Macroscopic evolution of mechanical and thermal energy in a harmonic chain

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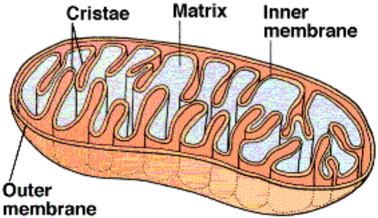
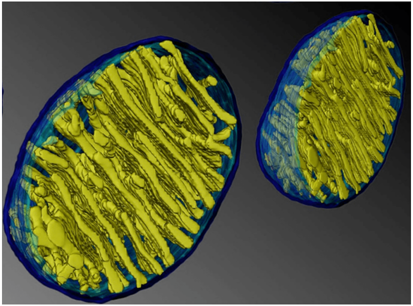
Heat production in mitochondria

The mitochondria: “powerhouse of the cells” (Siekevitz, 1957)



- actively respiring mitochondria **heat up**
- heat production occurs across the cristae membranes, which typically lie **in parallel**, potentially retaining heat $\simeq$ **radiator**



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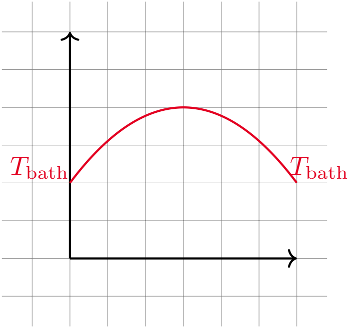

Temperature profile

Non-equilibrium phenomenon

[PLoS Biol 2017, 2018]

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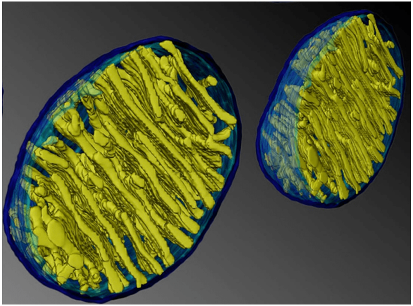

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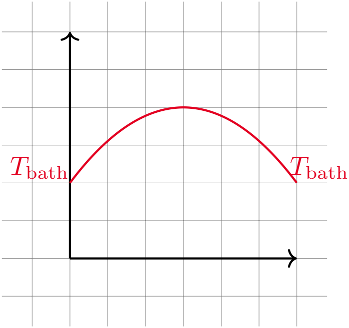

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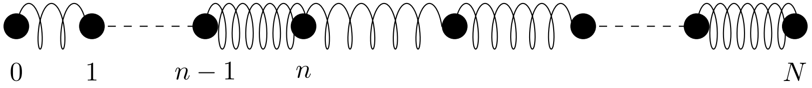
▷ Illustration of **conversion of work into heat**: microscopic model **?**

One-dimensional chain of oscillators

Microscopic model

- $1d$ chain of $N+1$ **unpinned coupled oscillators**



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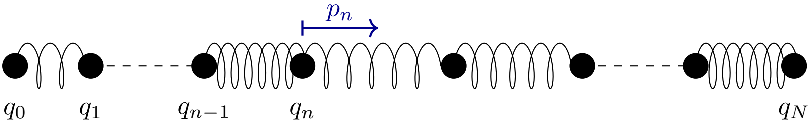

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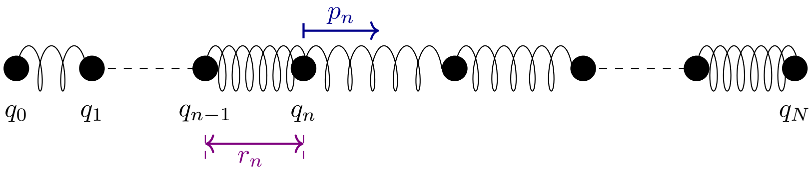

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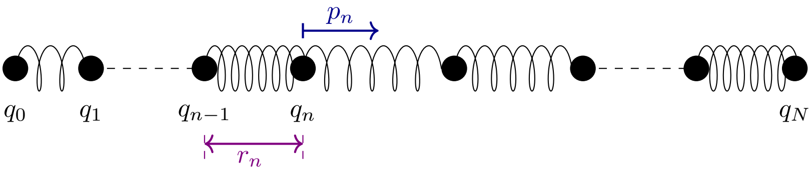

