Free energy landscape of glasses

Recall : Ferro :

$$P(m) \propto e^{-\beta N f(m)}$$ ← free energy functional: constrained free energy!

$$f(m,\beta) = -J\frac{m^2}{2} - \overset{(\beta^{-1})}{T}\cdot S(m)$$ ← $-\frac{1+m}{2}\ln\left(\frac{1+m}{2}\right) - \frac{1-m}{2}\log\left(\frac{1-m}{2}\right)$

Full free energy: $\frac{F}{N} = -T\log Z = -T\log\int_{-1}^{1} dm \; \overbrace{e^{-\beta N f(m)}}^{P(m)}$ (all possible m)

$$= N \min_{-1\le m\le 1} f(m)\,!$$

Note: $f(m,\beta)$ is analytic in β and m !

phase transition comes from argmin : $m^* = 0 \to m^* = \pm m_{eq}$ (non-analytic bifurcation).

⇒ Obtain $f(m,\beta)$ from a high T expansion.

"States" Aim : Find glass "states" as minima of some $f(m,\beta)$!

⟺ pure states of statistical mechanics:

Full Gibbs measure: $P_G(\{S\}) = \frac{1}{Z} e^{-\beta H(\{S\})}$

General theorem: can be decomposed into pure states: (defined in Th.D. limit via boundary conditions in fully connected models: via field selection)

$$P_G = \sum_{\alpha = \text{pure states}} w_\alpha \, P_\alpha(\{S\})$$

weight, pure state probability

pure states: clustering prop.: $\langle S_i S_j\rangle_{\alpha,\text{conn.}} = \sum_{\{S\}} S_i S_j P_\alpha(\{S\}) - \langle S_i\rangle\langle S_j\rangle_\alpha \xrightarrow[|i-j|\to\infty]{} 0$ (where $\sum_{\{S\}} S_i S_j P_\alpha(\{S\}) = \langle S_i S_j\rangle_\alpha$)

Special case of fully connected models (no space: everyone "equally far")

$\Rightarrow \langle S_i S_j \rangle_c = 0 \quad \forall i, j$

$\hookrightarrow P_\alpha(\{S\}) = \prod_i P_i^\alpha(\{S_i\}) = \prod_i \frac{1 + m_i^\alpha S_i}{2}$ ← $P_\alpha(S_i)$ characterized by m_i^α

$\Rightarrow$ Find the m_i^α that correspond to these pure states!, and their w_α!

as minima of a free energy functional. (Check for ferro!)

~~Probes of many state "picture"? Does P_α have many pure states~~

Remark about ZFC $\Leftrightarrow$ FC last time:

intrastate "overlap"

$$q_{EA} = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{N}\sum_i [S_i(t_0)\, S_i(t_0+t)]_\alpha \Rightarrow \frac{1}{N}\sum_i (m_i^\alpha)^2$$

↑ start close to $\{m^\alpha\}$ — α-independent "self-averaging"

$$\chi_{ZFC} = \beta(1 - q_{EA})$$

$\Leftrightarrow$ full susceptibility:

$$\chi_{FC} = \chi_{full} = \beta\Big(1 - \frac{1}{N}\sum_i \langle m_i\rangle_{full}^2\Big)$$

$$= \beta\Big(1 - \frac{1}{N}\sum_i \Big(\sum_\alpha w_\alpha m_i^\alpha\Big)^2\Big)$$

$$= \beta\Big(1 - \underbrace{\sum_{\alpha,\gamma} w_\alpha w_\gamma \underbrace{\frac{1}{N}\sum_i m_i^\alpha m_i^\gamma}_{q^{\alpha\gamma}}}\Big)$$

↑ inter-state overlap

$$= \beta(1 - q)$$

$q^{\alpha\gamma} < q^{\alpha\alpha}$ in general

C. Schw. $q^{\alpha\gamma} < \sqrt{q^{\alpha\alpha} q^{\gamma\gamma}} = q_{EA}$

$$q \neq (<!)\quad q_{EA} = \frac{1}{N}\sum_i (m_i^\alpha)^2$$

↖ usually 0 for $B_{ex} = 0$

$\Rightarrow \chi_{full} > \chi_{ZFC}$!

