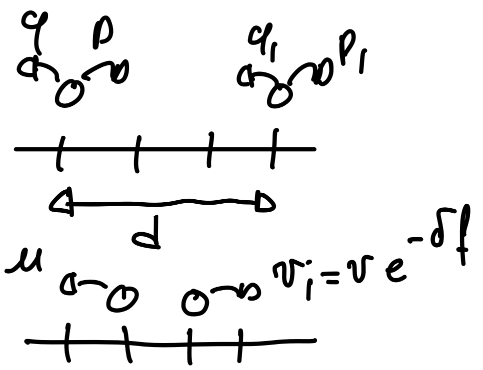
Average distance between two motors



$$p_1 = p\, e^{-\delta f} < p$$

$$q_1 = q\, e^{(1-\delta)f} > q$$

$$r = \frac{p_1+q}{p+q_1} < 1 \qquad r_1 = \frac{u+v_1}{p+q_1}$$

$$\Rightarrow P_d(1) = \frac{1-r}{1-r+r_1} \quad \& \quad P_d(k\geq 2) = \frac{r_1(1-r)}{1-r+r_1}\, r^{k-2}$$

Comment: $P_d(k) \underset{k\to\infty}{\sim} c\, e^{-k \ln r} \Rightarrow \langle k\rangle$ finite, scales as $\frac{1}{\ln r}$ as $r \to 1$

In this case, $\langle k\rangle$ finite $\Rightarrow$ the two motors go at the same average speed

Mean speed of the first motor

$$v_{2M} = \langle v\rangle = v_{isolated} \times p(isolated) + v_1 P_d(1)$$

$$= (p_1-q_1)\left[1-P_d(1)\right] + v_1 P_d(1)$$

$$= (p_1-q_1)\frac{r_1}{1-r+r_1} + v_1 \frac{1-r}{1-r+r_1} = \frac{(p_1-q_1)(u+v_1) + v_1(p+q_1-p_1-q)}{p+q_1-p_1-q+u+v_1}$$

$$=0$$

$$= \frac{u(p_1-q_1)+v_1(p-q)}{p+q_1-p_1-q+u+v_1}$$

Stall force f such that $V^{2M}(f)=0$

$$u\, e^{-\delta f}(p-q e^{f}) + v e^{-\delta f}(p-q) = 0 \Leftrightarrow u q e^{f} = up + vp - vq$$

$$f_s^{2M} = \ln\left[\frac{p}{q} + \frac{v}{u}\underbrace{\left(\frac{p}{q}-1\right)}_{>0}\right] > \ln\frac{p}{q} = f_s^{1M}$$

Whatever the interactions between the motors, the stall force to stop the 1^{st} motor is always larger when there is a 2^{nd} motor behind it. This is because the presence of the second motor prevents backward fluctuations of the 1^{st} motor. (2)

Speed of the first motor

The second motor increases the stall force, does it increase the speed? .

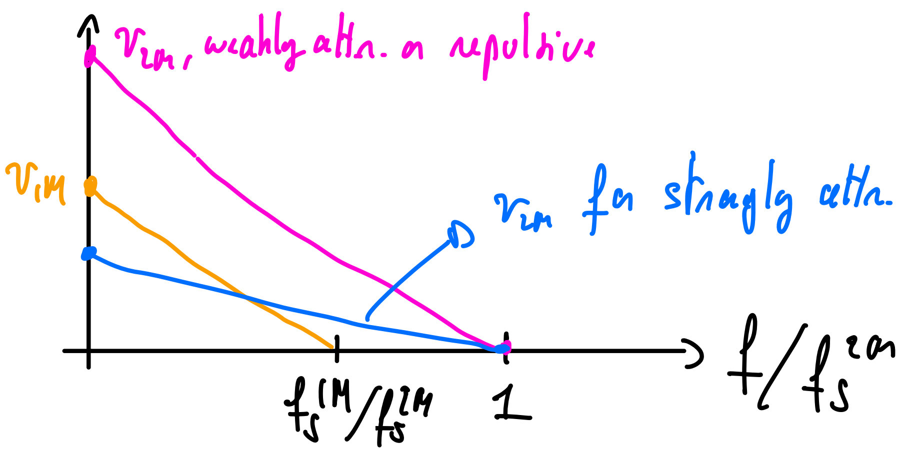
$$v_{2M} - v_{1M} = \frac{u(p_1-q_1) + v_1(p-q)}{p+q_1-p_1-q+u+v_1} - \frac{(p_1-q_1)(p+q_1-p_1-q+u+v_1)}{\underbrace{p-p_1}_{>0}+\underbrace{q_1-q}_{>0}+\underbrace{u+v_1}_{>0}} \Rightarrow \text{denominator is} > 0$$