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- **Dynamics** on the configurations of particles

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

Hamiltonian dynamics

Total energy = Hamiltonian

$$\mathcal{H}_N := \frac{p_0^2}{2} + \sum_{n=1}^{N} \mathcal{E}_n \qquad \text{with} \qquad \mathcal{E}_n := \frac{p_n^2}{2} + \underbrace{V(r_n)}_{\textbf{interaction}} + \underbrace{\cancel{W(q_n)}}_{\textbf{no pinning}}$$

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$$\begin{aligned} \dot{r}_n(t) &= p_n(t) - p_{n-1}(t) \\ \dot{p}_n(t) &= V'(r_{n+1})(t) - V'(r_n)(t) \end{aligned} \qquad (\star)$$

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3. Stochastic Langevin **thermostats**: ensure $\mathbb{E}\big[p_0^2\big] = T_-$, $\mathbb{E}[p_N^2] = T_+$.

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$$\sum_{n=1}^{N} \frac{p_n^2}{2} + V(r_n) \ \textbf{(energy)} \qquad \text{and} \qquad \sum_{n=1}^{N} r_n \ \textbf{(volume)}$$

Harmonic interactions

GOAL:

- Distribute $\{r_n(0), p_n(0)\}$ **randomly** $\sim \mu_0^N$

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HARD question with a **long** history!

- Quite **few results** for a generic choice of V
- Rigorous results with the **harmonic choice** $V(r) = \frac{r^2}{2}$

Harmonic potential and periodic b.c.

Harmonic case: $V(r) = \frac{r^2}{2}$ then... $\mathcal{E}_n = \frac{1}{2}(r_n^2 + p_n^2)$ and $(\star)$ is **linear!**

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- ❗ In the **harmonic** case there are much **more** conservation laws

$$\mathcal{R}_N = \sum r_n, \qquad \mathcal{H}_N = \sum \mathcal{E}_n, \qquad \text{but also } \mathcal{P}_N = \sum p_n, \dots$$

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- Thanks to linearity, one can use **Fourier transforms**

Towards diffusion of heat?

In the pure harmonic case, one can easily see

- transport of any **energy phonon** $\rightarrow$ **no diffusion**

  $\varphi(t,k) = 2|\sin(\pi k)|\widehat{q}(t,k) + i\widehat{p}(t,k), \qquad k \in \{0, \frac{1}{n}, \ldots, \frac{n-1}{n}\}$ (Fourier modes)

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Too many conservation laws! We add a **stochastic noise** which

- keeps **only two** conservation laws: **energy** and **volume**
- models the effect of **nonlinearity** in V'
- allows us to prove convergences rigorously

Harmonic chain with stochastic noise in the diffusive time scale

Stochastic perturbation

Property of the **stochastic noise**: have to preserve $\mathcal{H}_N$ and $\mathcal{R}_N$

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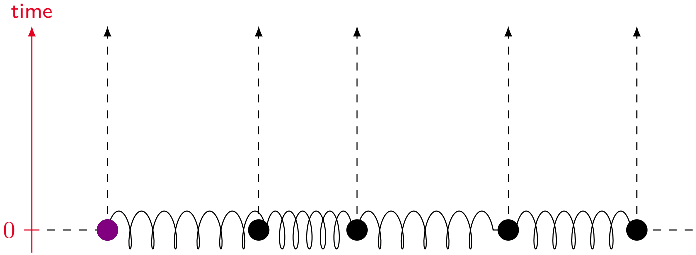

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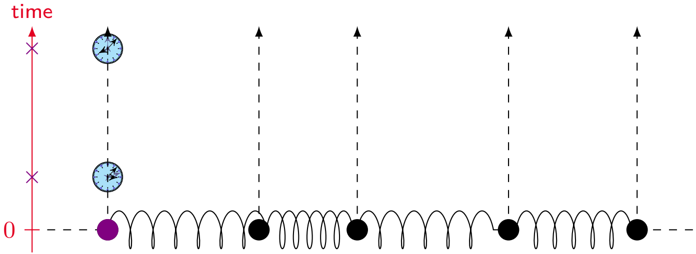

