Free enery landscape

Two universality classes of glasses

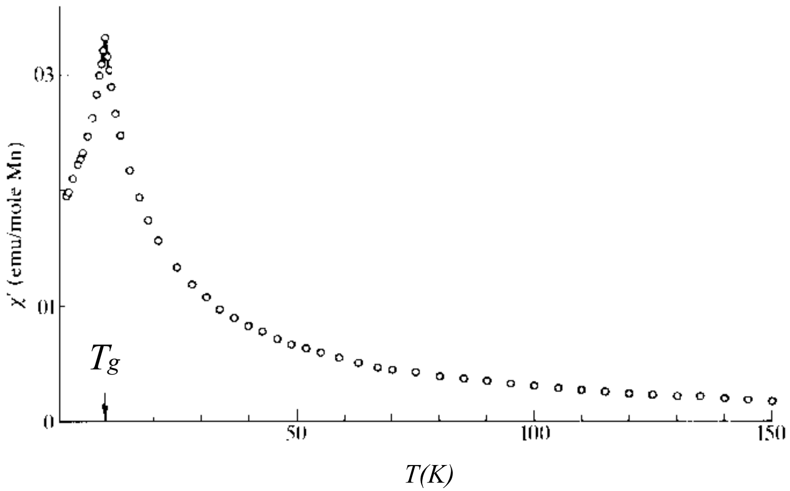
Two-spin interacting glasses: SK – model

versus

Multi-spin interactions: p-spin model

With very different phenomenology!

Signatures of the spin glass transition



AC-susceptibility in Cu-0.9%Mn

(Mulder et al., 1981, 1982)

$$\langle s_i \rangle = 0, \ T > T_g, \ \text{(paramagnet)}$$

$$\langle s_i \rangle \neq 0, \ T > T_g, \ \text{(spin glass)}$$

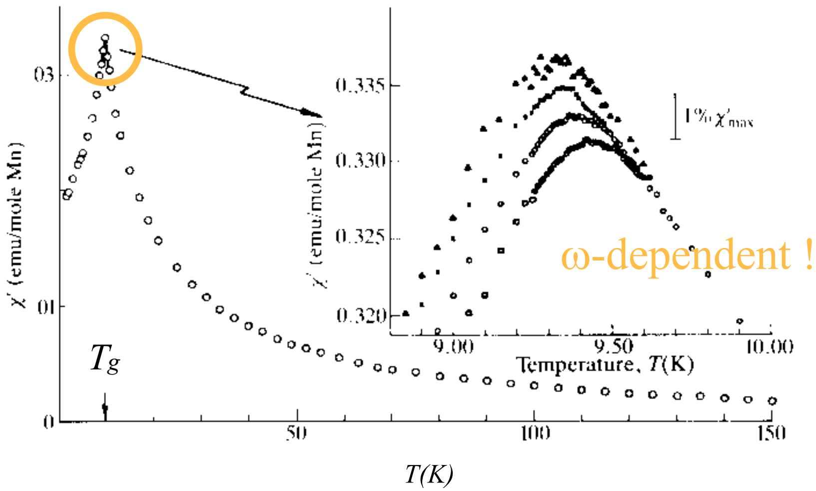
$$q_{EA} \equiv \frac{1}{N} \sum_i \langle s_i \rangle^2$$

$$\chi = \frac{T}{N} \sum_i \left(\langle s_i^2 \rangle - \langle s_i \rangle^2 \right)$$

$$\chi_{nl} = \frac{\beta^2}{N} \sum_{i,j} \langle s_i s_j \rangle^2 \xrightarrow{T \to T_g} \infty$$

Becomes critical, long ranged!

Signatures of the spin glass transition



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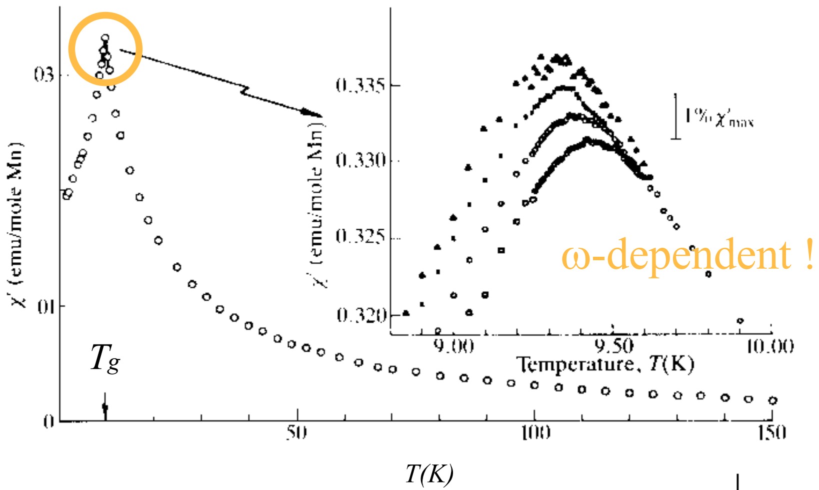

