# Nonequilibrium steady states of the aerogel dynamics

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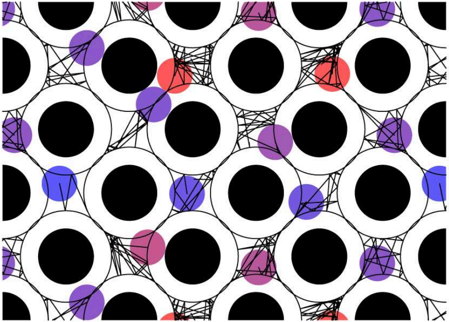
## Aerogels

- **Aerogels**: porous material derived from gels, in which gas molecules are confined in solid cells.
- Very low thermal conductivity, used in aeronautics and thermal isolation of buildings.

## Microscopic evolution

Microscopic model introduced by Gaspard and Gilbert (Phys. Rev. Lett., '08):



**Hamiltonian evolution** with $H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}|\mathbf{p}|^2 + V(\mathbf{q})$,

$$\boxed{V(\mathbf{q}) = \begin{cases} 0 & \text{if } q \in \Omega, \\ \infty & \text{if } q \notin \Omega, \end{cases}}$$

for $\Omega \subset (\mathbb{R}^d)^N$.

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(Prosen and Campbell, Chaos '05; Gilbert and Lefevere, Phys. Rev. Lett. '08)

- $d = 1$, $\Omega = \{q^1, \ldots, q^N \in [0,1], |q^i - q^{i+1}| \leq 1 - a\}$ for $0 < a < \dfrac{1}{2}$.
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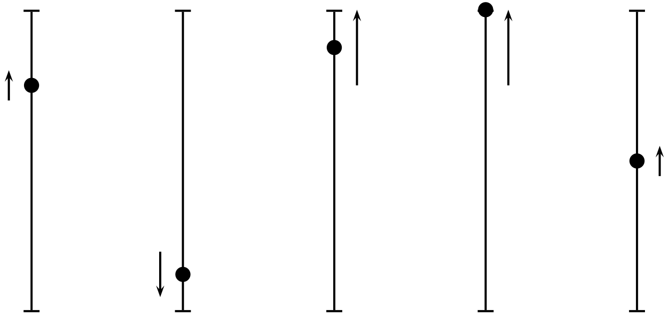

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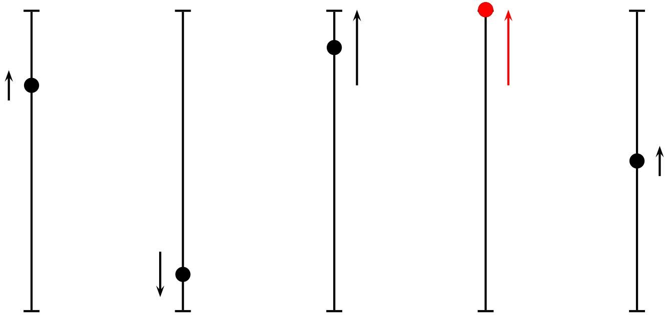

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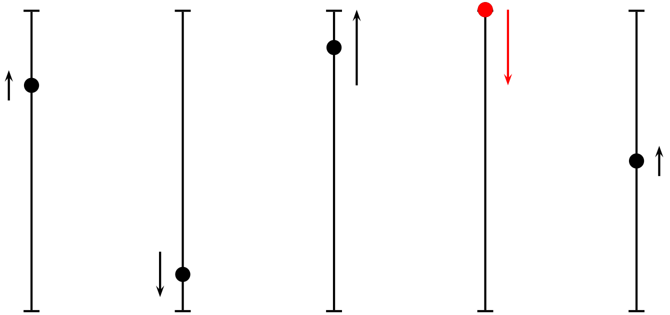

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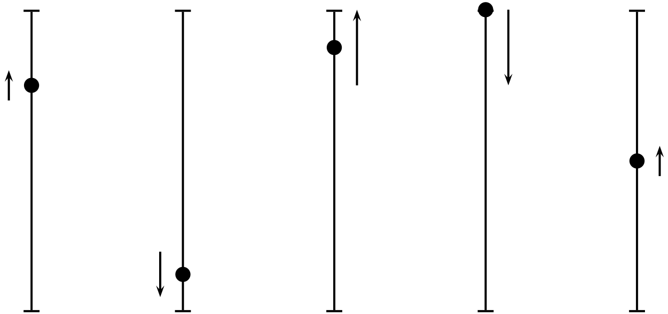

