Modelling of Complex Real-World Systems
Part A. General Methods

A2. Stochastic processes

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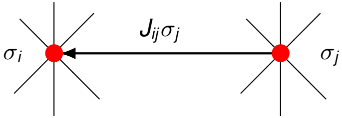
Discrete variables

Definitions

- discrete time steps, $\ell = 0, 1, 2, \ldots$
- binary dynamical variables: $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$, $\sigma_i = \pm 1$
- local 'forces' (or 'fields'):

$$h_i(\boldsymbol{\sigma}) = \sum_{j=1}^{N} J_{ij}\sigma_j + \theta_i \qquad \begin{array}{ll} J_{ij} & \text{interaction strengths} \\ \theta_i & \text{external fields} \end{array}$$



- effect of forces: if $h_i(\boldsymbol{\sigma}) > 0$ then $\sigma_i \to 1$
  if $h_i(\boldsymbol{\sigma}) < 0$ then $\sigma_i \to -1$

	$\sigma_i = 1$	$\sigma_i = -1$
magnetic systems	spin *i* up	spin *i* down
neural networks	neuron *i* firing	neuron *i* at rest
gene regulation	gene *i* switched on	gene *i* switched off
epidemics	person *i* infected	person *i* healthy
computer logic	Boolean var *i* is TRUE	Boolean var *i* is FALSE
image analysis	pixel *i* is black	pixel *i* is white
sociology	voter *i* favours republicans	voter *i* favours democrats
commerce	user *i* prefers Windows	user *i* prefers Apple Mac
financial markets	trader *i* sells shares	trader *i* buys shares
...	...	...

binary values often quite appropriate,
methods are easily generalized to $\sigma_i \in \{1, 2, \ldots, Q\}$
(if needed)

Stochastic evolution of $\boldsymbol{\sigma}$

- parallel dynamics:

$$\forall i: \qquad \sigma_i(\ell+1) = \mathrm{sgn}[h_i(\boldsymbol{\sigma}(\ell)) + T\eta_i(\ell)]$$

- sequential dynamics:

$$\text{pick } i_\ell \text{ randomly}: \qquad \begin{cases} \text{if } i \neq i_\ell: & \sigma_i(\ell+1) = \sigma_i(\ell) \\ \text{if } i = i_\ell: & \sigma_i(\ell+1) = \mathrm{sgn}[h_i(\boldsymbol{\sigma}(\ell)) + T\eta_i(\ell)] \end{cases}$$

$$\eta_i(\ell): \qquad \text{indep random vars, drawn from } w(\eta),$$
$$w(-\eta) = w(\eta),\ \langle \eta_i(\ell)\eta_j(\ell')\rangle = \delta_{ij}\delta_{\ell\ell'}$$

- noise parameter $T \geq 0$

  $T = 0$: parallel dynamics is deterministic,
  sequential dynamics has randomness in order of updates

  $T \to \infty$: fully random evolution of $\boldsymbol{\sigma}$

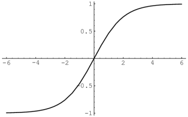
Probabilistic description

- use integrated noise distribution

$$g(z) = 2\int_0^z \mathrm{d}\eta\ w(\eta): \quad g(-z) = -g(z), \quad \lim_{z\to\pm\infty} g(z) = \pm 1, \quad \frac{\mathrm{d}}{\mathrm{d}z} g(z) \geq 0$$

$$w(\eta) = (2\pi)^{-\frac{1}{2}} \mathrm{e}^{-\frac{1}{2}\eta^2}: \qquad g(z) = \mathrm{Erf}(z/\sqrt{2})$$

$$w(\eta) = \frac{1}{2}[1 - \tanh^2(\eta)]: \qquad g(z) = \tanh(z)$$



- if $\sigma' = \mathrm{sgn}[h + T\eta]$:

$$\mathrm{Prob}(\sigma' = 1) = \int_{-h/T}^{\infty} \mathrm{d}\eta\ w(\eta) = \frac{1}{2} + \int_0^{h/T} \mathrm{d}\eta\ w(\eta) = \frac{1}{2} + \frac{1}{2} g(h/T)$$

$$\mathrm{Prob}(\sigma' = -1) = \frac{1}{2} - \frac{1}{2} g(h/T)$$

$$\mathrm{combined}: \quad \mathrm{Prob}(\sigma') = \frac{1}{2} + \frac{1}{2}\sigma' g(\beta h), \quad \beta = 1/T$$

- application to parallel evolution of $\boldsymbol{\sigma}$, define $\mathrm{Prob}(\sigma_i(\ell)=\sigma)=p_\ell(\sigma)$

$$\text{if } \boldsymbol{\sigma}(\ell) \text{ known}: \qquad \forall i: \quad p_{\ell+1}(\sigma_i|\boldsymbol{\sigma}(\ell)) = \frac{1}{2}+\frac{1}{2}\sigma_i g(\beta h_i(\boldsymbol{\sigma}(\ell)))$$

$$p_{\ell+1}(\boldsymbol{\sigma}|\boldsymbol{\sigma}(\ell)) = \prod_{i=1}^{N}\Big[\frac{1}{2}+\frac{1}{2}\sigma_i g(\beta h_i(\boldsymbol{\sigma}(\ell)))\Big]$$

$$\text{more generally}: \qquad p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')\prod_{i=1}^{N}\Big[\frac{1}{2}+\frac{1}{2}\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))\Big]$$

all σ_i can change state in one time unit
Markov chain representation:

$$p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_\ell(\boldsymbol{\sigma}'), \qquad W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \prod_{i=1}^{N}\Big[\frac{1}{2}+\frac{1}{2}\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))\Big]$$

$$h_i(\boldsymbol{\sigma}) = \sum_j J_{ij}\sigma_j + \theta_i$$

- application to sequential evolution of $\boldsymbol{\sigma}$, define $\mathrm{Prob}(\sigma_i(\ell) = \sigma) = p_\ell(\sigma)$

$$\boldsymbol{\sigma}(\ell) \text{ and } i_\ell \text{ known}: \quad \begin{cases} \text{if } i \neq i_\ell: & p_{\ell+1}(\sigma_i|\boldsymbol{\sigma}(\ell), i_\ell) = \delta_{\sigma_i,\sigma_i(\ell)} \\ \text{if } i = i_\ell: & p_{\ell+1}(\sigma_i|\boldsymbol{\sigma}(\ell), i_\ell) = \frac{1}{2}[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}(\ell)))] \end{cases}$$

$$p_{\ell+1}(\boldsymbol{\sigma}|\boldsymbol{\sigma}(\ell), i_\ell) = \Big[\prod_{j\neq i_\ell} \delta_{\sigma_j,\sigma_j(\ell)}\Big] \frac{1}{2}[1+\sigma_{i_\ell} g(\beta h_{i_\ell}(\boldsymbol{\sigma}(\ell)))]$$

$$\text{average over } \boldsymbol{\sigma}(\ell): \quad p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')\Big[\prod_{j\neq i_\ell} \delta_{\sigma_j,\sigma'_j}\Big] \frac{1}{2}[1+\sigma_{i_\ell} g(\beta h_{i_\ell}(\boldsymbol{\sigma}'))]$$

$$\text{average over } i_\ell: \quad p_{\ell+1}(\boldsymbol{\sigma}) = \frac{1}{N}\sum_i \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')\Big[\prod_{j\neq i} \delta_{\sigma_j,\sigma'_j}\Big] \frac{1}{2}[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))]$$

in one time unit: only one σ_i can change,
so noticeable system evolution only after $\mathcal{O}(N)$ time steps ...

- sequential dynamics,
  simplification using state-flip operators:

$$F_i \Phi(\boldsymbol{\sigma}) = \Phi(\sigma_1, \ldots, \sigma_{i-1}, -\sigma_i, \sigma_{i+1}, \ldots, \sigma_N)$$

$$\begin{aligned}
p_{\ell+1}(\boldsymbol{\sigma}) &= \frac{1}{N}\sum_i \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')\Big[\prod_{j\neq i}\delta_{\sigma_j,\sigma_j'}\Big]\frac{1}{2}\big[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))\big] \\
&= \frac{1}{N}\sum_i \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')[\delta_{\sigma_i,\sigma_i'}+\delta_{\sigma_i,-\sigma_i'}]\Big[\prod_{j\neq i}\delta_{\sigma_j,\sigma_j'}\Big]\frac{1}{2}\big[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))\big] \\
&= \frac{1}{N}\sum_i \sum_{\boldsymbol{\sigma}'} p_\ell(\boldsymbol{\sigma}')\Big[\delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}+\delta_{F_i\boldsymbol{\sigma},\boldsymbol{\sigma}'}\Big]\frac{1}{2}\big[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}'))\big] \\
&= \frac{1}{2N}\sum_i p_\ell(\boldsymbol{\sigma})\big[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}))\big] + \frac{1}{2N}\sum_i p_\ell(F_i\boldsymbol{\sigma})\big[1+\sigma_i g(\beta h_i(F_i\boldsymbol{\sigma}))\big]
\end{aligned}$$

introduce $w_i(\boldsymbol{\sigma}) = \frac{1}{2}\,[1-\sigma_i g(\beta h_i(\boldsymbol{\sigma}))]$:

$$\frac{1}{2}\big[1+\sigma_i g(\beta h_i(\boldsymbol{\sigma}))\big] = 1-w_i(\boldsymbol{\sigma}), \qquad \frac{1}{2}\big[1+\sigma_i g(\beta h_i(F_i\boldsymbol{\sigma}))\big] = w_i(F_i\boldsymbol{\sigma})$$

$$
\begin{aligned}
p_{\ell+1}(\boldsymbol{\sigma}) &= \frac{1}{N}\sum_i p_\ell(\boldsymbol{\sigma})[1-w_i(\boldsymbol{\sigma})] + \frac{1}{N}\sum_i p_\ell(F_i\boldsymbol{\sigma})w_i(F_i\boldsymbol{\sigma}) \\
&= p_\ell(\boldsymbol{\sigma}) + \frac{1}{N}\sum_i \Big[p_\ell(F_i\boldsymbol{\sigma})w_i(F_i\boldsymbol{\sigma}) - p_\ell(\boldsymbol{\sigma})w_i(\boldsymbol{\sigma})\Big]
\end{aligned}
$$

all σ_i can change state in $\mathcal{O}(N)$ time units
Markov chain representation:

$$p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_\ell(\boldsymbol{\sigma}')$$

$$W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} + \frac{1}{N}\sum_i w_i(\boldsymbol{\sigma}')\left[\delta_{F_i\boldsymbol{\sigma},\boldsymbol{\sigma}'} - \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}\right]$$

$$w_i(\boldsymbol{\sigma}) = \frac{1}{2}\left[1-\sigma_i g(\beta h_i(\boldsymbol{\sigma}))\right], \quad h_i(\boldsymbol{\sigma}) = \sum_j J_{ij}\sigma_j + \theta_i$$

notes:

(i) for finite β, parallel and sequential dynamics are both ergodic, so both always evolve to unique stationary states $p_\infty(\boldsymbol{\sigma})$

(ii) Markov chains of the general form $p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_\ell(\boldsymbol{\sigma}')$ have the following solution: $p_\ell(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W^\ell[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_0(\boldsymbol{\sigma}')$

- sequential dynamics,
  from discrete to continuous times

  assume *duration* of each iteration ℓ is random,

  $\pi_\ell(t) = \frac{1}{\ell!}(\frac{t}{\Delta})^\ell \mathrm{e}^{-t/\Delta}$: probability that at time $t \in [0, \infty)$ precisely ℓ updates have been made
  Poisson distr, $\langle \ell \rangle = t/\Delta$, $\langle \ell^2 \rangle = t/\Delta + t^2/\Delta^2$

  now

$$
\begin{aligned}
p_t(\boldsymbol{\sigma}) &= \sum_{\ell \geq 0} \pi_\ell(t) p_\ell(\boldsymbol{\sigma}) = \sum_{\ell \geq 0} \pi_\ell(t) \sum_{\boldsymbol{\sigma}'} W^\ell[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] \, p_0(\boldsymbol{\sigma}') \\
\Delta \frac{\mathrm{d}}{\mathrm{d}t} p_t(\boldsymbol{\sigma}) &= \Delta \sum_{\ell \geq 0} \frac{\mathrm{d}\pi_\ell(t)}{\mathrm{d}t} \sum_{\boldsymbol{\sigma}'} W^\ell[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] \, p_0(\boldsymbol{\sigma}') \\
&= \sum_{\ell \geq 0} \left[I[\ell > 0] \pi_{\ell-1}(t) - \pi_\ell(t) \right] \sum_{\boldsymbol{\sigma}'} W^\ell[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] \, p_0(\boldsymbol{\sigma}') \\
&= \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}; \boldsymbol{\sigma}'] \, p_t(\boldsymbol{\sigma}') - p_t(\boldsymbol{\sigma})
\end{aligned}
$$

  choose $\Delta = N^{-1}$: $\langle \ell \rangle = \mathcal{O}(N)$

combine

$$\frac{1}{N}\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W\left[\boldsymbol{\sigma};\boldsymbol{\sigma}'\right] p_t(\boldsymbol{\sigma}') - p_t(\boldsymbol{\sigma})$$

$$W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} + \frac{1}{N}\sum_i w_i(\boldsymbol{\sigma}')\left[\delta_{F_i\boldsymbol{\sigma},\boldsymbol{\sigma}'} - \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}\right]$$

so-called *master equation*
for sequential dynamics:

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'}\sum_i w_i(\boldsymbol{\sigma}')\left[\delta_{F_i\boldsymbol{\sigma},\boldsymbol{\sigma}'} - \delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} p_t(\boldsymbol{\sigma}')\right]$$

$$= \sum_i \left[w_i(F_i\boldsymbol{\sigma})p_t(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma})p_t(\boldsymbol{\sigma})\right]$$

(i) all σ_i can now change on timescales $t = \mathcal{O}(1)$

(ii) $w_i(\boldsymbol{\sigma}) = \frac{1}{2}[1 - \sigma_i g(\beta h_i(\boldsymbol{\sigma}))]$: *transition rates*

(iii) $\sqrt{\langle \ell^2\rangle_\pi - \langle \ell\rangle_\pi^2}/\langle \ell\rangle_\pi = 1/\sqrt{Nt}$,
hence uncertainty in nr of iterations vanishes for $N \to \infty$

Continuous variables

Definitions

- discrete time steps: $t_\ell = \ell\Delta$, $\ell = 0, 1, 2, \ldots$
- continuous dynamical variables: $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_N)$, $\sigma_i \in \mathbb{R}$
- local 'forces' $f_i(\boldsymbol{\sigma})$
- stochastic evolution

$$\forall i: \qquad \sigma_i(t_\ell+\Delta) = \sigma_i(t_\ell) + \Delta f_i(\boldsymbol{\sigma}(t_\ell)) + \sqrt{2T\Delta}\,\eta_i(\ell)$$

$$\eta_i(\ell): \quad \text{indep Gaussian random vars (noise),}$$

$$\langle \eta_i(\ell)\rangle = 0, \quad \langle \eta_i(\ell)\eta_j(\ell')\rangle = \delta_{ij}\delta_{\ell\ell'}$$

for $\Delta \downarrow 0$: *Langevin equation*
(with *continuous* time)

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_i(t) = f_i(\boldsymbol{\sigma}(t)) + \xi_i(t)$$

$$\text{Gaussian noise,} \quad \langle \xi_i(t)\rangle = 0, \quad \langle \xi_i(t)\xi_j(t)\rangle = 2T\delta_{ij}\delta(t-t')$$

to confirm this, rewrite

$$\frac{\sigma_i(t_\ell+\Delta)-\sigma_i(t_\ell)}{\Delta} = f_i(\boldsymbol{\sigma}(t_\ell)) + \xi_i(t_\ell), \qquad \text{Gaussian } \xi_i(t_\ell) = \frac{\sqrt{2T}}{\sqrt{\Delta}}\eta_i(\ell)$$

$$\Delta \downarrow 0: \qquad \frac{\mathrm{d}}{\mathrm{d}t}\sigma_i(t) = f_i(\boldsymbol{\sigma}(t)) + \xi_i(t), \qquad \langle \xi_i(t)\rangle = 0, \;\; \langle \xi_i(t)\xi_j(t)\rangle = 2T\delta_{ij}C(t,t')$$

$$C(t,t') = \lim_{\Delta\downarrow 0} C_\Delta(t,t'), \quad C_\Delta(t,t') = \frac{1}{\Delta}\langle \eta_i(\frac{t}{\Delta})\eta_i(\frac{t'}{\Delta})\rangle$$

noise correlations:

$$C_\Delta(t,t) = \Delta^{-1}, \quad C_\Delta(t,t+\tau) = 0 \text{ for } \tau > 0,$$

$$\begin{aligned}
\lim_{\Delta\downarrow 0}\int \mathrm{d}\tau\; C_\Delta(t,t+\tau) &= \lim_{\Delta\downarrow 0}\Delta\sum_\ell C_\Delta(t,t+\ell\Delta) \\
&= \lim_{\Delta\downarrow 0}\sum_\ell \langle \eta_i(\frac{t}{\Delta})\eta_i(\frac{t}{\Delta}+\ell)\rangle = \lim_{\Delta\downarrow 0}\sum_\ell \delta_{\ell 0} = 1
\end{aligned}$$

hence: $C(t,t') = \lim_{\Delta\downarrow 0} C_\Delta(t,t') = \delta(t-t')$

moment generating function
for Langevin equation

remember: $\xi_i(t_\ell) = \frac{\sqrt{2T}}{\sqrt{\Delta}}\eta_i(\ell)$

$$
\begin{aligned}
\langle \mathrm{e}^{\mathrm{i}\int \mathrm{d}t \sum_i \psi_i(t)\xi_i(t)} \rangle &= \lim_{\Delta\downarrow 0} \langle \mathrm{e}^{\mathrm{i}\Delta \sum_\ell \sum_i \psi_i(\ell\Delta)\xi_i(\ell\Delta)} \rangle \\
&= \lim_{\Delta\downarrow 0} \langle \mathrm{e}^{\mathrm{i}\sqrt{2T\Delta} \sum_\ell \sum_i \psi_i(\ell\Delta)\eta_i(\ell)} \rangle \\
&= \lim_{\Delta\downarrow 0} \prod_i \prod_\ell \langle \mathrm{e}^{\mathrm{i}\sqrt{2T\Delta}\psi_i(\ell\Delta)\eta_i(\ell)} \rangle \\
&= \lim_{\Delta\to 0} \prod_{i,\ell} \int \frac{d\eta}{\sqrt{2\pi}}\, \mathrm{e}^{-\frac{1}{2}\eta^2 + \mathrm{i}\eta\psi_i(\ell\Delta)\sqrt{2T\Delta}} \\
&= \lim_{\Delta\to 0} \prod_{i,\ell} \mathrm{e}^{-T\Delta\psi_i^2(\ell\Delta)} = \lim_{\Delta\to 0} \mathrm{e}^{-T\Delta \sum_\ell \sum_i \psi_i^2(\ell\Delta)} \\
&= \mathrm{e}^{-T\int \mathrm{d}t \sum_i \psi_i^2(t)}
\end{aligned}
$$