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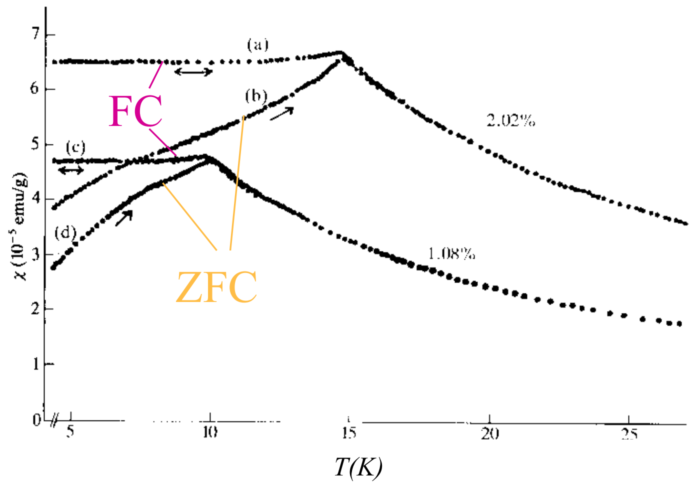
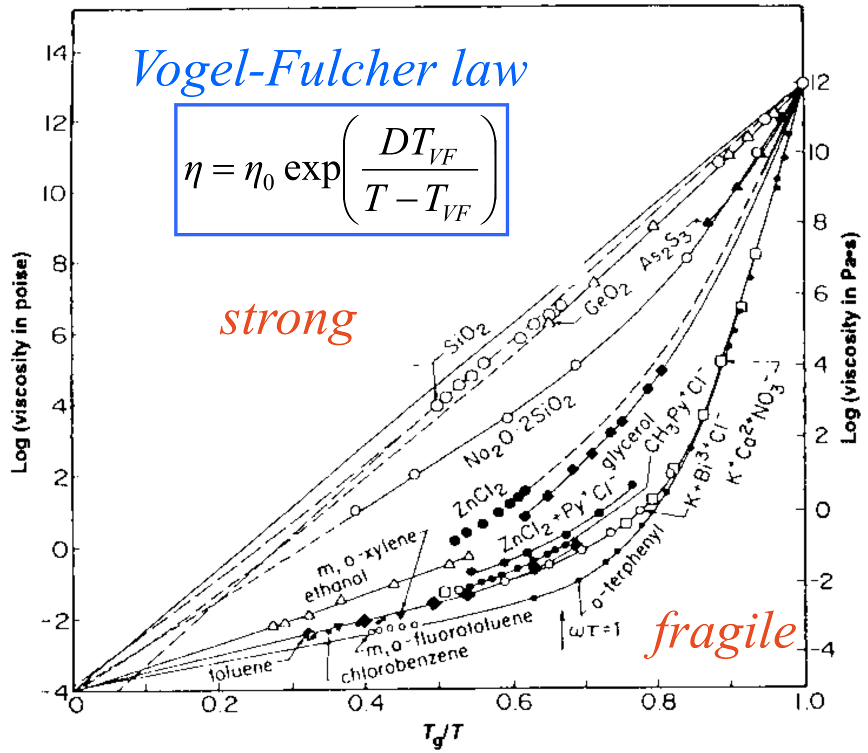


(Nagata et al., 1979)

Structural Glasses: viscous liquids

Structural Glass transition:Viscosity

Definition of T_g : $\eta(T_g) = 10^{14}\,\text{Poise} \;\leftrightarrow\; \tau_{rel} \approx 10^2 - 10^3\,\text{sec}$



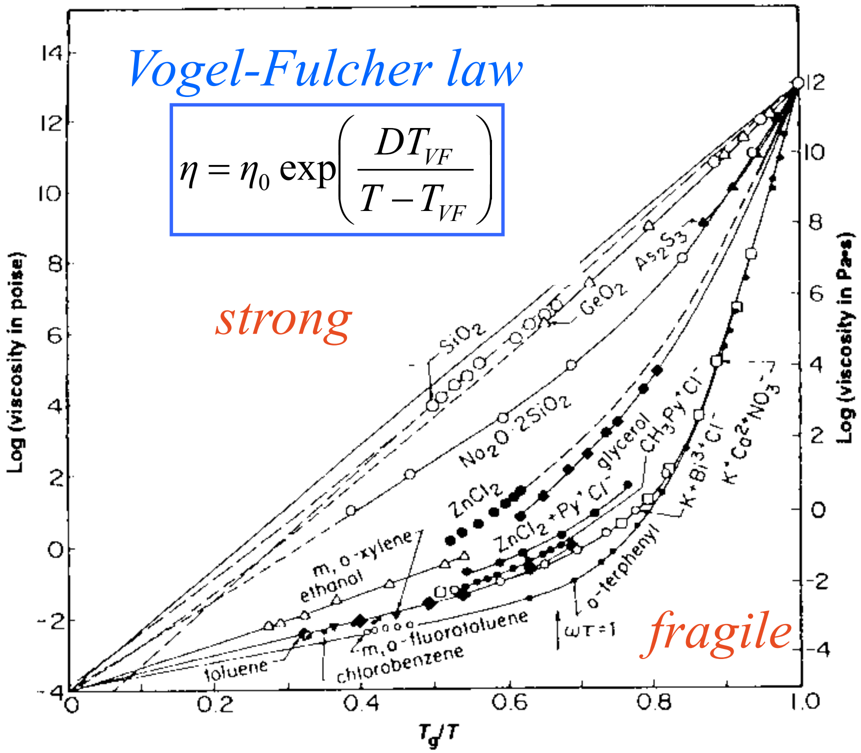
From C. A. Angell, Science, 1995

Glass transition:Viscosity

Definition of T_g : $\boxed{\eta(T_g) = 10^{14}\,\text{Poise} \leftrightarrow \tau_{rel} \approx 10^2 - 10^3\,\text{sec}}$

Strong glasses

- open networks
- robust against deformation
- barriers slowly increasing
- T_{VF} small, D large



$$\eta = \eta_0 \exp\left(\frac{DT_{VF}}{T - T_{VF}}\right)$$

Fragile glasses

- van der Waals liquids
- high plasticity above T_g
- barriers increase fast
- T_{VF} close to T_g D small

From C. A. Angell, Science, 1995

Free energy landscape

Study two universality classes of glasses

Two-spin interacting glasses: SK – model
versus
Multi-spin interactions: p-spin model

Motivation for multi-spin models:

- Optimization problems (3-SAT) have multi-spin interactions
- Langevin dynamics of mean field p-spin model is identical to mode-coupling approximation to supercooled liquids!