$$\begin{aligned}
\text{Sign}(v_{2M}-v_{1M}) &= \text{Sign}\left[v_1(p-q) - (p_1-q_1)(p+q_1-p_1-q) - v_1(p_1-q_1)\right] \\
&= \text{Sign}\left[(v_1-(p_1-q_1))(\underbrace{p-p_1}_{\geq 0}+\underbrace{q_1-q}_{\geq 0})\right] \\
&= \text{Sign}\left[v-p+qe^{f}\right]
\end{aligned}$$

* if $f > f_s^{2M}$, $v_{2M} = v_{1M} = 0$
* if $f_s^{2M} > f > f_s^{1M}$, $v_{2M} > 0 = v_{1M}$
* if $f_s^{1M} > f$, then $v_{2M} > v_{1M} \Leftrightarrow v > p - qe^{f} \underset{f=0}{\simeq} p-q$

If attractive forces are strong, $v < p-q$ & $v_{2M} < v_{1M}$

If ——— are weak, or interactions are repulsive $v_{2M} > v_{1M}$



N body: [O. Campas, et al Phys. Rev. Lett. 97, 038101 (2006)]

5 Detailed balance for Markov Processes

Langevin equations: continuous time & continuous space

Markov processes: continuous time & discrete space

(Markov chain: discrete time & discrete space)

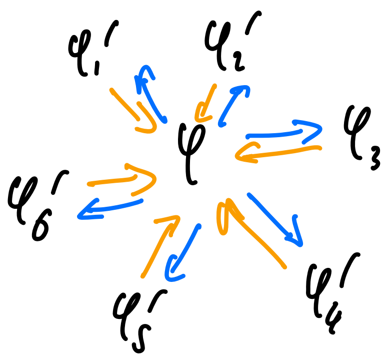
These can be seen as different level of coarse-graining, as above, or as dealing with observables of different nature (continuous position x vs discrete number of particles n_i).

The notion of time reversal symmetry & detailed balance extend to the discrete case.

5.1) Detailed balance at the rate level

$$\partial_t P(\varphi) = \sum_{\varphi' \neq \varphi} W(\varphi' \to \varphi) P(\varphi') - \sum_{\varphi' \neq \varphi} W(\varphi \to \varphi') P(\varphi)$$

Steady state: $\partial_t P(\varphi) = 0 \Rightarrow \forall \varphi,\ \underbrace{\sum_{\varphi' \neq \varphi} W(\varphi' \to \varphi) P(\varphi')}_{\text{probability flux into } \varphi} = \underbrace{\sum_{\varphi' \neq \varphi} W(\varphi \to \varphi') P(\varphi)}_{\text{probability flux out of } \varphi}$



This is called global balance, the sum of ingoing fluxes is balanced by the sum of outgoing fluxes, leaving $P(\varphi)$ constant.

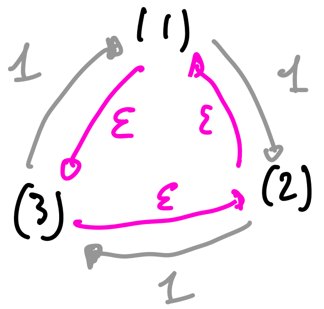
Detailed Balance (DB) is a stronger constraint: $W(\varphi' \to \varphi) P(\varphi') = W(\varphi \to \varphi') P(\varphi)$

It enforces the balance between each pair of state and guarantees that the dynamics is time reversible in the steady state since

$$P(\varphi,t';\varphi',t) = P(\varphi,t'|\varphi',t)\,P(\varphi',t) \underset{t'=t+dt}{\approx} W(\varphi'\to\varphi)\,dt\,P(\varphi',t)$$
$$= W(\varphi\to\varphi')\,dt\,P(\varphi,t)$$

Then DB $\Rightarrow P(\varphi,t+dt;\varphi',t) = P(\varphi',t+dt;\varphi,t)$

example: Invariance by rotation $\Rightarrow$ steady state $P(i)=\frac{1}{3}$



Let's check that it satisfies global balance

flux out of (i) : $(1+\varepsilon)\times\frac{1}{3}$
flux into (i) : $(1+\varepsilon)\times\frac{1}{3}$
} global balance

However $P(i)\,W(i\to i+1) = \frac{1}{3}\times 1 = \frac{1}{3}$ while $P(i+1)\,W(i+1\to i) = \varepsilon/3$

$\Rightarrow$ No detail balance if $\varepsilon \neq 1$.