Probabilistic description

from Langevin eqn for $\boldsymbol{\sigma}(t)$ to
Fokker-Planck eqn for $p_t(\boldsymbol{\sigma}) = \langle \delta[\boldsymbol{\sigma} - \boldsymbol{\sigma}(t)] \rangle$

- use (in distributional sense):

$$\delta(\mathbf{x}+\boldsymbol{\epsilon}) = \delta(\mathbf{x}) + \sum_i \epsilon_i \frac{\partial}{\partial x_i}\delta(\mathbf{x}) + \frac{1}{2}\sum_{ij} \epsilon_i \epsilon_j \frac{\partial^2}{\partial x_i \partial x_j}\delta(\mathbf{x}) + \mathcal{O}(|\boldsymbol{\epsilon}|^3)$$

- start with discrete time

$$\begin{aligned} p_{t+\Delta}(\boldsymbol{\sigma}) - p_t(\boldsymbol{\sigma}) &= \langle \delta\left[\boldsymbol{\sigma} - \boldsymbol{\sigma}(t) - \Delta \mathbf{f}(\boldsymbol{\sigma}(t)) - \sqrt{2T\Delta}\,\boldsymbol{\eta}(\tfrac{t}{\Delta})\right]\rangle - \langle \delta[\boldsymbol{\sigma} - \boldsymbol{\sigma}(t)]\rangle \\ &= -\sum_i \frac{\partial}{\partial \sigma_i} \langle \delta[\boldsymbol{\sigma} - \boldsymbol{\sigma}(t)] \left[\Delta f_i(\boldsymbol{\sigma}(t)) + \sqrt{2T\Delta}\,\eta_i(\tfrac{t}{\Delta})\right]\rangle \\ &\quad + T\Delta \sum_{ij} \frac{\partial^2}{\partial \sigma_i \partial \sigma_j} \langle \delta[\boldsymbol{\sigma} - \boldsymbol{\sigma}(t)]\eta_i(\tfrac{t}{\Delta})\eta_j(\tfrac{t}{\Delta})\rangle + \mathcal{O}(\Delta^{\frac{3}{2}}) \end{aligned}$$

- $\boldsymbol{\sigma}(t)$ depends only on those $\eta_j(t'/\Delta)$ with $t' < t$, so for any function $A(\boldsymbol{\sigma})$:

$$\langle A(\boldsymbol{\sigma}(t))\eta_i(\frac{t}{\Delta})\rangle = \langle A(\boldsymbol{\sigma}(t))\rangle\langle\eta_i(\frac{t}{\Delta})\rangle = 0$$

$$\langle A(\boldsymbol{\sigma}(t))\eta_i(\frac{t}{\Delta})\eta_j(\frac{t}{\Delta})\rangle = \langle A(\boldsymbol{\sigma}(t))\rangle\langle\eta_i(\frac{t}{\Delta})\eta_j(\frac{t}{\Delta})\rangle = \delta_{ij}\langle A(\boldsymbol{\sigma}(t))\rangle$$

$$\begin{aligned} & p_{t+\Delta}(\boldsymbol{\sigma}) - p_t(\boldsymbol{\sigma}) \\ &= -\Delta\sum_i \frac{\partial}{\partial\sigma_i}\langle\delta[\boldsymbol{\sigma}-\boldsymbol{\sigma}(t)]f_i(\boldsymbol{\sigma}(t))\rangle + T\Delta\sum_i\frac{\partial^2}{\partial\sigma_i^2}\langle\delta[\boldsymbol{\sigma}-\boldsymbol{\sigma}(t)]\rangle + \mathcal{O}(\Delta^{\frac{3}{2}}) \\ &= -\Delta\sum_i \frac{\partial}{\partial\sigma_i}\Big[\langle\delta[\boldsymbol{\sigma}-\boldsymbol{\sigma}(t)]\rangle f_i(\boldsymbol{\sigma})\Big] + T\Delta\sum_i\frac{\partial^2}{\partial\sigma_i^2}\langle\delta[\boldsymbol{\sigma}-\boldsymbol{\sigma}(t)]\rangle + \mathcal{O}(\Delta^{\frac{3}{2}}) \\ &= -\Delta\sum_i \frac{\partial}{\partial\sigma_i}\Big[p_t(\boldsymbol{\sigma})f_i(\boldsymbol{\sigma})\Big] + T\Delta\sum_i\frac{\partial^2}{\partial\sigma_i^2}p_t(\boldsymbol{\sigma}) + \mathcal{O}(\Delta^{\frac{3}{2}}) \end{aligned}$$

- $\Delta\downarrow 0$: Fokker-Planck eqn

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = -\sum_i\frac{\partial}{\partial\sigma_i}[p_t(\boldsymbol{\sigma})f_i(\boldsymbol{\sigma})] + T\sum_i\frac{\partial^2}{\partial\sigma_i^2}p_t(\boldsymbol{\sigma})$$

Detailed balance

Detailed balance for ergodic Markov chains

- our present Markov chains $$p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p_\ell(\boldsymbol{\sigma}'), \qquad \sum_{\boldsymbol{\sigma}} W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = 1 \ \forall \boldsymbol{\sigma}'$$

  detailed balance property (DB):

  $$\exists p(\boldsymbol{\sigma}) \geq 0 \text{ such that}: \quad W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p(\boldsymbol{\sigma}') = W[\boldsymbol{\sigma}';\boldsymbol{\sigma}]p(\boldsymbol{\sigma}) \quad \text{for all } \boldsymbol{\sigma},\boldsymbol{\sigma}'$$

  if DB: $p(\boldsymbol{\sigma})$ is invariant state of the process
  since process ergodic: $p_\infty(\boldsymbol{\sigma}) = \lim_{t\to\infty} p_t(\boldsymbol{\sigma}) = p(\boldsymbol{\sigma})$

  proof: $$\sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p(\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}';\boldsymbol{\sigma}]p(\boldsymbol{\sigma}) = p(\boldsymbol{\sigma})$$

notes:

(i) all ergodic Markov chains have unique stationary state, but not always DB
(ii) DB is often a useful route for finding the stationary state
(iii) interpretation: no currents in stationary state,
rates of transitions $\boldsymbol{\sigma} \to \boldsymbol{\sigma}'$ and $\boldsymbol{\sigma}' \to \boldsymbol{\sigma}$ are the same for all pairs $(\boldsymbol{\sigma},\boldsymbol{\sigma}')$

application to parallel dynamics

forces $h_i(\boldsymbol{\sigma}) = \sum_j J_{ij}\sigma_j + \theta_i$, noise $w(\eta) = \frac{1}{2}[1 - \tanh^2(\eta)]$

- now $g(z) = \tanh(z)$,
  use $1 + \tanh(z) = \mathrm{e}^z / \cosh(z)$

$$W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] = \prod_i \left[\frac{1}{2} + \frac{1}{2}\sigma_i \tanh(\beta h_i(\boldsymbol{\sigma}'))\right] = \prod_i \frac{\mathrm{e}^{\beta\sigma_i h_i(\boldsymbol{\sigma}')}}{2\cosh(\beta h_i(\boldsymbol{\sigma}'))}$$

DB:

$$\frac{\mathrm{e}^{\beta\sum_i \sigma_i h_i(\boldsymbol{\sigma}')} p(\boldsymbol{\sigma}')}{\prod_i \cosh[\beta h_i(\boldsymbol{\sigma}')]} = \frac{\mathrm{e}^{\beta\sum_i \sigma_i' h_i(\boldsymbol{\sigma})} p(\boldsymbol{\sigma})}{\prod_i \cosh[\beta h_i(\boldsymbol{\sigma})]} \quad \text{for all } \boldsymbol{\sigma}, \boldsymbol{\sigma}'$$