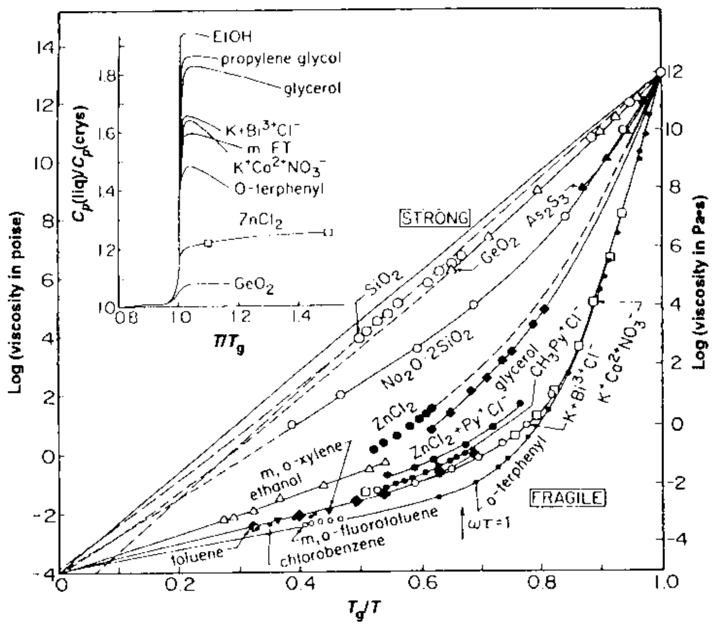
Free energy landscape

Simple model for supercooled liquids

Kirkpatrick, Thirumalai, Wolynes

Supercooled liquids:

Liquids that fail to crystallize, ansd thus remain amorphous and non-rigid but get very viscous and slow



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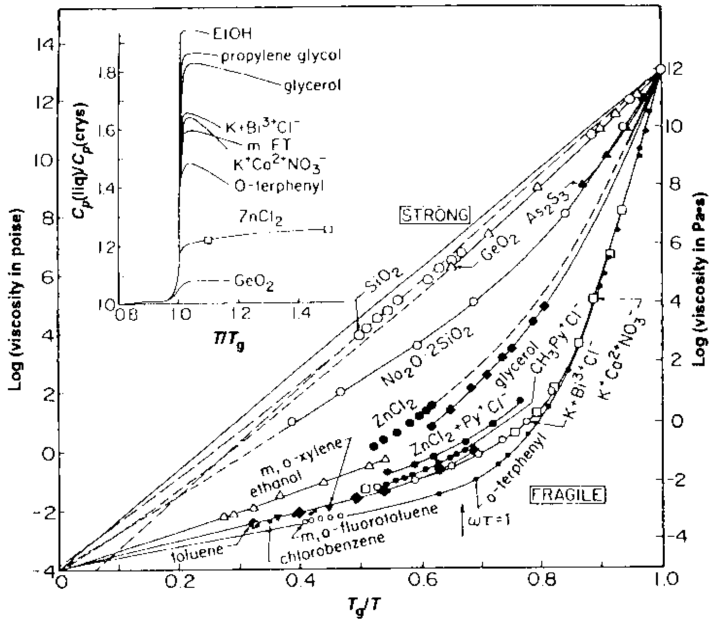
Liquids that fail to crystallize, ansd thus remain amorphous and non-rigid but get very viscous and slow

Relation with spin models??



Simple model for supercooled liquids

Kirkpatrick, Thirumalai, Wolynes

Simple liquid Hamiltonian $$H = \frac{\mu(t)}{2}\phi^2 + \frac{g}{p!}\phi^p$$ $\phi(r)$: local density

Langevin equation $$\frac{\partial \phi}{\partial t} = -\mu(t)\phi - \frac{g}{(p-1)!}\phi^{p-1} + \eta$$

The dynamical evolution equations for such a liquid are identical to those of a p-spin model (see later).

→ Conjecture / belief: The glass transition and the structure of the glass phase of models with interactions between p>2 spins captures the essence of the physics of structural glasses (that have no intrinsic but only **self-generated** disorder!)

The spherical p-spin model

Hamiltonian

$$H[\sigma] = -\frac{1}{p!}\sum_{i_1\cdots i_p} J_{i_1\ldots i_p}\sigma_{i_1}\cdots\sigma_{i_p} = -\sum_{i_1<i_2<\cdots<i_p} J_{i_1\ldots i_p}\sigma_{i_1}\cdots\sigma_{i_p}$$

Spherical constraint (easy to compute - but for p=2 trivializes the model)

$$\sum_i \sigma_i^2 = N$$

Gaussian disorder with zero mean and variance:

$$\overline{J^2_{i_1\cdots i_p}} = \frac{p!}{2N^{p-1}}$$

ensures O(1) local fields and O(N) total energy.

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$$\sum_i \sigma_i^2 = N$$

Free energy functional -- Zeroth order (entropy):

$$e^{A^0[m]} = \int d\sigma\delta\left(\sum_i \sigma_i^2 - N\right) e^{\sum_i \lambda_i^0(\sigma_i - m_i)} = \int_{-i\infty}^{i\infty}\frac{d\mu}{2\pi}\int d\sigma e^{-\mu\sum_i\sigma_i^2 + \mu N + \sum_i \lambda_i^0(\sigma_i - m_i)}$$

$$= \int_{-i\infty}^{i\infty}\frac{d\mu}{2\pi}\exp\left[N\mu + \frac{N}{2}\log\left(\frac{\pi}{\mu}\right) + \frac{1}{4\mu}\sum_i(\lambda_i^0)^2 - \sum_i\lambda_i^0 m_i\right].$$

