II) Mean field Theory (1985 - now)

History   1948 : Kauzmann's entropy crisis
1958 : Gibbs di Marzio
lattice polymer model with $T_K > 0$
(probably not true)
1965 Adam Gibbs
$S_{conf} \to \xi \to$ dynamics

1984 : density functional theory
1985 - 1992 : mean field spin glasses with glass transition
2000 : Lattice glass models Bethe lattice
2013 - 2020 : liquid State theory in $d \to \infty$

Book Parisi Urbani Zamponi,
Theory Simple Glass (2020)

a) Spherical p-spin model

$$H = - \underbrace{\sum_{i_1 \dots i_p}}_{\text{fully connected}} \underbrace{J_{i_1 \dots i_p}}_{\text{quenched disorder}} \underbrace{S_{i_1} \dots S_{i_p}}_{\text{p-spin interactions}}$$

$\begin{cases} S_i = \pm 1 & \text{Ising} \\ \text{Here } S_i \in \mathbb{R} & \text{with spherical constraint } \sum_{i=1}^{N} S_i^2 = N \end{cases}$

J's random variables $\overline{J} = 0$ and

variance $\overline{J_{i_1 \dots i_p}^2} = \frac{p!}{2 N^{p-1}}$ ensures proper thermodynamic limit

b) Dynamics

to enforce spherical constraint

Langevin $$\frac{dS_i(t)}{dt} = -\frac{\partial H}{\partial S_i} + \underbrace{\eta_i(t)}_{\text{thermal noise}} - \mu(t)\, S_i$$

$$\langle \eta_i(t)\,\eta_j(t')\rangle = 2T\,\delta_{ij}\,\delta(t-t')$$

MF $\Rightarrow$ exact dyn. eq. can be derived

for $C(t) = \frac{1}{N}\sum_{i=1}^{N} \langle S_i(t)\, S_i(0)\rangle$

assuming TTI + FDT = equilibrium

$$\begin{cases} \dfrac{dC(t)}{dt} = -T\,C(t) - \dfrac{p}{2T}\displaystyle\int_0^t dt'\, C^{p-1}(t-t')\,\frac{dC}{dt'}(t') \\ C(t=0)=1 \quad \rightarrow \text{can be solved} \end{cases}$$

Nonergodic if $C(t\to\infty) = q$

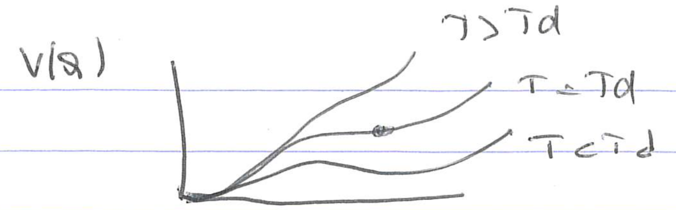
$$\Leftrightarrow \quad 0 = -Tq - \frac{p}{2T}\, q^{p-1}(q-1)$$

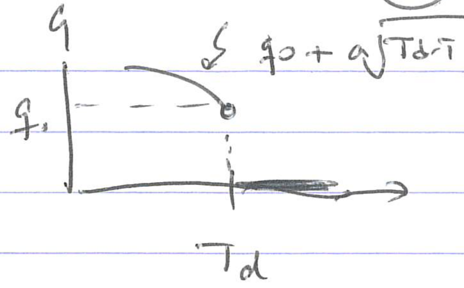
$$\Leftrightarrow \quad \frac{q}{1-q} = \frac{p}{2T^2}\, q^{p-1}$$

$$V(q) \equiv T\int_0^q dq'\left[\frac{q}{1-q} - \frac{p}{2T^2} q^{p-1}\right]$$

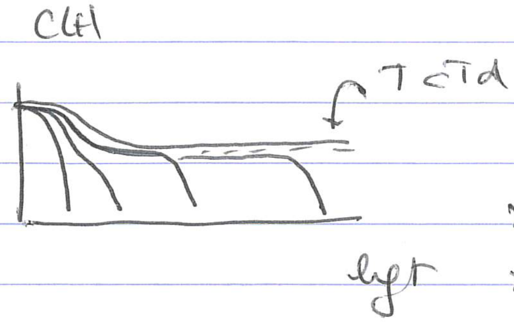
$$V(q) = T\left[-q - \log(1-q) - \frac{q^p}{2T^2}\right]$$

$\frac{\partial V}{\partial q} = 0$ solution of





Full time dependence



x 2 step decay
x stretched exp
$e^{-(t/\tau)^\beta}$
⇓
good.

x but $\tau \sim (T - T_d)^{-\gamma}$ ⇒ not good!

