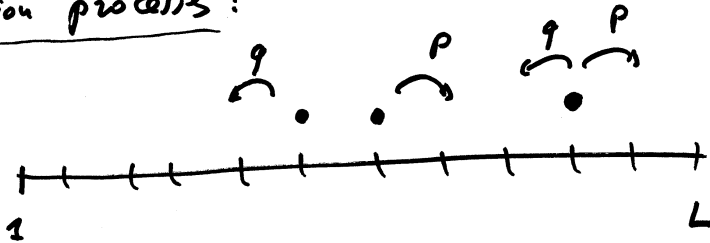


Lecture 2 - 30/11/2011

• MOTIVATIONS :

Exclusion process :



- Each site is either empty ($n_i = 0$) or occupied (\bullet , $n_i = 1$) by a particle
- Each particle can jump to its left (right) with rate q (p) provided the target site is empty (EXCLUSION RULE)

• This can model :

- car / pedestrian (in a queue) traffic, jam
- motion of motor proteins (e.g: dynein, kinesin) on microtubules

• Classification :

SSEP	(Symmetric)	$p = q$
ASEP	(asymmetric)	$p \neq q$
TASEP	(totally -)	$q = 0$ $p > 0$
WASEP	(weakly asymmetric)	$p - q = \frac{\epsilon}{L}$

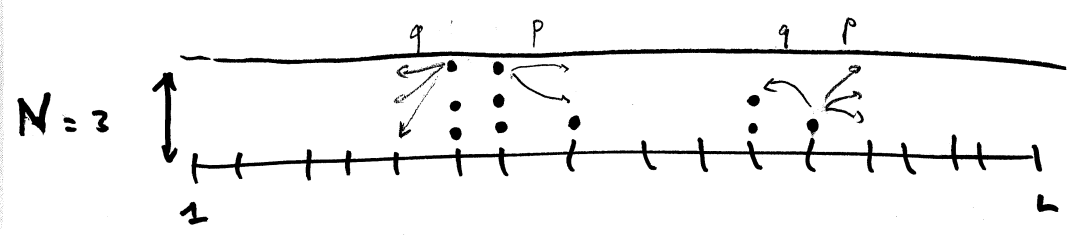
- This is the "Ising model" of non-equilibrium dynamics
- The (non-equilibrium) steady state \rightarrow (NESS) is known in various situations
 - closed boundary condition, or periodic
 - contact with reservoirs at the boundaries

The large deviation of current (activity) have been computed in the large size limit (with finite size correction) in the (WA)SEP.

• Partial Exclusion Process :

The ^{exclusion} condition is used: each site can contain between 0 and N particles

Each particle can jump to any of the empty site with rate p or q



in other words, in terms of particle number transition rates:

$$\begin{aligned}
 W(\dots n_i, n_{i+1}, \dots \rightarrow \dots n_i - 1, n_{i+1} + 1, \dots) &= p n_i (N - n_{i+1}) \\
 W(\dots n_i, n_{i+1}, \dots \xrightarrow{q} \dots n_i + 1, n_{i+1} - 1, \dots) &= q (N - n_i) n_{i+1}
 \end{aligned}$$

Annotations:
 - p : choice of the moving particle (jump to the right)
 - $(N - n_{i+1})$: choice of the target site
 - q : particle moving
 - $(N - n_i)$: target site

This implements the partial exclusion ($N - n = 0$ if the occupation # n of the target site is $n = N$ i.e. if the target site is full)

• Spin operators for stochastic processes :

One defines, for each site described by a vector $|n\rangle$ ($0 \leq n \leq N$)

$$\begin{aligned}
 S^+ |n\rangle &= (N - n) |n + 1\rangle \\
 S^- |n\rangle &= n |n - 1\rangle \\
 \hat{n} |n\rangle &= n |n\rangle
 \end{aligned}$$

or matrixially:
 $S^+ = \begin{pmatrix} 0 & & & \\ N & & & \\ & \ddots & & \\ & & 1 & \\ & & & 0 \end{pmatrix}$
 $S^- = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & n \\ & & & & 0 \end{pmatrix}$
 $\hat{n} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & n \end{pmatrix}$

One also reads from the matrices :

$$\begin{aligned}
 \langle n | S^+ &= \langle n - 1 | (N - n + 1) \\
 \langle n | S^- &= \langle n + 1 | (n + 1)
 \end{aligned}$$

where by convention one notes:
 $\langle -1 | = \langle N + 1 | = 0$

Commutation relations:

