

Modelling of Complex Real-World Systems Part B. Tools for Heterogeneous Systems

B1. Homogeneous systems

Ton Coolen

Department of Biophysics, Radboud University
module NWI-NM127, January 2021



Homogeneous systems

discrete

$$\frac{d}{dt} p_t(\sigma) = \sum_i [w_i(F_i \sigma) p_t(F_i \sigma) - w_i(\sigma) p_t(\sigma)], \quad w_i(\sigma) = \frac{1}{2} [1 - \sigma_i \tanh(\beta h_i(\sigma))]$$

$$p_{t+1}(\sigma) = \sum_{\sigma'} W[\sigma; \sigma'] p_t(\sigma'), \quad W[\sigma; \sigma'] = \prod_{i=1}^N \left[\frac{1}{2} + \frac{1}{2} \sigma_i \tanh(\beta h_i(\sigma')) \right]$$

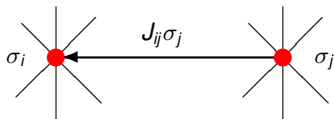
continuous

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

• forces

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

$$f_i(\sigma) = \sum_j J_{ij} \sigma_j + \theta_i + g(\sigma_i)$$



homogeneous, with $h_i(\sigma) = \mathcal{O}(1)$ for $N \rightarrow \infty$:

$$J_{ij} = J/N, \quad \theta_i = \theta:$$

$$h_i(\sigma) = Jm(\sigma) + \theta$$

$$f_i(\sigma) = Jm(\sigma) + \theta + g(\sigma_i)$$

$$m(\sigma) = \frac{1}{N} \sum_i \sigma_i$$

Sequential master equation

Dynamical solution

$$\frac{d}{dt} p_t(\sigma) = \sum_{i=1}^N [w_i(F_i \sigma) p_t(F_i \sigma) - w_i(\sigma) p_t(\sigma)], \quad w_i(\sigma) = \frac{1}{2} [1 - \sigma_i \tanh(\beta(Jm(\sigma) + \theta))]$$

key macroscopic object

$$m(\sigma) = \frac{1}{N} \sum_i \sigma_i, \quad P_t(m) = \sum_{\sigma} p_t(\sigma) \delta[m - m(\sigma)]$$

- macroscopic dynamics

$$\begin{aligned} \frac{d}{dt} P_t(m) &= \sum_{\sigma} \frac{d}{dt} p_t(\sigma) \delta[m - m(\sigma)] \\ &= \sum_i \sum_{\sigma} [w_i(F_i \sigma) p_t(F_i \sigma) - w_i(\sigma) p_t(\sigma)] \delta[m - m(\sigma)] \\ &= \sum_i \sum_{\sigma} p_t(\sigma) w_i(\sigma) \left(\delta[m - m(F_i \sigma)] - \delta[m - m(\sigma)] \right) \end{aligned}$$

- expand, using $m(F_i\sigma) = m(\sigma) - \frac{2}{N}\sigma_i$

$$\delta[m - m(F_i\sigma)] = \delta[m - m(\sigma)] + \frac{2\sigma_i}{N} \frac{d}{dm} \delta[m - m(\sigma)] + \mathcal{O}(N^{-2})$$

$$\begin{aligned} \frac{d}{dt} P_t(m) &= \sum_i \sum_{\sigma} p_t(\sigma) w_i(\sigma) \left\{ \frac{2\sigma_i}{N} \frac{d}{dm} \delta[m - m(\sigma)] + \mathcal{O}(N^{-2}) \right\} \\ &= \frac{1}{N} \frac{\partial}{\partial m} \sum_i \sum_{\sigma} p_t(\sigma) [1 - \sigma_i \tanh(\beta(Jm(\sigma) + \theta))] \sigma_i \delta[m - m(\sigma)] + \mathcal{O}\left(\frac{1}{N}\right) \\ &= \frac{\partial}{\partial m} \sum_{\sigma} p_t(\sigma) [m(\sigma) - \tanh(\beta(Jm(\sigma) + \theta))] \delta[m - m(\sigma)] + \mathcal{O}\left(\frac{1}{N}\right) \\ &= \frac{\partial}{\partial m} \sum_{\sigma} p_t(\sigma) [m - \tanh(\beta(Jm + \theta))] \delta[m - m(\sigma)] + \mathcal{O}\left(\frac{1}{N}\right) \\ &= \frac{\partial}{\partial m} \left\{ P_t(m) [m - \tanh(\beta(Jm + \theta))] \right\} + \mathcal{O}\left(\frac{1}{N}\right) \end{aligned}$$

$$N \rightarrow \infty: \quad \frac{d}{dt} P_t(m) = -\frac{\partial}{\partial m} \left\{ P_t(m) F(m) \right\}, \quad F(m) = \tanh(\beta(Jm + \theta)) - m$$

