The mathematical derivation of thermodynamic laws from interacting oscillators

Marielle Simon

Full microscopic description

Bulk dynamics $(j = 1, \dots, n)$

$$\mathrm{d}r_j(t) = (p_j(t) - p_{j-1}(t))\,\mathrm{d}t$$

$$\mathrm{d}p_j(t) = \underbrace{(r_{j+1}(t) - r_j(t))\,\mathrm{d}t}_{\text{hamiltonian}} \underbrace{- 2p_j(t^-)\,\mathrm{d}\mathcal{N}_j(\gamma t)}_{\text{flip of intensity } \gamma}, \qquad j \neq n$$

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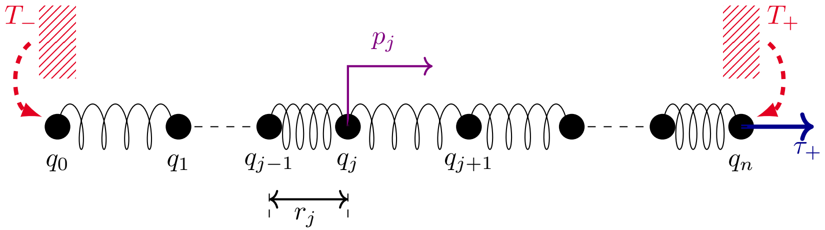
Boundary conditions? We add **two mechanisms**



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Langevin thermostat: Assume that $(q(t), p(t)) \in \mathbb{R} \times \mathbb{R}$ follows

$$\begin{cases} \mathrm{d}q(t) = p(t)\mathrm{d}t \\ \mathrm{d}p(t) = -V'(q(t))\mathrm{d}t \underbrace{-\sigma p(t)\mathrm{d}t}_{\text{dissipation}} + \underbrace{\sqrt{2\sigma\beta^{-1}}\,\mathrm{d}w(t)}_{\text{brownian fluctuation}} \end{cases}$$

then the invariant proba measure is the **equilibrium Gibbs measure**

$$\frac{\exp(-\beta\mathcal{H}(p,q))}{Z}\mathrm{d}q\mathrm{d}p \quad \text{at } \textbf{temperature } \beta^{-1} \quad \text{with } \mathcal{H} = \frac{p^2}{2} + V(q)$$

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$$\mathrm{d}p_0(t) = (r_1(t) - 0)\,\mathrm{d}t \underbrace{-2p_0(t^-)\,\mathrm{d}\mathcal{N}_0(\gamma t)}_{\text{flip of intensity } \gamma} \underbrace{-\,p_0(t)\,\mathrm{d}t + \sqrt{2T_-}\mathrm{d}w_0(t)}_{\text{Langevin at } T_- \text{ (intensity } \sigma = 1)},$$

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The local Gibbs initial measure

Let $\mathbf{r}_{\mathrm{ini}} : [0,1] \to \mathbb{R}$ and $T_{\mathrm{ini}} : [0,1] \to (0,+\infty)$ be **continuous**.

Then $\mathbf{e}_{\mathrm{ini}}(x) = T_{\mathrm{ini}}(x) + \frac{1}{2}\mathbf{r}_{\mathrm{ini}}^2(x)$ is the **total energy profile**.

A **typical example** of initial probability measure is

$$\mathrm{d}\nu_{\mathrm{ini}}^n = \frac{e^{-\frac{1}{2}p_0^2/T_0}}{\sqrt{2\pi T_0}} \prod_{j=1}^n \frac{e^{-\frac{1}{2}\left(p_j^2+(r_j-\mathbf{r}_{\mathrm{ini}}(\frac{j}{n}))^2\right)/T_j}}{2\pi T_j} \mathrm{d}p_j \mathrm{d}r_j, \quad T_j := T_{\mathrm{ini}}(\tfrac{j}{n})$$

i.e. the **local Gibbs measure**, which satisfies (indeed)

$$\frac{1}{n}\sum_{j=1}^n G\left(\tfrac{j}{n}\right)\mathbb{E}\left[r_j(0)\right] \xrightarrow[n\to\infty]{} \int_0^1 G(x)\mathbf{r}_{\mathrm{ini}}(x)\mathrm{d}x$$