- all $p_\infty(\boldsymbol{\sigma})$ non-zero
  (ergodicity), so define $p(\boldsymbol{\sigma}) = \mathrm{e}^{\beta[\sum_i \theta_i\sigma_i + K(\boldsymbol{\sigma})]} \prod_i \cosh[\beta h_i(\boldsymbol{\sigma})]$

  detailed balance

$$\forall(\boldsymbol{\sigma},\boldsymbol{\sigma}'):\quad \sum_i \sigma_i h_i(\boldsymbol{\sigma}') + \sum_i \theta_i\sigma_i' + K(\boldsymbol{\sigma}') = \sum_i \sigma_i' h_i(\boldsymbol{\sigma}) + \sum_i \theta_i\sigma_i + K(\boldsymbol{\sigma})$$

$$\sum_{ij} \sigma_i J_{ij}\sigma_j' + K(\boldsymbol{\sigma}') = \sum_{ij} \sigma_i' J_{ij}\sigma_j + K(\boldsymbol{\sigma})$$

- average over $\boldsymbol{\sigma}'$: $K(\boldsymbol{\sigma})+0=2^{-N}\sum_{\boldsymbol{\sigma}'}K(\boldsymbol{\sigma}')+0$ for all $\boldsymbol{\sigma}$,
  so K is a constant

$$\forall(\boldsymbol{\sigma},\boldsymbol{\sigma}'):\quad \sum_{ij}\sigma_i J_{ij}\sigma_j' = \sum_{ij}\sigma_i' J_{ij}\sigma_j \quad \text{i.e.} \quad \sum_{ij}\sigma_i\Big(J_{ij}-J_{ji}\Big)\sigma_j'=0$$

  hence $J_{ij}=J_{ji}$ for all (i,j),
  interaction matrix $\mathbf{J}=\{J_{ij}\}$ must be *symmetric*

- final picture for parallel dynamics
  - $\{J_{ij}\}$ non-symmetric: no DB, $p_\infty(\boldsymbol{\sigma})$ not generally known
  - $\{J_{ij}\}$ symmetric: DB holds,

$$p_\infty(\boldsymbol{\sigma})=\frac{1}{Z}e^{\beta\sum_i\theta_i\sigma_i}\prod_i\cosh\Big[\beta\Big(\sum_j J_{ij}\sigma_j+\theta_i\Big)\Big]$$

$$Z=\sum_{\boldsymbol{\sigma}}e^{\beta\sum_i\theta_i\sigma_i}\prod_i\cosh\Big[\beta\Big(\sum_j J_{ij}\sigma_j+\theta_i\Big)\Big]$$

(Peretto distribution)

application to sequential dynamics

forces $h_i(\boldsymbol{\sigma})=\sum_j J_{ij}\sigma_j+\theta_i$, noise $w(\eta)=\frac{1}{2}[1-\tanh^2(\eta)]$
exclude self-interactions, $J_{ii}=0$ for all i

- now $g(z)=\tanh(z)$,
  use $1-\tanh(z)=\mathrm{e}^{-z}/\cosh(z)$

$$W[\boldsymbol{\sigma};\boldsymbol{\sigma}']=\delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}+\frac{1}{N}\sum_i w_i(\boldsymbol{\sigma}')[\delta_{F_i\boldsymbol{\sigma},\boldsymbol{\sigma}'}-\delta_{\boldsymbol{\sigma}\boldsymbol{\sigma}'}]$$

  only need to inspect DB condition for $(\boldsymbol{\sigma},\boldsymbol{\sigma}')$ with $\boldsymbol{\sigma}'=F_i\boldsymbol{\sigma}$ for some i (trivially satisfied otherwise)

$$w_i(\boldsymbol{\sigma})=\frac{\mathrm{e}^{-\beta\sigma_i h_i(\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]},$$

$$\forall(\boldsymbol{\sigma},i):\quad w_i(F_i\boldsymbol{\sigma})p(F_i\boldsymbol{\sigma})=w_i(\boldsymbol{\sigma})p(\boldsymbol{\sigma})$$
$$\forall(\boldsymbol{\sigma},i):\quad \mathrm{e}^{\beta\sigma_i h_i(F_i\boldsymbol{\sigma})}p(F_i\boldsymbol{\sigma})=\mathrm{e}^{-\beta\sigma_i h_i(\boldsymbol{\sigma})}p(\boldsymbol{\sigma})$$
$$\forall(\boldsymbol{\sigma},i):\quad \mathrm{e}^{\beta\sigma_i h_i(\boldsymbol{\sigma})}p(F_i\boldsymbol{\sigma})=\mathrm{e}^{-\beta\sigma_i h_i(\boldsymbol{\sigma})}p(\boldsymbol{\sigma})$$

- all $p_\infty(\boldsymbol{\sigma})$ non-zero, so define

$$p(\boldsymbol{\sigma})=\mathrm{e}^{\beta[\sum_k\theta_k\sigma_k+\frac{1}{2}\sum_{k\ell}\sigma_k J_{k\ell}\sigma_\ell+K(\boldsymbol{\sigma})]}$$

- detailed balance

$$\forall(\boldsymbol{\sigma},i): \quad \sigma_i h_i(\boldsymbol{\sigma}) + \sum_k \theta_k F_i\sigma_k + \frac{1}{2}\sum_{k\ell} J_{k\ell}(F_i\sigma_k)(F_i\sigma_\ell) + K(F_i\boldsymbol{\sigma}) = -\sigma_i h_i(\boldsymbol{\sigma}) + \sum_k \theta_k\sigma_k + \frac{1}{2}\sum_{k\ell} J_{k\ell}\sigma_k\sigma_\ell + K(\boldsymbol{\sigma})$$

use $F_i\sigma_k = \sigma_k - 2\delta_{ik}\sigma_i$

$$\forall(\boldsymbol{\sigma},i): \quad \sum_k \theta_k(\sigma_k - 2\delta_{ik}\sigma_i) + \frac{1}{2}\sum_{k\ell} J_{k\ell}(\sigma_k - 2\delta_{ik}\sigma_i)(\sigma_\ell - 2\delta_{i\ell}\sigma_i) + K(F_i\boldsymbol{\sigma}) = -2\sigma_i\Big(\theta_i + \sum_j J_{ij}\sigma_j\Big) + \sum_k \theta_k\sigma_k + \frac{1}{2}\sum_{k\ell} J_{k\ell}\sigma_k\sigma_\ell + K(\boldsymbol{\sigma})$$

$$\forall(\boldsymbol{\sigma},i): \quad -\sigma_i\sum_{k\ell} J_{k\ell}\Big(\delta_{ik}\sigma_\ell + \delta_{i\ell}\sigma_k\Big) + K(F_i\boldsymbol{\sigma}) = -2\sigma_i\sum_j J_{ij}\sigma_j + K(\boldsymbol{\sigma})$$

$$\forall(\boldsymbol{\sigma},i): \quad (1-F_i)K(\boldsymbol{\sigma}) = \sigma_i\sum_\ell \Big(J_{i\ell} - J_{\ell i}\Big)\sigma_\ell$$

- apply to both sides $(1-F_j)$, with $j \neq i$:

$$\forall(\boldsymbol{\sigma}, i\neq j): \quad \overbrace{(1-F_i)(1-F_j)K(\boldsymbol{\sigma})}^{\text{symmetric in } (i,j)} = \overbrace{2\sigma_i\sigma_j(J_{ij} - J_{ji})}^{\text{antisymmetric in } (i,j)} \qquad \text{hence } \begin{cases} J_{ij} = J_{ji} \\ K(\boldsymbol{\sigma}) = K \end{cases}$$

- final picture for sequential dynamics
  without self-interactions
  - $\{J_{ij}\}$ non-symmetric: no DB, $p_\infty(\boldsymbol{\sigma})$ not generally known
  - $\{J_{ij}\}$ symmetric: DB holds,

$$p_\infty(\boldsymbol{\sigma}) = \frac{1}{Z}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}, \quad H(\boldsymbol{\sigma}) = -\frac{1}{2}\sum_{i\neq j}\sigma_i J_{ij}\sigma_j - \sum_i \theta_i\sigma_i$$

$$Z = \sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta H(\boldsymbol{\sigma})}$$

(Gibbs-Boltzmann distribution)

standard in statistical physics,
temperature $1/\beta$, *Hamiltonian* $H(\boldsymbol{\sigma})$, *partition function* Z

notes:

(i) sequential dynamics with self-interactions: only DB for pathological cases

(ii) alternative noise statistics $w(\eta) \neq \frac{1}{2}[1-\tanh^2(\eta)]$: no DB
(neither in parallel nor in sequential dynamics)

Detailed balance for Fokker-Planck equations

- FP-equation: $$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = -\sum_i \frac{\partial}{\partial \sigma_i}[p_t(\boldsymbol{\sigma})f_i(\boldsymbol{\sigma})] + T\sum_i \frac{\partial^2}{\partial \sigma_i^2}p_t(\boldsymbol{\sigma})$$

  rewrite
  $$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) + \sum_i \frac{\partial}{\partial \sigma_i}J_i(\boldsymbol{\sigma},t) = 0, \qquad J_i(\boldsymbol{\sigma},t) = \left(f_i(\boldsymbol{\sigma}) - T\frac{\partial}{\partial \sigma_i}\right)p_t(\boldsymbol{\sigma})$$

  stationary states: $\sum_i \frac{\partial}{\partial \sigma_i}J_i(\boldsymbol{\sigma},\infty) = 0$ (divergence-free current)

