Lecture 1.

29/11/2011

MOTIVATIONS:

- Classical thermodynamics provides a frame to understand the **mean-value** of macroscopic observables (energy, density, susceptibility, ...)
- Physical systems are composed of numerous but finite # of particles → one wants to understand **fluctuations** of those observables.

GENERIC SETUP:

- Set of configurations $\{\mathcal{C}\}$ (finite or discrete)
  e.g: occupation numbers $\{n_i\}$ on sites i of a network / lattice.
- Transition rates $W(\mathcal{C}\to\mathcal{C}')$ between rates $(\mathcal{C}\neq\mathcal{C}')$ (continuous-time dynamics)
- Evolution of the probability $P(\mathcal{C},t)$ of being in $\mathcal{C}$ at time t:

Master Equation

$$\boxed{\begin{aligned} \partial_t P(\mathcal{C},t) &= \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P(\mathcal{C}',t) - r(\mathcal{C})P(\mathcal{C},t) \\ \text{with } r(\mathcal{C}) &= \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}') \quad \text{(escape rate from conf. } \mathcal{C}) \end{aligned}}$$

one assumes $W(\mathcal{C}\to\mathcal{C})=0$

- Where does this come from? Come back to discrete time

$$P(\mathcal{C},t+dt) = \sum_{\mathcal{C}'} \underbrace{dt\, W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}',t)}_{\substack{\text{probability to have}\\ \text{jumped from } \mathcal{C}' \text{ to } \mathcal{C}\\ \text{between } t \text{ and } t+dt}} - \underbrace{\Big(1-dt\overbrace{\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')}^{r(\mathcal{C})}\Big)P(\mathcal{C},t)}_{\substack{\text{probability to have}\\ \text{remained in } \mathcal{C} \text{ btw}\\ t \text{ and } t+dt}}$$

To understand / remember / recover the second term, one remarks that it ensures probability conservation:

$$\sum_{\mathcal{C}} P(\mathcal{C},t+dt) = \sum_{\mathcal{C}} P(\mathcal{C},t)$$

PROPERTIES:

- *Conservation of probability*: one has

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) = 0$$

as directly checked. Since $\sum_{\mathcal{C}} P(\mathcal{C},0) = 1$ this property remains valid at all times

- *Steady state*:

[this is the case if one can reach any state from any other through $\{W(\mathcal{C}\to\mathcal{C}')\}$, and if there are no recurrent states]

One assumes there exist a unique steady state $P_{st}(\mathcal{C})$ solution of $\partial_t P(\mathcal{C},t)=0$

i.e. verifying the ~~detailed~~ global balance condition

$$\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')\, P_{st}(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P_{st}(\mathcal{C}') \qquad \forall\, \mathcal{C}$$

- *"Equilibrium dynamics": detailed balance condition*

$$W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C}) = W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') \qquad \forall\, \mathcal{C},\mathcal{C}'$$

  - the steady state is then called "equilibrium state" $\quad P_{st} = P_{eq}$
  - this condition is much more restrictive
  - interpretation 1: there is no current of probability in the steady state

$$0 = \sum_{\mathcal{C}'} \Big(\underbrace{W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') - W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C})}_{\text{current of probability in } \mathcal{C} \ (=0)} \Big)$$

  - interpretation 2: the dynamics starting from P_{eq} is **reversible**

using detailed balance condition

$$\underbrace{P_{eq}(\mathcal{C}_0)\, W(\mathcal{C}_0\to\mathcal{C}_1)\ldots W(\mathcal{C}_{K-1}\to\mathcal{C}_K)}_{\text{probability density of the history } \mathcal{C}_0\to\ldots\to\mathcal{C}_K \text{ of the system}} = \underbrace{P_{eq}(\mathcal{C}_K)\, W(\mathcal{C}_K\to\mathcal{C}_{K-1})\ldots W(\mathcal{C}_1\to\mathcal{C}_0)}_{\text{probability density of the time-reversed history } \mathcal{C}_K\to\ldots\to\mathcal{C}_0 \text{ of the system}}$$

Those probabilities are the same: reversibility, equilibrium.

OPERATOR NOTATION :

- One considers a vector space of basis $|\mathcal{C}\rangle$, $\mathcal{C}$ in the set of all configs.
- The space is orthonormal, the scalar product denoted $\langle\cdot|\cdot\rangle$:

$$\langle \mathcal{C}' | \mathcal{C} \rangle = \delta_{\mathcal{C}\mathcal{C}'} \qquad \text{(Kronecker delta)}$$

- Traduction of the Markov evolution : (master equation)

Defining the vector $|P(t)\rangle = \sum_{\mathcal{C}} P(\mathcal{C},t)\,|\mathcal{C}\rangle$ of components $P(\mathcal{C},t)$:

$$\partial_t |P(t)\rangle = \mathbb{W}\,|P(t)\rangle \quad \text{with} \quad \boxed{\mathbb{W}_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}}$$

$\mathbb{W}_{\mathcal{C}\mathcal{C}'}$ is the element $\mathcal{C}\mathcal{C}'$ of the matrix (or 'operator') $\mathbb{W}$.
named 'evolution operator'

- Traduction of the conservation of probability :

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) \iff \boxed{\langle - | \,\mathbb{W} = 0 \quad \text{with } \langle - | = \sum_{\mathcal{C}} \langle \mathcal{C} |}$$

in other words, the vector $\langle - |$ is a left eigen vector of $\mathbb{W}$ of eigenvalue 0 .

- Traduction of the steady state property :
  - the global balance condition rewrites $\boxed{\mathbb{W}|P_{st}\rangle = 0}$

    in other words the vector $|P_{st}\rangle$ is a right eigenvalue of $\mathbb{W}$ of e.v. 0.
  - It must exists if probability is conserved, since $\mathbb{W}$ and $\mathbb{W}^T$ have the same spectrum (and a left eigen vector of $\mathbb{W}$ corresponds to a right $\vec{ev}$ of $\mathbb{W}^T$)

- Remark: All other eigen values of $\mathbb{W}$ are of ~~modulus~~ real part <0 .

Lecture on Stoch process

- Traduction of the detailed balance condition:

$$W(\mathcal{C}'\to\mathcal{C})\,P_{eq}(\mathcal{C}') = W(\mathcal{C}\to\mathcal{C}')\,P_{eq}(\mathcal{C}) \qquad \forall \mathcal{C}\mathcal{C}'$$

$$\Leftrightarrow \quad \mathbb{W}_{\mathcal{C}\mathcal{C}'}\,P_{eq}(\mathcal{C}') = \mathbb{W}_{\mathcal{C}'\mathcal{C}}\,P_{eq}(\mathcal{C})$$

$$\Leftrightarrow \quad P_{eq}^{-1/2}(\mathcal{C})\,\mathbb{W}_{\mathcal{C}\mathcal{C}'}\,P_{eq}(\mathcal{C}')^{1/2} = P_{eq}(\mathcal{C}')^{-1/2}\,\mathbb{W}_{\mathcal{C}'\mathcal{C}}\,P_{eq}(\mathcal{C})^{1/2}$$

$$\Leftrightarrow \quad \boxed{\text{the 'symetrised operator' } \mathbb{W}^{sym} = \hat{P}_{eq}^{-1/2}\,\mathbb{W}\,\hat{P}_{eq}^{1/2} \text{ is symmetric}}$$

where $\hat{P}_{eq}$ is the diagonal operator of elements $P_{eq}(\mathcal{C})$.

In this case, $\mathbb{W}^{sym}$ (and hence $\mathbb{W}$) can be diagonalized.