(Liouville equation)

solve Liouville eqn

$$\frac{d}{dt} P_t(m) = -\frac{\partial}{\partial m} \left\{ P_t(m) F(m) \right\} \Rightarrow P_t(m) = \delta[m - m(t)], \quad \frac{d}{dt} m(t) = F(m(t))$$

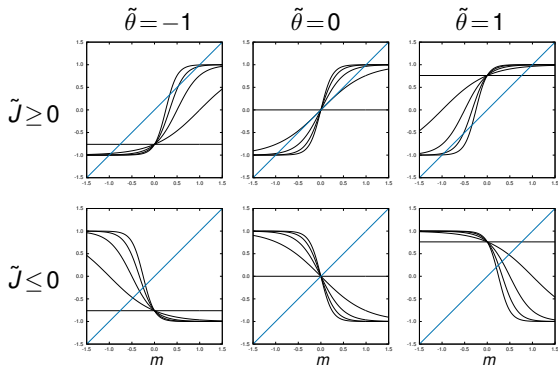
$N \rightarrow \infty$: $m(\sigma)$ evolves

deterministically, according to closed eqn

(see exercises)

$$\frac{d}{dt} m = \tanh(\tilde{J}m + \tilde{\theta}) - m, \quad \tilde{J} = \beta J = J/T, \quad \tilde{\theta} = \beta \theta = \theta/T$$

- stationary states:
 $m = \tanh(\tilde{J}m + \tilde{\theta})$



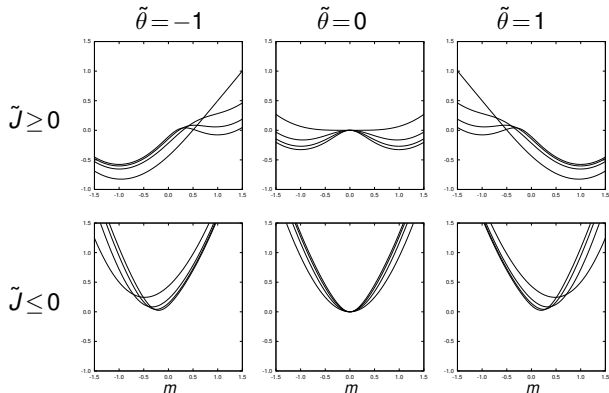
- process minimizes

$$\Phi(m) = \frac{1}{2}m^2 - \tilde{J}^{-1} \log \cosh(\tilde{J}m + \tilde{\theta})$$

proof:

since $dm/dt = -\partial\Phi(m)/\partial m$

$$\frac{d}{dt}\Phi(m) = \frac{\partial\Phi(m)}{\partial m} \frac{dm}{dt} = -\left(\frac{\partial\Phi(m)}{\partial m}\right)^2 \leq 0$$



Equilibrium solution

$$\begin{aligned} p(\boldsymbol{\sigma}) &= \frac{1}{Z} e^{-\beta H(\boldsymbol{\sigma})}, & H(\boldsymbol{\sigma}) &= -\frac{J}{2N} \sum_{i \neq j} \sigma_i \sigma_j - \theta \sum_i \sigma_i \quad (\text{Curie-Weiss model}) \\ & & &= \frac{1}{2} J - \frac{1}{2} J N m^2(\boldsymbol{\sigma}) - N \theta m(\boldsymbol{\sigma}) \end{aligned}$$

- generating function
(free energy density)

$$\begin{aligned} f &= -\frac{1}{\beta N} \log Z, & Z &= \sum_{\boldsymbol{\sigma}} e^{-\beta H(\boldsymbol{\sigma})}, \\ -\frac{\partial f}{\partial \theta} &= -\frac{1}{N Z} \sum_{\boldsymbol{\sigma}} \frac{\partial H(\boldsymbol{\sigma})}{\partial \theta} e^{-\beta H(\boldsymbol{\sigma})} = \frac{1}{Z} \sum_{\boldsymbol{\sigma}} m(\boldsymbol{\sigma}) e^{-\beta H(\boldsymbol{\sigma})} = \langle m(\boldsymbol{\sigma}) \rangle \end{aligned}$$