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Macroscopic evolution of volume and energy profiles

? Hydrodynamic limit ✚ Boundary conditions

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THEOREM: when $T_-, T_+ > 0$ **[Komorowski, Olla, S. 2020]**

$$\frac{1}{n}\sum_{j=0}^{n} G\big(\tfrac{j}{n}\big)\ \mathbb{E}\big[r_j(tn^2)\big] \xrightarrow[n\to\infty]{} \int_0^1 G(x)\ \mathbf{r}(t,x)\ \mathrm{d}x$$

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with $\mathbf{r}(0,\cdot) = \mathbf{r}_{\text{ini}}$, $\mathbf{e}(0,\cdot) = \mathbf{e}_{\text{ini}}$

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$$\partial_t \mathbf{r} = \frac{1}{2\gamma}\partial_{xx}\mathbf{r}, \qquad \partial_t \mathbf{e} = \frac{1}{4\gamma}\partial_{xx}\Big(\mathbf{e} + \frac{\mathbf{r}^2}{2}\Big)$$

and

$$\begin{cases} \mathbf{r}(t,0) = 0 \\ \mathbf{e}(t,0) = T_- \end{cases} \qquad \begin{cases} \mathbf{r}(t,1) = \tau_+ \\ \mathbf{e}(t,1) = T_+ + \frac{1}{2}\tau_+^2 \end{cases}$$

- **Elongation**

$$\partial_t \mathbf{r}(t,x) = \frac{1}{2\gamma}\partial_{xx}\mathbf{r}(t,x)$$

- **Total energy**

$$\boxed{\mathbf{e}(t,x) = \underbrace{\mathbf{e}^{\mathrm{th}}(t,x)}_{\text{temperature}} + \mathbf{e}^{\mathsf{mech}}(t,x)}$$

with

$$\mathbf{e}^{\mathsf{mech}}(t,x) = \frac{1}{2}\mathbf{r}^2(t,x)$$

$$\partial_t \mathbf{e}^{\mathrm{th}}(t,x) = \frac{1}{4\gamma}\partial_{xx}\mathbf{e}^{\mathrm{th}}(t,x) + \frac{1}{2\gamma}\underbrace{\big(\partial_x \mathbf{r}(t,x)\big)^2}_{\substack{\text{dissipation}\\ \text{of mechanical energy}\\ \text{into thermal energy}}}$$

Stationary profile

Stationary solutions: $\mathbf{r}_\infty(\cdot)$ and $\mathbf{e}^{\mathrm{th}}_\infty(\cdot)$

$$\mathbf{r}_\infty(x) = \tau_+ \, x$$

$$\mathbf{e}^{\mathrm{th}}_\infty(x) = \tau_+^2 \, x(1-x) + (T_+ - T_-)\, x + T_-$$

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heating inside the system

- and with **stationary current**

$$J_\infty = -\frac{1}{4\gamma}(T_+ - T_- + \tau_+^2) < 0 \quad \text{if} \quad T_- > T_+ \text{ and } \tau_+ \text{ is large}$$

uphill diffusion

A little flavour of the proof

A few elements of proof

1. Estimate **boundary terms**: for instance

$$\left| \int_0^t \mathbb{E}\big[p_0(sn^2)\big] \, \mathrm{d}s \right| \lesssim \frac{1}{n} \qquad \left| \int_0^t \mathbb{E}\big[p_n(sn^2)\big] \, \mathrm{d}s \right| \lesssim \frac{1}{n}$$

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2. $\mathbf{L}^2$ **bound** on averages:

$$\frac{1}{n} \sum_{j=0}^{n} \left[\Big(\mathbb{E}\big[r_j(sn^2)\big]\Big)^2 + \Big(\mathbb{E}\big[p_j(sn^2)\big]\Big)^2 \right] \lesssim 1$$