This fits our intuition: if $\varepsilon<1$, the CW rotation is more likely than the time reversed, CCW, rotation.

Comment: DB is a joint property of the rates and the steady state distribution.

5.2) At the trajectory level

Escape rate: $r(\varphi) = \sum_{\varphi'\neq\varphi} W(\varphi\to\varphi')$ is the total rate at which the system hops out of configuration φ.

Escape time: τ is the first time at which the system escapes φ, given that it is in φ at time 0. Q: $P(\tau) = ?$

$\tau = N dt$ & work in the limit $N\to\infty$, $dt\to 0$, $N dt = \tau$ constant

Proba($\varphi\to\varphi'$ during dt) $= W(\varphi\to\varphi')\,dt + O(dt^2)$

Proba(out of φ during dt) $= \sum_{\varphi'\neq\varphi} W(\varphi\to\varphi')\,dt + O(dt^2) \simeq r(\varphi)\,dt$

Proba(stay in φ during dt) $= 1 - r(\varphi)\,dt$

$$\text{Proba (1}^{st}\text{ escape in } [\tau, \tau+dt]) = \underbrace{[1 - r(q)\,dt]^N}_{\text{does not escape in the } N \text{ first time intervals}} \cdot \underbrace{r(q)\,dt}_{\text{then it escapes}}$$

$$\simeq e^{-N r(q)\,dt}\, r(q)\,dt = r(q)\, e^{-\tau r(q)}\, dt$$

$\Rightarrow$ the probability density to exit at τ is $\boxed{P(\tau) = r(q)\, e^{-\tau r(q)}}$

Comment: (i) $P(\tau > t) = \int_t^{\infty} d\tau\, P(\tau) = e^{-t r(q)}$ $\Rightarrow$ the probability to remain in q decreases exponentially in time.

(ii) $W(q \to q')\,dt$ is the probability that the system jumps out of q AND into q'.

Q: Given that the system hops out of q, what is the proba that it goes into a specific q'?

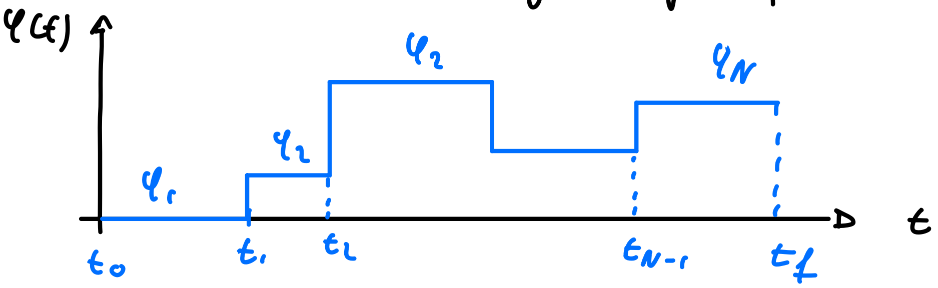
$$P(q \to q' \;\&\; \text{jump in the next } dt) = W(q \to q')\,dt = P(q \to q' \mid \text{jump}) \times \underbrace{P(\text{jump})}_{r(q)\,dt}$$

$$\Rightarrow P(q \to q' \mid \text{jump}) = \frac{W(q \to q')}{\sum_{q'' \neq q} W(q \to q'')}$$

This is the basis of the tower-sampling algorithm

Probability of a full trajectory

A trajectory is defined as a sequence of configurations q_i and jump times t_i, at which the system goes from q_i to q_{i+1}.



The probability to go from φ to φ' in $[t, t+dt]$ is $W(\varphi \to \varphi')\,dt$

→ independent from $\varphi(s \le t)$ → Markovian dynamics.