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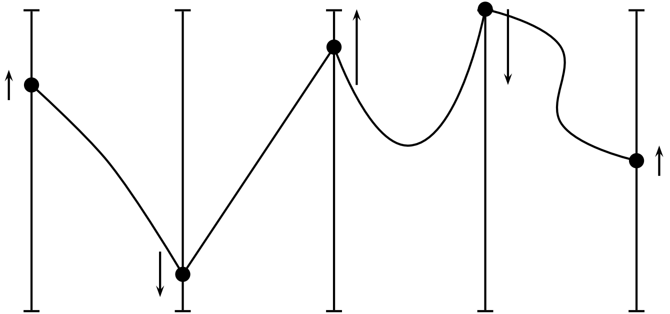

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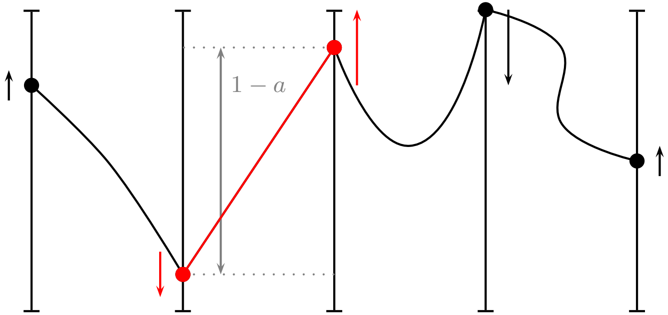

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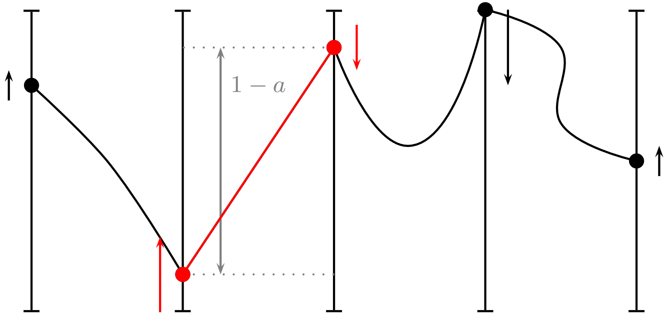

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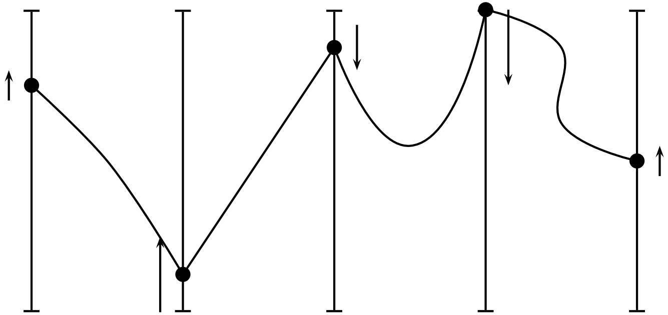

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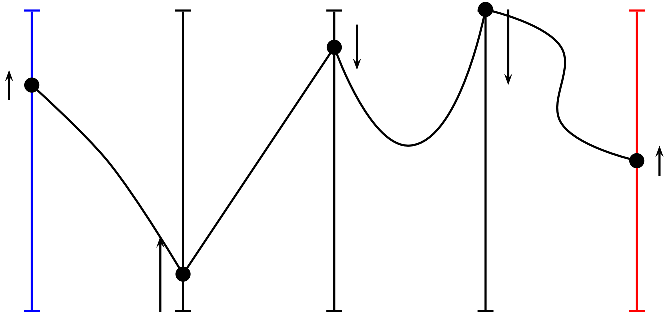


- Thermal baths: **stochastic velocity update** at the boundary of the cell for the leftmost and rightmost particles.