One defines $S^z = \hat{n} - \frac{1}{2}N$

$$= \begin{pmatrix} -\frac{N}{2} & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & \ddots & \\ & & & & \frac{N}{2} \end{pmatrix}$$

(2.3)
Lecture on
Stochastic processes

One checks directly that S^\pm, S^z obey the commutation relations

$$\boxed{[S^+, S^-] = \pm S^z \quad [S^+, S^z] = 2S^+ \quad [S^-, S^z] = 2S^-}$$

which are the same for quantum operators

Similarly, defining

$$S^x = \frac{1}{2}(S^+ + S^-)$$

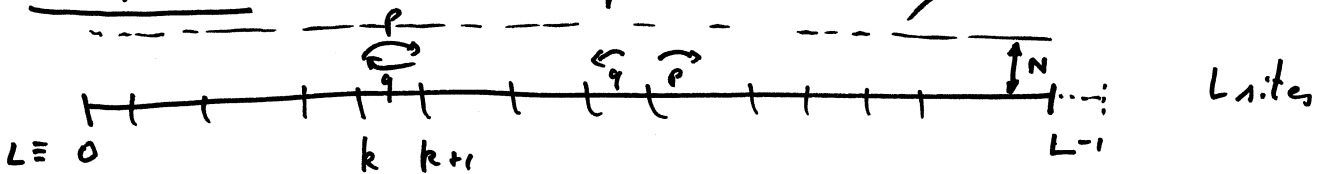
$$S^y = \frac{1}{2i}(S^+ - S^-)$$

one has $\boxed{[S^x, S^y] = iS^z}$ and similar cyclic permutation
(i : complex number $i^2 = -1$)

Let's e.g. show that $[S^+, S^-] = 2S^z = 2\hat{n} - N$:

$$\begin{aligned} [S^+, S^-] |n\rangle &= S^+ n |n-1\rangle - S^- (N-n) |n+1\rangle = [(N-n+1)n - (N-n)(n+1)] |n\rangle \\ &= (2n - N) |n\rangle \quad \text{hence the result} \end{aligned}$$

Example 1: ASEP with periodic boundary conditions



$$\partial_t P(\vec{n}, t) = \sum_{k=0}^{L-1} \left\{ p \binom{N-n_{k+1}}{n_{k+1}} P(n_{k+1}, n_{k+1}-1, t) + q \binom{N-n_k}{n_k} P(n_k-1, n_k+1, t) - q n_{k+1} (N-n_k) P(\vec{n}) - p n_k (N-n_{k+1}) P(\vec{n}) \right\}$$

$$\partial_t |P(t)\rangle = \sum_{\vec{n}} \sum_{k=0}^{L-1} \left\{ p \binom{N-n_{k+1}}{n_{k+1}} P(n_{k+1}, n_{k+1}-1, t) |\vec{n}\rangle + q \binom{N-n_k}{n_k} P(n_k-1, n_k+1, t) |\vec{n}\rangle - q n_{k+1} (N-n_k) P(\vec{n}) |\vec{n}\rangle - p n_k (N-n_{k+1}) P(\vec{n}) |\vec{n}\rangle \right\}$$

change of variable on \vec{n} so as to factorize by $P(\vec{n})$

$$= \sum_{\vec{n}} \sum_{k=0}^{L-1} \left\{ p n_k (N-n_{k+1}) |n_k-1, n_{k+1}\rangle + q (N-n_k) n_{k+1} |n_k+1, n_{k+1}-1\rangle - p n_k (N-n_{k+1}) |\vec{n}\rangle - q (N-n_k) n_{k+1} |\vec{n}\rangle \right\} P(\vec{n})$$

in the sum: $L \equiv 0$ (periodic b.c.)