Saddle point:

$$\frac{\partial A^0}{\partial \lambda_i^0} = 0 \to \lambda_i^0 = 2\mu m_i \qquad A^0[m] = N\mathrm{st}_\mu\left[\mu(1-q) + \frac{1}{2}\log\left(\frac{\pi}{\mu}\right)\right]$$

$$\mu = \frac{1}{2(1-q)} \qquad A^0[m] = N\frac{1}{2}\log(1-q)$$

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Hamiltonian

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Spherical constraint (easy to compute - but for p=2 trivializes the model)

$$\sum_i \sigma_i^2 = N$$

Free energy functional -- First order (mean energy):

$$\frac{dA^\beta}{d\beta} = -\langle H\rangle \xrightarrow{(\beta=0)} = \frac{1}{p!}\sum_{i_1\ldots i_p} J_{i_1\ldots i_p} m_{i_1}\cdots m_{i_p}$$

The spherical p-spin model

Hamiltonian

$$H[\sigma] = -\frac{1}{p!}\sum_{i_1\cdots i_p} J_{i_1\ldots i_p}\sigma_{i_1}\cdots\sigma_{i_p} = -\sum_{i_1<i_2<\cdots<i_p} J_{i_1\cdots i_p}\sigma_{i_1}\cdots\sigma_{i_p}$$

Spherical constraint (easy to compute - but for p=2 trivializes the model)

$$\textstyle\sum_i \sigma_i^2 = N$$

Free energy functional -- Second order (Onsager / vdW-like term):

$$\frac{d^2 A^\beta}{d\beta^2} = \langle U_0^2 \rangle$$

$$U = H - \langle H\rangle - \sum_i \partial_\beta \lambda_i^\beta(\sigma_i - m_i) \qquad \partial_\beta \lambda_i^\beta|_{\beta=0} = \frac{d}{dm_i}\langle H\rangle_0$$

$$\rightarrow \qquad U_0 = -\frac{1}{p!}\sum_{i_1\cdots i_p} J_{i_1\cdots i_p}[\sigma_{i_1}\cdots\sigma_{i_p} - m_{i_1}\cdots m_{i_p} - p(\sigma_{i_1} - m_{i_1})m_{i_2}\cdots m_{i_p}]$$

The spherical p-spin model

Hamiltonian

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$$\frac{d^2A^\beta}{d\beta^2} = \langle U_0^2\rangle = \langle U_0\,(H - \langle H\rangle_0)\rangle =$$

$$U = H - \langle H\rangle - \sum_i \partial_\beta\lambda_i^\beta(\sigma_i - m_i) \qquad \partial_\beta\lambda_i^\beta|_{\beta=0} = \frac{d}{dm_i}\langle H\rangle_0$$

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Use $\quad \langle U(\sigma_i - m_i)\rangle = 0$

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$$U = H - \langle H\rangle - \sum_i \partial_\beta\lambda_i^\beta(\sigma_i - m_i) \qquad \partial_\beta\lambda_i^\beta|_{\beta=0} = \frac{d}{dm_i}\langle H\rangle_0$$

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Use $\langle U(\sigma_i - m_i)\rangle = 0$ $\qquad q = q(\{m_i\}) = \frac{1}{N}\sum_i m_i^2$

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Spherical constraint (easy to compute - but for p=2 trivializes the model)

$$\sum_i \sigma_i^2 = N$$

Free energy functional: (0th +1st +2nd order)

$$\frac{G(\{m_i\})}{N} = -\frac{1}{2\beta}\log(1-q) - \frac{1}{p!N}\sum_{i_1\cdots i_p} J_{i_1\cdots i_p} m_{i_1}\cdots m_{i_p} - \frac{\beta}{4}[1 - pq^{p-1} + q^p(p-1)]$$

The spherical p-spin model

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Pure states = Minima of G !

free energy $N f_\alpha = G(\{m_i^\alpha\})$

weight of pure state in the full Gibbs measure $w_\alpha \propto \exp(-\beta N f_\alpha)$

The spherical p-spin model

Hamiltonian

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free energy $Nf_\alpha = G(\{m_i^\alpha\})$

weight of pure state in the full Gibbs measure $w_\alpha \propto \exp(-\beta N f_\alpha)$

Can show: metastable states capture the essential phase space: $\overline{\log(\sum_\alpha w_\alpha)} = \overline{\log(Z_{\text{full}})}$

The spherical p-spin model

Hamiltonian

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Pure states = Minima of G !

Write $\quad m_i = \sqrt{q}\, n_i \quad \sum n_i^2 = N$

The spherical p-spin model

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Peculiarity of spherical model:

(Minimum-maximum merger)

- Minimization of G wrt n_i is independent of T !
- Minima have constant "angular" texture n_i. Only $q = q(T)$ changes with T, until instability occurs at T*.

The spherical p-spin model

Hamiltonian

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Pure states = Minima of G !

Write $m_i = \sqrt{q}n_i$ $\sum n_i^2 = N$

$\partial G/\partial q = 0$ Has no solution anymore $\leftrightarrow$ (Minimum-maximum merger)

Peculiarity of spherical model:

- Minimization of G wrt n_i is independent of T !
- Minima have constant "angular" texture n_i. Only $q = q(T)$ changes with T, until instability occurs at T*.

