Hydrodynamic limit for a harmonic chain with random masses

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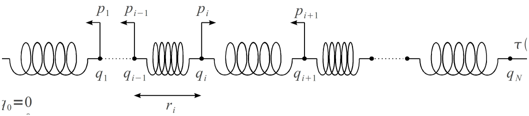
Chain of oscillators: infinite model



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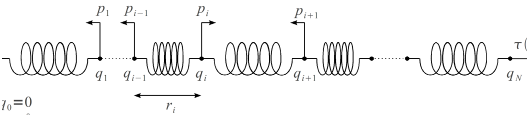

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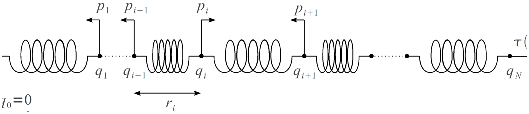

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We are interested in the *macroscopic* evolution of $(r_x(t), p_x(t), \mathcal{E}_x(t))$.

Gibbs measures and Thermodynamic Entropy

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

$$d\mu_{\beta,\tau,p} = \prod_x e^{-\beta(\mathcal{E}_x - \mathbf{p}p_x - \tau r_x) - \mathcal{G}(\beta,\tau,\mathbf{p})} dp_x dr_x$$

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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)

Theorem

(Fritz, Funaki, Lebowitz, PTRF 1994) Assume that probability ν *is translation invariant, stationary, finite entropy density, and the conditional measure* $\nu(dp|r)$ *is exchangeable.*
Then ν *is a convex combination of Gibbs measures* $d\mu_{\beta,\tau,p}$.

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- Chaoticity of the dynamics, due to the non-linearity of V, should give such ergodic property
- Adding conservative noise (stochastic collisions) to the dynamics one obtain ergodicity.

Hyperbolic Scaling, Euler equations

Local equilibrium: we expect the weak convergence to the hyperbolic system of PDE

$$r_{[Ny]}(Nt), p_{[Ny]}(Nt), \mathcal{E}_{[Ny]}(Nt) \rightharpoonup (r(y,t), p(y,t), \mathfrak{e}(y,t))$$

$$\begin{aligned}
\partial_t r(t,y) &= \partial_y p(t,y) \\
\partial_t p(t,y) &= \partial_y \tau[u(t,y), r(t,y)] \\
\partial_t \mathfrak{e}(t,y) &= \partial_y (\tau[u(t,y), r(t,y)] p(t,y))
\end{aligned}$$

$u = \mathfrak{e} - p^2/2$: internal energy.
For smooth solutions this is proven with conservative noise in the dynamics:

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

Harmonic Oscillators Chain

This is an example of a non-ergodic dynamics:

$$V(r) = r^2/2$$

in fact it is a *completely integrable dynamics*:

$$\dot{q}_x = p_x, \qquad \dot{p}_x = \Delta q_x = q_{x+1} + q_{x-1} - q_x,$$

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$$\hat{f}(k) = \sum_x f_x e^{i2\pi kx} \qquad k \in \Pi \sim [0,1]$$

$\omega(k) = |\sin(\pi k)|$ dispersion relation:

$$\mathcal{H} = \sum_x \mathcal{E}_x = \frac{1}{2} \int \left[\omega(k)^2 |\hat{q}(k)|^2 + |\hat{p}(k)|^2 \right] dk$$

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$$\frac{d}{dt}\hat{\psi}(t,k) = -i\omega(k)\hat{\psi}(t,k) \qquad \hat{\psi}(t,k) = e^{-i\omega(k)t}\hat{\psi}(0,k)$$

Harmonic Chain: Thermal Equilibrium

Consider the chain in *thermal* equilibrium: initial distribution with covariances

$$\langle\, r_x(0); r_{x'}(0) \,\rangle = \langle\, p_x(0); p_{x'}(0) \,\rangle = \beta^{-1}\delta_{x,x'}, \qquad \langle\, q_x; p_{x'} \,\rangle = 0,$$

for some inverse temperature β, while in *mechanical local equilibrium*:

$$\langle\, r_{[Ny]}(0) \,\rangle \longrightarrow r(0,y), \qquad \langle\, p_{[Ny]}(0) \,\rangle \longrightarrow p(0,y).$$

Harmonic Chain: Thermal Equilibrium

thermal equilibrium is conserved by the dynamics: for any $t \geq 0$

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Proof.