In the gain term of that equation, one recognizes

(2.4)
Lecture on
Stoch. process

$$\begin{cases} n_k (N - n_{k+1}) |n_{k-1}, n_{k+1}\rangle = S_k^- S_{k+1}^+ |\vec{n}\rangle \\ (N - n_k) n_{k+1} |n_{k+1}, n_{k+1}\rangle = S_k^+ S_{k+1}^- |\vec{n}\rangle \end{cases}$$

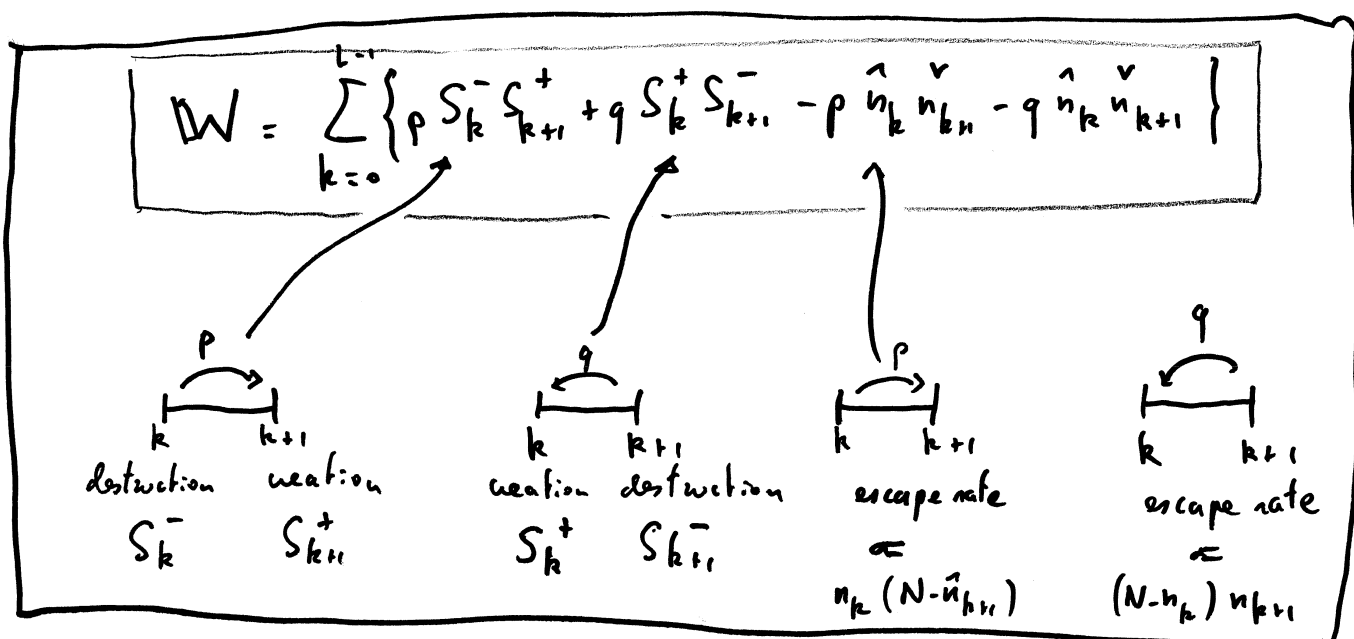
one notes $\hat{n}_k \equiv \hat{n}_k |\vec{n}\rangle = n_k |\vec{n}\rangle$

$$\hat{n}_k^v = N - \hat{n}_k$$

Thus:

$$\partial_t |P(t)\rangle = \sum_{k=0}^{L-1} \left\{ p S_k^- S_{k+1}^+ + q S_k^+ S_{k+1}^- - p \hat{n}_k^v \hat{n}_{k+1} - q \hat{n}_k^v \hat{n}_{k+1} \right\} \sum_{\vec{n}} P(\vec{n}) |\vec{n}\rangle$$

One identifies \mathbb{W} in $\partial_t |P(t)\rangle = \mathbb{W} |P(t)\rangle$ to:



One thus reads directly from the dynamics the form of \mathbb{W}

• Example 1 ^{bis}: s-modified operator of evolution $\mathbb{W}(s)$

* s conjugated to the activity κ :

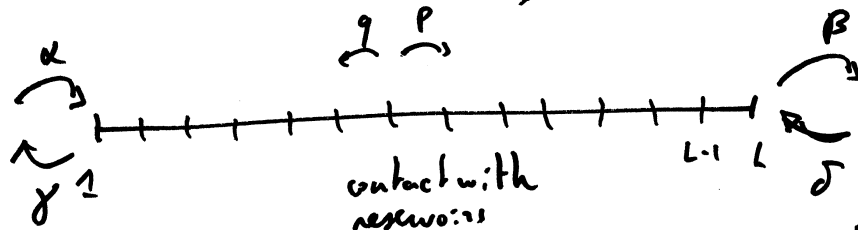
$$\mathbb{W}(s) = \sum_{k=0}^{L-1} \left\{ e^{-s} [p S_k^- S_{k+1}^+ + q S_k^+ S_{k+1}^-] - p \hat{n}_k^v \hat{n}_{k+1} - q \hat{n}_k^v \hat{n}_{k+1} \right\}$$