- detailed balance:
  $J_i(\boldsymbol{\sigma},\infty) = 0$ for all i (zero current)

  $$\mathrm{DB}: \qquad f_i(\boldsymbol{\sigma}) = T\frac{\partial}{\partial \sigma_i}\log p(\boldsymbol{\sigma})$$
  $$f_i(\boldsymbol{\sigma}) = -\frac{\partial}{\partial \sigma_i}H(\boldsymbol{\sigma}) \text{ for some } H(\boldsymbol{\sigma}), \qquad p(\boldsymbol{\sigma}) = \frac{1}{Z}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}$$

  forces must be *conservative*

  but since $\boldsymbol{\sigma} \in \mathbb{R}^N$,
  further requirement: $$p(\boldsymbol{\sigma}) \text{ normalisable}, \quad \int \mathrm{d}\boldsymbol{\sigma}\ \mathrm{e}^{-\beta H(\boldsymbol{\sigma})} < \infty$$

- example: conservative forces
  but no DB stationary state

$$f_i(\boldsymbol{\sigma}) = 0 \text{ for all } i : \qquad H(\boldsymbol{\sigma}) = C \text{ (constant)}, \quad p(\boldsymbol{\sigma}) = \frac{1}{Z}\mathrm{e}^{-\beta C} \quad \ldots$$

$$\text{actual solution : } p_t(\boldsymbol{\sigma}) = (4\pi T t)^{-N/2} \int \mathrm{d}\boldsymbol{\sigma}' \; p_0(\boldsymbol{\sigma}')\mathrm{e}^{-(\boldsymbol{\sigma}-\boldsymbol{\sigma}')^2/4Tt}$$

$$\lim_{t\to\infty} p_t(\boldsymbol{\sigma}) \text{ indeed does not exist}$$

- final picture for continuous variables
  described by Langevin or Fokker-Planck eqns
  - stationary state need not exist
  - $f_i(\boldsymbol{\sigma})$ non-conservative: no DB, $p_\infty(\boldsymbol{\sigma})$ not generally known
  - $f_i(\boldsymbol{\sigma})$ conservative: DB holds if $\int \mathrm{d}\boldsymbol{\sigma} \; \exp(-\beta H(\boldsymbol{\sigma})) < \infty$
    with $H(\boldsymbol{\sigma})$ defined by $f_i(\boldsymbol{\sigma}) = -\partial H(\boldsymbol{\sigma})/\partial \sigma_i$

$$p_\infty(\boldsymbol{\sigma}) = \frac{1}{Z}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}, \qquad Z = \int \mathrm{d}\boldsymbol{\sigma} \; \mathrm{e}^{-\beta H(\boldsymbol{\sigma})}$$

(Gibbs-Boltzmann distribution)

Examples of interacting continuous variables

$$\boldsymbol{\sigma} \in \mathbb{R}^N: \quad \frac{\mathrm{d}}{\mathrm{d}t}\sigma_i = f_i(\boldsymbol{\sigma}) + \xi_i(t), \qquad f_i(\boldsymbol{\sigma}) = \sum_j J_{ij} \tanh(\gamma\sigma_j) - \sigma_i + \theta_i$$

- forces conservative?

  note: if $f_i = -\partial H/\partial\sigma_i$ then $\partial f_i/\partial\sigma_j - \partial f_j/\partial\sigma_i = 0$

  here:

  $$\forall \boldsymbol{\sigma}: \qquad 0 = \frac{\partial f_i(\boldsymbol{\sigma})}{\partial\sigma_j} - \frac{\partial f_j(\boldsymbol{\sigma})}{\partial\sigma_i} = \gamma\Big(J_{ij}[1-\tanh^2(\gamma\sigma_j)] - J_{ji}[1-\tanh^2(\gamma\sigma_i)]\Big)$$
  $$\boldsymbol{\sigma} = \mathbf{0}: \quad \text{if conservative then } J_{ij} = J_{ji} \text{ for all } (i,j)$$

  if $\{J_{ij}\}$ symmetric:

  $$\forall \boldsymbol{\sigma}: \qquad 0 = \gamma J_{ij}\Big(\tanh^2(\gamma\sigma_i) - \tanh^2(\gamma\sigma_j)\Big)$$

  forces never conservative, unless $J_{ij} = 0$ for all $i \neq j$
  here $H(\boldsymbol{\sigma}) = \sum_i \left[\frac{1}{2}\sigma_i^2 - \theta_i\sigma_i - (J_{ii}/\gamma)\log\cosh(\gamma\sigma_i)\right]$
  (non-interacting variables)

The H-theorem

Boltzmann's $\mathcal{H}$-function

for detailed balance processes,
with $p_\infty(\boldsymbol{\sigma}) = Z^{-1} \exp[-\beta H(\boldsymbol{\sigma})]$

$$\text{discrete variables :} \qquad \mathcal{H}[p] = \sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma}) \left[H(\boldsymbol{\sigma}) + \beta^{-1} \log p(\boldsymbol{\sigma}) \right]$$

$$\text{continuous variables :} \qquad \mathcal{H}[p] = \int \mathrm{d}\boldsymbol{\sigma}\; p(\boldsymbol{\sigma}) \left[H(\boldsymbol{\sigma}) + \beta^{-1} \log p(\boldsymbol{\sigma}) \right]$$

generalizes free energy $F = U - TS$ in physics,
with Shannon entropy $S = -\sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma}) \log p(\boldsymbol{\sigma})$
(integral instead of summation for continuous $\boldsymbol{\sigma}$)

claims:

- $\mathcal{H}[p]$ is a *Lyapunov function* for standard stochastic processes that evolve to a Gibbs-Boltzmann equilibrium state
- so $\mathrm{d}\mathcal{H}[p_t]/\mathrm{d}t \leq 0$, and $\mathcal{H}[p]$ bounded from below
- $\mathrm{d}\mathcal{H}[p_t]/\mathrm{d}t = 0$ only at $p_\infty(\boldsymbol{\sigma}) = Z^{-1} \exp[-\beta H(\boldsymbol{\sigma})]$

lower bound of $\mathcal{H}[p]$

- discrete $\boldsymbol{\sigma}$

$$\begin{aligned}\mathcal{H}[p] &= \sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma})\left[H(\boldsymbol{\sigma}) + \frac{1}{\beta}\log p(\boldsymbol{\sigma})\right] = \frac{1}{\beta}\sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma})\log\left[\mathrm{e}^{\beta H(\boldsymbol{\sigma})} p(\boldsymbol{\sigma})\right] \\ &= -\frac{1}{\beta}\log Z + \frac{1}{\beta}\sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma})\log\left[\frac{p(\boldsymbol{\sigma})}{p_\infty(\boldsymbol{\sigma})}\right], \quad p_\infty(\boldsymbol{\sigma}) = \frac{1}{Z}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})} \\ &= -\frac{1}{\beta}\log Z + \frac{1}{\beta}D[p||p_\infty] \geq -\frac{1}{\beta}\log Z\end{aligned}$$

KL distance $D[p||q] = \sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma})\log[p(\boldsymbol{\sigma})/q(\boldsymbol{\sigma})] \geq 0$

- continuous $\boldsymbol{\sigma}$

  same argument, but with $\int \mathrm{d}\boldsymbol{\sigma}$ instead of $\sum_{\boldsymbol{\sigma}}$,
  and KL distance $D[p||q] = \int \mathrm{d}\boldsymbol{\sigma}\; p(\boldsymbol{\sigma})\log[p(\boldsymbol{\sigma})/q(\boldsymbol{\sigma})] \geq 0$

lower bound is achieved
if and only if $p(\boldsymbol{\sigma}) = p_\infty(\boldsymbol{\sigma})$

Evolution of $\mathcal{H}[p_t]$ for Fokker-Planck eqn with conservative forces

- if $f_i(\boldsymbol{\sigma}) = -\partial H(\boldsymbol{\sigma})/\partial\sigma_i$:

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(\boldsymbol{\sigma}) = \sum_i \frac{\partial}{\partial\sigma_i}\left[p_t(\boldsymbol{\sigma})\frac{\partial H(\boldsymbol{\sigma})}{\partial\sigma_i} + T\frac{\partial}{\partial\sigma_i}p_t(\boldsymbol{\sigma})\right], \qquad T = \frac{1}{\beta}$$

this gives (via integration by parts)

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p_t] &= \int \mathrm{d}\boldsymbol{\sigma}\,\left[H(\boldsymbol{\sigma}) + \frac{1}{\beta}\log p_t(\boldsymbol{\sigma}) + \frac{1}{\beta}\right]\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) \\
&= \int \mathrm{d}\boldsymbol{\sigma}\,\left[H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\right]\sum_i \frac{\partial}{\partial\sigma_i}\left[p_t(\boldsymbol{\sigma})\frac{\partial H(\boldsymbol{\sigma})}{\partial\sigma_i} + T\frac{\partial}{\partial\sigma_i}p_t(\boldsymbol{\sigma})\right] \\
&= \sum_i \int \mathrm{d}\boldsymbol{\sigma}\,\left[H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\right]\frac{\partial}{\partial\sigma_i}\left[p_t(\boldsymbol{\sigma})\frac{\partial}{\partial\sigma_i}\Big(H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\Big)\right] \\
&= \text{boundary terms} - \sum_i \int \mathrm{d}\boldsymbol{\sigma}\; p_t(\boldsymbol{\sigma})\left[\frac{\partial}{\partial\sigma_i}\Big(H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})\Big)\right]^2
\end{aligned}$$