# Long time behaviour

**Aim:** long time behaviour of the process $X(t) = (\mathbf{q}(t), \mathbf{p}(t)) \in \Omega \times \mathbb{R}^N$.

- Piecewise Deterministic Markov Process, in particular, non Feller process.
- 'Very little stochasticity' $\rightsquigarrow$ difficult problem in general.

**Remark:** the number of null velocities is conserved, but the corresponding subspaces

$$\mathcal{X}_k := \left\{ (\mathbf{q}, \mathbf{p}) \in \Omega \times \mathbb{R}^N : \sum_{i=1}^{N} \mathbb{1}_{\{p^i=0\}} = k \right\}$$

are negligible for $k \in \{1, \dots, n\}$.

## Ideal result: typical ergodicity

There exists a unique probability distribution $\pi$ on $\Omega \times \mathbb{R}^N$ such that, for $\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$-almost all initial data,

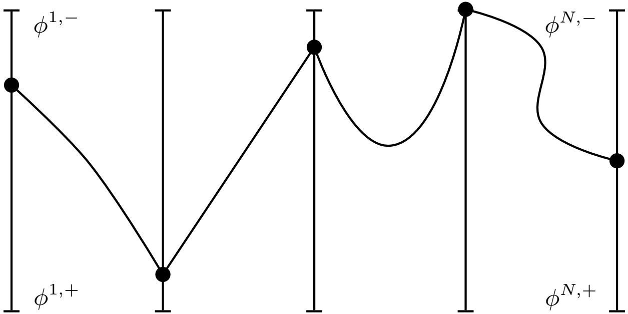
$$\mathrm{Law}(X(t)) \xrightarrow[t \to +\infty]{} \pi.$$

Then $\pi$ is a **nonequilbrium steady state**.

# Plan

# Thermal equilibrium

Let $\phi^{1,+}(p)$, $\phi^{1,-}(p)$, $\phi^{N,+}(p)$ and $\phi^{N,-}(p)$ refer to the density updates:



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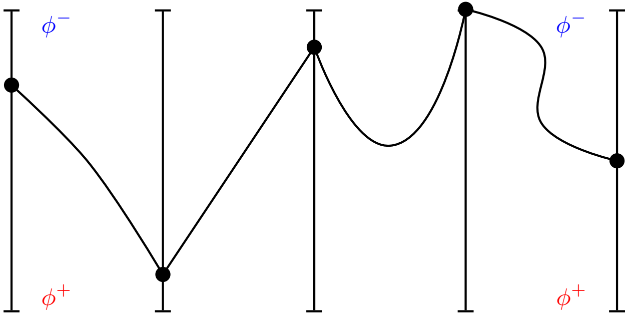
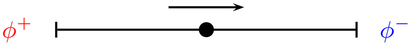



System at **thermal equilibrium** if $\phi^{1,+} = \phi^{N,+} = \phi^+$, $\phi^{1,-} = \phi^{N,-} = \phi^-$.
Then, a stationary probability distribution is given by

$$\boxed{\pi(\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}) = \frac{1}{|\Omega|}\mathbb{1}_{\{\mathbf{q}\in\Omega\}}\Phi(p^1)\cdots\Phi(p^N)\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p},}$$

where $\Phi(p)\mathrm{d}q\mathrm{d}p$ is the **steady state of an isolated particle**.

# Motion of a single particle




Stationary distribution for $(q(t), p(t))$: $\Phi(p)\mathrm{d}q\mathrm{d}p$, where

$$\boxed{\Phi(p) = \frac{1}{\mu^+ + \mu^-}\left(\mathbb{1}_{\{p>0\}}\frac{\phi^+(p)}{p} + \mathbb{1}_{\{p<0\}}\frac{\phi^-(-p)}{-p}\right)},$$

with $\mu^+ := \int_{p=0}^{+\infty} \frac{\phi^+(p)}{p}\mathrm{d}p$, $\mu^- := \int_{p=0}^{+\infty} \frac{\phi^-(p)}{p}\mathrm{d}p$.