- objective: find

$$\lim_{N \rightarrow \infty} f = -\lim_{N \rightarrow \infty} \frac{1}{\beta N} \log Z, \quad Z = \sum_{\boldsymbol{\sigma}} e^{-\frac{1}{2} \tilde{J} + \frac{1}{2} \tilde{J} N m^2(\boldsymbol{\sigma}) + N \tilde{\theta} m(\boldsymbol{\sigma})}$$

main obstacle: $\sum_{\boldsymbol{\sigma}}$

Route A: *Gaussian linearisation*

strategy:

- 1 use $\int \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2+ax} = e^{\frac{1}{2}a^2}$ to linearize the term quadratic in σ
- 2 ensure all terms in exponent of integral scale as $\mathcal{O}(N)$
- 3 use steepest descent integration

- 1 linearization

$$Z = \sum_{\sigma} e^{-\frac{1}{2}\tilde{J} + \frac{1}{2}\tilde{J}Nm^2(\sigma) + N\tilde{\theta}m(\sigma)} = e^{-\frac{1}{2}\tilde{J}} \sum_{\sigma} \int \frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2 + xm(\sigma)\sqrt{\tilde{J}N} + N\tilde{\theta}m(\sigma)}$$

- 2 scaling with N :
 $x \rightarrow y\sqrt{\tilde{J}N}$

$$\begin{aligned} Z &= e^{-\frac{1}{2}\tilde{J}} \left(\frac{\tilde{J}N}{2\pi}\right)^{\frac{1}{2}} \sum_{\sigma} \int dy e^{-\frac{1}{2}\tilde{J}Ny^2 + ym(\sigma)\tilde{J}N + N\tilde{\theta}m(\sigma)} \\ &= e^{-\frac{1}{2}\tilde{J}} \left(\frac{\tilde{J}N}{2\pi}\right)^{\frac{1}{2}} \int dy e^{-\frac{1}{2}\tilde{J}Ny^2} \sum_{\sigma} e^{(y\tilde{J} + \tilde{\theta}) \sum_i \sigma_i} \\ &= 2^N e^{-\frac{1}{2}\tilde{J}} \left(\frac{\tilde{J}N}{2\pi}\right)^{\frac{1}{2}} \int dy e^{-\frac{1}{2}\tilde{J}Ny^2} \cosh^N(y\tilde{J} + \tilde{\theta}) \end{aligned}$$

3 steepest descent

$$\begin{aligned}
 \lim_{N \rightarrow \infty} f &= - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \log \left\{ 2^N e^{-\frac{1}{2} \tilde{J}} \left(\frac{\tilde{J} N}{2\pi} \right)^{\frac{1}{2}} \int dy e^{-\frac{1}{2} \tilde{J} N y^2 + N \log \cosh(\tilde{J} y + \tilde{\theta})} \right\} \\
 &= -\frac{1}{\beta} \log 2 - \frac{1}{\beta} \max_y \left[\log \cosh(\tilde{J} y + \tilde{\theta}) - \frac{1}{2} \tilde{J} y^2 \right] \\
 &= -\frac{1}{\beta} \log 2 + \frac{1}{\beta} \min_y \left[\frac{1}{2} \tilde{J} y^2 - \log \cosh(\tilde{J} y + \tilde{\theta}) \right] \\
 &= -\frac{1}{\beta} \log 2 + J \min_y \Phi(y), \quad \Phi(y) = \frac{1}{2} y^2 - \tilde{J}^{-1} \log \cosh(\tilde{J} y + \tilde{\theta})
 \end{aligned}$$

solve $\Phi'(y) = 0$ $y = \tanh(\tilde{J} y + \tilde{\theta})$, soln: y^*

$$\begin{aligned}
 m = \langle m(\sigma) \rangle &= -\frac{\partial}{\partial \theta} f = -J \frac{\partial}{\partial \theta} \left[\frac{1}{2} y^{*2} - \tilde{J}^{-1} \log \cosh(\tilde{J} y^* + \tilde{\theta}) \right] \\
 &= -J \left[\Phi'(y^*) \frac{\partial y^*}{\partial \theta} - \beta \tilde{J}^{-1} \tanh(\tilde{J} y^* + \tilde{\theta}) \right] = \tanh(\tilde{J} y^* + \tilde{\theta}) = y^*
 \end{aligned}$$