~~Rk:~~

q / χ_{full} contains "inter valley" contributions

$$q_{EA} - q = \frac{(\chi_{full} - \chi_{ZFC})}{\beta}$$

$= \Delta$ "anomaly" measures ergodicity breaking

Simulations:

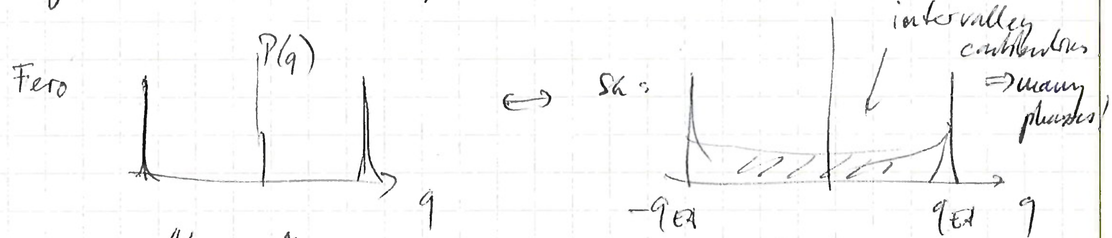
Sign of ergodicity breaking: "Probability of overlap":

$q^{\alpha\beta}$

$$P_J(q) := \sum_{\alpha\beta} w_\alpha w_\beta \, \delta(q - q^{\alpha\beta})$$

(⚠ Caution: not self-averaging! $P_J(q) \underset{N\to\infty}{\not\to} \overline{P_J(q)}$)

Disorder average: $\overline{P_J(q)} =: P(q)$



"trivial" "non-trivial" $P(q)$

Measure in simulations by working with two or more copies!

⇓

Now how to find these pure states?

$\Leftrightarrow m_i^\alpha = ?$

Construction of $f(\{m_i\})$

{ Plefka JPC 15, 1971 (1982)
Georges + Yedidia JPC (1991)

Constrained free energy

enforce mag. m_i by aux fields b_i;

| Eventually: "states ⟺ stable config that requires $b_i \to 0$ | Infinitesimal

$$-\beta F(\{b_i\}) := \log \sum_{\{s_i\}} \exp\left[-\beta H(s_i) + \beta \sum_i b_i s_i\right]$$

[Think of: $H = -\frac{1}{2}\sum_{ij} J_{ij} s_i s_j - h_i \sum s_i$]
$\uparrow$ real ext. field

$$\Rightarrow m_i(\{b\}) \equiv \langle s_i \rangle = -\frac{\partial F}{\partial b_i}$$

Susceptibility matrix: $\chi_{ij} \equiv \frac{\partial m_i}{\partial b_j} = -\frac{\partial^2 F}{\partial b_i \partial b_j} = \chi_{ji} = \beta \langle s_i s_j \rangle_c = \beta\left(\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle\right)$
$= \beta \langle (s_i - m_i)(s_j - m_j)\rangle$

χ_{ij} is positive definite: $\forall v$: $v \chi v = \sum_{ij} \beta \langle v_i (s_i - m_i) v_j (s_j - m_j)\rangle \geq 0$

Free energy functional $G(\{m_i\})$: Legendre trafo of $F(\{b_i\})$

$$-\beta G(\{m_i\}) := -\beta \overset{F''<0}{\max_{\{b_i\}}} \left(F(\{b_i\}) + \sum_i b_i m_i\right) \qquad (*)$$

$$= \min_{b_i} \log\left[\sum_{\{s\}} \exp\left(-\beta H(s) + \beta \sum_i b_i (s_i - m_i)\right)\right]$$

$\Updownarrow$

$$\partial_{b_i}(\ )\Big|_{b_i = b_i(\{m_i\})} = 0 \iff \langle s_i - m_i\rangle\Big|_{b_i} = 0 \iff m_i = \langle s_i\rangle_{b_i}$$

