Diffusive transport in non-acoustic chains.

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Macroscopic space-time scales

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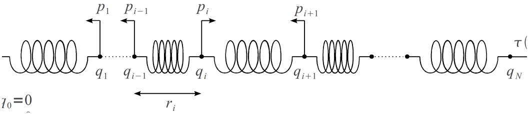
non-vanishing sound velocity $\Leftrightarrow$ acoustic chain.

Chain of oscillators with tension



Hamiltonian unpinned dynamics of FPU type: $j \in \mathbb{Z}$,

$$H = \sum_j \frac{p_j^2}{2} + V(\nabla q_j) = \sum_j \frac{p_j^2}{2} + V(r_j)$$

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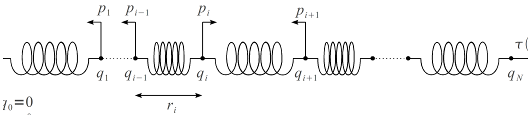

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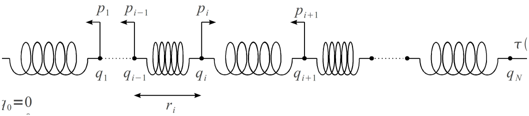

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momentum exchange For each couple of nearest neighbor particle, we randomly exchange momentum, $(p_i, p_{i+1}) \to (p_{i+1}, p_i)$, with intensity 1.

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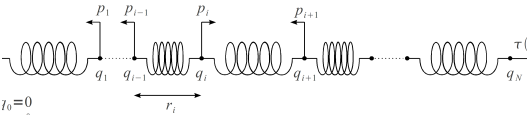

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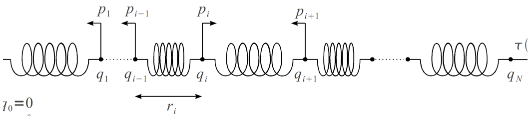

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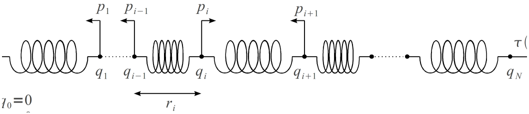

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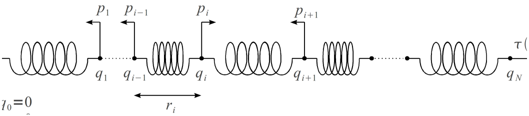

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Gibbs measures and Thermodynamic Entropy

$$\mathcal{E}_j = \frac{p_j^2}{2} + V(r_j) \qquad \text{energy of particle } j$$

Gibbs measure at temperature β^{-1}, tension τ and momentum p are:

$$d\mu_{\beta,\tau,p} = \prod_j e^{-\beta(\mathcal{E}_j - pp_j - \tau r_j) - \mathcal{G}(\beta,\tau,p)} dp_j dr_j$$

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Thermodynamic entropy is

$$S(u,r) = \inf_{\tau,\beta} \{-\beta\tau r + \beta u - \mathcal{G}(\beta,\tau,0)\}$$

$$\beta(u,r) = \partial_u S(u,r), \qquad \tau(u,r) = -\beta^{-1}\partial_r S(u,r).$$

Ergodicity (of the infinite system)

The stocastic perturbation of the dynamics is sufficient to give ergodicity:

Theorem

(Fritz, Funaki, Lebowitz, PTRF 1994)

Assume that ν *is translation invariant and stationary, with finite entropy density, and furthemore that*

$$\nu(dp|r)$$

is exchangeable.

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- $\nu(dp|r)$ maxwellian (Gallavotti-Verboven 1975)
- $\nu(dp|r)$ convex combination of maxwellians (Olla, Varadhan, Yau, 1993).