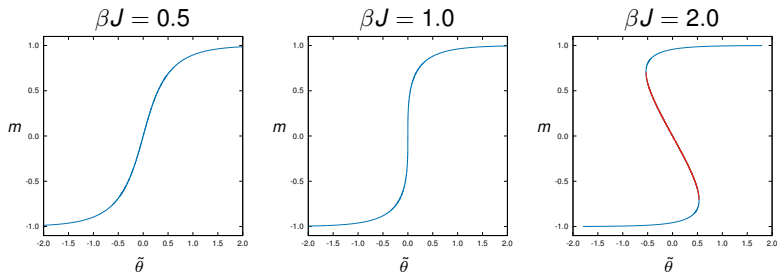
so

$$m = \tanh(\tilde{J} m + \tilde{\theta}), \quad m = \operatorname{argmin}_y \Phi(y)$$

disadvantage:
works only when H quadratic in $m(\sigma)$

Phenomenology

- spontaneous order and remanence



blue: stable solns of $m = \tanh(\tilde{J}m + \tilde{\theta})$

red: unstable solns of $m = \tanh(\tilde{J}m + \tilde{\theta})$

$\tilde{J} = \beta J > 1$: stable solns $m \neq 0$ even when $\tilde{\theta} = 0$
remanence (i.e. memory)

- no external forces, $\tilde{\theta}=0$:

$$\tilde{J} \leq 0: \quad m^2 = m \tanh(\tilde{J}m) = -|m| \tanh(|\tilde{J}m|) \leq 0 \quad \text{so } m = 0$$

$$\tilde{J} > 0: \quad m^2 = |m| \tanh(\tilde{J}|m|) = |m| \int_0^{\tilde{J}|m|} dx [1 - \tanh^2(x)] \leq \tilde{J}m^2$$

$$m^2(\tilde{J}-1) \geq 0 \quad \text{hence } m=0 \text{ for } \tilde{J} < 1$$

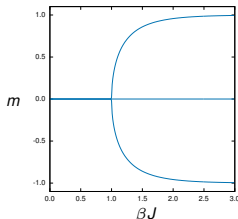
near $\tilde{J}=1$: $\tilde{J}=1+\epsilon$, $|m| \ll 1$, use $\tanh(x) = x - \frac{1}{3}x^3 + \mathcal{O}(x^5)$

$$m = \tanh(m(1+\epsilon)) = m(1+\epsilon) - \frac{1}{3}m^3 + \mathcal{O}(\epsilon m^3, m^5)$$

$$m=0 \quad \text{or} \quad \epsilon = \frac{1}{3}m^2 + \mathcal{O}(\epsilon m^2, m^4)$$

$$m=0 \quad \text{or} \quad m = \pm(3\epsilon)^{\frac{1}{2}} + \dots$$

$m \neq 0$ solns emerge at $\tilde{J}=1$
phase transition



- apparent paradoxes

- equilibrium analysis: $m = \operatorname{argmin}_y \Phi(y)$,
 $\tilde{J} > 1$ and $\tilde{\theta} \neq 0$: minimum has $m = |m| \operatorname{sgn}(\tilde{\theta})$,

yet if $|\tilde{\theta}|$ not too big: $\operatorname{sgn}(m(\infty)) = \operatorname{sgn}(m(0))$ (remanence) ...

- consider $\tilde{\theta} = 0$ for simplicity,
process is ergodic, all σ can in principle be reached,

yet if $\tilde{J} > 1$: $\operatorname{sgn}[m(\infty)] = \operatorname{sgn}[m(0)]$...

- consider $\tilde{\theta} = 0$ for simplicity,
 $p_\infty(\sigma) = p_\infty(-\sigma)$, hence $\langle \sigma_i \rangle = 0$ for all i ,

yet if $\tilde{J} > 1$: $m(\infty) = N^{-1} \sum_i \langle \sigma_i \rangle \neq 0$...