- Proof: based on **Renewal Theorem** (Lefevere and Zambotti, J. Math. Phys. '11).
- By the way: very interesting **large deviation principle** when $t \to +\infty$.
- If $\phi^+(p) = \phi^-(p) = \beta p \mathrm{e}^{-\frac{\beta p^2}{2}}$, then $\Phi(p)$ is the **Maxwell-Boltzmann distribution** at inverse temperature $\beta$.

# Plan

Thermal equilibrium and thermal baths

The stochastic billiard representation

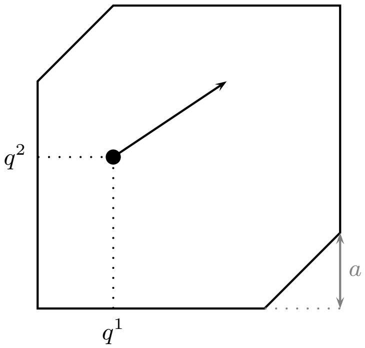
Ergodicity of the observed Markov chain

# The two particle model

We no longer assume thermal equilibrium.

- The problem is difficult.
- Drastic simplification: $N = 2$.

Then, the model rewrites in terms of a **stochastic billiard** on the table $\Omega$:



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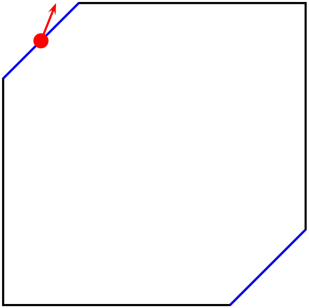

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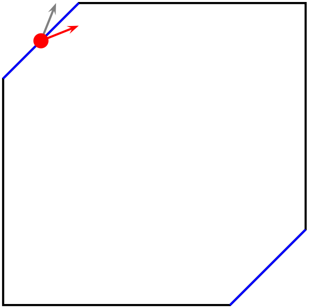

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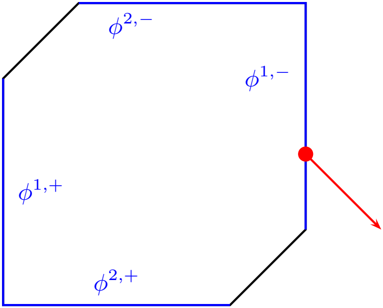


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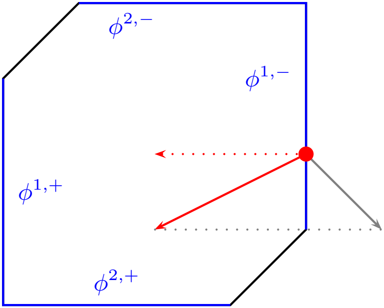


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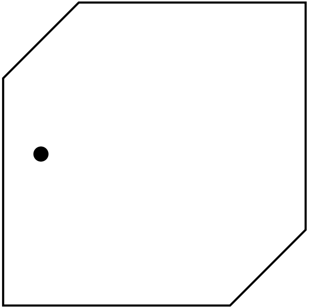

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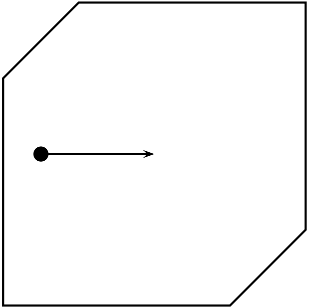

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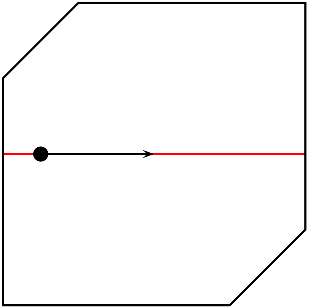

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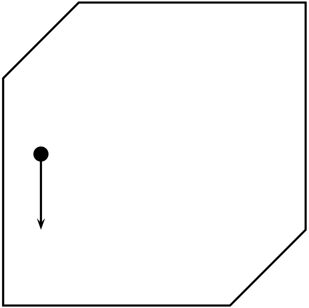

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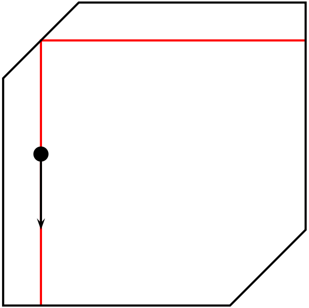