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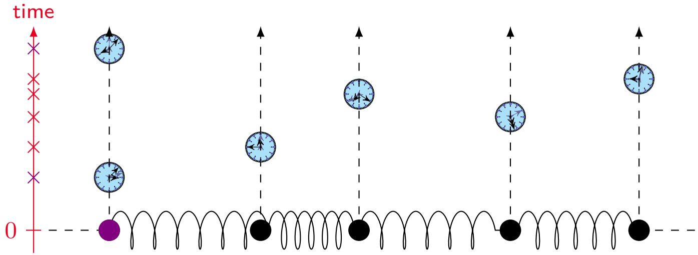

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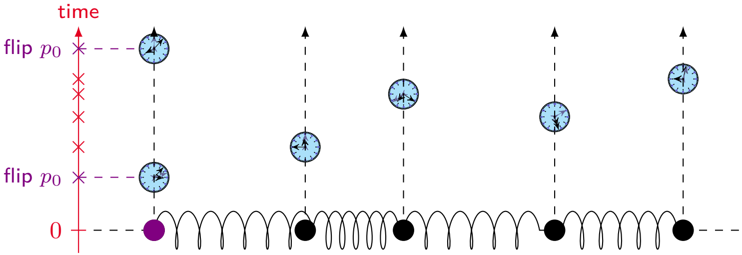

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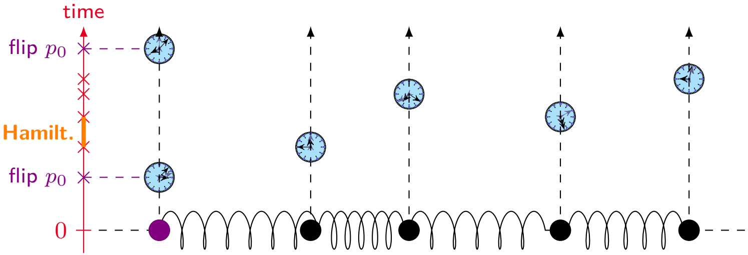

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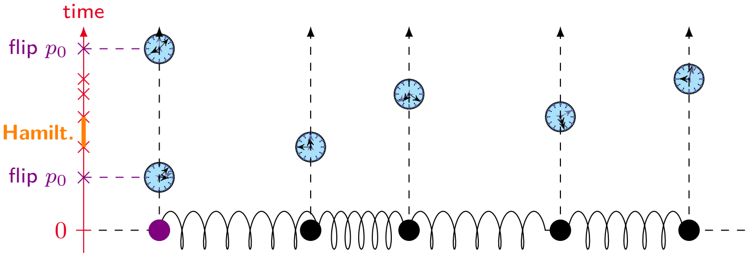

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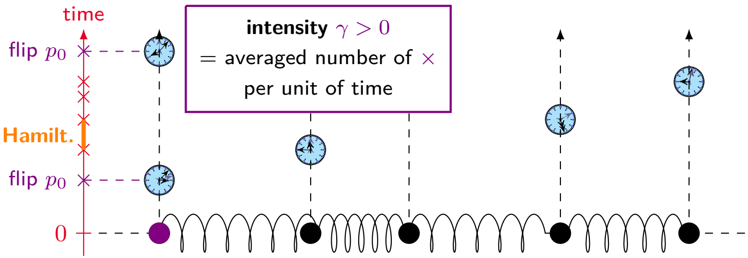

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Full microscopic description

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

$$\mathrm{d}r_n(t) = (p_n(t) - p_{n-1}(t))\,\mathrm{d}t$$

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

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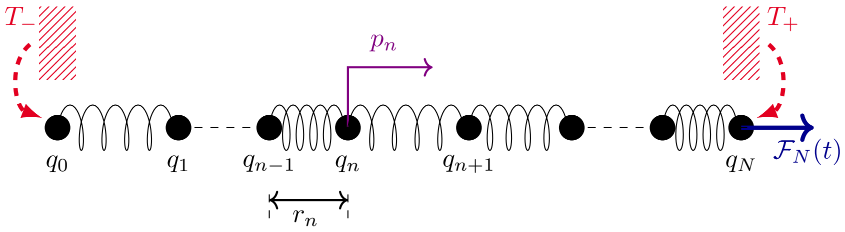
Boundary conditions? We add **two mechanisms**



Evolution at the boundaries?