- Formal solution through matrix exponentiation:

× form 1 : $\begin{cases} \partial_t|P(t)\rangle = \mathbb{W}\,|P(t)\rangle \\ |P(0)\rangle = 0 \end{cases}$ has a solution $|P(\mathcal{C},t)\rangle = e^{t\mathbb{W}}|P_0\rangle$

but this form is not very useful. $\displaystyle = \sum_{n\geq 0}\frac{t^n}{n!}\mathbb{W}^n|P_0\rangle$

× form 2 : description in terms of a jump process. To eliminate the diagonal term in $\displaystyle \partial_t\,|P(t)\rangle_{\mathcal{C}} = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\,|P(t)\rangle_{\mathcal{C}'} - r(\mathcal{C})|P(t)\rangle_{\mathcal{C}}$,

one sets $Q(\mathcal{C},t) = e^{-t\,r(\mathcal{C})}\,P(\mathcal{C},t)$ which verifies

$$(*) \quad \underline{\partial_t|Q(t)\rangle = W(t)\,|Q(t)\rangle} \quad \text{with} \quad W(t)_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C})\,e^{t(r(\mathcal{C}')-r(\mathcal{C}))}$$

this is a linear evolution with time-dependent operator $W(t)$

The solution is $|Q(t)\rangle = \mathcal{T}exp\left(\int_0^t W\right)|Q(0)\rangle$ $(**)$

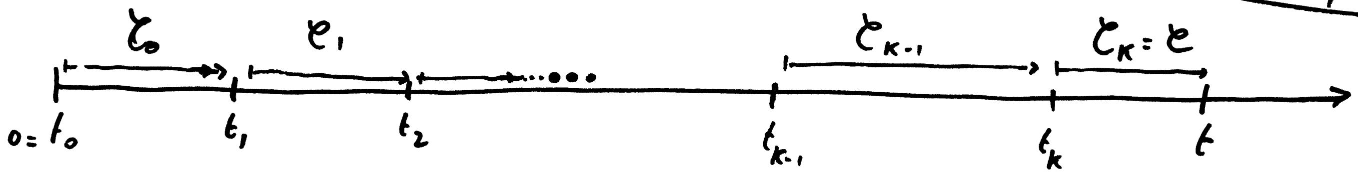
where the time-ordered exponential $\mathcal{T}exp$ writes $K\in\mathbb{N}$

$$\mathcal{T}exp\left(\int_0^t W\right) = \sum_{K\geq 0}\mathcal{T}\left(\int_0^t W\right)^K = \sum_{K\geq 0}\int_0^t dt_K\int_0^{t_{K-1}} dt_{K-1}\cdots\int_0^{t_2} dt_1\,W(t_K)\ldots W(t_1)$$

$$= \sum_{K\geq 0}\int_0^t dt_1\int_{t_1}^t dt_2\cdots\int_{t_{K-1}}^t dt_K\,W(t_K)\ldots W(t_1)$$

check that $(**)$ solves $(*)$ using this expression

Final form of the result: coming back to $P(\mathcal{C},t)$ from $Q(\mathcal{C},t)$:



sum over the number of jumps — sum over the histories of configurations — integrals over the time jump t_k's between $\mathcal{C}_{k-1}$ and $\mathcal{C}_K$

$$\boxed{\begin{aligned} P(\mathcal{C},t) = \sum_{K\geq 0} \sum_{\mathcal{C}_0\cdots\mathcal{C}_K} \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 \cdots \int_{t_{K-1}}^{t} dt_K \\ \text{Ⓐ}\rightarrow \quad r(\mathcal{C}_0)\, e^{-(t_1-t_0)\, r(\mathcal{C}_0)} \times \cdots \times r(\mathcal{C}_{K-1})\, e^{-(t_K-t_{K-1})\, r(\mathcal{C}_{K-1})}\, e^{-(t-t_K)\, r(\mathcal{C}_K)} \\ \text{Ⓑ}\rightarrow \quad \times \frac{W(\mathcal{C}_0\to\mathcal{C}_1)}{r(\mathcal{C}_0)} \times \cdots \times \frac{W(\mathcal{C}_{K-1}\to\mathcal{C})}{r(\mathcal{C}_{K-1})} \\ \times\, P_0(\mathcal{C}_0) \end{aligned}}$$

- in Ⓐ: • all the $r(\mathcal{C}_{k-1})\, e^{-(t_k-t_{k-1})\, r(\mathcal{C}_{k-1})}$ $(1\leq k\leq K)$ represent the probability that the time t_k of jump between $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$ is t_k.
  - $e^{-(t-t_K)\, r(\mathcal{C}_K)}$ represents the probability not to jump between t_K and t

  hence Ⓐ is the probability distribution of the times jump t_k.

- in Ⓑ: $\dfrac{W(\mathcal{C}_{k-1}\to\mathcal{C}_k)}{r(\mathcal{C}_{k-1})}$ represents the (normalised) probability to jump to $\mathcal{C}_k$ starting from $\mathcal{C}_{k-1}$.

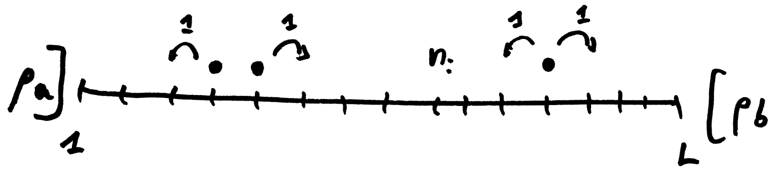
  hence Ⓑ represents the probability of the history of configurations $\mathcal{C}_0\to\cdots\to\mathcal{C}_K$

<u>Remark</u>: one can rewrite Ⓐ $= \prod_{k=0}^{K-1} r(\mathcal{C}_k)\,.\, e^{-\int_0^t dt'\, r(\mathcal{C}_{t'})}$

check that this is the correct solution when rates depend on time and hence r

LARGE DEVIATION FUNCTIONS

- Examples and motivation:



$n_i \in \{0,1\}$ occupation number

. total current on a time interval $[0,t]$: $Q = \#\left\{\begin{matrix}\text{jumps to}\\ \text{the right}\end{matrix}\right\} - \#\left\{\begin{matrix}\text{jumps to}\\ \text{the left}\end{matrix}\right\}$

in time: $Q \mapsto Q+1$ each time a particle jumps to the right
$Q \mapsto Q-1$ — — — left.

. total time and space integrated density:

$$\rho = \frac{1}{L}\int_0^t d\tau \sum_{i=1}^{L} n_i(t)$$

evolution in time: continuous (no jumps)
on each interval $[t_{k-1}, t_k]$ where the system does not change configurat°:

$$\rho \mapsto \rho + \frac{1}{L}\int_{t_{k-1}}^{t_k} d\tau \sum_{i=1}^{L} \overbrace{n_i(t_{k-1})}^{\text{constant}} = \rho + (t_k - t_{k-1})\,\frac{1}{L}\sum_{i=1}^{L} n_i(t_{k-1})$$

- 'dynamical activity' K: on a time interval $[0,t]$, $K = \#\left\{\begin{matrix}\text{change}\\ \text{of configurat°}\end{matrix}\right\}$

in time: $K \mapsto K+1$ each time a configuration changes

- 'integrated escape rate' R: configuration at time τ, constant $\mathcal{C}_\tau = \mathcal{C}_{k-1}$ for $\tau \in [t_{k-1}, t_k]$

$$R = \int_0^t d\tau\, r(\mathcal{C}_\tau)$$

$$R = \sum_{k=1}^{K} (t_k - t_{k-1})\, r(\mathcal{C}_{k-1}) + (t - t_K)\, r(\mathcal{C}_K)$$

- <u>Generic cases:</u> A_1 A_2 observables depending on the history of the system on $[0,t]$

A_1 defined as: $\begin{cases} A_1\big|_{t=0} = 0 \ , \quad A_1 \mapsto A_1 + a_1(\mathcal{C}\to\mathcal{C}') \\ \text{at each jump } \mathcal{C}\to\mathcal{C}' \end{cases}$

A_2 defined as $\quad A_2 = \int_0^t d\tau\, a_2(\mathcal{C}_\tau) = \sum_{k=1}^{K} (t_k - t_{k-1})\, a_2(\mathcal{C}_{k-1}) + (t-t_K)\, a_2(\mathcal{C}_K)$

- <u>Large deviation function:</u>

× <u>in direct space:</u> for A an observable of type A_1 or A_2:

. the probability density of being in $\mathcal{C}$ at time t, having observed a value A of the observable, is denoted $P(\mathcal{C}, A, t)$.