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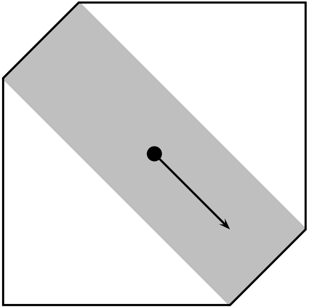

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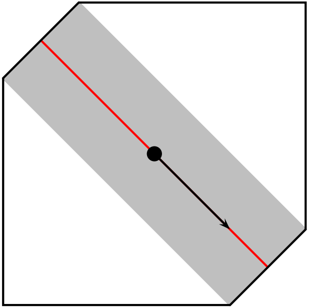

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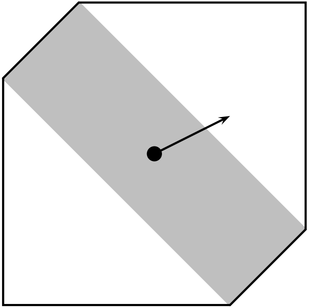

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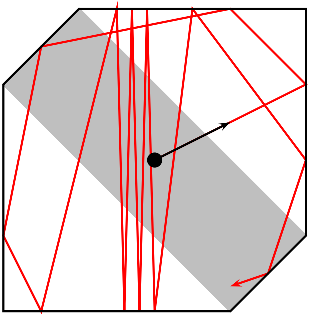

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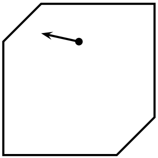

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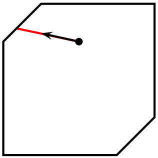

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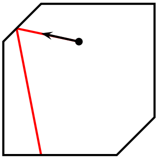

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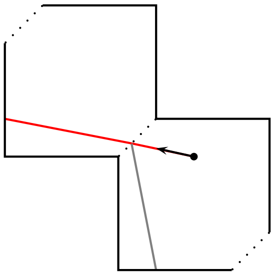

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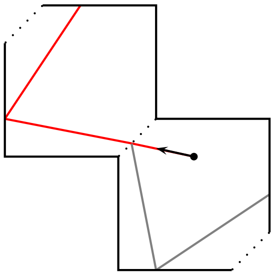

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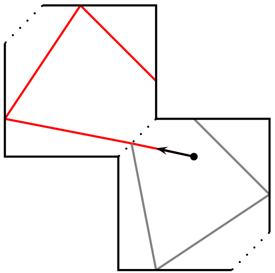

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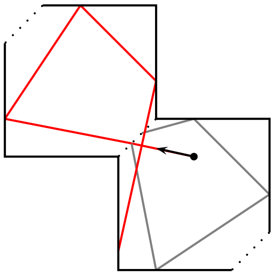

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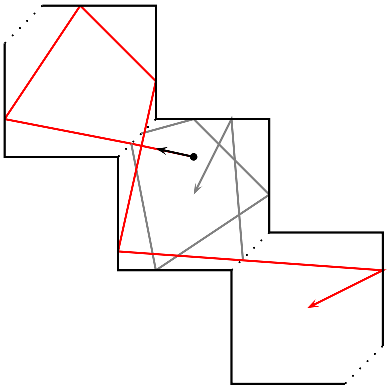

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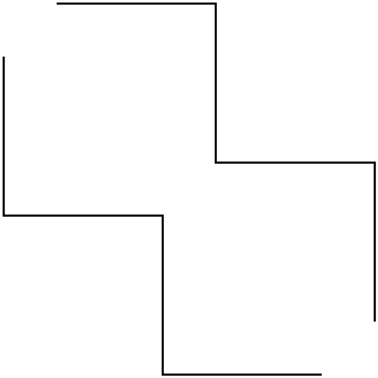

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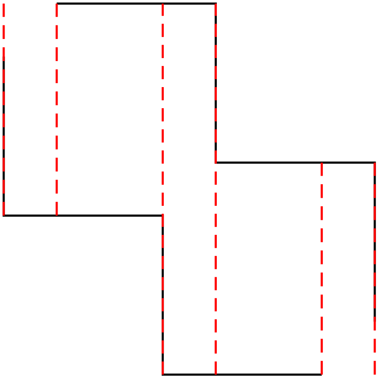