Legendre trafo properties:

$$m_i(b) = -\frac{\partial F}{\partial b_i} \text{ (above)} \iff b_i(m) = \frac{\partial G}{\partial m_i}$$

$$\frac{\partial b_i}{\partial m_j} \equiv \left(\frac{\partial m_k}{\partial b_\ell}\right)^{-1}_{ij} = (\chi^{-1})_{ij} = \frac{\partial^2 G}{\partial m_i \partial m_j} = -\left(\frac{\partial^2 F}{\partial b_k \partial b_\ell}\right)^{-1}_{ij} \overset{F''<0}{\geq} 0$$

$$\Rightarrow \quad -\beta F(\{b_i\}) = -\beta \min_{m_i}\left[G(m_i) - \sum_i b_i m_i\right] \qquad \text{(back trafo)}$$

Interest in b_i = aux. field = 0 $\Leftrightarrow$ spontaneously stable $\{m_i\}$!

$\Leftrightarrow$ search for minima of $G(\{m_i\})$ — 0 !

BUT: By construction: (Legendre) : $G = \min_{b_i}(\ldots)$ $\Rightarrow$ $G(\{m_i\})$ is convex

$\Rightarrow$ what about local minima?

$\Rightarrow$ Do not necessarily impose global minimum! Just local: $G_{b_i} = 0$, $\frac{\partial^2 G}{\partial m_i \partial m_j} \geq 0$!

$\Rightarrow$ Inspired from Ferro: $f(m) \equiv G(m_i = m)$: analytic in β $\Rightarrow$ high T expansion ($\equiv$ exp. in J!) ↳ good at large N!

$\Rightarrow$ follow $G(\{m_i\};\beta)$ even when local minima appear!

Calculation

Def. $A(\{m_i\};\beta) \equiv -\beta G(m_i) \qquad \lambda_i^\beta \equiv \beta b_i$

$$A \equiv \log\left[\sum_{\{S\}} e^{-\beta H(S) + \sum_i \lambda_i^\beta (S_i - m_i)}\right]\Bigg|_{\lambda_i^\beta \text{ s.th. } \langle S_i - m_i\rangle = 0 \,!}$$

Note: $-\frac{\partial A}{\partial m_i} = \lambda_i^\beta$!

in the end $\lambda_i^\beta = 0$! $\Leftrightarrow$ $\frac{\partial A}{\partial m} = 0$ (minima of G) + impose $\partial^2 A \leq 0$!

6

Expansion: $A(\beta; m) = A(\beta=0) + \beta\partial_\beta A(\beta=0) + \frac{\beta^2}{2}\partial_\beta^2 A(\beta=0)$ $\boxed{\text{at fixed } m_i}$

0^{th} order: $\underline{A(\beta=0)}$. ($\beta=0 \Leftrightarrow$ interaction irrelevant $\Rightarrow -\beta G =$ entropy)

$$= \log \sum_{\{s\}} \exp \sum_i \lambda_i^{\beta=0}(s_i - m_i) = \sum_i \left[-\lambda_i^{\beta=0} m_i + \log 2\cosh \lambda_i^0\right] \quad \boxed{\text{Ising}}$$

constraint: $\langle s_i - m_i\rangle_{\beta=0} = 0 \Leftrightarrow \frac{\partial A}{\partial \lambda_i} = 0 \to m_i = \tanh \lambda_i^0$

plug $\lambda_i^{(0)}$ into $A^{\beta=0}$ $\Rightarrow$

$$A(\beta=0) = -\sum_i \left(p_i \log p_i + (1-p_i)\log(1-p_i)\right) = \sum_i S_0(m_i)$$

$$p_i = \frac{1+m_i}{2}$$

1^{st} order: (Expect: $A = -\beta G = -\frac{1}{T}(E - TS) = S - \beta E$)

$$\partial_\beta A_\lambda^\beta = \partial_\beta \log \sum_s e^{-\beta H + \sum\lambda(s-m)}$$

$$= \langle -H + \sum_i \partial_\beta \lambda_i \underbrace{(s_i - m_i)}_{\langle s_i - m_i\rangle = 0}\rangle = -\langle H\rangle \quad \forall \beta!$$