1975 - 1985 liquid state theory ⇒ mode coupling theory

Approximate closure of dyn. eq for $F(\vec{q}, t)$

$$\frac{dF(\vec{q},t)}{dt} = -\frac{D q^2}{S(q)} F(\vec{q},t) - \int_0^t dt' \frac{\partial F}{\partial t'}(\vec{q},t') \, M(\vec{q}, t-t')$$

with $M = M[S(q), F(\vec{q},t)]$
↑ functional

(Note $S(q) \to$ controls all behaviour!)

Same mathematical form → same solutions.

Connection MCT - pspin suggests MCT is "mean field"
(1987 - 1989)
NOT QUITE!

It holds only for dynamics as MCT has no statics
p-spin also has interesting static properties
↳ phase transition.

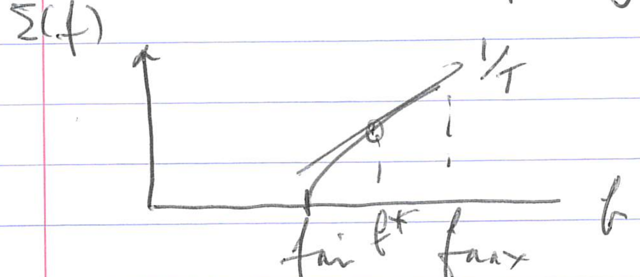
c) Metastable states

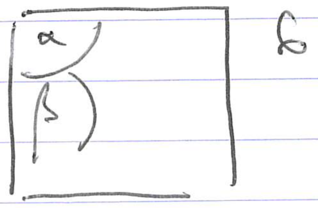
free Energy minima can be computed
(Thouless Anderson Palmer, TAP)

for given f (free energy), $\exists$ exponential number of minima $\mathcal{N}(f) = \exp(N\Sigma(f))$

$[f, f+df)$ $\mathcal{N}(f)df$

$\Sigma(f) \equiv$ Complexity; or Configurational Entropy





$$Z \simeq \sum_\alpha e^{-N\beta f_\alpha}$$

$$= \sum_\alpha \left[\int df\, \delta(f - f_\alpha) \right] e^{-\beta N f_\alpha}$$

$$= \int df \left[\sum_\alpha \delta(f - f_\alpha) \right] e^{-\beta N f}$$

$$= \int df\; e^{N\Sigma(f) - \beta N f}$$

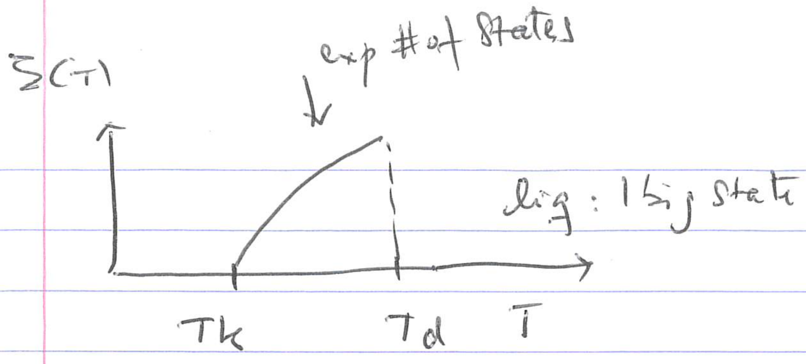
$$= \int df\; e^{-N\beta\underline{[f - T\Sigma]}}$$