Acoustic Chains: Hyperbolic Scaling, Euler equations

3 conserved quantities:

volume stretch $\mathcal{R}_N(t)[G] = \frac{1}{N}\sum_i G(i/N) r_i(Nt)$

momentum $\pi_N(t)[G] = \frac{1}{N}\sum_i G(i/N) p_i(Nt)$

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$$(\mathcal{R}_N(t), \pi_N(t), \mathfrak{e}_N(t)) \longrightarrow (r(x,t)dx, \pi(x,t)dx, \mathfrak{e}(x,t)dx)$$

$$\boxed{\begin{array}{ccc} \partial_t r = \partial_x \pi & \partial_t \pi = \partial_x \tau & \partial_t \mathfrak{e} = \partial_x(\tau\pi) \\ \pi(0,t) = 0, & \tau(r(1,t), U(1,t)) = \tau_1(t) & \end{array}}$$

$U = \mathfrak{e} - \pi^2/2$: internal energy. For smooth solutions this is proven in:

- N. Even, S.O., ARMA (2014)
- S.O., SRS Varadhan, HT Yau, CMP (1993)

entropy evolution

$$\partial_t r = \partial_x \pi \qquad \partial_t \pi = \partial_x \tau \qquad \partial_t \mathfrak{e} = \partial_x(\tau\pi)$$
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When shocks will appear, we will have dissipation and

$$\frac{d}{dt}\int_0^1 S(r(x,t), U(x,t))dx > 0$$

and (eventually) *convergence* to a **mechanical** equilibrium, characterized by constant tension and momentum.

Acoustic Chains: Mechanical Equilibrium

In particular starting with smooth initial profiles such that

$$p_0(x) = 0, \qquad \tau(u_0(x), r_0(x)) = \tau_0 = \text{cost}$$

$u_0(x) = e_0(x) - \frac{p^2(x)}{2} = e_0(x)$
and non constant entropy profile $S(u_0(x), r_o(x))$
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This means that they evolve towards *thermal equilibrium* at a larger time scale:

- diffusive scaling $(N^2 t, Nx)$, if thermal conductivity is finite, with heat equation governing the evolution of the temperature profile,
- superdiffusive scaling $(N^\alpha t, Nx), 1 < \alpha < 2$, if thermal conductivity is infinite.

If $\partial_r \tau(u, r) > 0$ (acoustic chains), we expect superdiffusion of heat, confirmed by many numerical experiments.

Acoustic Chains: Energy Superdiffusion

Consider the Harmonic chain with noise conserving energy and momentum.

$$V(r) = \frac{r^2}{2}, \qquad \tau(r, U) = r, \qquad S = 1 + \log(\pi\beta^{-1})$$

$$\mathfrak{e}(x,0) = \frac{1}{2} r(x,0)^2 + \frac{1}{2}\pi(x,0)^2 + \beta^{-1}(x,0)$$

In the hyperbolic space-time scale limit we have

$$\boxed{\partial_t r = \partial_x \pi \qquad \partial_t \pi = \partial_x r \qquad \partial_t \mathfrak{e} = \partial_x(r\pi)}$$

linear wave equation: no shocks! no dissipation!
Profiles of **temperature** and **entropy** do not change in time:

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Since microscopically the noise made the dynamic 'ergodic', the convergence to equilibrium should happen in another space-time scale.

Acoustic Chains: Temperature profile

In the infinite space case, in the hyperbolic scale, after $t \to \infty$, all the phonon modes go to infinity, and the *phonon energy*

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This temperature profile will start to evolve at a larger time scale, supediffusive, shorter than the diffusive one.

Acoustic Chains: What superdiffusion?

Assume $V(r) = \frac{\alpha r^2}{2}$, and centered initial conditions:

$$< p_j(0) >= 0, \qquad < r_j(0) >= 0$$

This is maintained at any positive time t.

Theorem (Jara-Komorowski-Olla, CMP 2015)

Assume $\frac{1}{N}\sum_x \langle \mathcal{E}_i(0) \rangle < C$, $G \in \mathcal{C}_0(\mathbb{R})$:

$$\frac{1}{N}\sum_i G(i/N)\left\langle \mathcal{E}_i(N^{3/2}t)\right\rangle \underset{N\to\infty}{\longrightarrow} \int_{\mathbb{R}} G(x)\; T(t,x)dx$$

$$\boxed{\partial_t T(x,t) \;=\; -\hat{c}|\Delta_x|^{3/4} T(x,t)} \qquad \hat{c} = \frac{\alpha^{3/4}}{2^{9/4}(3\gamma)^{1/2}}$$

$T(x,0) = \beta^{-1}(x,0)$.