$\beta = 0$: $\partial_\beta A_\lambda^\beta\big|_{\beta=0} = -\langle H\rangle_0 = \frac{1}{2}\sum_{ij} J_{ij}\underbrace{\langle s_i s_j\rangle}_{\substack{\langle s_i\rangle\langle s_j\rangle \\ m_i m_j}} + h\sum_i \underbrace{\langle s_i\rangle}_{m_i}$

2^{nd} order.

disconnected part $\partial\lambda\langle s - m\rangle = 0$

$$\partial_\beta^2 A_\lambda^\beta = -\partial_\beta\langle H\rangle = \langle H\left(H - \sum\partial_\beta\lambda(s-m)\right)\rangle - \langle H\rangle^2$$

$$= \langle H(\underbrace{H - \sum\partial_\beta\lambda(s-m) - \langle H\rangle}_{=U}))\rangle$$

"fluctuational part of H"

Now show that $= \langle U^2\rangle$!

general:

$$\partial_\beta\langle O\rangle = \langle(\partial_\beta O)\rangle - \langle OU\rangle$$

Easy: $\langle U\rangle = 0 \quad \Leftarrow \quad \langle s-m_i\rangle = 0$

Use
$$\frac{dm_i}{d\beta} = 0 = \frac{d}{d\beta}\langle S_i\rangle \overset{\text{On-relation}}{=} -\langle s_i U\rangle \underset{\langle U\rangle=0}{=} -\langle (s_i-m_i)U\rangle$$

$$\Rightarrow \quad \underline{\partial_\beta^2 A^\beta = \langle U^2\rangle}$$

$$\underline{U_{\beta=0}} = H - \langle H\rangle - \sum_i \partial_\beta A_i^\beta\big|_{\beta=0}(s_i-m_i) \quad \Leftarrow \quad \partial_\beta A_i^\beta\big|_{\beta 0} = -\partial_\beta \partial_{m_i} A^\beta\big|_{\beta=0}$$

$$= +\partial_{m_i}\langle H\rangle\big|_{\beta=0} \quad \text{SK}$$

$$= -\sum_{j(\neq i)} J_{ij} m_j - h$$

SK

$$= -\frac{1}{2}\sum_{i\neq j} J_{ij}(s_i s_j - m_i m_j) - \sum_i h(s_i-m_i) + \sum_i (s_i-m_i)\Big(\sum_{j\neq i} J_{ij}m_j + h\Big)$$

$$= -\frac{1}{2}\sum_{i\neq j} J_{ij}(s_i-m_i)(s_j-m_j) = -\sum_{\langle ij\rangle} J_{ij}(s_i-m_i)(s_j-m_j)$$

$$\partial_\beta^2 A^\beta\big|_0 = \langle U_{\beta=0}^2\rangle_0 = \sum_{\substack{\langle ij\rangle \\ \langle kl\rangle}} \langle J_{ij} J_{kl}(s_i-m_i)(s_j-m_j)(s_k-m_k)(s_l-m_l)\rangle_0$$

$$= \sum_{\substack{\langle ij\rangle \\ (=\langle kl\rangle)}} J_{ij}^2 \underbrace{\langle (s_i-m_i)^2\rangle}_{(1-m_i^2)} \underbrace{\langle (s_j-m_j)^2\rangle}_{(1-m_j^2)} = \frac{1}{2}\sum_{i\neq j} J_{ij}^2 (1-m_i^2)(1-m_j^2)$$

only paired indices survive

$\Rightarrow$ Summing up:

$$A^\beta = -\beta G(m) = \sum_i S_0(m_i) + \frac{\beta}{2}\sum_{i\neq j} J_{ij} m_i m_j + \beta h \sum_i m_i$$
$$+ \frac{\beta^2}{4}\sum_{i\neq j} J_{ij}^2 (1-m_i^2)(1-m_j^2) + O(\beta^3)$$

$x_i J_{ij}^2 x_j \Rightarrow$ like v.d.W! $\leftarrow$ T-dependent energy $\Rightarrow$ G(m) explicitly T dependent!