. the probability distribution of A at time t is

$$P(A,t) = \sum_{\mathcal{C}} P(\mathcal{C}, A, t) \quad \text{and scales as}$$

$$\boxed{P(A,t) \sim \exp\left(+t\,\pi(A/t)\right)} \quad \text{as } t\to\infty$$

π is a dynamical equivalent of the entropy

. π is difficult to determine in general ("microcanonical problem")
one prefers to go to the "canonical dynamical ensemble"

× in <u>Laplace space:</u> one has the $t\to\infty$ scaling

$$\boxed{\langle e^{-sA} \rangle \sim \exp\left(t\,\psi(s)\right)} \quad \text{as } t\to\infty$$

average taken on histories on time interval $[0,t]$

$\psi(s)$ is the cumulant generating function: (ψ is a "dynamical free energy")

$$\boxed{\partial_s^k \psi\big|_{s=0} = (-1)^k \frac{1}{t}\langle A^k\rangle_c} \quad \langle A^k\rangle_c \text{ is the } k^{th} \text{ cumulant of } A.$$

lecture on Stoch. processes

- <u>Interpretation of s; link between $\psi(s)$ and $\pi(k)$:</u>

× Starting from $\langle e^{-sA}\rangle = \int dA\, P(A,t)\, e^{-sA}$ $\qquad A = at$

$$e^{+t\psi(s)} \sim \int da\, e^{\underbrace{t[\pi(a)-sa]}}$$

in the $t\to\infty$ limit, one may use the saddle point theorem

One has $\boxed{\psi(s) = \max_a (\pi(a) - sa)}$ $\quad \psi$ and π are legendre transformed.

If π is convex, one may perform the inverse laplace transform:

$$\boxed{\pi(a) = \min_s (\psi(s) + sa)}$$

× If $a^*(s)$ is the a where the $\max_a$ is reached
or if $s^*(a)$ — s —— $\min_s$ ——) one says that $a^*(s)$ and s / $s^*(a)$ and a are 'conjugated'

× ⚠ s plays a role similar to the inverse temperature β:
it fixes the average value of A (in the same way as β fixes the average value of the energy)

× <u>Indeed</u>, in the large time limit: the mean value of an observable $\mathcal{O}$ in the 's-state' writes

$$\langle \mathcal{O}(\mathcal{C})\rangle_s \equiv \frac{\langle \mathcal{O}(\mathcal{C}(t))e^{-sA}\rangle}{\langle e^{-sA}\rangle} = \frac{1}{\langle e^{-sA}\rangle}\sum_{\mathcal{C},A} \overbrace{P(\mathcal{C},A,t)}^{\sim e^{t\pi(A/t)}\tilde{P}(\mathcal{C},A/t)}\, \mathcal{O}(\mathcal{C})\, e^{-sA} \qquad A = at$$

$$\sim \frac{\int da \sum_{\mathcal{C}} \tilde{P}(\mathcal{C},a)\mathcal{O}(\mathcal{C})\, e^{t(\pi(a)-sa)}}{\int da\; e^{t(\pi(a)-sa)}}$$

the saddle is reached at the same value $a = a^*(s)$

$$\langle \mathcal{O}(\mathcal{C})\rangle_s \sim \sum_{\mathcal{C}} \tilde{P}(\mathcal{C}, a^*(s))\mathcal{O}(\mathcal{C}) \quad \text{i.e.} \quad \boxed{\langle \mathcal{O}(\mathcal{C})\rangle_s \overset{t\to\infty}{=} \langle \mathcal{O}(\mathcal{C})\rangle\Big|_{A = a^*(s)t}}$$

mean value in the s-state, of $\mathcal{O}(\mathcal{C})$ at final time

Mean value of $\mathcal{O}(\mathcal{C})$ at final time for histories with $A = a^*(s)t$

In the same way, if $\pi(a)$ is convex: by inverse Legendre transform

$$\boxed{\left\langle \mathcal{O}(\mathcal{C}) \right\rangle \Big|_{A=at} \overset{t\to\infty}{=} \left\langle \mathcal{O}(\mathcal{C}) \right\rangle_{s=s^*(a)}}$$

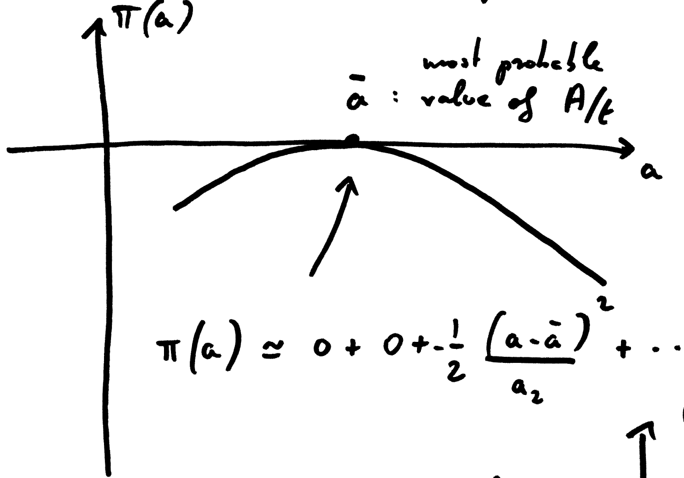
Mean value of $\mathcal{O}(\mathcal{C})$ at final time for histories with a value $A=at$ of the observable A

Mean value in the s-state of $\mathcal{O}(\mathcal{C})$ at final time:

$$\langle \mathcal{O}(\mathcal{C})\rangle_s = \frac{\langle \mathcal{O}(\mathcal{C}(t))\, e^{-sA}\rangle}{\langle e^{-sA}\rangle}$$

In other words, to characterize the value of the observable $\mathcal{O}$ in histories with a value $A\sim at$ of the observable A, one has to compute $\langle \mathcal{O}(\mathcal{C})\rangle_s$ at $s=s^*(a)$.

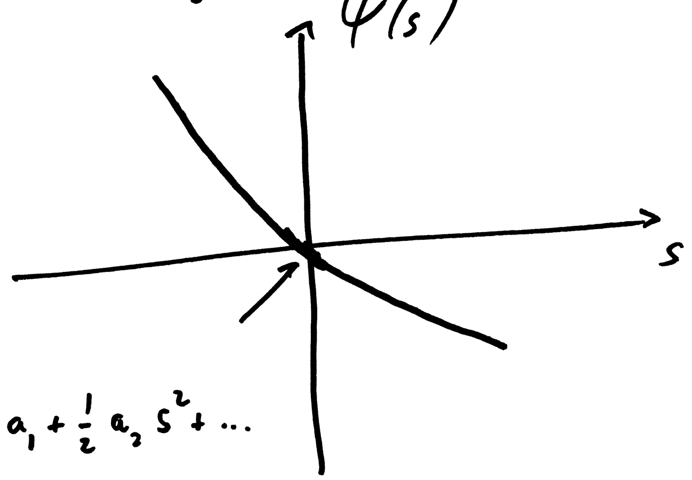
- Generic shape of the functions $\pi(a)$ and $\psi(s)$:



$$\pi(a) \simeq 0 + 0 - \frac{1}{2}\frac{(a-\bar{a})^2}{a_2} + \dots$$

$a_1 = \dfrac{\langle A\rangle}{t}$ mean value

$a_2 = \dfrac{\langle A^2\rangle_c}{t}$ second cumulant



$$\psi(s) \simeq -s a_1 + \frac{1}{2} a_2 s^2 + \dots$$

• Large deviation functions as maximal eigenvalues

1. Cases of observables of type A_1

* Time evolution for $P(\mathcal{C},A_1,t)$:

$$\partial_t P(\mathcal{C},A_1,t) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}', A_1 - a_1(\mathcal{C}'\to\mathcal{C}), t) - r(\mathcal{C}) P(\mathcal{C},A_1,t)$$

this evolution is non-diagonal in the direction A_1
the operator of evolution is very difficult to diagonalize.