* s conjugated to the total current Q :

$$\mathbb{W}(s) = \sum_{k=0}^{L-1} \left\{ e^{-s} p S_k^- S_{k+1}^+ + e^s q S_k^+ S_{k+1}^- - p \hat{n}_k^v \hat{n}_{k+1} - q \hat{n}_k^v \hat{n}_{k+1} \right\}$$

• Example 2: with boundary conditions with reservoirs

lecture 2.5
Stoch. processes



$$W = W_{\text{bulk}} + W_{\text{res}} \quad \text{where } W_{\text{bulk}} = \sum_{k=1}^{L-1} \left\{ p S_k^- S_{k+1}^+ + q S_k^+ S_{k+1}^- - p \hat{n}_k \hat{n}_{k+1}^v - q \hat{n}_k^v \hat{n}_{k+1} \right\}$$

* from the rules given previously one expects:

$$W_{\text{res}} = \alpha (S_1^+ - \hat{n}_1^v) + \delta (S_L^+ - \hat{n}_L^v) + \gamma (S_1^- - \hat{n}_1) + \beta (S_L^- - \hat{n}_L)$$

* let's for instance check explicitly the left (α) boundary term:

$$\partial_t P(\vec{n}, t) \stackrel{\alpha \gamma}{=} \alpha (N - n_1) P(n_1, t) + \gamma (n_1 + 1) P(n_1 + 1, t) - \alpha (N - n_1) P(n_1, t) - \gamma n_1 P(n_1, t)$$

$$\partial_t |P(t)\rangle = \sum_{\vec{n}} \left(\alpha \overbrace{(N - n_1 + 1) P(n_1, t)}^{n_1 \rightarrow n_1 + 1} |\vec{n}\rangle + \gamma \overbrace{(n_1 + 1) P(n_1 + 1, t)}^{n_1 \rightarrow n_1 - 1} |\vec{n}\rangle - \alpha (N - n_1) P(n_1, t) |\vec{n}\rangle - \gamma n_1 P(n_1, t) |\vec{n}\rangle \right)$$

change of variable on \vec{n}
so as to factorize $P(\vec{n}, t)$

$$= \sum_{\vec{n}} \left(\alpha \overbrace{(N - n_1) |n_1 + 1\rangle}^{S_1^+ |\vec{n}\rangle} + \gamma \overbrace{n_1 |n_1 - 1\rangle}^{S_1^- |\vec{n}\rangle} - \alpha (N - n_1) |\vec{n}\rangle - \gamma n_1 |\vec{n}\rangle \right) P(\vec{n}, t)$$

$$= \underbrace{(\alpha (S_1^+ - \hat{n}_1^v) + \gamma (S_1^- - \hat{n}_1))}_{\text{this is the left term of the boundary operator}} \underbrace{\sum_{\vec{n}} P(\vec{n}, t) |\vec{n}\rangle}_{|P(t)\rangle}$$

this is the left term of the boundary operator

W_{res} that we expected

• Analogy with quantum mechanics

What is the link between the S^\pm, S^z and the quantum ones?

• Quantum operators; Σ^\pm, Σ^z verify

$$\begin{cases} \Sigma^+ |n\rangle = \sqrt{(n+1)(N-n)} |n+1\rangle \\ \Sigma^- |n\rangle = \sqrt{n(N-n+1)} |n-1\rangle \\ \Sigma^z |n\rangle = (n - \frac{1}{2}N) |n\rangle \end{cases} \rightarrow \Sigma^z = S^z$$

Besides, they are hermitian-adjoint: $(\Sigma^+)^\dagger = \Sigma^-$

• From quantum to statistical operators:

Consider $Q = \binom{N}{n}^{-1/2}$ (binomial coefficient) $\binom{N}{n} = \frac{N!}{n!(N-n)!}$

and let's show that

$$\boxed{S^\pm = Q^{-1} \Sigma^\pm Q}$$

$$\frac{(n+1)!(N-n-1)!}{n!(N-n)!} = \frac{n+1}{N-n}$$

$$\begin{aligned} Q^{-1} \Sigma^+ Q |n\rangle &= \binom{N}{n}^{-1/2} Q^{-1} \sqrt{(n+1)(N-n)} |n+1\rangle = \sqrt{(n+1)(N-n)} \left(\frac{\binom{N}{n}}{\binom{N}{n+1}} \right)^{-1/2} |n+1\rangle \\ &= \sqrt{\frac{(n+1)(n+1)(N-n)}{(N-n)^{-1}}} |n+1\rangle = (N-n) |n+1\rangle = S^+ |n\rangle \quad \text{OK} \end{aligned}$$

$$\begin{aligned} Q^{-1} \Sigma^- Q |n\rangle &= \binom{N}{n}^{-1/2} Q^{-1} \sqrt{n(N-n+1)} |n-1\rangle = \sqrt{n(N-n+1)} \left(\frac{\binom{N}{n}}{\binom{N}{n-1}} \right)^{-1/2} |n-1\rangle \\ &= \sqrt{\frac{n(N-n+1)n}{N-n+1}} |n-1\rangle \left(\frac{n!(N-n)!}{(n-1)!(N-n+1)!} \right)^{-1/2} = \left(\frac{n}{N-n+1} \right)^{-1/2} |n-1\rangle \\ &= n |n-1\rangle = S^- |n-1\rangle \quad \text{OK} \end{aligned}$$

• To summarize: S^\pm are (non-unitary) similarity transformations through Q of the quantum spin operators Σ^\pm

Since the transformation is not unitary: $(S^+)^\dagger \neq S^-$ while $(\Sigma^+)^\dagger = \Sigma^-$

Indeed $(S^+)^\dagger = Q^\dagger \Sigma^- Q^{-\dagger} = \underbrace{Q^\dagger Q}_{\neq \mathbb{1}} S^- \underbrace{Q^{-1} Q^{-\dagger}}_{\neq \mathbb{1}}$ since Q is not unitary

• Steady state in equilibrium for the symmetric S.E.P. (L.7)
Lecture on
Stoch. processes

Fix a density $0 < p < 1$ and consider the eq. distrib. product of Bernoulli laws

$$P_{eq}^p(\vec{n}) = \prod_{k=1}^L \binom{N}{n_k} p^{n_k} (1-p)^{N-n_k}$$

x case of a single site: $|B^p\rangle = \sum_{n=0}^N P_{eq}^p(n) |n\rangle = \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} |n\rangle$

action of S^+ :

$$\begin{aligned} S^+ |B^p\rangle &= \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} (N-n) |n+1\rangle = \sum_{n=0}^N \binom{N}{n-1} p^{n-1} (1-p)^{N-n+1} |n\rangle \\ &= \sum_{n=0}^N n \frac{1-p}{p} \binom{N}{n} p^n (1-p)^{N-n} |n\rangle \quad \text{we used } (N-n+1) \binom{N}{n-1} = n \binom{N}{n} \\ &= \frac{1-p}{p} \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} \underbrace{n}_{\hat{n}} |n\rangle = \frac{1-p}{p} \hat{n} |B^p\rangle \end{aligned}$$

$$\boxed{S^+ |B^p\rangle = \frac{1-p}{p} \hat{n} |B^p\rangle}$$

action of S^- :

$$\begin{aligned} S^- |B^p\rangle &= \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} n |n-1\rangle = \sum_{n=0}^N \binom{N}{n+1} p^{n+1} (1-p)^{N-n-1} |n\rangle \\ &= \sum_{n=0}^N (N-n) \left(\frac{1-p}{p}\right) \binom{N}{n} p^n (1-p)^{N-n} |n\rangle \quad \text{when we used } (n+1) \binom{N}{n+1} = (N-n) \binom{N}{n} \\ &= \frac{p}{1-p} \sum_{n=0}^N \binom{N}{n} p^n (1-p)^{N-n} (N-n) |n\rangle = \frac{p}{1-p} (N - \hat{n}) |B^p\rangle \end{aligned}$$

$$\boxed{S^- |B^p\rangle = \frac{p}{1-p} \hat{n} |B^p\rangle}$$

x case of Product law on the sites with p.b.c. and $p=q$: $W = \sum_{k=1}^L \{ S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ - \hat{n}_k \hat{n}_{k+1} - \hat{n}_{k+1} \hat{n}_k \}$

Thus $W |B^p\rangle = \sum_{k=1}^L \left\{ \frac{p}{1-p} \frac{1-p}{p} \hat{n}_k \hat{n}_{k+1} + \frac{p}{1-p} \frac{1-p}{p} \hat{n}_{k+1} \hat{n}_k - \hat{n}_k \hat{n}_{k+1} - \hat{n}_{k+1} \hat{n}_k \right\} |B^p\rangle$

and one finds $W |B^p\rangle = 0$: $|B^p\rangle$ is the steady state with p fixed by the total # of particles

• Eq. steady state in contact with reservoirs:

(2.8)
Lecture on
stoch. processes

Now, the # of particles is not fixed.