- boundary terms:

$$\mathrm{BT} \;=\; \frac{1}{2}\sum_i \int \prod_{j\neq i} \mathrm{d}\sigma_j \left[p_t(\boldsymbol{\sigma}) \frac{\partial}{\partial \sigma_i}\Big(H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma}) \Big)^2 \right]_{\sigma_i=-\infty}^{\sigma_i=\infty}$$

if $p_t(\boldsymbol{\sigma})|_{\sigma_i\to\pm\infty}$ sufficiently fast: BT=0,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p_t] \;=\; -\sum_i \int \mathrm{d}\boldsymbol{\sigma}\; p_t(\boldsymbol{\sigma}) \Big[\frac{\partial}{\partial \sigma_i}\Big(H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma}) \Big) \Big]^2 \leq 0$$

- stationarity requires

$$\begin{aligned}
\forall\boldsymbol{\sigma}: &\quad p(\boldsymbol{\sigma}) = 0 \quad \text{or} \quad H(\boldsymbol{\sigma}) + T\log p(\boldsymbol{\sigma}) \;\text{ is constant} \\
\forall\boldsymbol{\sigma}: &\quad p(\boldsymbol{\sigma}) = 0 \quad \text{or} \quad \mathrm{e}^{\beta H(\boldsymbol{\sigma})} p(\boldsymbol{\sigma}) \;\text{ is constant} \\
\forall\boldsymbol{\sigma}: &\quad p(\boldsymbol{\sigma}) = 0 \quad \text{or} \quad p(\boldsymbol{\sigma}) = Z^{-1}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}
\end{aligned}$$

Evolution of $\mathcal{H}[p_t]$ for discrete variables described by detailed balance master eqn

- master eqn

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = \sum_i \Big[w_i(F_i\boldsymbol{\sigma})p_t(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma})p_t(\boldsymbol{\sigma})\Big]$$

evolution of $\mathcal{H}[p_t]$ (use $\sum_{\boldsymbol{\sigma}} \frac{\mathrm{d}}{\mathrm{d}t}p_t(\boldsymbol{\sigma}) = 0$)

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p_t] &= \sum_{\boldsymbol{\sigma}} [H(\boldsymbol{\sigma}) + T\log p_t(\boldsymbol{\sigma})] \sum_i \Big[w_i(F_i\boldsymbol{\sigma})p_t(F_i\boldsymbol{\sigma}) - w_i(\boldsymbol{\sigma})p_t(\boldsymbol{\sigma})\Big] \\ &= \sum_i \sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma})w_i(\boldsymbol{\sigma})\Big[[H+T\log p_t]_{F_i\boldsymbol{\sigma}} - [H+T\log p_t]_{\boldsymbol{\sigma}}\Big]\end{aligned}$$

- rewrite transition rates

$$w_i(\boldsymbol{\sigma}) = \frac{1}{2}[1-\tanh[\beta\sigma_i h_i(\boldsymbol{\sigma})]] = \frac{\mathrm{e}^{-\beta\sigma_i h_i(\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]} = \frac{\mathrm{e}^{\frac{1}{2}\beta H(\boldsymbol{\sigma}) - \frac{1}{2}\beta H(F_i\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]}$$

since, if all $J_{ii} = 0$ and $J_{ij} = J_{ji}$:

$$H(F_i\boldsymbol{\sigma}) - H(\boldsymbol{\sigma}) = 2\sigma_i h_i(\boldsymbol{\sigma}) \qquad \text{(see exercises)}$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p_t] &= \sum_i \sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma}) \frac{\mathrm{e}^{\frac{1}{2}\beta H(\boldsymbol{\sigma}) - \frac{1}{2}\beta H(F_i\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]} \Big[[H + T\log p_t]_{F_i\boldsymbol{\sigma}} - [H + T\log p_t]_{\boldsymbol{\sigma}} \Big] \\
&= \frac{1}{2} \sum_i \sum_{\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma}) \frac{\mathrm{e}^{\frac{1}{2}\beta H(\boldsymbol{\sigma}) - \frac{1}{2}\beta H(F_i\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]} \Big[[H + T\log p_t]_{F_i\boldsymbol{\sigma}} - [H + T\log p_t]_{\boldsymbol{\sigma}} \Big] \\
&\quad + \frac{1}{2} \sum_i \sum_{\boldsymbol{\sigma}} p_t(F_i\boldsymbol{\sigma}) \frac{\mathrm{e}^{\frac{1}{2}\beta H(F_i\boldsymbol{\sigma}) - \frac{1}{2}\beta H(\boldsymbol{\sigma})}}{2\cosh[\beta h_i(\boldsymbol{\sigma})]} \Big[[H + T\log p_t]_{\boldsymbol{\sigma}} - [H + T\log p_t]_{F_i\boldsymbol{\sigma}} \Big] \\
&= \sum_i \sum_{\boldsymbol{\sigma}} \frac{[H + T\log p_t]_{F_i\boldsymbol{\sigma}} - [H + T\log p_t]_{\boldsymbol{\sigma}}}{4\cosh[\beta h_i(\boldsymbol{\sigma})]} \\
&\qquad \times \Big[p_t(\boldsymbol{\sigma}) \mathrm{e}^{\frac{1}{2}\beta H(\boldsymbol{\sigma}) - \frac{1}{2}\beta H(F_i\boldsymbol{\sigma})} - p_t(F_i\boldsymbol{\sigma}) \mathrm{e}^{\frac{1}{2}\beta H(F_i\boldsymbol{\sigma}) - \frac{1}{2}\beta H(\boldsymbol{\sigma})} \Big] \\
&= \sum_i \sum_{\boldsymbol{\sigma}} \frac{[\beta H + \log p_t]_{F_i\boldsymbol{\sigma}} - [\beta H + \log p_t]_{\boldsymbol{\sigma}}}{4\beta\cosh[\beta h_i(\boldsymbol{\sigma})]} \mathrm{e}^{-\frac{1}{2}\beta H(\boldsymbol{\sigma}) - \frac{1}{2}\beta H(F_i\boldsymbol{\sigma})} \\
&\qquad \times \Big[p_t(\boldsymbol{\sigma}) \mathrm{e}^{\beta H(\boldsymbol{\sigma})} - p_t(F_i\boldsymbol{\sigma}) \mathrm{e}^{\beta H(F_i\boldsymbol{\sigma})} \Big] \\
&= -\sum_i \sum_{\boldsymbol{\sigma}} \frac{\mathrm{e}^{-\frac{1}{2}\beta[H(\boldsymbol{\sigma}) + H(F_i\boldsymbol{\sigma})]}}{4\beta\cosh[\beta h_i(\boldsymbol{\sigma})]} \\
&\qquad \times \Big[[\beta H + \log p_t]_{F_i\boldsymbol{\sigma}} - [\beta H + \log p_t]_{\boldsymbol{\sigma}} \Big] \Big[\mathrm{e}^{[\beta H + \log p_t]_{F_i\boldsymbol{\sigma}}} - \mathrm{e}^{[\beta H + \log p_t]_{\boldsymbol{\sigma}}} \Big]
\end{aligned}
$$

- final step

$$(x-y)(\mathrm{e}^x-\mathrm{e}^y)\geq 0, \quad \text{with equality if and only if} \quad x=y$$

hence $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p_t]\geq 0$

- stationarity requires

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}[p]=0: \qquad \text{for all } i: \quad \beta H(F_i\boldsymbol{\sigma})+\log p(F_i\boldsymbol{\sigma})=\beta H(\boldsymbol{\sigma})+\log p(\boldsymbol{\sigma})$$

$$\beta H(\boldsymbol{\sigma})+\log p(\boldsymbol{\sigma}) \text{ is constant}$$

$$\mathrm{e}^{\beta H(\boldsymbol{\sigma})}p(\boldsymbol{\sigma}) \text{ is constant}$$

$$p(\boldsymbol{\sigma})=Z^{-1}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}$$

Correlation and response functions

Definitions

- add time-dependent perturbations,
  $\theta_i \to \theta_i + \theta_i(t)$ or $f_i(\boldsymbol{\sigma}) \to f_i(\boldsymbol{\sigma}) + \theta_i(t)$

  $$C_{ij}(t,t') = \langle \sigma_i(t)\sigma_j(t')\rangle \qquad G_{ij}(t,t') = \frac{\partial\langle\sigma_i(t)\rangle}{\partial\theta_j(t')} \quad (t > t')$$

  stationary state

  $$C_{ij}(t,t') = C_{ij}(t-t'), \qquad G_{ij}(t,t') = G_{ij}(t-t')$$

- detailed balance equilibrium:
  fluctuation-dissipation theorems (FDT)

  $$\text{discrete } \boldsymbol{\sigma},\ \text{parallel dynamics:} \qquad G_{ij}(\tau>0) = -\beta[C_{ij}(\tau+1) - C_{ij}(\tau-1)]$$

  $$\text{discrete } \boldsymbol{\sigma},\ \text{sequential dynamics:} \qquad G_{ij}(\tau) = -\beta\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}C_{ij}(\tau)$$

  $$\text{continuous } \boldsymbol{\sigma}: \qquad G_{ij}(\tau) = -\beta\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}C_{ij}(\tau)$$