* Going to the s-state : Laplace transform

One introduces $\hat{P}(\mathcal{C},s,t) = \sum_{A_1} e^{-sA_1} P(\mathcal{C},A_1,t)$

It verifies $\langle e^{-sA_1}\rangle = \sum_{\mathcal{C},A_1} e^{-sA_1} P(\mathcal{C},A_1,t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)$

* Time evolution : from the time evolution of $P(\mathcal{C},A_1,t)$ one finds

$$\partial_t \hat{P}(\mathcal{C},s,t) = \sum_{\mathcal{C}'} e^{-sa_1(\mathcal{C}'\to\mathcal{C})} W(\mathcal{C}'\to\mathcal{C})\, \hat{P}(\mathcal{C}',s,t) - r(\mathcal{C})\hat{P}(\mathcal{C},s,t)$$

This time, the operator is diagonal in direction s. Putting $|\hat{P}(t)\rangle = \sum_{\mathcal{C}} \hat{P}(\mathcal{C},s,t)|\mathcal{C}\rangle$

one has

$$\boxed{\begin{aligned} \partial_t |\hat{P}(s,t)\rangle &= \mathbb{W}(s)\, |\hat{P}(s,t)\rangle \\ \left(\mathbb{W}(s)\right)_{\mathcal{C}\mathcal{C}'} &= \underbrace{e^{-sa_1(\mathcal{C}'\to\mathcal{C})}}\, W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'} \end{aligned}}$$

here, only the non-diagonal part of the evolution operator is modified by s

* Largest eigenvalue of $\mathbb{W}(s)$: one has $\langle e^{-sA_1}\rangle = \sum_{\mathcal{C}} \underbrace{\hat{P}(\mathcal{C},s,t)}$

but $|\hat{P}(s,t)\rangle = e^{t\mathbb{W}(s)} |\hat{P}_0\rangle \underset{t\to\infty}{\sim} e^{t \underbrace{\max \mathrm{Sp}\, \mathbb{W}(s)}_{\text{maximal eigenvalue of } \mathbb{W}(s)}} \Rightarrow \sim e^{t\max \mathrm{Sp}\,\mathbb{W}(s)}$

Hence $\langle e^{-sA_1}\rangle \sim e^{t\max \mathrm{Sp}\,\mathbb{W}(s)}$ and by definit°

$$\boxed{\psi(s) = \max \mathrm{Sp}\, \mathbb{W}(s)}$$

it is the largest eigenvalue of $\mathbb{W}(s)$

2. Case of observable of type A_2

$\partial_t P(\mathcal{C}, A_2, t)$ is not as directly obtained as previously.

* first approach: time discretization

ok up to order dt

$$P(\mathcal{C}, A_2, t+dt) = \sum_{\mathcal{C}'} dt\, W(\mathcal{C}' \to \mathcal{C})\, P(\mathcal{C}', A_2, t) + (1 - dt\, r(\mathcal{C}))\, \underbrace{P\Big(\mathcal{C},\ A_2 - \overbrace{\int_{t-dt}^{t} d\tau\, a_2(\mathcal{C}(\tau))}^{\simeq dt\, a_2(\mathcal{C})}\Big)}_{P(\mathcal{C}, A_2, t) - dt\, \partial_{A_2} P(\mathcal{C}, A_2, t)\, a_2(\mathcal{C})}$$

Hence, in the $dt \to 0$ limit:

$$\boxed{\partial_t P(\mathcal{C}, A_2, t) = \sum_{\mathcal{C}'} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', A_2, t) - \big(r(\mathcal{C}) P(\mathcal{C}, A_2, t) + a_2(\mathcal{C}) \partial_{A_2} P(\mathcal{C}, A_2, t)\big)}$$

Or, introducing $\hat{P}(\mathcal{C}, s, t) = \int dA_2\, e^{-sA_2} P(\mathcal{C}, A_2, t)$

one again has $\langle e^{-sA_2} \rangle = \int dA_2 \sum_{\mathcal{C}} P(\mathcal{C}, A_2, t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t)$

The equation of evolution is thus (by integration by part)

$$\partial_t \hat{P}(\mathcal{C}, s, t) = \sum_{\mathcal{C}'} W(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s, t) - \big(r(\mathcal{C}) + s\, a_2(\mathcal{C})\big) \hat{P}(\mathcal{C}, s, t)$$

Or, in vector notation:

$$\boxed{\begin{aligned} \partial_t |\hat{P}(s,t)\rangle &= \mathbb{W}(s)\, |\hat{P}(s,t)\rangle \\ \big(\mathbb{W}(s)\big)_{\mathcal{C}\mathcal{C}'} &= W(\mathcal{C}' \to \mathcal{C}) - \underbrace{\big(r(\mathcal{C}) + s\, a_2(\mathcal{C})\big)\, \delta_{\mathcal{C}\mathcal{C}'}} \end{aligned}}$$

this time, it is the diagonal part of the operator of evolution which is modified by s

× second derivation of the result:

One has $A_2 = \sum_{k=1}^{K} (t_k - t_{k-1})\, a_2(\mathcal{C}_{k-1}) + (t - t_K)\, a_2(\mathcal{C}_K)$

Thus, using the expression previously obtained for the probability of an history

$$\left\langle e^{-sA_2} \right\rangle = \sum_{K\geq 0} \sum_{\mathcal{C}_0 \cdots \mathcal{C}_K} \int_{t_0}^{t} dt_1 \cdots \int_{t_{K-1}}^{t} dt_K \; e^{-\sum_{k=1}^{K}(t_k - t_{k-1})\left(r(\mathcal{C}_{k-1}) + s a(\mathcal{C}_{k-1})\right) - (t - t_K)\left(r(\mathcal{C}_K) - r(\mathcal{C}_{K-1})\right)} \times \prod_{k=1}^{K} W(\mathcal{C}_{k-1} \to \mathcal{C}_k) \quad P_0(\mathcal{C}_K)$$

And one recognizes precisely the expression of

$$\langle - | \; T\exp \underbrace{\mathbb{W}_s(t)} \; | P_0 \rangle$$

time dependent operator of evolution
corresponding precisely to $\mathbb{W}(s)$ for s associated to A_2

which is compatible with $|\hat{P}(s,t)\rangle = T\exp \mathbb{W}_s(t) \, |P_0\rangle$

- **Remark**: mixed observables:

The l.d.f. $\psi(s_1, s_2) = \lim_{t\to\infty} \frac{1}{t} \log \langle e^{-s_1 A_1 - s_2 A_2} \rangle$ is the max e.v. of

$$\boxed{\left(\mathbb{W}(s_1, s_2)\right)_{\mathcal{C}\mathcal{C}'} = \underbrace{e^{-s_1 a_1(\mathcal{C}' \to \mathcal{C})}\, W(\mathcal{C}' \to \mathcal{C}) - \left(r(\mathcal{C}) + s_2 a_2(\mathcal{C})\right)\delta_{\mathcal{C}\mathcal{C}'}}_{}}$$

both diagonal and non-diagonal parts of the operator of evolution are modified, respectively by s_2 and s_1

- Time reversal symmetry and fluctuation theorem:

[Lebowitz & Spohn]

Consider the observable $Q_{LS} = \log \frac{W(\mathcal{C}_0\to\mathcal{C}_1)\ \ldots\ W(\mathcal{C}_{K-1}\to\mathcal{C}_K)}{W(\mathcal{C}_K\to\mathcal{C}_{K-1})\ldots W(\mathcal{C}_1\to\mathcal{C}_0)}$ ("entropy current")

Upon a jump $\mathcal{C}\to\mathcal{C}'$ one has $Q_{LS} \mapsto Q_{LS} + \log \frac{W(\mathcal{C}\to\mathcal{C}')}{W(\mathcal{C}'\to\mathcal{C})}$

The modified operator of evolution for s associated to Q_{LS} is

$$\left(\mathbb{W}(s)\right)_{\mathcal{C}\mathcal{C}'} = e^{-s\log\frac{W(\mathcal{C}'\to\mathcal{C})}{W(\mathcal{C}\to\mathcal{C}')}}\, W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}$$

$$= W(\mathcal{C}'\to\mathcal{C})^{1-s}\, W(\mathcal{C}\to\mathcal{C}')^{s} - r(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}$$