⇒ $P[\text{trajectory } \varphi(t)] = \prod_k P[\text{transition from } \varphi_k \text{ to } \varphi_{k+1}]$

Let us denote by $P(\varphi)$ the steady state proba to be in φ and compare the probability of $\varphi(t)$ & $\varphi^R(t) = \varphi(t^R = t_f - t)$.

$$P(\{\varphi(t)\}) = \underbrace{P(\varphi_1)}_{\text{start at } \varphi_1} \times \underbrace{r(\varphi_1)\, e^{-r(\varphi_1)(t_1 - t_0)}}_{\text{jump out at } t_1} \cdot \underbrace{\frac{W(\varphi_1 \to \varphi_2)}{r(\varphi_1)}}_{\text{go to } \varphi_2} \times \underbrace{r(\varphi_2)\, e^{-r(\varphi_2)(t_2 - t_1)} \cdot \frac{W(\varphi_2 \to \varphi_3)}{r(\varphi_2)}}_{\text{same for } \varphi_2 \to \varphi_3}$$

$$\times \cdots \times \underbrace{r(\varphi_{N-1})\, e^{-r(\varphi_{N-1})(t_{N-1} - t_{N-2})} \cdot \frac{W(\varphi_{N-1} \to \varphi_N)}{r(\varphi_{N-1})}}_{\text{same for } \varphi_{N-1} \to \varphi_N} \cdot \underbrace{e^{-r(\varphi_N)(t_f - t_{N-1})}}_{\text{stay in } \varphi_N \text{ in } [t_{N-1}, t_f]}$$

The factors $r(\varphi_i)$ cancel out.

$$P(\{\varphi(t)\}) = P(\varphi_1) \times \prod_{i=1}^{N-1} W(\varphi_i \to \varphi_{i+1}) \times \prod_{i=1}^{N} e^{-r(\varphi_i)(t_i - t_{i-1})} \quad \text{with } t_N \equiv t_f$$

Detailed balance $P(\varphi_i)\, W(\varphi_i \to \varphi_{i+1}) = W(\varphi_{i+1} \to \varphi_i)\, P(\varphi_{i+1})$

$$\underbrace{P(\varphi_1)\, W(\varphi_1 \to \varphi_2)}_{W(\varphi_2 \to \varphi_1)\, P(\varphi_2)}\, W(\varphi_2 \to \varphi_3) \cdots W(\varphi_{N-1} \to \varphi_N)$$

$$W(\varphi_2 \to \varphi_1)\, \underbrace{P(\varphi_2)\, W(\varphi_2 \to \varphi_3)}_{W(\varphi_3 \to 2)\, P(\varphi_3)}$$

$$\cdots \quad W(\varphi_N \to \varphi_{N-1})\, P(\varphi_N)$$

$$\Rightarrow \underbrace{P(\varphi_1)}_{\text{proba to start in } \varphi_1}\ \underbrace{\prod_i W(\varphi_i \to \varphi_{i+1})}_{\text{proba of forward transitions}} = \underbrace{\prod_i W(\varphi_{i+1} \to \varphi_i)}_{\text{Proba of backward transitions}}\ \underbrace{P(\varphi_N)}_{\text{proba to start in } \varphi_N}$$

$$\Rightarrow P(\{\varphi(t)\}) = P(\varphi_N) \times \prod_{i=1}^{N-1} W(\varphi_{i+1} \to \varphi_i) \times \prod_{i=1}^{N} e^{-\lambda(\varphi_i)(t_i - t_{i-1})} \qquad (*)$$

Reversed traj

(i) transitions $\qquad \varphi_1^R = \varphi_N,\ \varphi_2^R = \varphi_{N-1},\ \dots,\ \varphi_N^R = \varphi_1$

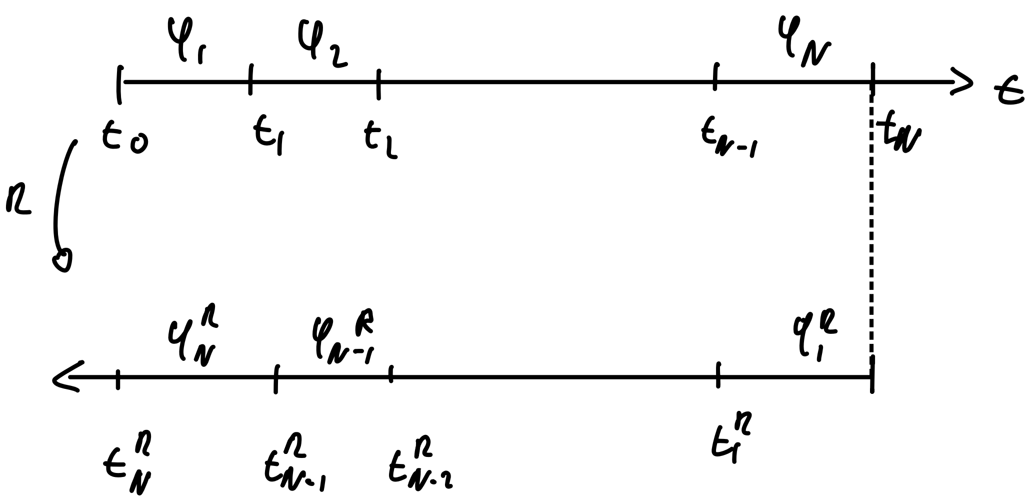
$$\Rightarrow \prod_{i=1}^{N-1} W(\varphi_{i+1} \to \varphi_i) = \prod_{i=1}^{N-1} W(\varphi_i^R \to \varphi_{i+1}^R)$$