FDT for discrete variables and detailed balance

- Markov chain

$$p_{\ell+1}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] p_\ell(\boldsymbol{\sigma}')$$

  probability of path
  $\boldsymbol{\sigma}(\ell') \to \boldsymbol{\sigma}(\ell'{+}1) \to \ldots \to \boldsymbol{\sigma}(\ell{-}1) \to \boldsymbol{\sigma}(\ell)$

$$\mathrm{Prob}[\boldsymbol{\sigma}(\ell'),\ldots,\boldsymbol{\sigma}(\ell)] = \Big(\prod_{k=\ell'}^{\ell-1} W[\boldsymbol{\sigma}(k{+}1);\boldsymbol{\sigma}(k)]\Big) p_{\ell'}(\boldsymbol{\sigma}(\ell'))$$

- expressions for C and G

$$\begin{aligned} C_{ij}(\ell,\ell') &= \sum_{\boldsymbol{\sigma}(\ell')} \cdots \sum_{\boldsymbol{\sigma}(\ell)} \mathrm{Prob}[\boldsymbol{\sigma}(\ell'),\ldots,\boldsymbol{\sigma}(\ell)] \sigma_i(\ell)\sigma_j(\ell') \\ &= \sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}'} \sigma_i \sigma_j' W^{\ell-\ell'}[\boldsymbol{\sigma};\boldsymbol{\sigma}'] p_{\ell'}(\boldsymbol{\sigma}') \\ G_{ij}(\ell,\ell') &= \sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}'\boldsymbol{\sigma}''} \sigma_i W^{\ell-\ell'-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}''] \left[\frac{\partial}{\partial\theta_j} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\right] p_{\ell'}(\boldsymbol{\sigma}') \end{aligned}$$

- differentiate stationarity eqn

$$\frac{\partial}{\partial\theta_j}p(\boldsymbol{\sigma}) = \frac{\partial}{\partial\theta_j}\sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}']p(\boldsymbol{\sigma}')$$

$$\frac{\partial}{\partial\theta_j}p(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'}\left\{\frac{\partial W[\boldsymbol{\sigma};\boldsymbol{\sigma}']}{\partial\theta_j}p(\boldsymbol{\sigma}') + W[\boldsymbol{\sigma};\boldsymbol{\sigma}']\frac{\partial}{\partial\theta_j}p(\boldsymbol{\sigma}')\right\}$$

- detailed balance

$$p(\boldsymbol{\sigma}) = Z^{-1}\mathrm{e}^{-\beta H(\boldsymbol{\sigma})}: \qquad \frac{\partial p(\boldsymbol{\sigma})}{\partial\theta_j} = -\left[\frac{1}{Z^2}\frac{\partial Z}{\partial\theta_j} + \beta\frac{\partial H(\boldsymbol{\sigma})}{\partial\theta_j}\right]p(\boldsymbol{\sigma})$$

insert into above eqn

$$-\left[\frac{1}{Z^2}\frac{\partial Z}{\partial\theta_j} + \beta\frac{\partial H(\boldsymbol{\sigma})}{\partial\theta_j}\right]p(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'}\frac{\partial W[\boldsymbol{\sigma};\boldsymbol{\sigma}']}{\partial\theta_j}p(\boldsymbol{\sigma}') - \sum_{\boldsymbol{\sigma}'}W[\boldsymbol{\sigma};\boldsymbol{\sigma}']\left[\left(\frac{1}{Z^2}\frac{\partial Z}{\partial\theta_j} + \beta\frac{\partial H(\boldsymbol{\sigma}')}{\partial\theta_j}\right)p(\boldsymbol{\sigma}')\right]$$

$$\beta\frac{\partial H(\boldsymbol{\sigma})}{\partial\theta_j}p(\boldsymbol{\sigma}) = -\sum_{\boldsymbol{\sigma}'}\frac{\partial W[\boldsymbol{\sigma};\boldsymbol{\sigma}']}{\partial\theta_j}p(\boldsymbol{\sigma}') + \beta\sum_{\boldsymbol{\sigma}'}W[\boldsymbol{\sigma};\boldsymbol{\sigma}']\frac{\partial H(\boldsymbol{\sigma}')}{\partial\theta_j}p(\boldsymbol{\sigma}')$$

$$\sum_{\boldsymbol{\sigma}'} \frac{\partial W[\boldsymbol{\sigma};\boldsymbol{\sigma}']}{\partial \theta_j} p(\boldsymbol{\sigma}') = \beta \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma};\boldsymbol{\sigma}'] \frac{\partial H(\boldsymbol{\sigma}')}{\partial \theta_j} p(\boldsymbol{\sigma}') - \beta \frac{\partial H(\boldsymbol{\sigma})}{\partial \theta_j} p(\boldsymbol{\sigma})$$

- response function $G_{ij}(\ell - \ell')$ with $\ell > \ell'$

$$\begin{aligned} G_{ij}(\ell) &= \sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''} \sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}''] \sum_{\boldsymbol{\sigma}'} \frac{\partial W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']}{\partial \theta_j} p_{\ell'}(\boldsymbol{\sigma}') \\ &= \beta \sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''} \sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}''] \left\{ \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}'] \frac{\partial H(\boldsymbol{\sigma}')}{\partial \theta_j} p(\boldsymbol{\sigma}') - \frac{\partial H(\boldsymbol{\sigma}'')}{\partial \theta_j} p(\boldsymbol{\sigma}'') \right\} \end{aligned}$$

compare to

$$C_{ij}(\ell) - C_{ij}(\ell - 1) = \sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''} \sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}''] \left\{ \sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}'] \sigma_j' p(\boldsymbol{\sigma}') - \sigma_j'' p(\boldsymbol{\sigma}'') \right\}$$

discrete variables, sequential dynamics

- work out $\partial H/\partial\theta_j$

$$H(\boldsymbol{\sigma}) = -\frac{1}{2}\sum_{k\neq\ell} J_{k\ell}\sigma_k\sigma_\ell - \sum_k \theta_k\sigma_k, \qquad \frac{\partial H(\boldsymbol{\sigma})}{\partial\theta_j} = -\sigma_j$$

hence

$$\begin{aligned} G_{ij}(\ell) &= -\beta\sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''}\sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}'']\left\{\sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\sigma_j' p(\boldsymbol{\sigma}') - \sigma_j'' p(\boldsymbol{\sigma}'')\right\} \\ &= -\beta\left[C_{ij}(\ell) - C_{ij}(\ell-1)\right] \end{aligned}$$

- master eqn version, large N: $\ell \to Nt + \mathcal{O}(\sqrt{N})$
  - $C_{ij}(\ell) - C_{ij}(\ell-1) \to N^{-1}\frac{\mathrm{d}}{\mathrm{d}t}C_{ij}(t)$
  - rescale perturbations $\theta_i(t) \to N\theta_i(t)$
  - $G_{ij}(\ell) \to N^{-1}G_{ij}(t)$

$$G_{ij}(t) = -\beta\frac{\mathrm{d}}{\mathrm{d}t}C_{ij}(t)$$

rescaling of $\theta_i(t)$ inevitable because
perturbation lasts only for $\Delta t = \mathcal{O}(N^{-1})$

discrete variables, parallel dynamics

- work out $\partial H/\partial\theta_j$

$$H(\boldsymbol{\sigma}) = -\frac{1}{\beta}\sum_k \log\cosh(\beta h_k(\boldsymbol{\sigma})) - \sum_k \theta_k\sigma_k, \quad h_k(\boldsymbol{\sigma}) = \sum_\ell J_{k\ell}\sigma_\ell + \theta_k$$

$$\frac{\partial H(\boldsymbol{\sigma})}{\partial\theta_j} = -\sigma_j - \tanh(\beta h_j(\boldsymbol{\sigma}))$$

hence

$$G_{ij}(\ell) = -\beta\sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''}\sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}'']\left\{\sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\sigma_j' p(\boldsymbol{\sigma}') - \sigma_j'' p(\boldsymbol{\sigma}'')\right\}$$

$$-\beta\sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''}\sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}'']\left\{\sum_{\boldsymbol{\sigma}'} W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\tanh(\beta h_j(\boldsymbol{\sigma}'))p(\boldsymbol{\sigma}') - \tanh(\beta h_j(\boldsymbol{\sigma}''))p(\boldsymbol{\sigma}'')\right\}$$

- final identity, via DB

$$\tanh[\beta h_j(\boldsymbol{\sigma}')]p(\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}''}\sigma_j'' W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']p(\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}''}\sigma_j'' W[\boldsymbol{\sigma}';\boldsymbol{\sigma}'']p(\boldsymbol{\sigma}'')$$

$$\tanh[\beta h_j(\boldsymbol{\sigma}')]p(\boldsymbol{\sigma}') = \sum_{\boldsymbol{\sigma}''} \sigma_j'' W[\boldsymbol{\sigma}';\boldsymbol{\sigma}'']p(\boldsymbol{\sigma}'')$$