Conjectured result for FPUT dynamics

This behavior at large space-time scale (diffusive for phonon and superdiffusive for heat mode) is also conjectured for the *equilibrium fluctuations* dynamics for the Fermi-Pasta-Ulam-Tsingou model

$$V(r) = r^2 + \alpha r^3 + \beta r^4$$

Recent *fluctuation hydrodynamics and mode coupling* calculation by Herbert Spohn (JSP 2014) for the deterministic FPU dynamics:

- If V symmetric ($\alpha = 0$ or β-FPU), and $\tau = 0$: then diffusion for phonons and $|\Delta|^{3/4}$-superdiffusion for heat (temperature),
- If V asymmetric (α-FPU), or symmetric but tension $\tau \neq 0$, then phonon KPZ-superdiffuse, and $|\Delta|^{5/6}$-superdiffusion for heat.

Non-acoustic chains

These are *tensionless* chains, obtained by considering also non-nearest neighbor interactions, for example:

$$\mathcal{H} = \sum_j \left[\frac{p_j^2}{2} + V(\Delta q_j) \right], \qquad \Delta q_j = q_{j+1} + q_{j-1} - 2q_j$$

Here the relevant balanced quantity is not the volume strain $r_j = q_j - q_{j-1}$, but the *curvature* $\kappa_j = \Delta q_j$ (*Beam problem*). Equilibrium measures are parametrized by temperature β^{-1}, momentum p and bending stress τ_2:

$$d\mu_{\beta,\tau,p} = \prod_j e^{-\beta(\mathcal{E}_j - p p_j - \tau_2 \kappa_j) - \mathcal{G}(\beta,\tau,p)} dp_j d\kappa_j$$

$$\mathcal{E}_j = \frac{p_j^2}{2} + V(\kappa_j)$$

Non-acoustic chains: macroscopic behavior

T. Komorowski, S.O., 2016

For the harmonic dynamics

$$V(\Delta q_x) = \frac{\alpha}{2}(\Delta q_x)^2$$

with random moment exchange we obtain:

- Thermal conductivity is finite! (This provides a first rigorous counterexample for a one dimensional system with momentum conservation).
- Mechanical and thermal modes evolve at the same macroscopic time scale (diffusive). There is a direct macroscopic transfer of energy from the mechanical to the thermal modes.

Non-acoustic chains: mechanical and thermal non-equilibrium

With a non constant initial profiles of curvature and momentum and temperature, everything evolves on the diffusive scale

$$\left(\kappa_{[Nx]}(N^2 t), p_{[Nx]}(N^2 t), e_{[Nx]}(N^2 t)\right) \rightharpoonup (\kappa(x,t), p(x,t), e(x,t))$$

The temperature profile is defined by

$$T(x,t) = e(x,t) - \frac{\alpha\kappa(x,t)^2 + p(x,t)^2}{2}$$

and the macroscopic equations are the *damped Euler-Bernoulli beam equations*

Non acoustic: Damped Euler-Bernoulli beam equation

$$\partial_t \kappa(x,t) = -\partial_x^2 p(x,t),$$
$$\partial_t p(x,t) = \alpha \partial_x^2 \kappa(x,t) + \gamma \partial_x^2 p(x,t)$$
$$\partial_t T(x,t) = D_\gamma \partial_x^2 T(x,t) + \frac{\gamma}{2}(\partial_x p)^2$$

$$D_\gamma = \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{3}}\right)\frac{\alpha}{\gamma} + \gamma\right]$$

Non acoustic: Damped Euler-Bernoulli beam equation

$$\begin{aligned}
\partial_t \kappa(x,t) &= -\partial_x^2 p(x,t), \\
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\end{aligned}$$

$$D_\gamma = \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{3}}\right)\frac{\alpha}{\gamma} + \gamma\right]$$