Saddle point $1 = T \dfrac{\partial \Sigma}{\partial f} \to$ graphic

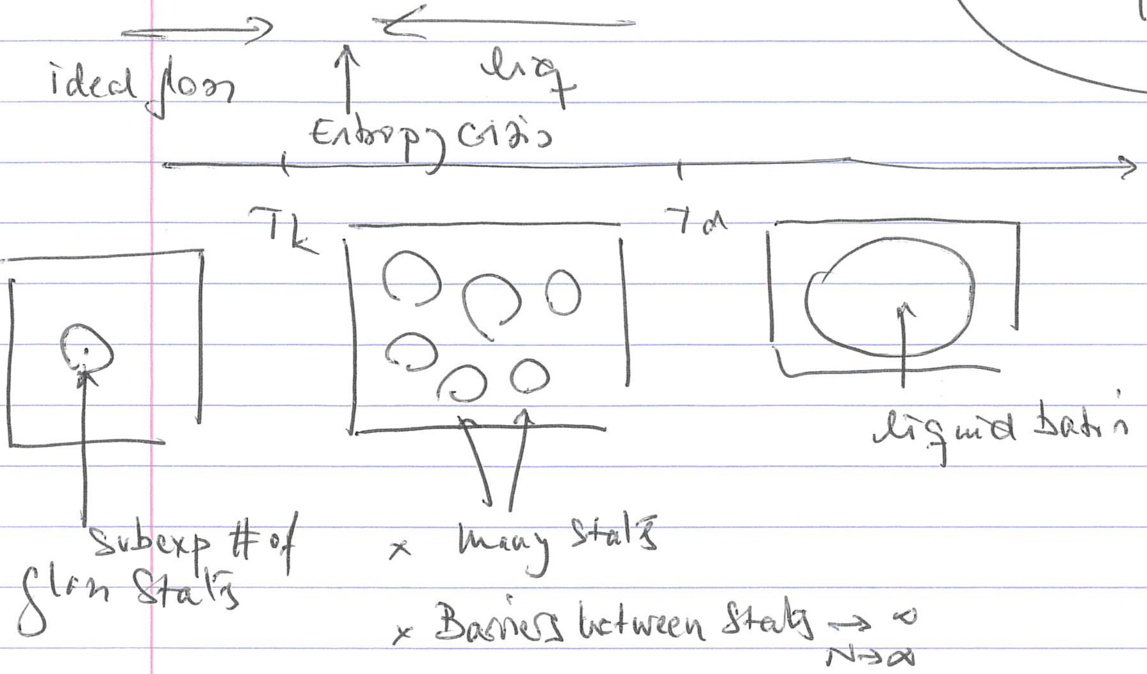
$$\boxed{F_{eq} = -(\beta N)^{-1} \log Z = f^* - T\Sigma(f^*)}$$

Smaller f^* have smaller Σ
larger f^* have larger Σ

eq = compromise between low f^* and large Σ



Mean field picture



not ergodic

d) Computing $\Sigma(T)$ in microscopic model

Monasson (1995) → use m replicas coupling them to force them to explore same state
Mézard Parisi (1999)

$$Z_m = \sum_\alpha e^{-\beta N m f_\alpha}$$

$$= \int df \, e^{N(\Sigma - \beta m f)}$$

Saddle point: $\dfrac{d\Sigma}{df} = \beta m$ (→ explore $\Sigma(f)$ changing m)

$$\phi(m,T) = \frac{-1}{\beta N} \log Z_m = -T\Sigma(f^*) + m f^*$$

$$\frac{\partial \phi}{\partial m}(m,T) = f^*, \quad \Sigma(m,T) = \Sigma(f^*) = -m^2 \frac{\partial}{\partial m}\left(\frac{\beta\phi}{m}\right)$$

Recipe: thermo of m coupled replicas

$\hookrightarrow \phi(m,T)$

$\hookrightarrow \Sigma(T)$

- If $m=1$ glass for $T \le T_K$
- If $m<1$ glass for $T < T_K^{(m)} < T_K$

glass thermodynamics can be computed $\rightarrow$

$$f_{glass}(T<T_K) = \phi(m^*,T)/m^*$$

with $m^* < 1$

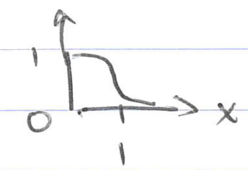
$T_K^{(m^*)} = T < T_K$

c) Glass Order parameter: overlap

Defined for pairs of configurations

- spins $Q_{12} = \frac{1}{N} \sum S_i^1 S_i^2$
- liquids

$$Q(\underbrace{\vec{r}^N}_{1}, \underbrace{\vec{r}_2^N}_{2}) = \frac{1}{N} \sum_{ij} w\left(\frac{|\vec{r}_i - \vec{r}_j|}{a}\right)$$

with $w(x) =$ 

and $a \approx 0.2\sigma$

In both cases if 1 ~ 2 $Q_{12} \sim 1$

1 and 2 uncorrelated $Q_{12} \sim 0$

- Why the overlap?

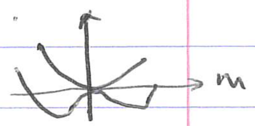
many states above T_K $\quad Q_{12} \sim 0$
$\quad$ Gibbs configs $\quad Q_{12} \sim 1$

again not the density profile ($\rho(\vec{r})$)
but their number!

f) The Franz-Parisi potential (FP, PRL, 1997)

→ use the overlap to define free energy (order parameter)
as in Landau theory of phase transitions

$m \to \phi(m)$



- Take $\{\vec{r}_0^{\,N}\}$ a ref config at equilibrium, T

- Define second config $\{\vec{r}^{\,N}\} \to Q(\vec{r}^{\,N}, \vec{r}_0^{\,N})$
$\to P(Q)$: proba distrib of Q