- explanation: non-commutation of limits

equilibrium calculations: $t \rightarrow \infty$ before $N \rightarrow \infty$

dynamical solution: $N \rightarrow \infty$ before $t \rightarrow \infty$

spontaneous symmetry breaking,
timescales required to see ergodicity diverge as $N \rightarrow \infty$

Route B: *integral representation of δ -function*

strategy:

- 1 insert $1 = \int dm \delta[m - m(\sigma)]$ to relocate $m(\sigma)$
- 2 use integral representation of δ
- 3 ensure all terms in exponent of integral scale as $\mathcal{O}(N)$
- 4 use steepest descent integration

- 1 more general $H(\sigma) = NE[m(\sigma)]$

$$\begin{aligned} Z &= \sum_{\sigma} e^{-\beta NE[m(\sigma)]} = \sum_{\sigma} \int dm \delta[m - m(\sigma)] e^{-\beta NE[m(\sigma)]} \\ &= \int dm e^{-\beta NE[m]} \sum_{\sigma} \delta[m - m(\sigma)] \end{aligned}$$

- 2 use $\delta(x) = (2\pi)^{-1} \int dk e^{ikx}$

$$Z = \int \frac{dm dk}{2\pi} e^{ikm - \beta NE[m]} \sum_{\sigma} e^{-ikm(\sigma)}$$

- 3 scaling with N :
 $k \rightarrow Ny$

$$\begin{aligned} Z &= \frac{N}{2\pi} \int dm dy e^{iNym - \beta NE[m]} \sum_{\sigma} e^{-iy \sum_i \sigma_i} \\ &= 2^N \frac{N}{2\pi} \int dm dy e^{iNym - \beta NE[m]} \cos^N(y) \end{aligned}$$

- 4 steepest descent

$$\begin{aligned} \lim_{N \rightarrow \infty} f &= - \lim_{N \rightarrow \infty} \frac{1}{\beta N} \log \left\{ 2^N \frac{N}{2\pi} \int dm dy e^{iNym - \beta NE[m] + N \log \cos(y)} \right\} \\ &= - \frac{1}{\beta} \log 2 - \frac{1}{\beta} \text{extr}_{(m,y)} \left[iym - \beta E[m] + \log \cos(y) \right] \\ &= - \frac{1}{\beta} \log 2 + \Phi(m^*, y^*), \quad \Phi(m, y) = E[m] - \frac{1}{\beta} \left(\log \cos(y) + iym \right) \end{aligned}$$

(m^*, y^*) : soln of $\frac{\partial \Phi}{\partial m} = \frac{\partial \Phi}{\partial y} = 0$

$$\frac{d}{dm} E[m] - iy/\beta = 0, \quad \tan(y) - im = 0$$

to solve : $\frac{d}{dm} E[m] - iy/\beta = 0, \quad \tan(y) - im = 0$

- identify correct saddle point

$$E[m] \in \mathbb{R}, \text{ so } y = i\beta x, \quad x \in \mathbb{R} : \quad \frac{d}{dm} E[m] + x = 0, \quad \tanh(\beta x) = m$$

$$\Rightarrow \quad m = \tanh\left(-\beta \frac{d}{dm} E[m]\right)$$

$$\lim_{N \rightarrow \infty} f = -\frac{1}{\beta} \log 2 + E[m] - \beta^{-1} \log \cosh(\beta x) + xm$$

$$= -\frac{1}{\beta} \log 2 + E[m] + \frac{1}{\beta} c^*(m),$$

$$c^*(m) = \frac{1}{2} [(1+m) \log(1+m) + (1-m) \log(1-m)]$$

(see exercises)

- present model:

$$E[m] = -\frac{1}{2} Jm^2 - \theta m$$

$$m = \tanh(\beta(Jm + \theta)), \quad \lim_{N \rightarrow \infty} f = -\frac{1}{\beta} \log 2 + \frac{1}{\beta} c^*(m) - \frac{1}{2} Jm^2 - \theta m$$

Parallel Markov chain

Dynamical solution

$$p_{t+1}(\sigma) = \sum_{\sigma'} W[\sigma; \sigma'] p_t(\sigma'), \quad W[\sigma; \sigma'] = \prod_{i=1}^N \frac{e^{\beta \sigma_i [Jm(\sigma') + \theta]}}{2 \cosh[\beta (Jm(\sigma') + \theta)]}$$

define

$$m(\sigma) = \frac{1}{N} \sum_i \sigma_i, \quad P_t(m) = \sum_{\sigma} p_t(\sigma) \delta[m - m(\sigma)]$$