- insert into $G_{ij}(\ell)$

$$\begin{aligned}
G_{ij}(\ell) &= -\beta\big[C_{ij}(\ell)-C_{ij}(\ell-1)\big] \\
&\quad -\beta\sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''}\sigma_i W^{\ell-1}[\boldsymbol{\sigma};\boldsymbol{\sigma}'']\Big\{\sum_{\boldsymbol{\sigma}'}W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\sum_{\boldsymbol{\sigma}'''}\sigma_j''' W[\boldsymbol{\sigma}';\boldsymbol{\sigma}''']p(\boldsymbol{\sigma}''') \\
&\qquad\qquad -\sum_{\boldsymbol{\sigma}'''}\sigma_j''' W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}''']p(\boldsymbol{\sigma}''')\Big\} \\
&= -\beta\big[C_{ij}(\ell)-C_{ij}(\ell-1)\big] \\
&\quad -\beta\sum_{\boldsymbol{\sigma}\boldsymbol{\sigma}''}\sigma_i W^{\ell}[\boldsymbol{\sigma};\boldsymbol{\sigma}'']\Big\{\sum_{\boldsymbol{\sigma}'}W[\boldsymbol{\sigma}'';\boldsymbol{\sigma}']\sigma_j' p(\boldsymbol{\sigma}') - \sigma_j'' p(\boldsymbol{\sigma}'')\Big\} \\
&= -\beta\big[C_{ij}(\ell)-C_{ij}(\ell-1)\big] - \beta\big[C_{ij}(\ell+1)-C_{ij}(\ell)\big] \\
&= -\beta\big[C_{ij}(\ell+1)-C_{ij}(\ell-1)\big]
\end{aligned}$$

$$G_{ij}(\ell>0) = -\beta[C_{ij}(\ell+1)-C_{ij}(\ell-1)], \qquad G_{ij}(\ell\leq 0)=0$$

FDT for continuous variables and detailed balance

- Fokker-Planck eqn in operator form

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t = \mathcal{L}p_t, \qquad \mathcal{L}(\boldsymbol{\sigma},\boldsymbol{\sigma}') = -\sum_i \frac{\partial}{\partial\sigma_i}\Big[f_i(\boldsymbol{\sigma}) - T\frac{\partial}{\partial\sigma_i}\Big]\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}')$$

$$\text{solution}: \quad p_t(\boldsymbol{\sigma}) = \int \mathrm{d}\boldsymbol{\sigma}'\,(\mathrm{e}^{t\mathcal{L}})(\boldsymbol{\sigma},\boldsymbol{\sigma}')p_0(\boldsymbol{\sigma}'), \qquad \mathrm{e}^{t\mathcal{L}} = \sum_{n\geq 0}\frac{t^n}{n!}\mathcal{L}^n$$

- conditional probability density

$$t \geq t': \qquad p_t(\boldsymbol{\sigma}|\boldsymbol{\sigma}(t')=\boldsymbol{\sigma}') = \Big(\mathrm{e}^{(t-t')\mathcal{L}}\Big)(\boldsymbol{\sigma},\boldsymbol{\sigma}')$$

$$C_{ij}(t,t') = \int d\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\;\sigma_i\,\mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\sigma_j'\;p_{t'}(\boldsymbol{\sigma}')$$

- response function

$$\text{during interval } [t',t'+\epsilon]: \quad \tilde{f}_i(\boldsymbol{\sigma}) = f_i(\boldsymbol{\sigma}) + \epsilon^{-1}\delta_{ij}\tilde{\theta}, \quad \tilde{\mathcal{L}} = \mathcal{L} + \epsilon^{-1}\Delta\mathcal{L}$$

$$\Delta\mathcal{L}(\boldsymbol{\sigma},\boldsymbol{\sigma}') = -\tilde{\theta}\frac{\partial}{\partial\sigma_j}\delta(\boldsymbol{\sigma}-\boldsymbol{\sigma}')$$

$$G_{ij}(t,t') = \lim_{\tilde{\theta}\to 0}\lim_{\epsilon\downarrow 0}\frac{\partial}{\partial\tilde{\theta}}\int \mathrm{d}\boldsymbol{\sigma}\;\sigma_i p_{t'}(\boldsymbol{\sigma})$$

- this gives

$$
\begin{aligned}
G_{ij}(t,t') &= \lim_{\tilde{\theta}\to 0}\lim_{\epsilon\downarrow 0}\frac{\partial}{\partial\tilde{\theta}}\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \overbrace{\mathrm{e}^{(t-t'-\epsilon)\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')}^{\text{propagate } t'+\epsilon\to t}\int \mathrm{d}\boldsymbol{\sigma}''\ \overbrace{\mathrm{e}^{\epsilon\tilde{\mathcal{L}}}(\boldsymbol{\sigma}',\boldsymbol{\sigma}'')}^{\text{propagate } t'\to t'+\epsilon}\ p_{t'}(\boldsymbol{\sigma}'') \\
&= \lim_{\tilde{\theta}\to 0}\lim_{\epsilon\downarrow 0}\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t'-\epsilon)\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\frac{\partial}{\partial\tilde{\theta}}\int \mathrm{d}\boldsymbol{\sigma}''\mathrm{e}^{\epsilon\tilde{\mathcal{L}}}(\boldsymbol{\sigma}',\boldsymbol{\sigma}'')p_{t'}(\boldsymbol{\sigma}'') \\
&= \lim_{\tilde{\theta}\to 0}\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\frac{\partial}{\partial\tilde{\theta}}\int \mathrm{d}\boldsymbol{\sigma}''\mathrm{e}^{\Delta\mathcal{L}}(\boldsymbol{\sigma}',\boldsymbol{\sigma}'')p_{t'}(\boldsymbol{\sigma}'')
\end{aligned}
$$

work out

$$
\begin{aligned}
\int \mathrm{d}\boldsymbol{\sigma}''\mathrm{e}^{\Delta\mathcal{L}}(\boldsymbol{\sigma}',\boldsymbol{\sigma}'')p_{t'}(\boldsymbol{\sigma}'') &= \mathrm{e}^{-\tilde{\theta}\frac{\partial}{\partial\sigma_j'}}p_{t'}(\boldsymbol{\sigma}') \\
&= \sum_{n\geq 0}\frac{(-\tilde{\theta})^n}{n!}\frac{\partial^n}{\partial(\sigma_j')^n}p_{t'}(\boldsymbol{\sigma}')\ =\ p_{t'}(\boldsymbol{\sigma}'-\tilde{\theta}\hat{\mathbf{e}}^j)
\end{aligned}
$$

$$
\begin{aligned}
G_{ij}(t,t') &= \lim_{\tilde{\theta}\to 0}\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\frac{\partial}{\partial\tilde{\theta}}p_{t'}(\boldsymbol{\sigma}'-\tilde{\theta}\hat{\mathbf{e}}^j) \\
&= -\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\frac{\partial}{\partial\sigma_j'}p_{t'}(\boldsymbol{\sigma}')
\end{aligned}
$$

always

$$C_{ij}(t,t') = \int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\sigma_j'\ p_{t'}(\boldsymbol{\sigma}')$$
$$G_{ij}(t,t') = -\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{(t-t')\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\frac{\partial}{\partial\sigma_j'}p_{t'}(\boldsymbol{\sigma}')$$

- detailed balance equilibrium

$$f_i(\boldsymbol{\sigma}) = -\frac{\partial H(\boldsymbol{\sigma})}{\partial\sigma_i}, \quad \left[f_i(\boldsymbol{\sigma}) - T\frac{\partial}{\partial\sigma_i}\right]p(\boldsymbol{\sigma}) = 0\ \forall i, \qquad \begin{aligned} C_{ij}(t,t') &= C_{ij}(t-t') \\ G_{ij}(t,t') &= G_{ij}(t-t') \end{aligned}$$

$$\begin{aligned}
-\beta\frac{\mathrm{d}}{\mathrm{d}\tau}C_{ij}(\tau) &= -\beta\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{\tau\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\int \mathrm{d}\boldsymbol{\sigma}''\ \mathcal{L}(\boldsymbol{\sigma}',\boldsymbol{\sigma}'')\sigma_j'' p(\boldsymbol{\sigma}'') \\
&= \beta\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{\tau\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\sum_k \frac{\partial}{\partial\sigma_k'}\left[f_k(\boldsymbol{\sigma}') - T\frac{\partial}{\partial\sigma_k'}\right]\left[\sigma_j' p(\boldsymbol{\sigma}')\right]
\end{aligned}$$
$$= \beta\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{\tau\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\sum_k \frac{\partial}{\partial\sigma_k'}\left[\sigma_j'\left(f_k(\boldsymbol{\sigma}')p(\boldsymbol{\sigma}') - T\frac{\partial}{\partial\sigma_k'}p(\boldsymbol{\sigma}')\right) - T\delta_{jk}p(\boldsymbol{\sigma}')\right]$$
$$= -\int \mathrm{d}\boldsymbol{\sigma}\mathrm{d}\boldsymbol{\sigma}'\ \sigma_i\ \mathrm{e}^{\tau\mathcal{L}}(\boldsymbol{\sigma},\boldsymbol{\sigma}')\sum_k \frac{\partial}{\partial\sigma_k'}\left[\delta_{jk}p(\boldsymbol{\sigma}')\right] = G_{ij}(\tau)$$