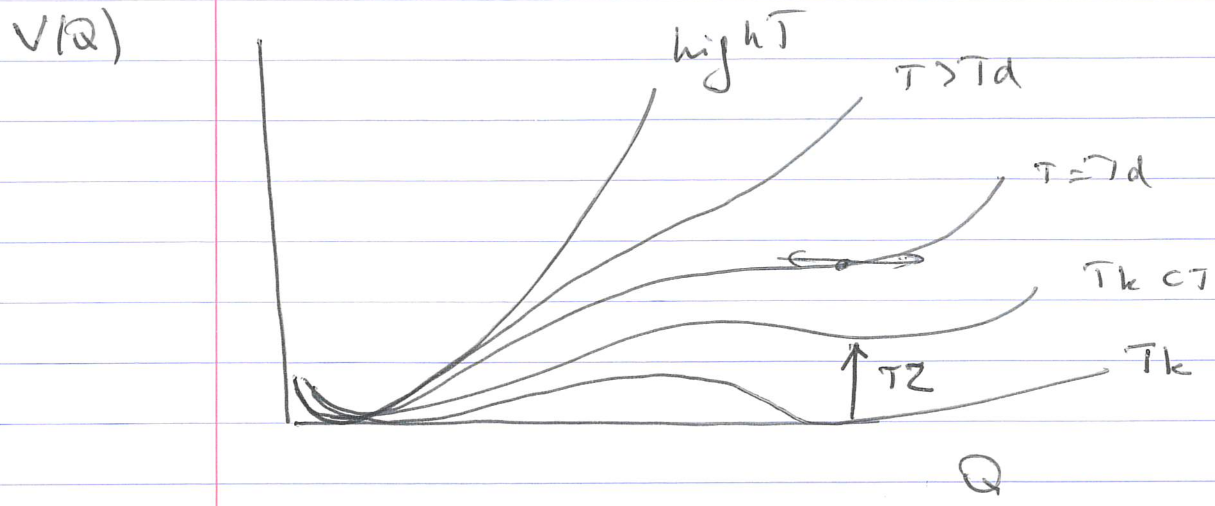
$$\boxed{V(Q) = -\frac{k_B T}{N} \overline{\log P[Q, \vec{r}_0^{\,N}]}}$$
→ average over $\vec{r}_0^{\,N}$

$\left(P \sim e^{-N\beta V(Q)} \right)$ = Free energy cost to have a fluct. of Q =

Formally:

$$V(Q) = -\frac{k_B T}{N} \int d\vec{r}_0^{\,N} \frac{e^{-\beta H(\vec{r}_0^{\,N})}}{Z} \log \int d\vec{r}^{\,N} e^{-\beta H(\vec{r}^{\,N})} \delta(Q - Q(\vec{r}_0^{\,N}, \vec{r}^{\,N}))$$

Mean field behavior of V(Q)



* (Td, Tk) again appear

* Similarity with dynamics

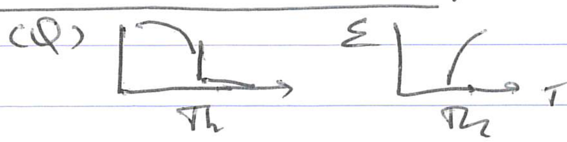
* Glass phase metastable. $T \gtrsim T_k$ at large Q

$$\boxed{V(Q_{glass}) - V(Q_{liquid}) = T\,\Sigma(T)}$$

Free energy difference between liquid (eq) and metastable glass!

* Discontinuous transition at Tk when $\Delta V \to 0$

Random First Order Transition (RFOT)



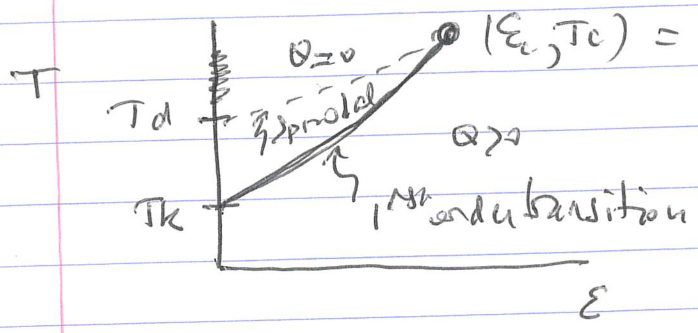
* Stat mech of constrained liquids

$$\underline{H} = H_0(\vec{r}^N) - \varepsilon\, Q(\vec{r}_0^N, \vec{r}^N)$$

contains disorder ($\vec{r}_0^N$)

cf Legendre transf $Q \leftrightarrow \varepsilon$ [like (P, v) etc.]