One thus has $\left(\mathbb{W}(s)\right)_{\mathcal{C}\mathcal{C}'} = \left(\mathbb{W}(1-s)\right)_{\mathcal{C}'\mathcal{C}}$

$$\mathbb{W}(s)^T = \mathbb{W}(1-s)$$

Since those to operators have the same spectrum, one has $\boxed{\psi(s) = \psi(1-s)}$

This symmetry is an instance of 'Gallavotti-Cohen relation'
(or 'Fluctuation Theorem')

- Numerical algorithm for large deviation function: s conjugated to $A = A_1$

By writing $W_s(\mathcal{C}\to\mathcal{C}') = e^{-s\,a(\mathcal{C}\to\mathcal{C}')}W(\mathcal{C}\to\mathcal{C}')$; $r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C}\to\mathcal{C}')$

$$\left(\mathbb{W}(s)\right)_{\mathcal{C}\mathcal{C}'} = \underbrace{W_s(\mathcal{C}'\to\mathcal{C}) - r_s(\mathcal{C})\,\delta_{\mathcal{C}\mathcal{C}'}}_{\text{(probability-conserving) evolution with modified rates } W_s(\mathcal{C}\to\mathcal{C}')} + \underbrace{\left(r_s(\mathcal{C}) - r(\mathcal{C})\right)\delta_{\mathcal{C}\mathcal{C}'}}_{\text{cloning with rate } r_s(\mathcal{C}) - r(\mathcal{C})}$$

one can device an algorithm to measure $\psi(s)$ numerically:

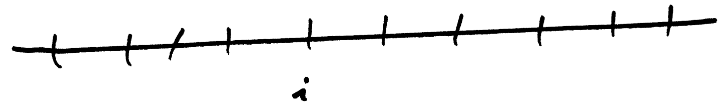
- evolution with rate $W_s(\mathcal{C}\to\mathcal{C}')$ of each copy
- cloning/pruning of copies with rate $r_s(\mathcal{C}) - r(\mathcal{C})$

then the global increase/decrease rate of the population is $\psi(s)$

[there are tricks to keep the population size constant – see Refs.]

Doi - Peliti Formalism for Lattice Gases -

- **Settings :**



lattice with sites i

Each site is described by an occupation number $n_i = 0, 1, \dots$

Dynamics : on each site i, a particle jumps to any neighbor j with rate $W_{i\to j}(\vec{n})$ which depends on the configuration of the whole system $\vec{n} = \{n_i\}$

Hence, in terms of particle occupations, rates write

number of particles that can jump.

$$W(\dots n_i \dots n_j \dots \to \dots n_i - 1 \dots n_j + 1) = n_i \, W_{i\to j}(\vec{n})$$

Example : biased diffusion in dimension 1 $\begin{cases} W_{i\to i+1} = p & \text{jump to the right} \\ w_{i\to i-1} = q & \text{jump to the left} \end{cases}$

$$\begin{cases} W(\dots n_i \, n_{i+1} \dots) \to \dots n_i - 1 \; n_{i+1} + 1 \dots) = p \, n_i \\ W(\dots n_i n_i \dots) \to \dots n_{i-1}+1 \; n_i - 1 \dots) = q \, n_i \end{cases}$$

- **Equation of evolution :** (boundary conditions may add terms)

occupation number before the jump

$$\partial_t P(\vec{n}, t) = \sum_i \sum_{j \text{ neighb. } i} \Big\{ (n_i + 1) \, w_{i\to j}(\dots n_i + 1, n_j - 1 \dots) \, P(\dots n_i + 1, n_j - 1 \dots)$$
$$- n_i w_{i\to j}(\dots n_i \, n_j \dots) \, P(\dots n_i \, n_j \dots) \Big\} \quad (*)$$

Written in this form, it is quite complex to use.

One introduces a (Fock) base $|\vec{n}\rangle$ and $|P(t)\rangle = \sum_{\vec{n}} P(\vec{n}, t) |\vec{n}\rangle$

By changing variables in $(*)$ one has : $(n_i \to n_i - 1 \, , \; n_j \to n_j + 1)$

$$\partial_t |P(t)\rangle = \sum_{\vec{n}} \sum_i \sum_{j \text{ neighb. } i} \left\{ \begin{array}{l} n_i \, w_{i\to j}(\vec{n}) \, P(\vec{n}, t) \, |\dots n_i - 1, n_j + 1 \dots\rangle \\ - n_i \, w_{i\to j}(\vec{n}) \, P(\vec{n}, t) \, |\vec{n}\rangle \end{array} \right\}$$

- Doi-Peliti operators of creation and annihilation a and a^+:

on a single site: $\boxed{\begin{array}{ll} a|n\rangle = n|n-1\rangle & (\text{with } a|0\rangle = 0) \\ a^+|n\rangle = |n+1\rangle & \end{array}}$

on each site: $a_i|\vec{n}\rangle = n_i|\dots n_i-1\dots\rangle \qquad a_i^+|\vec{n}\rangle = |\dots n_i+1\dots\rangle$

One also define a number operator $\hat{n}_i = a_i^+ a_i$, diagonal: $\hat{n}_i|\vec{n}\rangle = n_i|\vec{n}\rangle$

and also for a function $f(n)$ a diagonal operator $f(\hat{n})$ such that $f(\hat{n}_i)|\vec{n}\rangle = f(n_i)|\vec{n}\rangle$
$f(\vec{n})$ $\quad f(\hat{\vec{n}})$ $\quad f(\hat{\vec{n}})|\vec{n}\rangle = f(\vec{n})|\vec{n}\rangle$

- Expression of the operator of evolution:

$$\partial_t|P(t)\rangle = \sum_{\vec{n}}\sum_i\sum_{j\,\text{neighb}\,i}\Big\{\underbrace{\underbrace{w_{i\to j}(\vec{n})}\,P(\vec{n},t)\,a_i\,a_j^+\,\underbrace{|\vec{n}\rangle}}_{=\,w_{i\to j}(\hat{\vec{n}})|\vec{n}\rangle} - w_{i\to j}(\vec{n})P(\vec{n},t)\,|\vec{n}\rangle\Big\}$$

⚠ ordering ⚠

$$= \sum_i\sum_{j\,\text{neighb}\,i}\left(a_j^+a_i\,w_{i\to j}(\hat{\vec{n}}) - \hat{n}_i\,w_{i\to j}(\hat{\vec{n}})\right)\underbrace{\sum_{\vec{n}}P(\vec{n},t)|\vec{n}\rangle}_{=\,|P(t)\rangle \text{ by definit}}$$

Finally: $\boxed{\begin{array}{l}\partial_t|P(t)\rangle = \mathbb{W}|P(t)\rangle \text{ with} \\ \mathbb{W} = \sum_i\sum_{j\,\text{neighb}\,i}\left\{a_j^+a_i\,w_{i\to j}(\hat{\vec{n}}) - \hat{n}_i\,w_{i\to j}(\hat{\vec{n}})\right\}\end{array}}$

This is the Doi-Peliti form of the operator of evolution
If one is able to diagonalize $\mathbb{W}$ one knows all the dynamics

Remark: The ordering is important.
If rates for particles are of the form $w_{i\to j}(\vec{n})\cdot v_{i\to j}(\vec{n}')$ ($\vec{n}$: before; $\vec{n}'$: after the jump)

the term in the equ^n for P is $(n_i+1)w_{i\to j}(n_i+1\;n_j-1)\,v_{i\to j}(n_i\,n_j)\,P(n_i+1\;n_j-1)$

— $|P\rangle$ is $n_i\,w_{i\to j}(\vec{n})\,v_{i\to j}(n_i-1\;n_j+1)\,|\dots n_i-1\;n_j+1\dots\rangle$

— $\mathbb{W}$ is: $\boxed{v_{i\to j}(\hat{\vec{n}})\,a_j^+a_i\,w_{i\to j}(\hat{\vec{n}})}$
after jump $\qquad$ before jump