It can be rewritten as

$$\begin{aligned}
\partial_t^2 \kappa(x,t) &= -\alpha \partial_x^4 \kappa(x,t) - \gamma \partial_x^2 p(x,t), \\
\partial_t T(x,t) &= D_\gamma \partial_x^2 T(x,t) + \frac{\gamma}{2} (\partial_x p)^2 \\
p(x,t) &= \partial_t \kappa(x,t)
\end{aligned}$$

Non-acoustic chain: non-linear interaction

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And V non linear.
Preliminar numerical simulations seems to confirm this conjecture (*G. Stoltz, J. Roussel*).

Wave function and Wigner distribution

Proofs of these results do not use relative entropy but L^2 norms in Fourier coordinates.

$$k_x = -\Delta q_x = 2q_x - q_{x+1} - q_{x-1}$$

Wave function and Wigner distribution

$$k_x = -\Delta q_x = 2q_x - q_{x+1} - q_{x-1}$$

$$\begin{aligned} \dot{k}_{xx}(t) &= -\Delta p_x(t) \\ dp_x(t) &= \Delta k_x dt \ + \gamma \Delta p_x(t) dt + dM_x(t), \end{aligned}$$

Dispersion function:

$$\omega(k) = 2\sqrt{\alpha} \sin^2(\pi k), \qquad k \in \mathbb{T}.$$

Wave function

$$\hat{f}(k) = \sum_{y \in \mathbb{Z}} f(y) e^{-i 2\pi y k}$$

Complex wave function in Fourier space:

$$\boxed{\hat{\psi}(t,k) := \sqrt{\alpha}\hat{k}(t,k) + i\hat{p}(t,k)}$$

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$$d\hat{\psi}(t,k) := -i\sqrt{\alpha}\sin^2(k)\hat{\psi}(t,k)dt - \gamma\sin^2(k)[\hat{\psi}(t,k) - \hat{\psi}(t,-k)^*]dt$$
$$+ \gamma^{1/2} i \int_{\mathbb{T}} r(k,k')[\hat{\psi}(k-k') - \hat{\psi}(-k+k')^*] d\hat{M}(t,k')$$

Wigner distribution

$$\widehat{W}_\epsilon(\eta, k, t) = \langle \psi^*(k - \epsilon\eta, t)\psi(k + \epsilon\eta, t)\rangle$$

$$W_\epsilon(y, k, t) = \epsilon \int_{(\mathbb{T}/\epsilon)} e^{i2\pi y\eta}\widehat{W}_\epsilon(\eta, k, t)\, d\eta$$

This is different from the energy $< \mathcal{E}_{[\epsilon^{-1}y]} >$, but can be proven that

$$W_\epsilon(y, k, t) - < \mathcal{E}_{[\epsilon^{-1}y]}(t) > \underset{\epsilon \to 0}{\longrightarrow} 0.$$

Mechanical and thermal energy

$$\partial_t \kappa(t,x) = -\partial_x^2 p(t,x),$$
$$\partial_t p(t,x) = \alpha \partial_x^2 \kappa(t,x) + \gamma \partial_x^2 p(t,x)$$

The macroscopic mechanical energy is:

$$e_{mech}(t,x) = \frac{\alpha}{2}\kappa(t,x)^2 + \frac{1}{2}p(t,x)^2$$

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The Macroscopic thermal energy is $e_{th}(t,x) = T(t,x)$:

$$\partial_t e_{th}(x,t) \ = \ D_\gamma \partial_x^2 e_{th}(t,x) + \ \frac{\gamma}{2}\left(\partial_x p(t,x)\right)^2$$

Theorem

$$W_\epsilon(t,dy,dk) \ \underset{\epsilon\to 0}{\longrightarrow} \ W(t,dy,dk)$$
$$W(t,dy,dk) = e_{th}(t,y)\ dk\ dy + e_{mech}(t,y)\delta_0(dk)\ dy$$