(ii) waiting times

The waiting times are symmetric so we expect $\prod_i e^{-\lambda(\varphi_i)(t_i - t_{i-1})}$ to transform symmetrically into $\prod_i e^{-\lambda(\varphi_i^R)(t_i^R - t_{i-1}^R)}$

① $\lambda(\varphi_i) = \lambda(\varphi^R_{N-i+1})$

② $|t_i - t_{i-1}| = |t^R_{N-i} - t^R_{N-i+1}|$



$$e^{-\lambda(\varphi_i)(t_i - t_{i-1})} = e^{-\lambda(\varphi_i)|t_i - t_{i-1}|} = e^{-\lambda(\varphi^R_{N+1-i})|t^R_{N-i} - t^R_{N-i+1}|} = e^{-\lambda(\varphi^R_{N+1-i})(t^R_{N+1-i} - t^R_{N-i})}$$

$$\Rightarrow \prod_i e^{-\lambda(\varphi_i)(t_i - t_{i-1})} = \prod_i e^{-\lambda(\varphi_i^R)(t_i^R - t_{i-1}^R)}$$

Thus $(*)$ reads:

$$P(\{\varphi(t)\}) = P(\varphi_1^R) \cdot \prod_{i=1}^{N-1} W(\varphi_i^R \to \varphi_{i+1}^R) \times \prod_{i=1}^{N} e^{-\lambda(\varphi_i^R)(t_i^R - t_{i-1}^R)} = P(\{\varphi^R(t)\})$$

DB at the rates level thus imposes reversibility at the trajectory level!

Comments If we sum over all possible trajectories between q_1 & q_N, we find

$$P_{ss}(q_1, t_0)\, P(q_N, t_f \mid q_1, t_0) = P_{ss}(q_N, t_f)\, P(q_1, t_f \mid q_N, 0)$$

5.3) At the transition matrix level

Vector $|P(t)\rangle$ of dimension cardinal $(\{q\})$ whose i^{th} component is

$$P_i(t) \equiv P(q_i, t) \equiv P_{q_i}(t)$$

Master equation:

$$\partial_t P(q,t) = \sum_{q' \neq q} W(q' \to q)\, P(q', t) - \Big[\sum_{q' \neq q} W(q \to q')\Big] P(q,t)$$

$$\Leftrightarrow \partial_t P_q = \sum_{q'} M_{qq'} P_{q'} \quad \text{with} \quad M_{qq} = -\sum_{q' \neq q} W(q \to q')$$

$$\text{and} \quad M_{qq'} = W(q' \to q) \text{ if } q' \neq q$$

$\Leftrightarrow \partial_t |P\rangle = M\, |P\rangle$ $\Rightarrow$ like a Fokker Planck equation in finite dimension.

Detailed balance

$$\forall q \neq q', \quad P(q)\, W(q \to q') = P(q')\, W(q' \to q)$$

$$\Leftrightarrow \quad M_{q'q} P_q = M_{qq'} P_{q'} \quad \Leftrightarrow \quad M_{q'q} = P_q^{-1} M_{qq'} P_{q'}$$

$$\Leftrightarrow \quad M_{qq'}^{\dagger} = P_q^{-1} M_{qq'} P_{q'} \qquad (**)$$

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Let's define $\mathbb{P} = \text{diag}(p_q)$, then (**) can be rewritten as

$$M^{+} = \mathbb{P}^{-1} M \, \mathbb{P} \qquad (\Leftrightarrow \; H^{+} = P^{-1} H P)$$

Similarly: $M^{h} = \mathbb{P}^{-1/2} M \, \mathbb{P}^{1/2}$ is hermitian $\Rightarrow$ diagonalizable with real eigenvalues in an orthonormal basis.

$\Rightarrow$ M is diagonalizable, with real eigenvalues, but not in an orthonormal basis.