- Including large deviation parameter s:

× 1st case : s associated to $A = A_1$

One assumes that $A_1 \mapsto A_1 + a_1(i \to j)$ when a jump $i \to j$ occurs { which does not depend on the occupation number (this is easily generalized)

Then, in the equation for $\hat{P}(\vec{n}, s, t)$ one has:

$$\ldots (n_i+1)\, e^{-s a_1(i\to j)}\, w_{i\to j}(\ldots n_i+1, n_j-1 \ldots)\, P(\ldots n_i+1\ n_j-1 \ldots)$$

The operator of evolution is then

$$\boxed{\mathbb{W}(s) = \sum_i \sum_{j\,\text{neighb}\,i} \left\{ a_j^+ a_i\, e^{-s a_1(i\to j)}\, w_{i\to j}(\hat{\vec{n}}) - n_i w_{i\to j}(\hat{\vec{n}}) \right\}}$$

× 2nd case : s associated to $A = A_2$

In this case, only the diagonal term of $\mathbb{W}$ is affected:

$$\boxed{\mathbb{W}(s) = \sum_i \sum_{j\,\text{neighb}\,i} \left\{ a_j^+ a_i\, w_{i\to j}(\hat{\vec{n}}) - \left(\hat{n}_i w_{i\to j}(\hat{\vec{n}}) + s a_2(\hat{\vec{n}})\right) \right\}}$$

$\hat{n}_i = a_i^+ a_i$

- Remark on conservation of probability:

When $s=0$, one writes $\mathbb{W} = \sum_i \sum_{j\,n\,i} (a_j^+ - a_i^+)\, a_i\, w_{i\to j}(\vec{n})$

We now use the identity $\langle n | a^+ = \langle n-1|$ (for a single site)) see later why.
$\langle \vec{n} | a_i^+ = \langle \ldots n_i - 1 \ldots |$

Then $\langle - | \mathbb{W} = \sum_{\vec{n}} \sum_{i\,\text{neighb}\,j} \langle - | (a_j^+ - a_i^+)\, a_i w_{ij}(\hat{\vec{n}}) = \sum_{\vec{n}} \sum_{ij} \left(\langle \ldots n_j - 1 \ldots | - \langle \ldots n_i - 1 \ldots | \right) a_i w_{ij}$

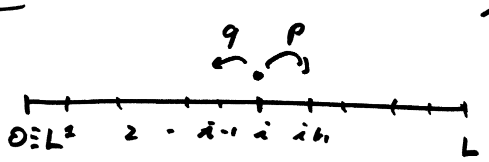
$$\overset{\text{changing } n}{=} \sum_{\vec{n}} \sum_{ij} \underbrace{\left(\langle n| - \langle n| \right)}_{0} a_i w_{ij}(\vec{n})$$

$\underline{\langle - | \mathbb{W} = 0}$ Probability is conserved.

EXAMPLES – (At last!)

- **(Biased) Diffusion in dimension 1:** with various boundary conditions

  - periodic boundary conditions:



a) $$\mathbb{W} = \sum_{i=1}^{L} \left\{ q\, a_i^+ a_{i+1} + p\, a_{i+1}^+ a_i - q\, a_{i+1}^+ a_{i+1} - p\, a_i^+ a_i \right\}$$

unbiased case: symmetric diffusion

$$\mathbb{W} = \sum_{i=1}^{L} a_i^+ (a_{i+1} - a_i) + a_{i+1}^+ (a_i - a_{i+1}) = -\sum_{i=1}^{L} \overbrace{(a_{i+1}^+ - a_i^+)(a_{i+1} - a_i)}^{\text{"}\nabla a^+ \nabla a\text{"}}$$

or: $$\mathbb{W} = \sum_{i=1}^{L} a_i^+ (a_{i+1} + a_{i-1} - a_i - a_i) = \sum_{i=1}^{L} \underbrace{a_i^+ (a_{i+1} + a_{i-1} - 2a_i)}_{\text{"}a^+ \Delta a\text{"}}$$

b) With s conjugated to the current Q: $\quad Q \mapsto \begin{cases} Q+1 & \text{if } \curvearrowright \\ Q-1 & \text{if } \curvearrowleft \end{cases}$

$$\mathbb{W}(s) = \sum_{i=1}^{L} \left\{ e^{s}\, q\, a_i^+ a_{i+1} + e^{-s}\, p\, a_{i+1}^+ a_i - (p+q)\, a_i^+ a_i \right\}$$

c) With s conjugated to the activity K: $\quad K \mapsto K+1$ at each jump

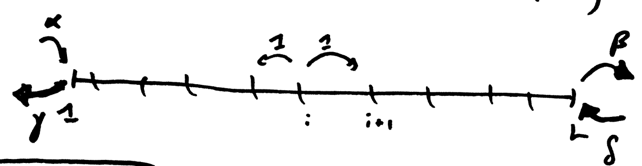
$$\mathbb{W}(s) = \sum_{i=1}^{L} \left\{ e^{s} \left[q\, a_i^+ a_{i+1} + p\, a_{i+1}^+ a_i \right] - (p+q)\, a_i^+ a_i \right\}$$

$$N = \int_0^t d\tau \sum_i n_i$$

d) With s conjugated to the total particle number: $\hat{n}_{tot} = \sum_i \hat{n}_i$

$$\mathbb{W}(s) = \sum_{i=1}^{L} \left\{ q\, a_i^+ a_{i+1} + p\, a_{i+1}^+ a_i - (p+q)\, a_i^+ a_i - s\, a_i^+ a_i \right\}$$

- boundary condition: reservoirs



⚠ correct indexing is important!

$$\mathbb{W} = \underbrace{\sum_{i=1}^{L-1} \left\{ a_{i+1}^+ a_i + a_i^+ a_{i+1} - a_i^+ a_i - a_{i+1}^+ a_{i+1} \right\}}_{\text{bulk dynamics}} + \underbrace{\alpha (a_1^+ - 1) + \beta (a_L - a_L^+ a_L) + \gamma (a_1 - a_1^+ a_1) + \delta (a_L^+ - 1)}_{\text{contact with reservoirs}}$$

- Annihilation / creation :

On a single site : n = occupation number $n \in \mathbb{N}$

Dynamics : $\begin{cases} \cdot \text{ creation at rate } c \\ \cdot \text{ annihilation of each particle at rate } 1 \cdot c) \end{cases}$

Hence : for particle number $\begin{cases} W(n \to n+1) = c \\ W(n \to n-1) = n. \end{cases}$

Equation for $P(n,t)$:

$$\partial_t P(n,t) = (n+1) P(n+1,t) + c\, P(n-1,t) - (\quad n + c) P(n)$$

$$\partial_t |P\rangle = \sum_n \left\{ \quad n\, P(n,t) |n-1\rangle + c\, P(n,t) |n+1\rangle - (\quad n + c) P(n) |n\rangle \right\}$$

$$\boxed{\mathbb{W} = \quad a + c\, a^{+} - (\quad a^{+} a + c)}$$

a and a^+ directly represent reaction and annihilation

Remark : check that $\begin{cases} \cdot \text{ probability is conserved : } \langle - | \mathbb{W} = 0 \\ \cdot \text{ the equilibrium state is Poissonian: } |P_{eq}\rangle = e^{-c} \sum_{n \geq 0} \frac{c^n}{n!} |n\rangle \end{cases}$

- Reaction $A + A \xrightarrow{k} 0$ (k is the reaction rate)

$$W(n \to n-2) = k\, n(n-1)$$

$\begin{pmatrix} n : \text{ choice for the first particle} \\ n-1 : \text{ 2nd} \end{pmatrix}$

$$\partial_t P(n,t) = \sum_n \left\{ k(n+2)(n+1) P(n+2,t) - k\, n(n-1) P(n,t) \right\}$$

$$\partial_t |P\rangle = \sum_n \left\{ k\, n(n-1) P(n) |n-2\rangle - k\, n(n-1) P(n) |n\rangle \right\}$$