$\Leftrightarrow$ DPRM!

$$\boxed{\text{Free energy functional for } \underline{\text{any}} \text{ Ising model!}}$$

$\mathcal{O}(\beta^3)$ terms: $\sim \beta^3 \Big[\sum_{i \neq j} J_{ij}^3 \, m_i (1-m_i^2)\, m_j (1-m_j^2) \Big]$

$$+ \beta^3 \sum_{i \neq j \neq k} J_{ij} J_{jk} J_{ki} \, (1-m_i^2)(1-m_j^2)(1-m_k^2)$$

SK:

$J_{ij}^2 \cdot (J_{ij} m_i m_j) \sim J_{ij}^2$

1. term: N^2 terms $O(N^{-\cancel{3/2}})$ $\sim N^{\cancel{0}} \ll N$

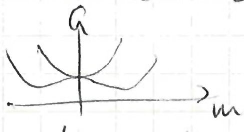
2. term N^3 terms $O(N^{-3/2})$ random signed $\sim N^{3/2} \cdot N^{-3/2} \sim O(1) \Rightarrow$ neglect! ? N^0

$\Rightarrow$ SK: expansion terminates (apparently at 2^{nd} order!)

$$\Longrightarrow \quad \mathcal{F}_{SK}(\{m_i\})$$

Apply to Ferro: $J_{ij} = J/N$: $G(m) = -TS_0(m) + E(m) = -TS_0(m) - \frac{Jm^2}{2} - hm$
fully-conn.

only 0^{th} + 1^{st} term $\Rightarrow$ indeed find



not convex!

Minima of free energy functional: $\Leftrightarrow$ i) T.A.P. equations

$$\beta h_i = \lambda_i^\beta = 0 \quad \Leftrightarrow \quad \frac{\partial G}{\partial m_i} = 0$$

$$\Leftrightarrow \quad 0 = \underset{\partial_{m_i} S^0(m_i)}{\underset{\parallel}{\operatorname{atanh}(m_i)}} - \beta h - \beta \sum_{j(\neq i)} J_{ij} m_j + \beta m_i \sum_{j \neq i} J_{ij}^2 \big[\beta(1-m_j^2)\big] + O(\beta^3)$$

$$\Rightarrow m_i = \tanh(\beta y_i)$$

$y_i =$ "thermodynamic" field

$$= \underbrace{\sum_{j(\neq i)} J_{ij} m_j + h}_{\text{usual mean field}} \underbrace{- m_i \sum_{j(\neq i)} J_{ij}^2 \underbrace{\beta(1-m_j^2)}_{\chi_{jj}}}_{\text{Onsager reaction}} + O(\beta^2)$$

$$y_i = h_{ext} \sum_{j(\neq i)} J_{ij}\, m_j^{(i)}$$

where $m_j^{(i)} = m_j - m_i J_{ij} \chi_{jj}$: magnetization that would be on j in absence of site i! ($J_{ij}=0$)

or $m_j = m_j^{(i)} + m_i J_{ij} \chi_{jj}$ as seen from here!

When m_i forms it polarizes environment further ⇒ this extra polarization should not be included in the mean field expression

(Ferro layed: ~~T_c~~ $h_{loc} = J \cdot z\, m$ interpret ~~term~~ high T expansion as 1/d expansion

$T_c \sim h$ $\quad \frac{h_{loc}}{T_c} \approx m \Rightarrow T_c = J \cdot z$

$h_{loc} = Jz\,(m - m\, J \frac{1}{T}) \Rightarrow \quad T_c = Jz\left(1 - \frac{J}{Jz}\right) = Jz - J = \underline{J(z-1)}$

$z = 2d \to T_c \simeq (2d-1)J$

$$\frac{T_c}{2dJ} = \left(1 - \frac{1}{2d} - \frac{1}{3d^2} - \frac{13}{24d^3}, \dots\right)$$

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ii) Minima: Solutions $\qquad$ high T: $m=0$ paramagnet! Unphysical $S<0$ at low T!

Assume: m_i^α sets in continuously ⇒ instability?

$$G_{para} = G(m_i = 0) = \underbrace{-T \log 2}_{-TS_0} + \underbrace{E_0}_{0} - \frac{\beta}{4} J^2$$

Onsager / v.d.W.