The spherical p-spin model

Solutions to the angular equations:

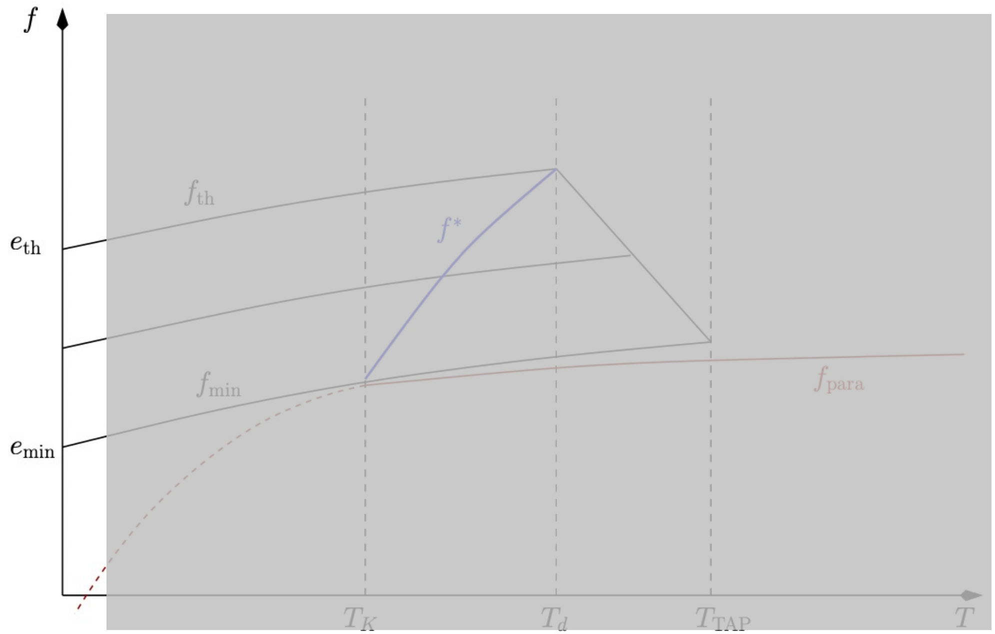
T = 0 :

- minima exist with energies $e \in [e_{\min}, e_{\mathrm{th}}]$

$e > e_{th}$: energy landscape dominated by saddles, not by minima

Threshold Marginal states

Ground state



The spherical p-spin model

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- There is an exponential number of them $\mathcal{N}(e) = \exp(N\Sigma(e))$
- $\Sigma(e_{min}) = 0$, and Σ is concave, increases with e

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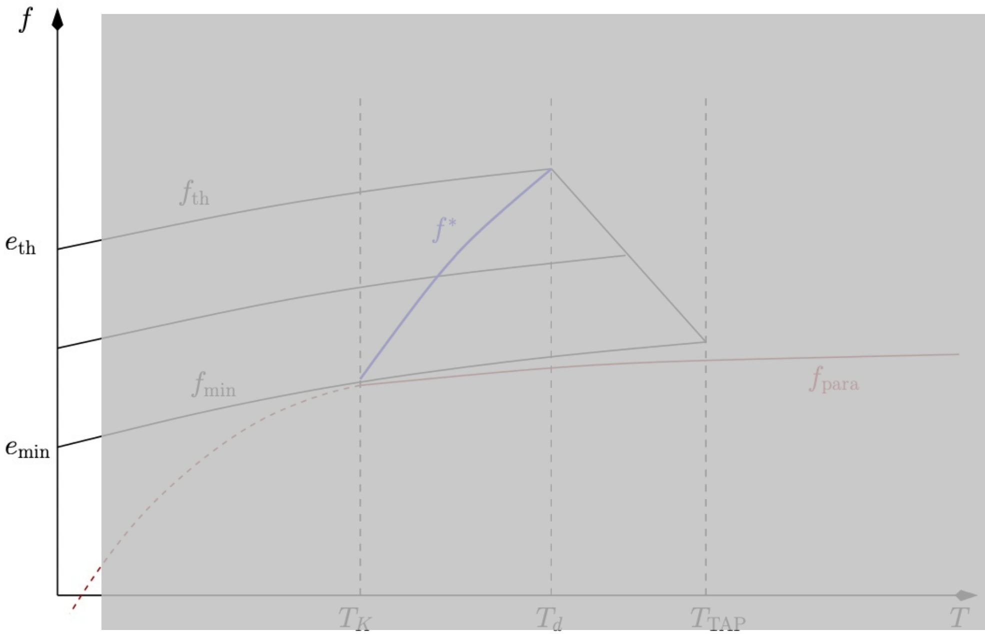

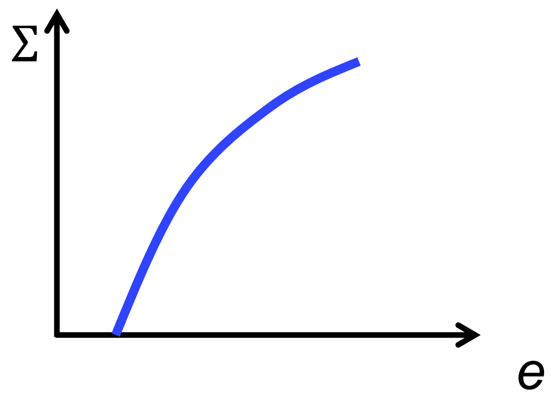

The spherical p-spin model

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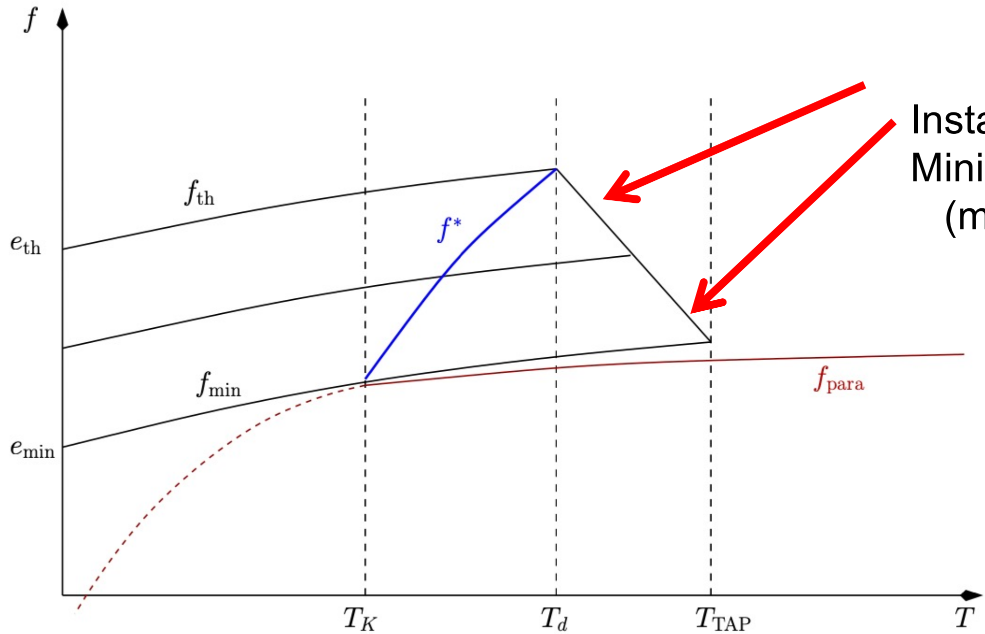