$F(\varepsilon) = V(Q) - \varepsilon Q$ large $\varepsilon \to$ large Q



(ε_c, T_c) = new critical point

RFIM univ. class

{ "van der waals picture" = MF theory
liquid gas }

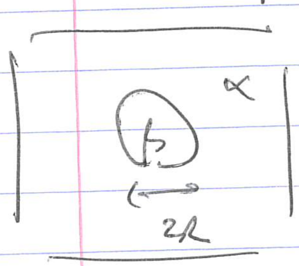
g) Finite dimensional effects on RFOT

① A system in finite dimension cannot have an exp. # of states $\Sigma(f)$!

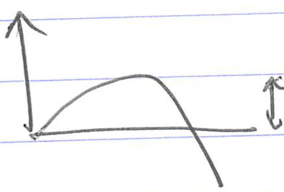
Demo: Imagine it does – prepare state α; f_α

– transition to β? $f_\beta < f_\alpha$

Nucleation (not possible as $d \to \infty$)



$$\Delta F = [f_\beta - f_\alpha] R^d + \sigma R^{d-1}$$



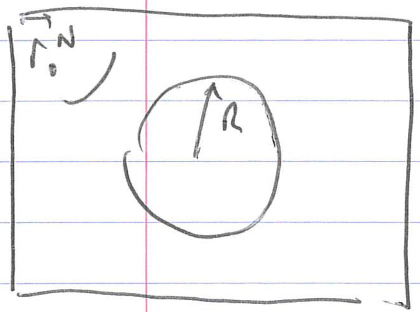
↕ barrier finite
→ go to β with
→ α does not exist!

• $\Sigma(f)$ does not exist because rearrangement can be local (in finite)

(2) Conjecture: dynamic transition at T_d
cannot exist either!
"MCT transition" at best a crossover
"dynamic transition"

(1) and (2) are strongest (and justified)
criticisms of MF theory

(3) A Point to Set lengthscale exists



- $\vec{r}_0^N$ at equilibrium
- freeze out side cavity
- thermalize inside

cavity stays inside state r_0^N or leaves?

Cost of leaving $\Delta F = \underbrace{-T\Sigma R^d}_{\text{explore states}} + \underbrace{\Upsilon(T) R^{d-1}}_{\text{surface cost}}$

$\Delta F \sim 0$ when $\boxed{R = \xi_{PTS} = \frac{\Upsilon(T)}{T\Sigma(T)}}$

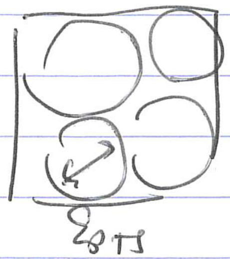
- $R < \xi_{PTS}$ $\quad Q \sim 1$ $\quad \tau = \infty$
- $R > \xi_{PTS}$ $\quad Q \sim 0$ state disappears

$\Rightarrow$ ξ_{PTS}: limit of validity of MF picture

$\Rightarrow$ $\propto \frac{1}{T\Sigma(T)}$: How to see "order" when $\xi\downarrow$

(4) A note to the dynamics

- $T > T_d$: MF-like dynamics
- $T_k < T < T_d$ ξ_{PTS} opens and grows



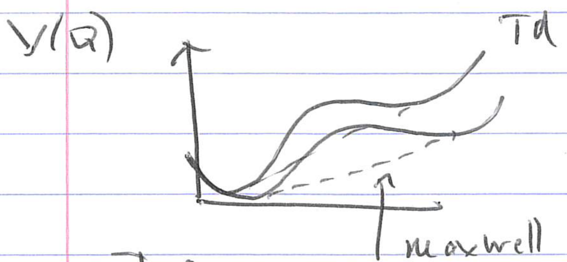
"mosaic"

$$\log \tau_\alpha(T) \sim \frac{\xi_{PTS}^4}{T} \sim \frac{1}{(T S_{conf})^4}$$

Decrease of S_{conf} ⇒ growth of τ_α (via ξ_{PTS})

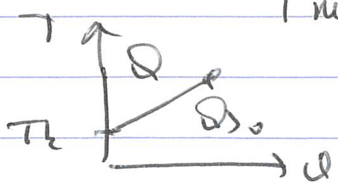
[Close to Adam Gibbs 1965 picture!]

(5) FP potential



can't exist

maxwell construction using interfaces.



can survive ...

Conclusion : MF should be cases exact in $d \to \infty$

- finite d corrections expected.
- Is anything true in real systems $d = 2, 3$?

↳ models and simulations
(3) (4)