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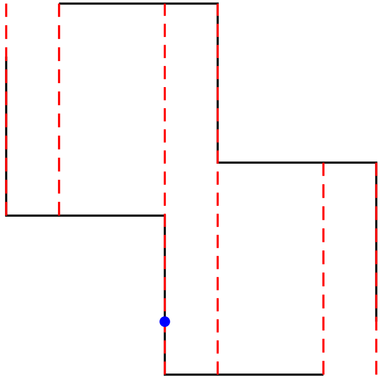

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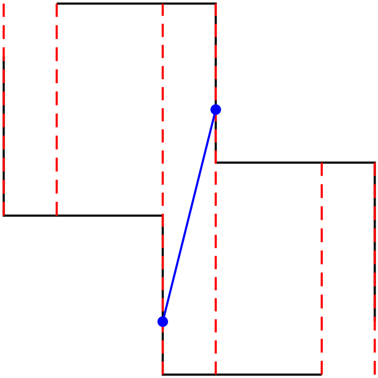

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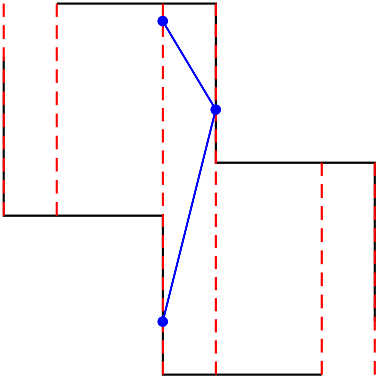

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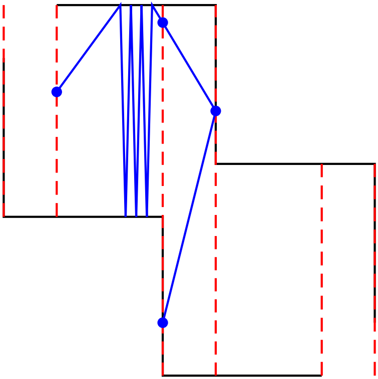

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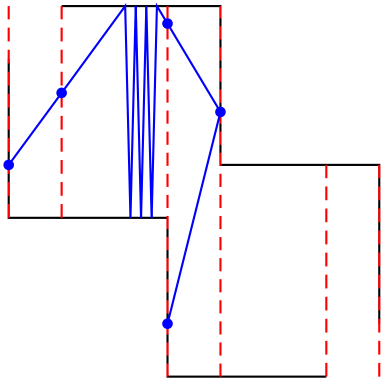

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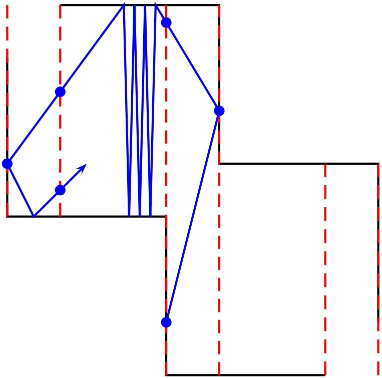
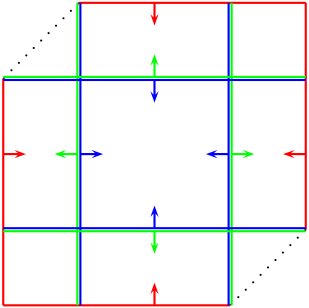


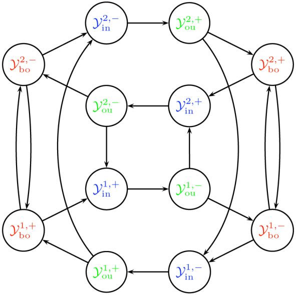
Let $(\tau_n)_{n\geq 0}$ be the sequence of observation times, $Y_n := X(\tau_n)$.
**Crucial remark:** on $[\tau_n, \tau_{n+1})$, the components evolve **independently**!