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

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

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

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

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Finally, at the **boundaries**,

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

$$\mathrm{d}p_N(t) = -\,\big(r_N(t) - \mathcal{F}_N(t)\big)\,\mathrm{d}t \underbrace{-2p_N(t^-)\,\mathrm{d}\mathcal{N}_N(\gamma t)}_{\text{flip of intensity } \gamma}$$

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From the microscopic description to macroscopic equations

Full dynamics in the diffusive time scale:

Hamiltonian + Flip noise + Boundary force and thermostats

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Initial measure μ_0^N: Given some profiles $\mathbf{r}_{\text{ini}}(\cdot)$ and $\mathbf{e}_{\text{ini}}(\cdot)$

$$\frac{1}{N}\sum_{n=0}^{N} G\big(\tfrac{n}{N}\big)\mathbb{E}\big[r_n(0)\big] \xrightarrow[N\to\infty]{} \int_0^1 G(x)\mathbf{r}_{\text{ini}}(x)\mathrm{d}x$$

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+ initial second moment and entropy bounds

Macroscopic evolution of volume and energy profiles

? Hydrodynamic limit $\simeq$ **law of large numbers** $\rightarrow$ **diffusion of energy?**

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

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▷ **Elongation**

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Stationary profile

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

$$\mathbf{r}_\infty(x) = \overline{F}\, x$$

$$e_\infty^{\mathrm{heat}}(x) = \overline{F}^2\, x(1-x) + (T_+ - T_-)\, x + T_-$$

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- and with **stationary current**

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- and with **stationary current**

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

uphill diffusion

A new boundary condition when $T_+ \equiv 0$

The **boundary force** writes

$$\mathcal{F}_N(t) = \underbrace{\overline{F}}_{\text{average}} + \underbrace{\widetilde{\mathcal{F}}_N(t)}_{\text{periodic}} \qquad \text{with } \widetilde{\mathcal{F}}_N(t) = \frac{1}{\sqrt{N}} \sum_{\ell \neq 0} \widehat{\mathcal{F}}(\ell) e^{i\ell\omega t}$$

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The **macroscopic equations** become:

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NB ✎ $(\overline{F}\partial_x r(t,1) + 4\gamma \mathbb{W}^{\text{heat}})$ comes from the **total work** by the force and $\mathbb{W}^{\text{heat}}$ comes from the **fluctuating** part $\widetilde{\mathcal{F}}_N$.

Total work done by the force

We define the **average work** done in the **diffusive time** scale:

$$W_N(t) = \frac{1}{N}\int_0^{tN^2} \mathcal{F}_N(s)\,\mathbb{E}[p_N](s)\mathrm{d}s$$

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- In the **bulk**, the **mechanical energy** is transformed into the **thermal one** at the rate $\frac{1}{2\gamma}(\partial_x r(t,x))^2$
- **Stationary profile:** still a parabola with

$$e_\infty^{\text{heat}}(0) = T_-, \qquad e_\infty^{\text{heat}}(1) = \overline{F}^2 + 4\gamma\mathbb{W}^{\text{heat}} + T_-$$

A little flavour of the proof

A few elements of proof

1. Estimate boundary terms: for instance

$$\left| \int_0^t \mathbb{E}\big[p_0(sN^2)\big] \, \mathrm{d}s \right| \leqslant \frac{C(t+1)}{N} \qquad \left| \int_0^t \mathbb{E}\big[p_N(sN^2)\big] \, \mathrm{d}s \right| \leqslant \frac{C(t+1)}{N}$$

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2. L^2 bound on averages:

$$\frac{1}{N}\sum_{n=0}^{N} \Big[\big(\mathbb{E}\big[r_n(s)\big]\big)^2 + \big(\mathbb{E}\big[p_n(s)\big]\big)^2 \Big] \leqslant C$$

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3. **Energy bound (via control of entropy production):**

$$\frac{1}{N} \sum_{n=0}^{N} \mathbb{E}\big[\mathcal{E}_n(tN^2)\big] \leqslant C(t+1)$$

Time evolution of averages

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

$$\overline{p}_n(t) := \mathbb{E}[p_n(t)], \qquad \overline{r}_n(t) := \mathbb{E}[r_n(t)]$$

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and at the **boundaries**:

$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p}_0(t) = N^2\overline{r}_1(t) - N^2(2\gamma+1)\overline{p}_0(t)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\overline{p}_N(t) = -N^2\overline{r}_N(t) + N^2\,\mathcal{F}_N(t) - N^2(2\gamma+1)\overline{p}_N(t)$$