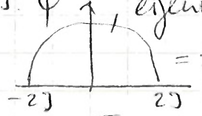
Prove existence of a transition?

$$S_{para} = -\frac{\partial G}{\partial T} = S_0 + \frac{\partial}{\partial T}\left(\frac{J^2}{4T}\right) = S_0 - \frac{J^2}{4T^2} \to < 0 \quad \text{for } T < \frac{\sqrt{\ln 2}\, J}{2}$$

Instability? $|m_i| \ll 1$

T.A.P. : $m_i \simeq \underbrace{\overset{\tanh(\beta y) \simeq \beta y}{\beta \sum_{j \neq i} J_{ij} m_j}}_{\text{random matrix}} - m_i (\beta J)^2 + O(m^3) + \cancel{\beta h}$ 0 no symmetry breaking

$\psi_i^{(\lambda)} : \sum_j J_{ij} \psi_j^{(\lambda)} = \lambda \psi_i^{(\lambda)}$ eigenvectors $\psi^{(\lambda)}$, eigenvalues

$\rho(\lambda) =$  $= \frac{1}{2\pi J^2}\sqrt{4J^2 - \lambda^2}$

$\Rightarrow \quad m_\lambda := \langle \psi^{(\lambda)} | m \rangle := \sum_i m_i \psi_i^{(\lambda)}$ $\sum_i [\psi_i^{(\lambda)}]^2 = 1$

Project linearized TAP. Eqs on $\psi^{(\lambda)}$

$$(1 + (\beta J)^2) m_\lambda = \beta \lambda m_\lambda + O(m^3) + \beta h_\lambda$$

$$\Rightarrow m_\lambda = \frac{\beta h_\lambda}{(1+(\beta J)^2) - \lambda \beta}$$ ← divergence of susceptibility

$m_{\lambda_{max}}$ becomes unstable first, when $1 + (\beta_c J)^2 = \lambda_{max} \beta = 2J \beta_c$

$$\Rightarrow \beta_c^{(SK)} = \frac{1}{J} \Leftrightarrow T_c = J$$

Note: Naive MF $m_i = \tanh(\sum J_{ij} m_j) \Rightarrow T_c = 2J$ wrong!

$\Rightarrow$ Fluctuations (Onsager) reduce T_c by factor of 2, despite mean-field situation!

Low T

TAP Eq.: $m_i = \tanh\left[\beta \sum_{j\neq i} J_{ij}\left(m_j - m_i J_{ij}\beta(1-m_j^2)\right)\right] \quad \forall i$

Validity? • Check that these are local minima: $\frac{\partial^2 G}{\partial m_i \partial m_j} \geq 0$

Recall: only local minima, since $\Gamma(m)$ would have to be convex (global minimum)

↳ There can be exponentially many local minima not only $O(N)$.

BUT: $m=0$ is still a solution and $\left.\frac{d^2 G}{dm_i dm_j}\right|_{m=0} = \left(\beta + \frac{1}{\beta}\right)\delta_{ij} - J_{ij}$

is positive at $T<T_c$ ⇒ What's going on?

Root of Problem: subleading terms in N can only be dropped if they don't diverge.

But: $\overline{(\beta J \chi_{ii})^2} = \overline{\left(\beta J \beta(1-m_i^2)\right)^2}^{\,i} \overset{!}{\leq} 1$

otherwise fluctuations diverge (sum of ring diagrams: $\chi J \chi J + \chi J \chi J \chi + \dots$)

variance: $J_{ij}^2 \chi_{jj}^2 \to \sum_j = N \frac{J^2}{N} \overline{\chi_{jj}^2} \overset{!}{<} 1$

$\boxed{m=0: \ (J\beta)^2 > 1 \ \text{for } T<T_c \Rightarrow m=0 \text{ is unphysical!}}$

Solutions of TAP

Very difficult! N non-linear Eqs.; exponentially many solutions exist. BUT: essentially all have a super-soft mode the higher β, the more (can be counted) in SK model: $\to \{m_i\}$

dynamics seems not to care!

kind of pathological ⇒ ~~both~~ related to marginal stability