$[a, a^+] = 1$

$$\mathbb{W} = k (a)^2 - k\, a^+ a (a^+ a - 1)$$

$\begin{cases} a a^+ = 1 + a^+ a \\ a^+ a (a^+ a - 1) = a^+ (1 + a^+ a) a - a^+ a = a^{+2} a^2 \end{cases}$

$$\boxed{\mathbb{W} = k \left(1 - a^{+2} \right) a^2}$$

Hence for instance the reaction-diffusion operator on a 1d lattice :

$$\mathbb{W} = - \sum_i \left(a^+_{i+1} - a^+_i \right) \left(a_{i+1} - a_i \right) + k \sum_i \left(1 - a_i^{+2} \right) a_i^2$$

- <u>Chemical reaction btw species</u> : $\begin{cases} B \xrightarrow{k_1} A \\ A+B \xrightarrow{k_2} 2B \end{cases}$

operators a, a^+ for A
b, b^+ for B

think that this part is diagonal, and equal to the escape rate

$$\mathbb{W} = k_1 \left(a^+ b - b^+ b \right) + k_2 \left(b^{+2} a b - a^+ a\, b^+ b \right)$$

$$\boxed{\mathbb{W} = k_1 \left(a^+ - b^+ \right) b + k_2 \left(b^{+2} - a^+ b^+ \right) a b}$$

- <u>Kinetically constrained models (KCM)</u> (Bosonic version) on a 1d lattice

$\circ : n_i = 0$ $\quad \circ \xrightarrow{c} \bullet$

$\bullet : n_i = 1$ $\quad \bullet \xrightarrow{(1-c)} \circ$

with rates proportional to the number of active neighbors before the jump

$$\begin{cases} W(n_i \to n_i + 1) = c\,(n_{i+1} + n_{i-1}) \\ W(n_i \to n_i - 1) = (1-c)\, n_i\, (n_{i+1} + n_{i-1}) \end{cases}$$

$$\boxed{\mathbb{W} = \sum_i \left[c\, a_i^+ + (1-c)\, a_i - \left(c + (1-c)\, a_i^+ a_i \right) \right] \left(a_{i+1}^+ a_{i+1} + a_{i-1}^+ a_{i-1} \right)}$$

- <u>Mean-Field version</u> : n is the number of active sites

choice

n-1 neighbors to the one which decays

$$\begin{cases} W(n \to n+1) = c\, n \\ W(n \to n-1) = (1-c)\, n\, (n-1) \end{cases}$$

$$\mathbb{W} = c\left(a^{+2} a - a^+ a \right) + (1-c) \Big[\underbrace{a\,(a^+ a - 1)}_{a^+ a^2} + a^+ a \underbrace{(a^+ a - 1)}_{a^+ a^2} \Big]$$

$(a^+ a + 1) a - a$

$$\boxed{\mathbb{W} = c\, a^+ (a^+ - 1) a + (1-c)\, a^+ (1 + a^+) a^2}$$

- Technical remark 1: useful similarity transformations:

Lectures on Stoch. processes (1.20)

1) $\varphi(\ell) = e^{-\ell\hat{n}} a\, e^{\ell\hat{n}}$: $\begin{cases} \varphi(0) = a \\ \varphi'(\ell) = e^{-\ell\hat{n}} \underbrace{(-\hat{n}a + a\hat{n})}_{aa^+a - a^+aa = (aa^+ - a^+a)a = a} e^{\ell n} = e^{-\ell\hat{n}} a\, e^{\ell\hat{n}} = \varphi(\ell) \end{cases}$

thus $\varphi(\ell) = e^{\ell}\varphi(0) = e^{\ell} a$ $\boxed{e^{-\ell\hat{n}} a\, e^{\ell\hat{n}} = e^{\ell} a}$

2) $\varphi(\ell) = e^{-\ell\hat{n}} a^+ e^{\ell\hat{n}}$: $\begin{cases} \varphi(0) = a^+ \\ \varphi'(\ell) = e^{-\ell\hat{n}} \underbrace{(-\hat{n}a^+ + a^+\hat{n})}_{a^+a^+a - a^+aa^+ = a^+(a^+a - aa^+) = -a^+} e^{\ell\hat{n}} = -e^{\ell\hat{n}} a^+ e^{\ell\hat{n}} = -\varphi(\ell) \end{cases}$

thus $\varphi(\ell) = e^{-\ell}\varphi(0) = e^{-\ell} a^+$ $\boxed{e^{-\ell\hat{n}} a^+ e^{\ell\hat{n}} = e^{-\ell} a^+}$

1+2) : On thus have found a similarity transformation $Q = e^{+\ell\hat{n}}$ such that

$$\boxed{\begin{cases} Q^{-1} a\, Q = z\, a \\ Q^{-1} a^+ Q = \frac{1}{z} a^+ \end{cases}}$$

(one has set $z = e^{\ell}$)

(Any similarity transformation does not modify the spectrum.)

3) $\varphi(\ell) = e^{-\ell a^+} a\, e^{\ell a^+}$ $\left.\begin{cases} \varphi(0) = a \\ \varphi'(\ell) = e^{-\ell a^+}(aa^+ - a^+a)e^{\ell a^+} = 1 \end{cases}\right\}$ $\varphi(\ell) = a + \ell$

in this case, setting $Q = e^{-\ell a^+}$ one has $\boxed{\begin{cases} Q^{-1} a\, Q = a + \ell \\ Q^{-1} a^+ Q = a^+ \end{cases}}$

4) Similarly $Q = e^{+\ell a}$ yields $\boxed{\begin{cases} Q^{-1} a\, Q = a \\ Q^{-1} a^+ Q = a^+ + \ell \end{cases}}$

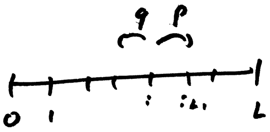
Remark: 1) and 2) can also be obtained directly:

$$z^{+\hat{n}} a\, z^{-\hat{n}} |n\rangle = z^{+\hat{n}} z^{-n} a|n\rangle = z^{+\hat{n}} z^{-n}\, n\, |n-1\rangle = z^{+(n-1)-n} a|n\rangle = z^{-1} a|n\rangle$$

$$z^{-\hat{n}} a^+ z^{+\hat{n}} |n\rangle = z^{-\hat{n}} z^{n} |n+1\rangle = z^{-(n+1)} z^{n} |n+1\rangle = z^{-1} a^+ |n\rangle$$

• <u>Technical remark 2</u>: Consequence of particle conservation

Let's consider the (biased) walk



with s conjugated $\begin{cases} \text{to the total current} \to \mathbb{W}_{tot}(s) \\ \text{to the current through the bond } 1 \leftrightarrow 2 \,{\scriptstyle (L-1 \leftrightarrow L)} : \mathbb{W}_1(s) \end{cases}$

One has
$$\mathbb{W}_{tot}(s) = \sum_{i=0}^{L-1} e^{s} q\, a_i^{+} a_{i+1} + e^{s} p\, a_{i+1}^{+} a_i - q\, a_{i+1}^{+} a_{i+1} - p\, a_i^{+} a_i$$

$$\mathbb{W}_1(s) = \begin{cases} \sum_{i=0}^{L-2} q\, a_i^{+} a_{i+1} + p\, a_{i+1}^{+} a_i - q\, a_{i+1}^{+} a_{i+1} - p\, a_i^{+} a_i \\ \quad + q e^{+s} a_{L-1}^{+} a_L + p\, a_L^{+} a_{L-1} e^{-s} - q\, \hat{n}_L - p\, \hat{n}_{L-1} \end{cases}$$

$\hookrightarrow$ (!) $a_L^{+} = a_0^{+}$ $\quad a_L = a_0$

One sets $\hat{Q} = e^{s \sum_{i=0}^{L-1} i \hat{n}_i}$

one has for $0 \leq i \leq L-2$
$$\begin{cases} \hat{Q}^{-1} a_i^{+} a_{i+1} \hat{Q} = e^{is} e^{-(i+1)s} a_i^{+} a_{i+1} = e^{-s} a_i^{+} a_{i+1} \\ \hat{Q}^{-1} a_{i+1}^{+} a_i \hat{Q} = e^{(i+1)s} e^{-is} a_{i+1}^{+} a_i = e^{s} a_{i+1}^{+} a_i \end{cases}$$