Let's see how α β γ δ are determined, and fix ρ :

$$W_{\text{reservoir}} = \alpha (S_1^+ - \hat{n}_1) + \delta (S_2^+ - \hat{n}_2) \\ + \gamma (S_1^- - \hat{n}_1) + \beta (S_2^- - \hat{n}_2)$$

$$W_{\text{res}} |BP\rangle = \alpha \left(\frac{1-\rho}{\rho} \hat{n}_1 - \hat{n}_1 \right) + \delta \left(\frac{1-\rho}{\rho} \hat{n}_2 - \hat{n}_2 \right) \\ + \gamma \left(\frac{\rho}{1-\rho} \hat{n}_1 - \hat{n}_1 \right) + \beta \left(\frac{\rho}{1-\rho} \hat{n}_2 - \hat{n}_2 \right) \\ = \left(\alpha \frac{1-\rho}{\rho} - \gamma \right) \hat{n}_1 + \left(\delta \frac{1-\rho}{\rho} - \beta \right) \hat{n}_2 \\ + \left(\gamma \frac{\rho}{1-\rho} - \alpha \right) \underbrace{\hat{n}_1}_{(N-\hat{n}_1)} + \left(\beta \frac{\rho}{1-\rho} - \delta \right) \underbrace{\hat{n}_2}_{(N-\hat{n}_2)}$$

For all those terms to vanish one needs:

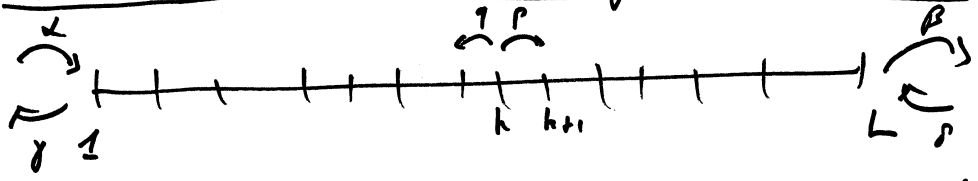
$$\begin{cases} \alpha \frac{1-\rho}{\rho} = \gamma \\ \delta \frac{1-\rho}{\rho} = \beta \end{cases}$$

ie $\boxed{\begin{matrix} \rho = \frac{\alpha}{\alpha + \gamma} \\ \rho = \frac{\delta}{\delta + \beta} \end{matrix}}$ $\left. \begin{matrix} \text{equality implies} \\ \frac{\alpha}{\delta} = \frac{\gamma}{\beta} \end{matrix} \right\}$

The solution for the steady state is thus $|BP\rangle$

with $\rho = \frac{\alpha}{\alpha + \gamma} = \frac{\delta}{\delta + \beta}$ provided $\frac{\alpha}{\gamma} = \frac{\delta}{\beta}$

• Symmetry 1: conservation of particle number:



Let's relate the operator $W_{tot}(s)$ for the total current to the one $W_1(s)$ for the current at the right boundary:

$$W_{tot}(s) = \sum_{k=1}^{L-1} \left\{ p S_k^- S_{k+1}^{+s} + q S_k^+ S_{k+1}^- e^s - p \hat{n}_k \hat{n}_{k+1}^v - q \hat{n}_k^v \hat{n}_{k+1} \right\} + \alpha (S_1^+ - \hat{n}_1) + \delta (S_L^+ - \hat{n}_L) + \gamma (S_1^- - \hat{n}_1) + \beta (S_L^- - \hat{n}_L)$$

* Let's find a similarity transform Q such that $Q^{-1} S^\pm Q = (z)^\pm S^\pm$:

$$\begin{aligned} z^{+\hat{n}} S^+ z^{-\hat{n}} |n\rangle &= z^{+\hat{n}} z^{-(n+1)} (n+1) |n+1\rangle = z S^+ |n\rangle \\ z^{-\hat{n}} S^- z^{+\hat{n}} |n\rangle &= z^{-\hat{n}} z^{-(n-1)} n |n-1\rangle = z^{-1} S^- |n\rangle \end{aligned} \quad \text{) thus } \underline{Q = z^{-\hat{n}} \text{ works}}$$