Control of covariances

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

$$\int_0^t \frac{1}{N}\sum_{n=0}^{N} G\big(\tfrac{n}{N}, s\big)\ \mathbb{E}\Big[\big(r_n - \overline{r}_n\big)^2 - \underbrace{\big(p_n - \overline{p}_n\big)^2}_{\sim\ \text{thermal}}\Big](sN^2)\ ds \xrightarrow[N\to\infty]{} 0.$$

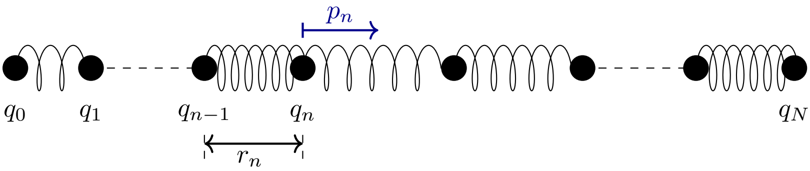
▷ Thanks to a good **control of covariances**. Let

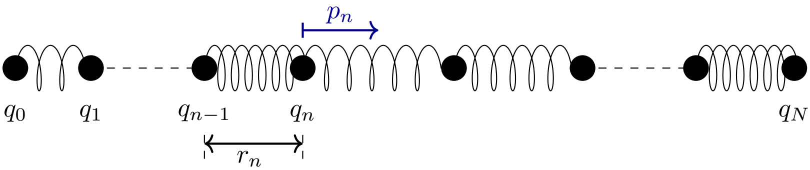
$$\mathcal{C}_N(t) := \frac{1}{N}\sum_{n,k=0}^{N}\Big(\mathrm{Cov}(p_n, r_k)^2 + \mathrm{Cov}(p_n, p_k)^2 + \mathrm{Cov}(r_n, r_k)^2\Big)(tN^2)$$

Then

$$\boxed{\mathcal{C}_N(t) \lesssim \mathcal{C}_N(0) + Ct\log^2(N)}$$

Conclusion





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

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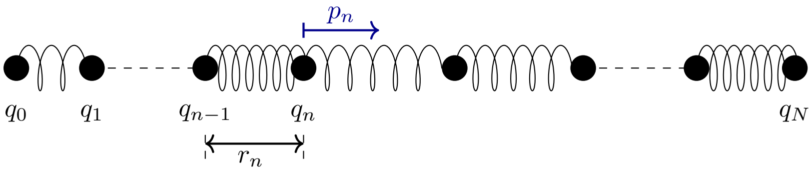

1) **Purely harmonic** chain $\rightarrow$ **transport** of energy phonons

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

$$\partial_t \mathbf{e}(t,x) = \frac{1}{4\gamma}\partial_{xx}\big(\mathbf{e} + \tfrac{1}{2}\mathbf{r}^2\big), \qquad \mathbf{e} = \tfrac{1}{2}\mathbf{r}^2 + e^{\text{heat}}$$

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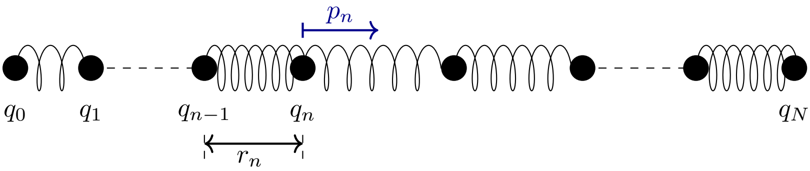

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3) Conversion of **work** into **heat** via a simple **microscopic model**
→ derivation of different boundary conditions
→ in particular, the **uphill phenomenon**

Thank you for your attention!

Komorowski T., Olla S. and Simon M.

- **Heat flow in a periodically forced, unpinned thermostatted chain**, *Electron. J. Probab.* 30 (2025), 1–48
  Hal: 04614909
- **Hydrodynamic limit for a chain with thermal and mechanical boundary forces**, *Electron. J. Probab.* 26 (2021), 1–49
  Hal: 02538469
- **An open microscopic model of heat conduction: evolution and non-equilibrium stationary states**, *Communications in Mathematical Sciences* 3 (2020), 18, 751–780