But: for $i = L-1$:
$$\hat{Q}^{-1} a_{L-1}^{+} a_L \hat{Q} = \hat{Q}^{-1} a_{L-1}^{+} a_0 \hat{Q} = e^{(L-1)s} a_{L-1}^{+} a_0$$
$$\hat{Q}^{-1} a_L^{+} a_{L-1} \hat{Q} = \hat{Q}^{-1} a_0^{+} a_{L-1} \hat{Q} = e^{-(L-1)s} a_0^{+} a_{L-1}$$

<u>Hence</u>:
$$\hat{Q}^{-1} \mathbb{W}_{tot}(s) \hat{Q} = \sum_{i=0}^{L-2} q\, a_i^{+} a_{i+1} + p\, a_{i+1}^{+} a_i - q\, a_{i+1}^{+} a_{i+1} - p\, a_i^{+} a_i$$
$$\quad + q e^{Ls} a_{L-1}^{+} a_L + p e^{-Ls} a_L^{+} a_{L-1} - q\, \hat{n}_L - p\, \hat{n}_{L-1}$$

$$\hat{Q}^{-1} \mathbb{W}_{tot}(s) \hat{Q} = \mathbb{W}_1(Ls)$$ thus, since spectra are the same:

$$\boxed{\psi_{tot}(s) = \psi_1(Ls)}$$

We thus have shown that the large deviation function for the total current is simply related to that of the current through one bond.

• Technical remark 3:

a^+ is not the adjoint of a, contrary to the situation in quantum mech.

× Reminder on quantum mechanics

The quantum creation and annihilation operators (denoted α, α^+ here) are such that
$$\begin{cases} \alpha\,|n\rangle = \sqrt{n}\,|n-1\rangle \\ \alpha^+|n\rangle = \sqrt{n+1}\,|n+1\rangle \end{cases}$$

α^+ is the hermitian conjugate of α. Indeed:

$$\langle n|\alpha^+ = \langle n|\underbrace{\alpha^+\sum_m |m\rangle}\langle m| = \sum_m \underbrace{\langle n|\sqrt{m+1}\,|m+1\rangle}_{\delta_{m+1,n}}\langle m| = \sqrt{n}\,\langle n-1|$$
$$= \left(\sqrt{n}\,|n-1\rangle\right)^+$$

$$\boxed{\langle n|\alpha^+ = (\alpha|n\rangle)^+}$$

× Similarity transformation from α, α^+ to a, a^+:

The quantum operator number $\alpha^+\alpha$ is equal to $a^+a = \hat{n}$: $\alpha^+\alpha|n\rangle = \alpha^+\sqrt{n}|n-1\rangle = n|$

One sets:
$$\boxed{\begin{cases} a = (\hat{n}!)^{-1/2}\,\alpha\,(\hat{n}!)^{1/2} \\ a^+ = (\hat{n}!)^{-1/2}\,\alpha^+(\hat{n}!)^{1/2} \end{cases}}$$

Then:
$$a|n\rangle = (\hat{n}!)^{-1/2}(n!)^{1/2}\sqrt{n}\,|n-1\rangle = \overbrace{\left(\frac{n!}{(n-1)!}\right)^{1/2}}^{\sqrt{n}}\sqrt{n}\,|n-1\rangle = n|n-1\rangle \quad \text{ok}$$

$$a^+|n\rangle = (\hat{n}!)^{-1/2}(n!)^{1/2}\sqrt{n+1}\,|n+1\rangle = \underbrace{\left(\frac{n!}{(n+1)!}\right)^{1/2}}_{1/\sqrt{n+1}}\sqrt{n+1}\,|n+1\rangle = |n+1\rangle \quad \text{ok}$$

The expressions above are thus correct representations of a, a^+

→ In other words the (statistical physics) Doi-Peliti operators a, a^+ are (non-unitary) similarity transformed of the quantum creation and annihilation operators α, α^+.

The non-unitarity explains why $(a)^+ \neq a^+$.

$\boxed{\text{Lecture on Stoch. processes}}$

- Technical remark 4: how can one transpose a, a^+ ?

$$\langle n|a^+ = \langle n|a^+ \overbrace{\sum_m |m\rangle\langle m|}^{\mathbb{1}\ (\text{identity})} = \sum_m \overbrace{\langle n|m+1\rangle}^{\delta_{n,m+1}}\langle m| = \langle n-1| \Rightarrow \boxed{\langle n|a^+ = \langle n-1|}$$

$$\langle n|a = \langle n|a \sum_m |m\rangle\langle m| = \sum_m \overbrace{\langle n|m|m-1\rangle}^{m\,\delta_{n,m-1}}\langle m| = \langle n+1|(n+1) \Rightarrow \boxed{\langle n|a = \langle n-1|(n+1)}$$

- Technical remark 5: What is the meaning of the eigen vectors associated to $\mathbb{W}(s)$?

. Let's call $|R\rangle$ and $\langle L|$ the left and right eigen vectors associated to the maximum eigen value $\psi(s)$ of $\mathbb{W}(s)$

One knows that at $s=0$: $\langle L| = \langle -| = \sum_{\mathcal{C}} \langle \mathcal{C}|$ and $|R\rangle = \underset{\text{steady state}}{|P_{st}\rangle}$.

. One can normalize $|R\rangle$ such that $\langle -|R\rangle = 1$ (ie $\sum_{\mathcal{C}} R(\mathcal{C}) = 1$: R is normalized).

Consider an observable $O(\mathcal{C})$ depending on the configuration.

. Final-time average in the s-state: diagonal operator of elements $O(\mathcal{C})$: $\hat{O} = \sum_{\mathcal{C}} O(\mathcal{C})|\mathcal{C}\rangle\langle\mathcal{C}|$

$$\langle O\rangle_s^{final} = \lim_{t\to\infty} \langle O(\mathcal{C}(t))\rangle_s = \lim_{t\to\infty} \frac{\langle -|\hat{O} e^{t\mathbb{W}(s)}|P_0\rangle}{\langle -|\underbrace{e^{t\mathbb{W}(s)}|P_0\rangle}_{\text{in the long time limit: } \sim e^{t\psi(s)}|R\rangle}} \leftarrow \text{initial configuration}$$

$$= \frac{\langle -|\hat{O} e^{t\psi(s)}|R\rangle}{\langle -| e^{t\psi(s)}|R\rangle} \quad \text{Hence: } \boxed{\langle O\rangle_s^{final} = \langle -|\hat{O}|R\rangle}$$

. Intermediate-time average in the s-state: let "$0 \ll \tau \ll t$"

$$\langle O\rangle_s^{interm.} = \lim_{\tau\to\infty}\lim_{t\to\infty} \langle O(\mathcal{C}(\tau))\rangle_s = \lim_{\tau\to\infty}\lim_{t\to\infty} \frac{\langle -|e^{(t-\tau)\mathbb{W}(s)}\hat{O}e^{\tau\mathbb{W}(s)}|P_0\rangle}{\underbrace{\langle -|e^{(t-\tau)\mathbb{W}(s)}}_{\sim \langle L|e^{(t-\tau)\psi(s)}} \underbrace{e^{\tau\mathbb{W}(s)}|P_0\rangle}_{\sim e^{\tau\psi(s)}|R\rangle}}$$

$$\boxed{\langle O\rangle_s^{final} = \langle L|\hat{O}|R\rangle}$$

. Other demonstration: consider the average of the time-integrated O:

$$\langle O\rangle_s^{integ} = \lim_{t\to\infty} \left\langle \frac{1}{t}\int_0^t d\tau\, O(\mathcal{C}(\tau))\right\rangle_s = \lim_{t\to\infty} \partial_t \partial_h \Big|_{h=0} \langle -|\underbrace{e^{t(\mathbb{W}(s)+h\hat{O})}}_{\text{on utilise une théorie de perturbation}}|P_0\rangle$$

$$= \langle L|\hat{O}|R\rangle$$