Instability: *T*=T*(e)*
Minima disappear at too high T (merging with maxima)

The spherical p-spin model

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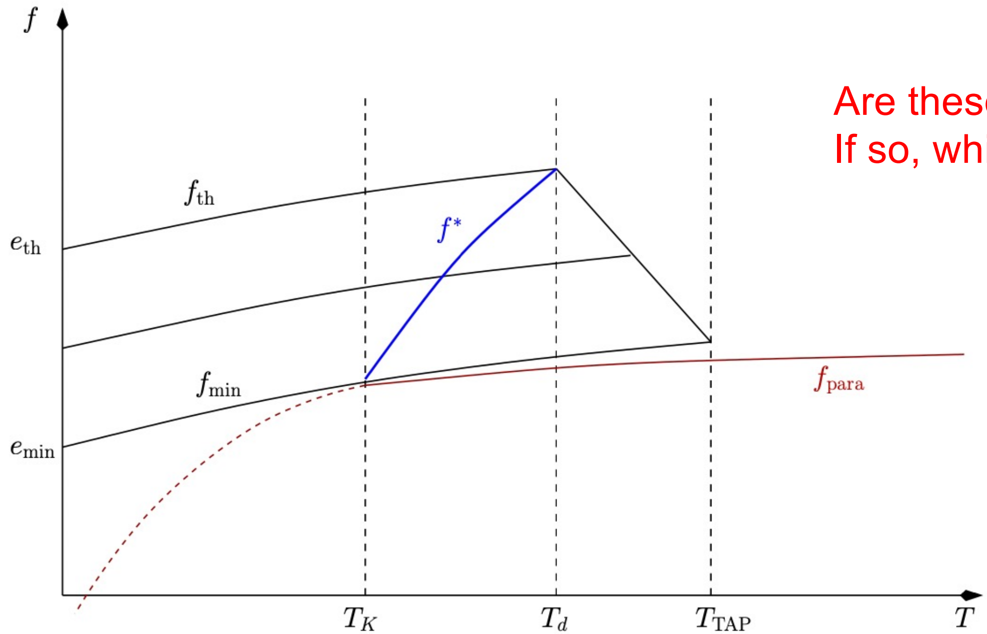

Are these minima relevant?
If so, which ones?

The spherical p-spin model

Solutions to the angular equations:

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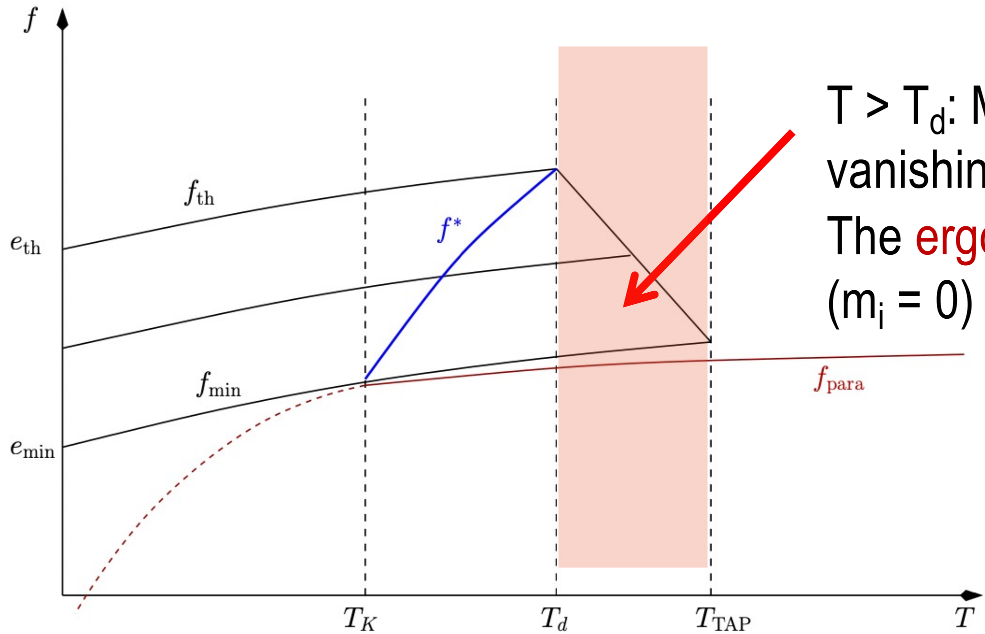

T > T_d: Minima exist, but occupy a vanishing fraction of phase space. The ergodic paramagnetic solution (m_i = 0) dominates

The spherical p-spin model

Solutions to the angular equations:

T = 0 :