Thermal equilibrium is Fourier space is:

$$\langle\, \hat\psi(k,0)^*; \hat\psi(k',0) \,\rangle = 2\beta^{-1}\delta(k-k'), \qquad \langle\, \hat\psi(k,0); \hat\psi(k',0) \,\rangle = 0.$$

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Consequently

$$\langle\, \hat\psi(k,t)^*; \hat\psi(k',t) \,\rangle = e^{i(\omega(k)-\omega(k'))t} \langle\, \hat\psi(k,0)^*; \hat\psi(k',0) \,\rangle = 2\beta^{-1}\delta(k-k'$$

$$\langle\, \hat\psi(k,t); \hat\psi(k',t) \,\rangle = e^{-i(\omega(k)+\omega(k'))t} \langle\, \hat\psi(k,0); \hat\psi(k',0) \,\rangle = 0.$$

□

Harmonic Chain: Thermal Equilibrium implies Euler Equation limit

$r_{[Ny]}(Nt)$ and $p_{[Ny]}(Nt)$ converge weakly to the solution of the linear wave equation

$$\partial_t \mathbf{r}(y,t) = \partial_y \mathbf{p}(y,t), \qquad \partial_t \mathbf{p}(y,t) = \partial_y \mathbf{r}(y,t).$$

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For the energy, because of the thermal equilibrium, for any $t \geq 0$:

$$\langle \mathcal{E}_x(t) \rangle = \beta^{-1} + \frac{1}{2}\left(\langle p_x(t) \rangle^2 + \langle r_x(t) \rangle^2\right)$$

$$\langle \mathcal{E}_{[Ny]}(Nt) \rangle \longrightarrow \mathbf{e}(y,t) = \beta^{-1} + \frac{1}{2}\left(\mathbf{p}^2(y,t) + \mathbf{r}^2(y,t)\right),$$

$$\partial_t \mathbf{e}(y,t) = \partial_y \left(\mathbf{p}(y,t)\,\mathbf{r}(y,t)\right).$$

Harmonic Chain: Local Thermal Equilibrium is not conserved

The argument fails dramatically if the system is not in thermal equilibrium, even local thermal Gibbs

$$\langle\, r_x(0); r_{x'}(0)\, \rangle = \langle\, p_x(0); p_{x'}(0)\, \rangle = \beta^{-1}\left(\frac{x}{N}\right)\delta_{x,x'}, \quad \langle\, q_x(0); p_{x'}(0)\, \rangle = 0 \tag{1}$$

is not conserved, and correlations between $p_x(t)$ and $r_x(t)$ build up in time.

No autonomous macroscopic equation for the energy!

There are infinite many conservation laws.

Wigner distribution

$\xi \in \mathbb{R},\ k \in [0,1]$,

$$\widehat{W}_N(\xi, k, t) \ := \ \frac{2}{N} \left\langle\!\!\left\langle \hat{\psi}^* \left(Nt, k - \frac{\xi}{2N}\right) \hat{\psi}\left(Nt, k + \frac{\xi}{2N}\right) \right\rangle\!\!\right\rangle$$

$$W_N(y, k, t) = \int \widehat{W}_N(t, \eta, k) e^{-i2\pi\xi y} \, d\eta, \qquad y \in \mathbb{R},$$

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$$W_N(y, k, t) = \int \widehat{W}_N(t, \eta, k) e^{-i2\pi\xi y} \, d\eta, \qquad y \in \mathbb{R},$$

In the limit it decompose in a thermal and a mechanical part:

$$\lim_{N\to\infty} \widehat{W}_N(\xi, k, t) = \widehat{W}_{th}(\xi, k, t) + \widehat{W}_m(\xi, t) \, \delta_0(dk) \qquad (2)$$

The mechanical part $\widehat{W}_m(\xi, t)$ is the Fourier transform of the mechanical energy

$$\widehat{W}_m(\xi, t) = \int \frac{1}{2} \left(\mathbf{p}^2(y, t) + \mathbf{r}^2(y, t) \right) e^{i2\pi\xi y} \, dy,$$

Wigner distribution

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$$\partial_t W_{th}(y,k,t) + \frac{\omega'(k)}{2\pi}\partial_y W_{th}(y,k,t) = 0.$$

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in fact for $k \neq 0$

$$\begin{aligned} \widehat{W}_N(\xi,k,t) \; &:= \; e^{i\left[\omega\left(k-\frac{\xi}{2N}\right)-\omega\left(k+\frac{\xi}{2N}\right)\right]Nt}\,\widehat{W}_N(\xi,k,0) \\ &\underset{N\to\infty}{\sim} \; e^{-i\omega'(k)\eta t}\,\widehat{W}_{th}(0,\eta,k) \end{aligned}$$

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$$W(t,y,k) = W(0, y - \frac{\omega'(k)}{2\pi}t, k)$$

Phonon of wave number k moves freely with velocity $\frac{\omega'(k)}{2\pi}$.

Wigner distribution

Consequently the thermal energy $\tilde{\mathbf{e}}(y,t)$ (i.e. temperature) evolves non autonomously following the equation

$$\partial_t \tilde{\mathbf{e}}(y,t) + \partial_y J(y,t) = 0, \qquad J(y,t) = \int \omega'(k) W_{th}(y,k,t)\, dk.$$

We say that the system is in *local equilibrium* if $W_{th}(y,k) = \beta^{-1}(y)$ constant in k.
Starting in thermal equilibrium means $W_{th}(y,k,0) = \beta^{-1}$ and trivially $W_{th}(y,k,t) = \beta^{-1}$ for any $t > 0$.
But starting with local equilibrium, i.e. $W(y,k,0) = \beta^{-1}(y)$ constant in k, we have a non autonomous evolution of $\tilde{e}(y,t)$.