* Apply $Q^{-1} \cdot Q$ with $Q = e^{-s \sum_{k=1}^L k \hat{n}_k}$:

$$\text{using } \begin{cases} Q^{-1} S_k^- S_{k+1}^+ Q = e^{-sk} e^{s(k+1)} S_k^- S_{k+1}^+ = e^s S_k^- S_{k+1}^+ \\ Q^{-1} S_k^+ S_{k+1}^- Q = e^{sk} e^{-s(k+1)} S_k^+ S_{k+1}^- = e^{-s} S_k^+ S_{k+1}^- \end{cases} \quad \begin{cases} Q^{-1} S_1^\pm Q = e^{\pm s} S_1^\pm \\ Q^{-1} S_L^\pm Q = e^{\pm Ls} S_L^\pm \end{cases}$$

One finds: s has disappeared from the bulk and remains at the right boundary

$$Q^{-1} W_{tot}(s) Q = \sum_{k=1}^{L-1} \left\{ p S_k^- S_{k+1}^+ + q S_k^+ S_{k+1}^- - p \hat{n}_k \hat{n}_{k+1}^v - q \hat{n}_k^v \hat{n}_{k+1} \right\} + \alpha (S_1^+ - \hat{n}_1) + \delta (e^{s(L+1)} S_L^+ - \hat{n}_L) + \gamma (S_1^- - \hat{n}_1) + \beta (e^{-s(L+1)} S_L^- - \hat{n}_L)$$

$$\boxed{Q^{-1} W_{t.f.}(s) Q = W_1((L+1)s)}$$

and the same relation thus holds for the large deviation functions

$$\boxed{\Psi_{tot}(s) = \Psi_1((L+1)s)}$$

This means that determining the statistics of the total current is equivalent to determining the statistics of the current to the right reservoir, which is in general more simple.

• Symmetry 2: invariance by rotation

lecture 12.10
stoch. processes

in periodic boundary conditions: let's explicit the $S^{x,y,z}$ operators:

$$\begin{cases} S^\pm = S^x \pm i S^y & \text{ie: } S^x = \frac{S^+ + S^-}{2} & S^y = \frac{S^+ - S^-}{2i} \\ \hat{n} = \frac{N}{2} + S^z \\ \hat{v} = \frac{N}{2} - S^z \end{cases}$$

$p=q=1$

$$\begin{aligned} W &= \sum_{k=1}^L \left\{ S_k^+ S_{k+1}^- + S_k^- S_{k+1}^+ - \hat{n}_k \hat{v}_{k+1} - \hat{v}_k \hat{n}_{k+1} \right\} \\ &= \sum_{k=1}^L \left\{ (S_k^x + i S_k^y)(S_{k+1}^x - i S_{k+1}^y) + (S_k^x - i S_k^y)(S_{k+1}^x + i S_{k+1}^y) - \left(\frac{N}{2} + S_k^z\right)\left(\frac{N}{2} - S_{k+1}^z\right) \right. \\ &\quad \left. - \left(\frac{N}{2} - S_k^z\right)\left(\frac{N}{2} + S_{k+1}^z\right) \right\} \\ &\quad \underbrace{2 \left\{ S_k^x S_{k+1}^x + S_k^y S_{k+1}^y + S_k^z S_{k+1}^z \right\}}_{\text{denoted by } \vec{S}_k \cdot \vec{S}_{k+1}} \end{aligned}$$

$$W = 2 \sum_{k=1}^L \vec{S}_k \cdot \vec{S}_{k+1}$$

$$\vec{S} = \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix}$$

R : matrix of rotation in 3D. $R \vec{S}$ is again a set of 3 spin operators

Besides: $(R \vec{S}_k) \cdot (R \vec{S}_{k+1}) = \vec{S}_k \cdot \vec{S}_{k+1}$ (invariant by rotation of the scalar product)

One thus have an invariant by rotation of the spin operators \vec{S}

It does not affect the bulk part of W to apply R .

• Use: for $W_s(s)$ in open boundary conditions, R modifies these boundary terms.

After the rotation one can reinterpret them, for $s \neq 0$

as a system in contact with different chem. potentials (eg. at eq.)

→ Mapping Btw equilibrium and non-equilibrium