- minima exist with energies $e \in [e_{\min}, e_{\mathrm{th}}]$
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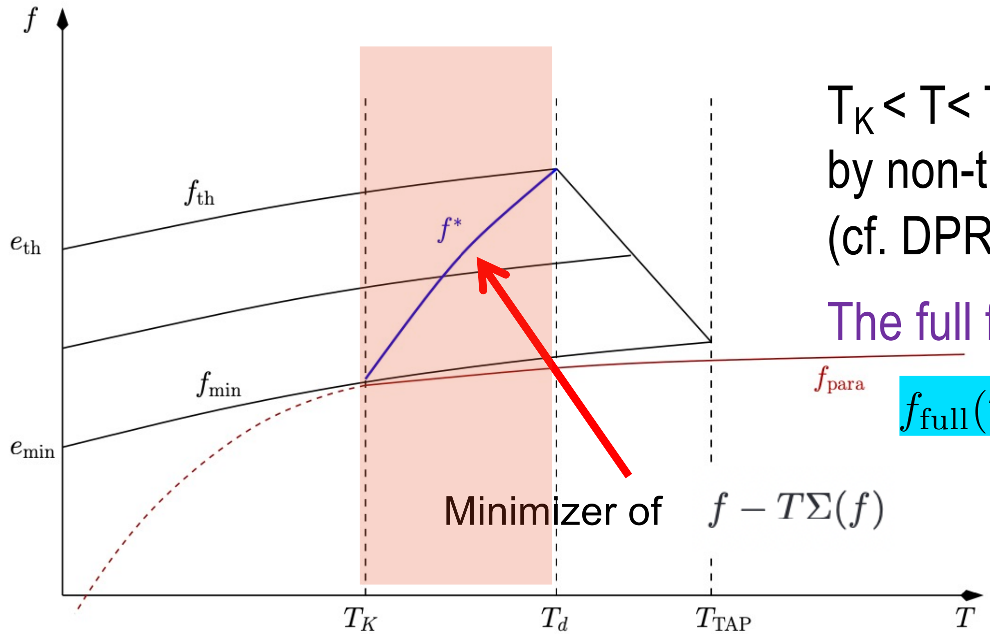
- $\Sigma(e_{min}) = 0$, and Σ is concave, increases with e



$T_K < T < T_d$: Gibbs weight is dominated by non-trivial minima f*
(cf. DPRM and REM)

The full free energy remains analytic:

$$f_{\mathrm{full}}(T) = f^* - T\Sigma(f^*) \stackrel{!}{=} f_{\mathrm{para}}(T)$$

The spherical p-spin model

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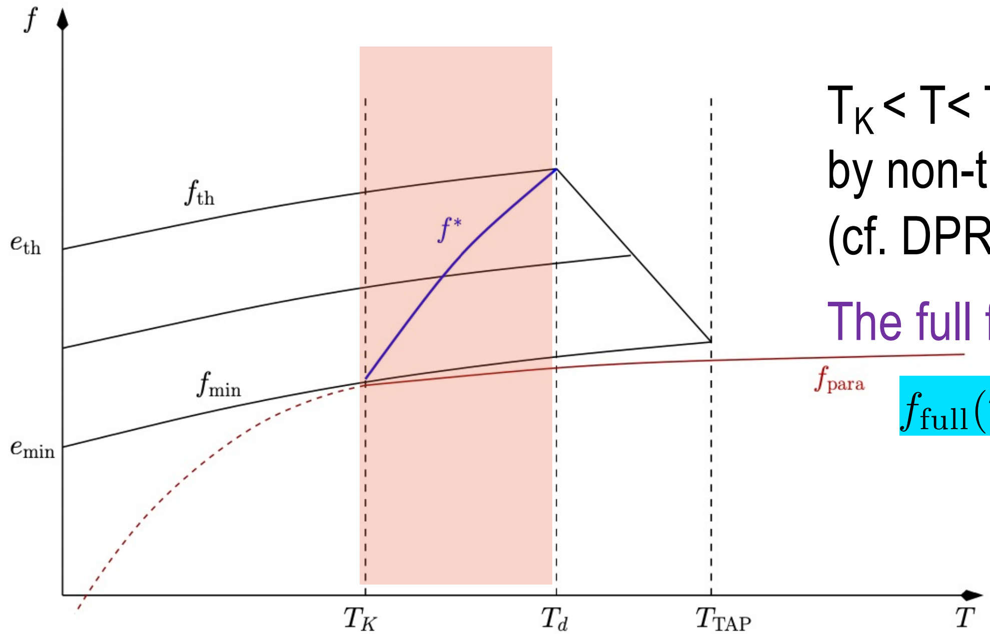

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(cf. DPRM and REM)

The full free energy remains analytic:

$$f_{\text{full}}(T) = f^* - T\Sigma(f^*) \stackrel{!}{=} f_{\text{para}}(T)$$

BUT: dynamics gets stuck in pure states $\rightarrow$ non-ergodic

The spherical p-spin model

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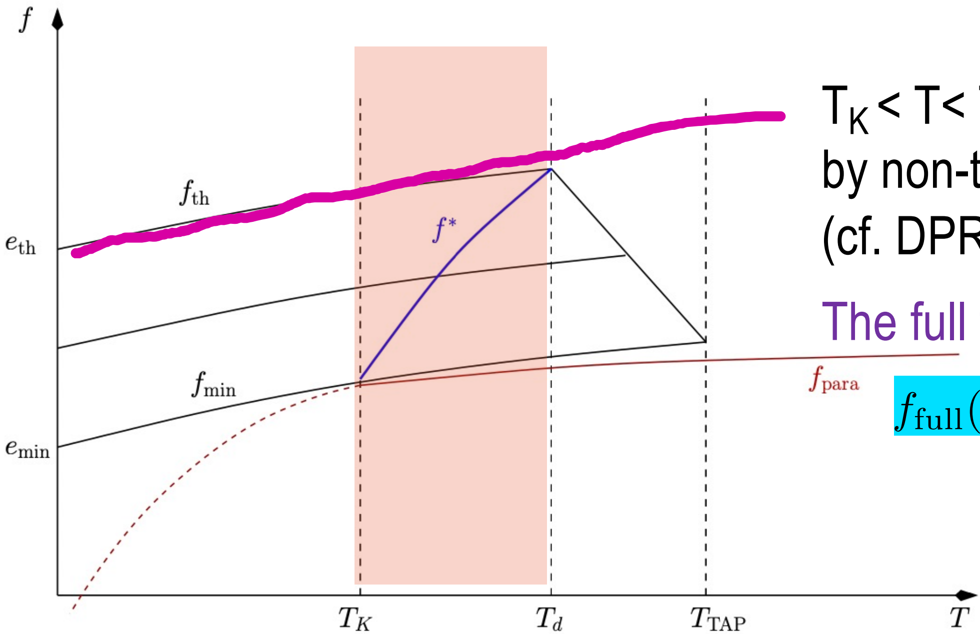