Harmonic Chain with Random Masses

The problem with the harmonic chain is that thermal waves of wavenumber k *move* with speed $\omega'(k)$, if they are not uniformed distributed (i.e. the system is not in thermal equilibrium), the temperature profile will not remain constant, as it should be following the Euler equations.

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If the masses are random, the thermal modes remains localized (frozen), by Anderson localization. This allows to close the energy equation, **without local equilibrium**.

Harmonic Chain with Random Masses

(F. Huveneers, C. Bernardin, S.Olla, 2017)

$\{m_x\}$ i.i.d. with absolutely continuous distribution,
$0 < m_- \leq m_x \leq m_+$,
$\overline{m} = \mathbb{E}(m_x)$.

$$m_x \dot{q}_x(t) = p_x(t), \qquad \dot{p}_x(t) = \Delta q_x(t), \qquad x = 1, \dots, N$$

with $q_0 = q_1$ and $q_{N+1} = q_N$ as boundary conditions.

Gibbs States, Local Gibbs States

The Gibbs states are characterized by three parameters: $\beta > 0$ and $p, r \in \mathbb{R}$. Its probability density writes

$$\prod_{x=1}^{N} \frac{e^{-\frac{\beta m_x}{2}\left(\frac{p_x}{m_x} - \frac{p}{\bar{m}}\right)^2 - \frac{\beta}{2}(r_x - r)^2}}{Z(\beta, p, r, m_x)}.$$

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We start with a local Gibbs state:

$$\prod_{x=1}^{N} \frac{e^{-\frac{\beta(x/N) m_x}{2}\left(\frac{p_x}{m_x} - \frac{p(x/N)}{\overline{m}}\right)^2 - \frac{\beta(x/N)}{2}(r_x - r(x/N))^2}}{Z(\beta(x/N), p(x/N), r(x/N), m_x)}.$$

Harmonic Chain with Random Masses: hydrodynamic limit

Almost surely with respect to $\{m_x\}$:

$$< r_{[Ny]}(Nt) >, < p_{[Ny]}(Nt) >, < \mathcal{E}_{[Ny]}(Nt) > \rightharpoonup (\mathbf{r}(y,t), \mathbf{p}(y,t), \mathfrak{e}(y,t))$$

$$\begin{aligned} \partial_t \mathbf{r}(t,y) &= \frac{1}{\overline{m}} \partial_y \mathbf{p}(t,y) \\ \partial_t \mathbf{p}(t,y) &= \partial_y \mathbf{r}(t,y) \\ \partial_t \mathfrak{e}(t,y) &= \frac{1}{\overline{m}} \partial_y \left(\mathbf{r}(t,y) \mathbf{p}(t,y) \right) \end{aligned}$$

with initial conditions:

$$\mathbf{r}(y,0) = r(y), \qquad \mathbf{p}(y,0) = p(y), \qquad \mathfrak{e}(y,0) = \frac{1}{\beta(y)} + \frac{p^2(y)}{2\overline{m}} + \frac{r^2(y)}{2}.$$

Random Masses: Localization of Thermal Modes

Equation of motion can be written as

$$\ddot{r}_x = -(\nabla^* M^{-1} \nabla r)_x \quad (1 \le x \le N-1), \qquad \ddot{p}_x = \left(\Delta M^{-1} p\right)_x \quad (1 \le x \le N),$$

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$$M^{-1/2}(-\Delta) M^{1/2} \varphi^k = \omega_k^2 \, \varphi^k, \qquad k = 0, \dots, N-1.$$

$$\psi^k = M^{-1/2} \varphi^k, \qquad M^{-1} \Delta \psi^k = \omega_k^2 \psi_k$$

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$$r(t) = \sum_{k=1}^{N-1} \left(\frac{\langle \nabla \psi^k, r(0) \rangle}{\omega_k} \cos \omega_k t + \langle \psi^k, p(0) \rangle \sin \omega_k t \right) \frac{\nabla \psi^k}{\omega_k},$$

$$p(t) = \sum_{k=0}^{N-1} \left(\langle \psi^k, p(0) \rangle \cos \omega_k t - \frac{\langle \nabla \psi^k, r(0) \rangle}{\omega_k} \sin \omega_k t \right) M \psi^k.$$

Localization of Thermal Modes

Localization length ξ_k diverges with N:

$$\xi_k^{-1} \sim \omega_k^2 \sim \left(\frac{k}{N}\right)^2,$$

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More precisely: for $0 < \alpha < \frac{1}{2}$

$$\mathbb{E}\left(\sum_{k=N^{1-\alpha}}^{N-1} |\psi_x^k \psi_{x'}^k|\right) \le Ce^{-cN^{-2\alpha}|x-x'|}.$$

This estimate is enough to prove that thermal modes remains localized and do not *move* macroscopically.