- macroscopic dynamics

$$\begin{aligned} P_{t+1}(m) &= \sum_{\sigma} p_{t+1}(\sigma) \delta[m - m(\sigma)] \\ &= \sum_{\sigma, \sigma'} \delta[m - m(\sigma)] \frac{e^{\beta \sum_i \sigma_i [Jm(\sigma') + \theta]}}{2^N \cosh^N[\beta (Jm(\sigma') + \theta)]} p_t(\sigma') \\ &= D(m) \sum_{\sigma'} \left(\frac{e^{\beta m (Jm(\sigma') + \theta)}}{2 \cosh[\beta (Jm(\sigma') + \theta)]} \right)^N p_t(\sigma') \end{aligned}$$

$$\text{with } D(m) = \sum_{\sigma} \delta[m - m(\sigma)]$$

- insert $1 = \int dm' \delta[m' - m(\sigma')]$

$$\begin{aligned}
 P_{t+1}(m) &= D(m) \int dm' \left(\frac{e^{\beta m(Jm' + \theta)}}{2 \cosh[\beta(Jm' + \theta)]} \right)^N \sum_{\sigma'} p_t(\sigma') \delta[m' - m(\sigma')] \\
 &= D(m) \int dm' \left(\frac{e^{\beta m(Jm' + \theta)}}{2 \cosh[\beta(Jm' + \theta)]} \right)^N P_t(m')
 \end{aligned}$$

equivalently

$$\begin{aligned}
 P_{t+1}(m) &= \int dm' e^{N\Phi(m, m')} P_t(m') \\
 \Phi(m, m') &= \frac{1}{N} \log D(m) + \log \left(\frac{e^{\beta m(Jm' + \theta)}}{2 \cosh[\beta(Jm' + \theta)]} \right)
 \end{aligned}$$

- $N \rightarrow \infty$: steepest descent integration

$$P_{t+1}(m) = P_t(m^*(m)),$$

$$m^*(m) = \operatorname{argmax}_{m'} \lim_{N \rightarrow \infty} \Phi(m, m')$$

$$= \operatorname{argmax}_x \left[m(\tilde{J}x + \tilde{\theta}) - \log \cosh(\tilde{J}x + \tilde{\theta}) \right]$$

$N \rightarrow \infty$: if $P_t(m) = \delta[m - m(t)] \Rightarrow P_{t+1}(m) = \delta[m - m(t+1)]$
 $m(\sigma)$ evolves *deterministically*

- link between $m(t)$ and $m(t+1)$,
solve

$$m(t) = \operatorname{argmax}_x \left[m(t+1) [\tilde{J}x + \tilde{\theta}] - \log \cosh(\tilde{J}x + \tilde{\theta}) \right]$$

differentiate wrt x : $m(t+1) = \tanh(\tilde{J}x + \tilde{\theta})$

result

$$m(t+1) = \tanh(\tilde{J}m(t) + \tilde{\theta})$$

- phenomenology

- fixed-point eqn: same as for sequential dynamics
- stability of fixed-points: different when $\tilde{J} < 0$!

$\tilde{\theta} = 0$:

$\tilde{J} \in [-1, 0)$: $m = 0$ stable

$\tilde{J} \in (-\infty, -1)$: $m = 0$ unstable, system entering oscillation

large times: $m(t) = (-1)^t m^*$, $m^* = \tanh(|\tilde{J}|m^*)$

Fokker-Planck equation

Dynamical solution

$$\frac{d}{dt} p_t(\boldsymbol{\sigma}) = - \sum_i \frac{\partial}{\partial \sigma_i} [p_t(\boldsymbol{\sigma}) f_i(\boldsymbol{\sigma})] + T \sum_i \frac{\partial^2}{\partial \sigma_i^2} p_t(\boldsymbol{\sigma}), \quad f_i(\boldsymbol{\sigma}) = Jm(\boldsymbol{\sigma}) + \theta + g(\sigma_i)$$

assume $p_t(\boldsymbol{\sigma})$ decays sufficiently fast for $|\boldsymbol{\sigma}| \rightarrow \infty$,
so that we need not worry about boundary terms