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$\Rightarrow$ Hydrodynamic limit for the **volume** and **mechanical energy**:

$$\frac{1}{n} \sum_{j=0}^{n} G\big(\tfrac{j}{n}\big) \, \mathbb{E}\big[r_j(tn^2)\big] \xrightarrow[n\to\infty]{} \int_0^1 G(x) \, \mathbf{r}(t,x) \, \mathrm{d}x$$

$$\frac{1}{n} \sum_{j=0}^{n} G\big(\tfrac{j}{n}\big) \, \underbrace{\tfrac{1}{2}\Big(\mathbb{E}[r_j]^2 + \mathbb{E}[p_j]^2\Big)(tn^2)}_{\mathcal{E}_j^{\mathrm{mech}}(tn^2)} \xrightarrow[n\to\infty]{} \int_0^1 G(x) \, \underbrace{\tfrac{1}{2}\mathbf{r}^2(t,x)}_{\mathbf{e}^{\mathrm{mech}}} \, \mathrm{d}x$$

A few elements of proof (bis)

4. Try to **close the equation for the energy**

$$\frac{1}{n}\sum_{j=0}^{n} G(\tfrac{j}{n})\mathbb{E}\big[e_j(tn^2) - e_j(0)\big]$$

$$= -\frac{n^2}{n}\sum_{j=0}^{n} G(\tfrac{j}{n})\int_0^t \mathbb{E}\big[\big(\underbrace{\mathbf{J}_{j,j+1}}_{\text{current}} - \mathbf{J}_{j-1,j}\big)(sn^2)\big]\mathrm{d}s$$

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NB: after recentering, everything goes to 0 *except* $\mathbb{E}[r_j]\mathbb{E}[r_{j+1}] \sim \mathbf{r}^2(t,\frac{j}{n})$

We need **new ingredients!**

6. An **energy** bound:

$$\sup_{s\in[0,t]} \frac{1}{n}\sum_{j=0}^{n} \mathbb{E}\big[e_j(sn^2)\big] \lesssim 1$$

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7. The **control of covariances**, for instance

$$\frac{1}{n}\sum_{j=0}^{n} G(\tfrac{j}{n}) \int_0^t \mathbb{E}\big[p_j p_{j+1}(sn^2)\big]\mathrm{d}s \xrightarrow[n\to+\infty]{} 0$$

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and **new limits at the boundaries** like e.g.

$$\frac{1}{t}\int_0^t \underbrace{\mathbb{E}\big[(p_1-\mathbb{E}[p_1])^2(sn^2)\big]}_{\text{variance of } p_1}\mathrm{d}s \xrightarrow[n\to+\infty]{} T_-.$$

How? 1. and 2. $\rightarrow$ Time evolution of averages

We have a closed system of evolution for the **averages**:

$$\overline{p}_j(t) := \mathbb{E}[p_j(t)], \qquad \overline{r}_j(t) := \mathbb{E}[r_j(t)]$$

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In the **bulk**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{r}_j(t) = n^2\big(\overline{p}_j(t) - \overline{p}_{j-1}(t)\big)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p}_j(t) = n^2\big(\overline{r}_{j+1}(t) - \overline{r}_j\big) - 2\gamma n^2\ \overline{p}_j(t)$$

and at the **boundaries**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p}_0(t) = n^2\overline{r}_1(t) - n^2(2\gamma+1)\overline{p}_0(t)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p}_n(t) = -n^2\overline{r}_n(t) + n^2\ \overline{\tau}_+ - n^2(2\gamma+1)\overline{p}_n(t)$$

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$$\frac{\mathrm{d}S}{\mathrm{d}t}(t) = -A_\gamma S(t) - S(t)A_\gamma^{\mathrm{T}} + 4\gamma \begin{pmatrix} 0 & 0 \\ 0 & D \end{pmatrix}$$