# Markov renewal process

**Fact:** the sequence $(Y_n, \tau_n)_{n \geq 0}$ is a **Markov renewal process**.
(i.e. $(Y_n, \tau_{n+1} - \tau_n)_{n \geq 0}$ is a Markov chain with transition depending only on $Y_n$)
In particular, $(Y_n)_{n \geq 0}$ is a **time homogeneous** Markov chain, with values in the space of **sections**

$$\mathcal{Y} := \bigcup_{(i,\varepsilon) \in \{1,2\} \times \{+,-\}} \mathcal{Y}_{\mathrm{bo}}^{i,\varepsilon} \cup \mathcal{Y}_{\mathrm{in}}^{i,\varepsilon} \cup \mathcal{Y}_{\mathrm{ou}}^{i,\varepsilon}$$





# Plan

# Markov Renewal Theorem

The **Markov Renewal Theorem** allows to derive the long time behaviour of $(X(t))_{t\geq 0}$ from **ergodic properties** of $(Y_n)_{n\geq 0}$.

## Markov Renewal Theorem (roughly)

If $(Y_n)_{n\geq 0}$ is **positive Harris recurrent**, then $(X(t))_{t\geq 0}$ is typically ergodic.

## Harris recurrence (roughly)

$(Y_n)_{n\geq 0}$ is **Harris recurrent** if there exist $R \subset \mathcal{Y}$, $\varepsilon > 0$ and $\lambda(\cdot)$ such that:

- Recurrence: $\forall y \in \mathcal{Y}$, $\mathbb{P}_y(\exists n \geq 1 : Y_n \in R) = 1$,
- Minorization: $\forall y \in R$, $\mathbb{P}_y(Y_1 \in \cdot) \geq \varepsilon\lambda(\cdot)$.

- Harris recurrence $\Longrightarrow$ existence and $\propto$-uniqueness of $\sigma$-**finite stationary distribution**.
- In addition, positivity $\Longleftrightarrow$ existence of (a unique) **stationary probability distribution**.

We only explain how to **construct** $R$ and prove the **minorization condition**.

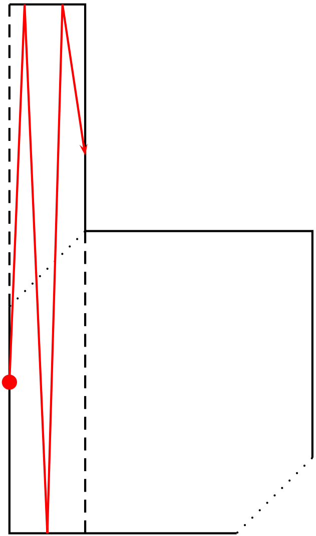
# The set $R$

Let us look at the unfolded process

- starting from a boundary section,
- arriving on a boundary section at the first observation time.

At the observation time:

- the horizontal component is fresh,
- the vertical component is close to its equilibrium **if it has had enough time to mix**.



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Let us look at the unfolded process

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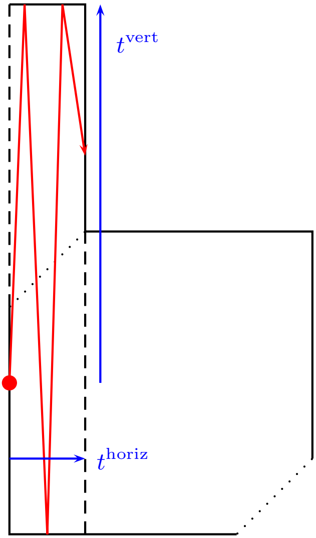
Let $\gamma := t^{\text{horiz}} - t^{\text{vert}}$.
**Renewal theorem:** if $\gamma$ is large enough, then **the minorization condition is satisfied**.

$\rightsquigarrow$ $\boxed{R \simeq \textbf{razing collisions}.}$



# Conclusion

**Sequel of the proof:**

- recurrence condition: tedious but OK,
- positivity: not OK yet (apart from thermal equilibrium)...

**Conclusion:**

- Unfolding the process allows to make interactions transparent for the dynamics,
- and provides a natural regenerative set $R$ by analyzing the action of thermal baths.
- Extension of the argument to general $N$ particle case: first requires to find a similar unfolding procedure.

**Thank you for your attention!**