$$\begin{aligned} \frac{d}{dt} \langle G \rangle &= \int d\boldsymbol{\sigma} G(\boldsymbol{\sigma}) \frac{d}{dt} p_t(\boldsymbol{\sigma}) \\ &= \sum_i \int d\boldsymbol{\sigma} G(\boldsymbol{\sigma}) \left[- \frac{\partial}{\partial \sigma_i} [p_t(\boldsymbol{\sigma}) f_i(\boldsymbol{\sigma})] + T \frac{\partial^2}{\partial \sigma_i^2} p_t(\boldsymbol{\sigma}) \right] \\ &= \sum_i \int d\boldsymbol{\sigma} \left[p_t(\boldsymbol{\sigma}) f_i(\boldsymbol{\sigma}) \frac{\partial}{\partial \sigma_i} G(\boldsymbol{\sigma}) + T p_t(\boldsymbol{\sigma}) \frac{\partial^2}{\partial \sigma_i^2} G(\boldsymbol{\sigma}) \right] \\ &= \sum_i \left\langle f_i \frac{\partial}{\partial \sigma_i} G \right\rangle + T \sum_i \left\langle \frac{\partial^2}{\partial \sigma_i^2} G \right\rangle \end{aligned}$$

no longer closed eqn for $m(\boldsymbol{\sigma}) \dots$

Macroscopic dynamics

observables $\Omega(\phi) = (\Omega_1(\sigma), \dots, \Omega_n(\sigma))$,

macroscopic, so $\partial\Omega_\mu(\sigma)/\partial\sigma_i = \mathcal{O}(N^{-1})$

$$P_t(\Omega) = \int d\sigma \rho_t(\sigma) \delta[\Omega - \Omega(\sigma)] = \langle \delta[\Omega - \Omega(\sigma)] \rangle$$

- evolution of $P_t(\Omega)$

$$\frac{d}{dt} P_t(\Omega) = \sum_i \left\langle f_i(\sigma) \frac{\partial \delta[\Omega - \Omega(\sigma)]}{\partial \sigma_i} \right\rangle + T \sum_i \left\langle \frac{\partial^2 \delta[\Omega - \Omega(\sigma)]}{\partial \sigma_i^2} \right\rangle$$

$$\frac{\partial \delta[\Omega - \Omega(\sigma)]}{\partial \sigma_i} = - \sum_{\mu=1}^n \frac{\partial \delta[\Omega - \Omega(\sigma)]}{\partial \Omega_\mu} \frac{\partial \Omega_\mu(\sigma)}{\partial \sigma_i}$$

$$\frac{\partial^2 \delta[\Omega - \Omega(\sigma)]}{\partial \sigma_i^2} = \sum_{\mu=1}^n \left[\sum_{\nu=1}^n \frac{\partial^2 \delta[\Omega - \Omega(\sigma)]}{\partial \Omega_\mu \partial \Omega_\nu} \overbrace{\frac{\partial \Omega_\mu(\sigma)}{\partial \sigma_i} \frac{\partial \Omega_\nu(\sigma)}{\partial \sigma_i}}^{\mathcal{O}(N^{-2})} - \frac{\partial \delta[\Omega - \Omega(\sigma)]}{\partial \Omega_\mu} \overbrace{\frac{\partial^2 \Omega_\mu(\sigma)}{\partial \sigma_i^2}}^{\mathcal{O}(N^{-1})} \right]$$

$$\frac{d}{dt} P_t(\Omega) = - \sum_{\mu=1}^n \frac{\partial}{\partial \Omega_\mu} \left\langle \left[\sum_i f_i(\sigma) \frac{\partial \Omega_\mu(\sigma)}{\partial \sigma_i} + T \sum_i \frac{\partial^2 \Omega_\mu(\sigma)}{\partial \sigma_i^2} \right] \delta[\Omega - \Omega(\sigma)] \right\rangle + \mathcal{O}\left(\frac{1}{N}\right)$$

- $N \rightarrow \infty$: Liouville eqn

$$\begin{aligned} \frac{d}{dt} P_t(\Omega) &= - \sum_{\mu=1}^n \frac{\partial}{\partial \Omega_{\mu}} \left\langle \left[\sum_i f_i(\sigma) \frac{\partial \Omega_{\mu}(\sigma)}{\partial \sigma_i} + T \sum_i \frac{\partial^2 \Omega_{\mu}(\sigma)}{\partial \sigma_i^2} \right] \delta[\Omega - \Omega(\sigma)] \right\rangle \\ &= - \sum_{\mu=1}^n \frac{\partial}{\partial \Omega_{\mu}} [F_{\mu}(\Omega, t) P_t(\Omega)] \end{aligned}$$