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with A_γ only depends on γ and

$$D = \mathrm{Diag}\big(T_-, \mathbb{E}[p_1^2], \ldots, \mathbb{E}[p_n^2]\big).$$

Thanks to the control of covariances

An interesting **additional** result is the following **equipartition** between **fluctuations** of distances and momenta

$$\int_0^t \frac{1}{n} \sum_{j=0}^{n} G\big(s, \tfrac{j}{n}\big)\ \mathbb{E}\Big[\big(r_j - \overline{r}_j\big)^2 - \big(p_j - \overline{p}_j\big)^2\Big](sn^2)\ \mathrm{d}s \xrightarrow[n\to\infty]{} 0.$$

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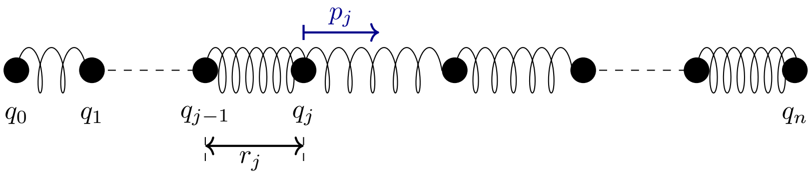
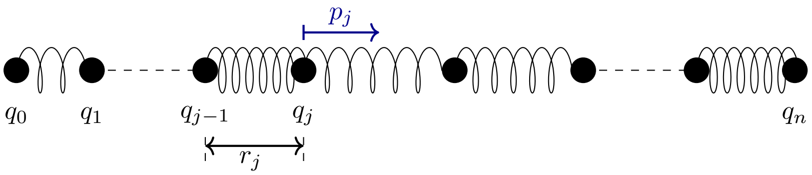
▷ This allows us to identify the **thermal energy** as the limit

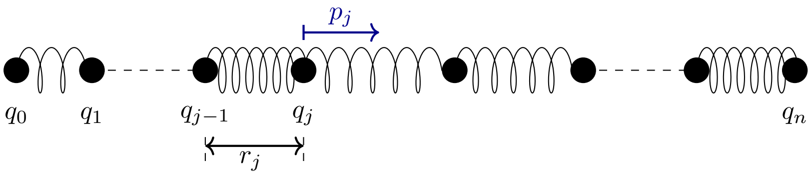
$$\int_0^t \frac{1}{n}\sum_{j=0}^{n} G(s, \tfrac{j}{n})\mathbb{E}\big[p_j^2(sn^2)\big]\mathrm{d}s \xrightarrow[n\to+\infty]{} \int_0^t \int_0^1 G(s,x)\mathbf{e}^{\mathrm{th}}(s,x)\mathrm{d}x\mathrm{d}s.$$

Conclusion





1) Purely harmonic chain $\rightarrow$ **transport** of energy phonons



1) **Purely harmonic** chain $\rightarrow$ **transport** of energy phonons

2) Add **stochastic FLIP noise** $\rightarrow$ **diffusion of total energy**

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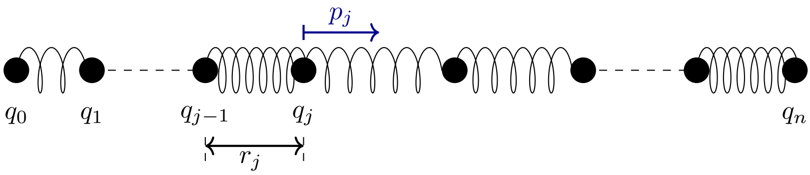
Conclusion



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3) Add **stochastic EXCHANCE noise** $\to$ **fractional diffusion**

$$\partial_t e^{\text{th}}(t,x) = -\frac{\kappa}{\sqrt{\gamma}}|\partial_x|^{3/4} e^{\text{th}}(t,x)$$

Thank you for your attention!

  

▷ T. Komorowski, S. Olla, M. Simon. **Hydrodynamic limit for a chain with thermal and mechanical boundary forces**

Electron. J. Probab. 26 (2021), 1–49

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