^{e,e}(\beta,0) \geq 0$$

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

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

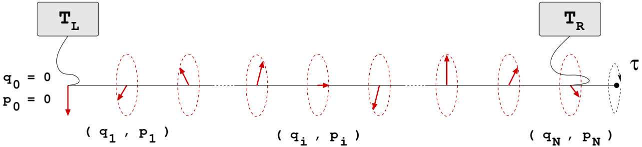
Non-stationary macroscopic evolution of $p - T$ profiles

$$\partial_t p = \partial_x \left[D^p(T) \partial_x p \right]$$
$$C_v(T) \partial_t T = \partial_x \left[K^e(T) \partial_x T \right] + D^p(T) \left[\partial_x p \right]^2.$$

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

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

Rotors: Non-equilibrium Stationary State



Currents of conserved quantities are constant in space:

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

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

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

Rotors: stationary profiles

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

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

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

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

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

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

Stationary State: some relations

Energy balance gives:

$$\tau < p_N > + \tilde{\gamma} \left(T_L - < p_1^2 >_{ss} \right) + \tilde{\gamma} \left(T_R - < p_N^2 >_{ss} \right) = 0$$

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Entropy production gives:

$$\tilde{\gamma} T_L^{-1} \left(T_L - < p_1^2 >_{ss} \right) + \tilde{\gamma} T_R^{-1} \left(T_R - < p_N^2 >_{ss} \right) + \tau < p_N >_{ss} \geq 0.$$

or

$$\tilde{\gamma} \left(T_L^{-1} - T_R^{-1} \right) \left(T_L - < p_1^2 >_{ss} \right) + \tau < p_N >_{ss} \geq 0.$$

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or

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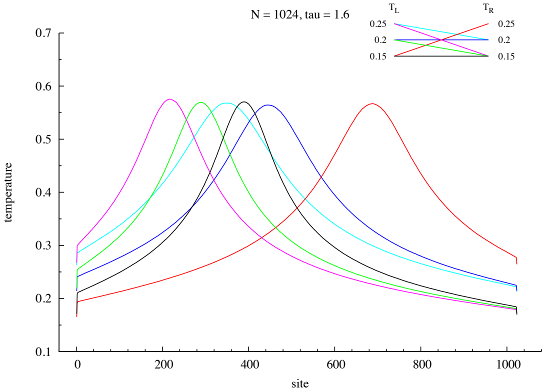
If $T_L = T_R$, then $\tau < p_N >_{ss} \geq 0$.

Rotors: stationary state very far from equilibrium

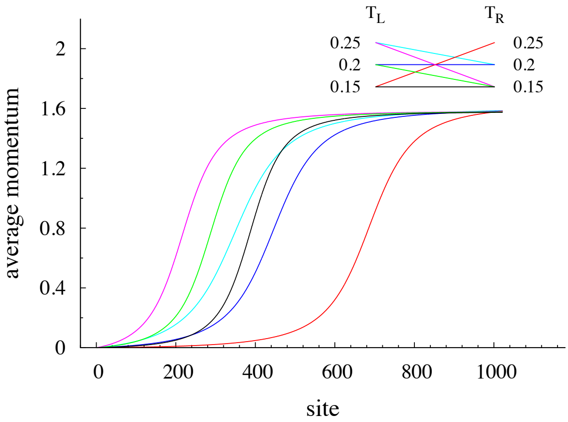
Dynamical simulations:
A. Iacobucci, F. Legoll, S. Olla, G. Stoltz, *Negative Thermal Conductivity in Rotor model*, **Phys. Rev. E** 2011.

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



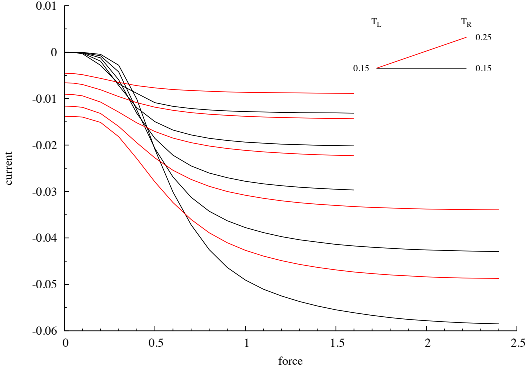
Local equilibrium is verified to high accuracy.

Rotors: average momentum profile



Rotors: negative linear response

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

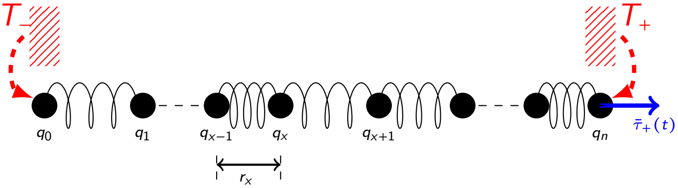


decreasing system sizes N = 2048, 1024, 512, 256, 128

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

Harmonic chain with velocity random flip

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



Chain of n harmonic springs,

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

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

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

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

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

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

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

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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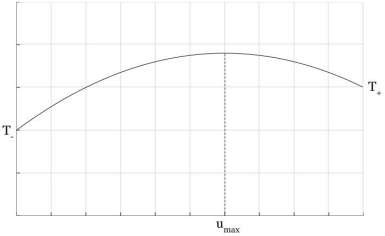
Explicit solution

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



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:

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

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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?