with

$$\begin{aligned} F_{\mu}(\Omega, t) &= \lim_{N \rightarrow \infty} \left\langle \sum_i f_i(\sigma) \frac{\partial \Omega_{\mu}(\sigma)}{\partial \sigma_i} + T \sum_i \frac{\partial^2 \Omega_{\mu}(\sigma)}{\partial \sigma_i^2} \right\rangle_{\Omega, t} \\ \langle G(\phi) \rangle_{\Omega, t} &= \frac{\int d\sigma \rho_t(\sigma) \delta[\Omega - \Omega(\sigma)] G(\sigma)}{\int d\sigma \rho_t(\sigma) \delta[\Omega - \Omega(\sigma)]} \end{aligned}$$

deterministic soln,

$$P_t(\Omega) = \delta[\Omega - \Omega(t)],$$

in which $\Omega(t)$ is soln of

$$\frac{d}{dt} \Omega = \lim_{N \rightarrow \infty} \left\langle \sum_i f_i(\sigma) \frac{\partial \Omega(\sigma)}{\partial \sigma_i} + T \sum_i \frac{\partial^2 \Omega(\sigma)}{\partial \sigma_i^2} \right\rangle_{\Omega, t}$$

Choice of macroscopic observables $\Omega(\sigma)$

- key macroscopic object

$$\varrho(\sigma|\sigma) = \frac{1}{N} \sum_i \delta(\sigma - \sigma_i), \quad \sigma \in \mathcal{S}, \quad \mathcal{S} = \{\sigma \mid \sigma = \ell\epsilon, \ell \in \mathbb{Z}, |\ell| < 1/\epsilon^2\}$$

$\epsilon \downarrow 0$ at end of calculation

$$\frac{\partial}{\partial \sigma_i} \varrho(\sigma|\sigma) = -\frac{1}{N} \delta'(\sigma - \sigma_i), \quad \frac{\partial^2}{\partial \sigma_i^2} \varrho(\sigma|\sigma) = \frac{1}{N} \delta''(\sigma - \sigma_i)$$

dynamics

$$\begin{aligned} \frac{d}{dt} \varrho(\sigma) &= \lim_{N \rightarrow \infty} \left\langle \sum_i f_i(\sigma) \frac{\partial \varrho(\sigma|\sigma)}{\partial \sigma_i} + T \sum_i \frac{\partial^2 \varrho(\sigma|\sigma)}{\partial \sigma_i^2} \right\rangle_{e,t} \\ &= - \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \left\langle f_i(\sigma) \delta'(\sigma - \sigma_i) \right\rangle_{e,t} + T \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \left\langle \delta''(\sigma - \sigma_i) \right\rangle_{e,t} \\ &= - \frac{\partial}{\partial \sigma} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \left\langle f_i(\sigma) \delta(\sigma - \sigma_i) \right\rangle_{e,t} + T \frac{\partial^2}{\partial \sigma^2} \varrho(\sigma) \end{aligned}$$

- remaining term

$$\begin{aligned}
 \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \langle f_i(\sigma) \delta(\sigma - \sigma_i) \rangle_{e,t} &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \langle [Jm(\sigma) + \theta + g(\sigma_i)] \delta(\sigma - \sigma_i) \rangle_{e,t} \\
 &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \langle [J \int d\sigma' \sigma' \varrho(\sigma' | \sigma) + \theta + g(\sigma)] \delta(\sigma - \sigma_i) \rangle_{e,t} \\
 &= \lim_{N \rightarrow \infty} [J \int d\sigma' \sigma' \varrho(\sigma') + \theta + g(\sigma)] \langle \frac{1}{N} \sum_i \delta(\sigma - \sigma_i) \rangle_{e,t} \\
 &= [J \int d\sigma' \sigma' \varrho(\sigma') + \theta + g(\sigma)] \varrho(\sigma)
 \end{aligned}$$

$$\frac{d}{dt} \varrho_t(\sigma) = -\frac{\partial}{\partial \sigma} \left[\left(J \int d\sigma' \sigma' \varrho_t(\sigma') + \theta + g(\sigma) \right) \varrho_t(\sigma) \right] + T \frac{\partial^2}{\partial \sigma^2} \varrho_t(\sigma)$$

- stationary soln, let $g(\sigma) = G'(\sigma)$

$$\varrho(\sigma) = \frac{1}{Z} e^{\beta[\sigma(Jm + \theta) + G(\sigma)]}, \quad m = \int d\sigma \sigma \varrho(\sigma), \quad Z = \int d\sigma e^{\beta[\sigma(Jm + \theta) + G(\sigma)]}$$

(see exercises)