T_K < T< T_d: Gibbs weight is dominated by non-trivial minima f* (cf. DPRM and REM)

The full free energy remains analytic:

$$f_{\mathrm{full}}(T) = f^* - T\Sigma(f^*) \stackrel{!}{=} f_{\mathrm{para}}(T)$$

BUT: dynamics gets stuck in pure states $\rightarrow$ non-ergodic

The spherical p-spin model

Solutions to the angular equations:

T = 0 :

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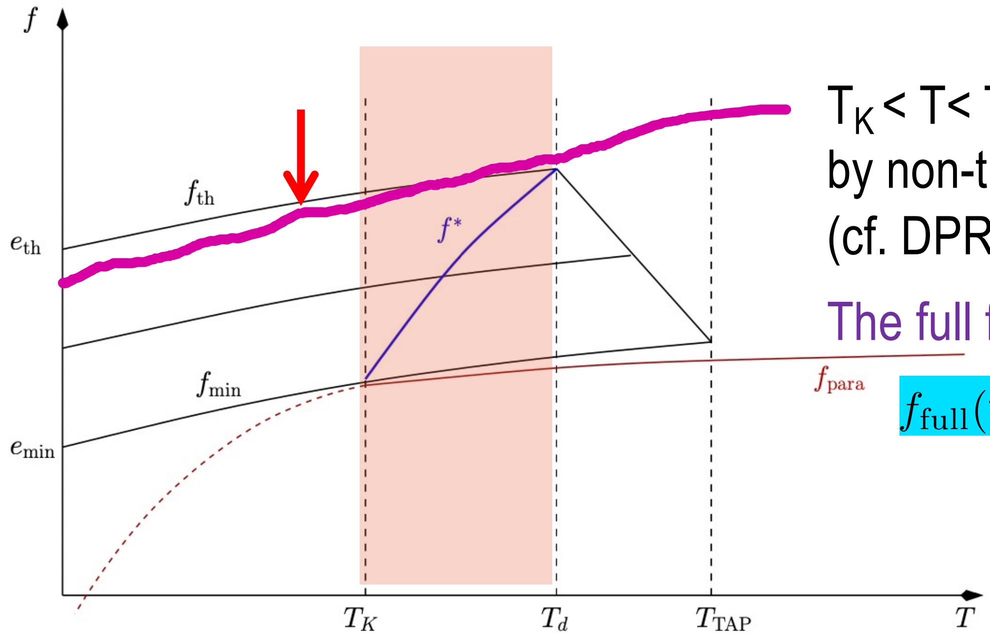

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Beyond mean field: onset of activated dynamics across (finite barriers)

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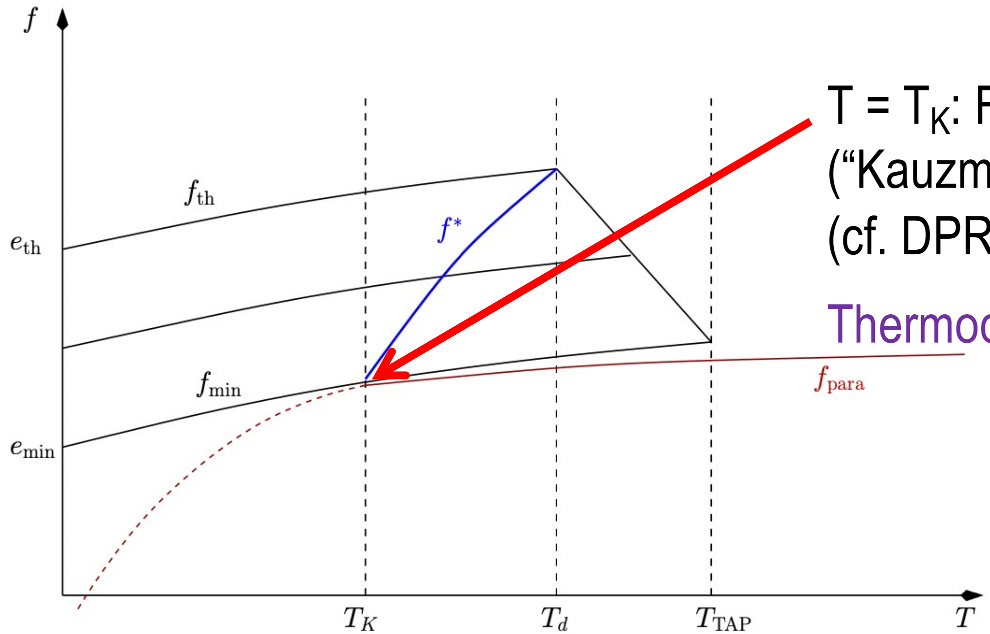

T = T_K: Freezing transition ("Kauzmann temperature"): (cf. DPRM and REM)

Thermodynamic transition

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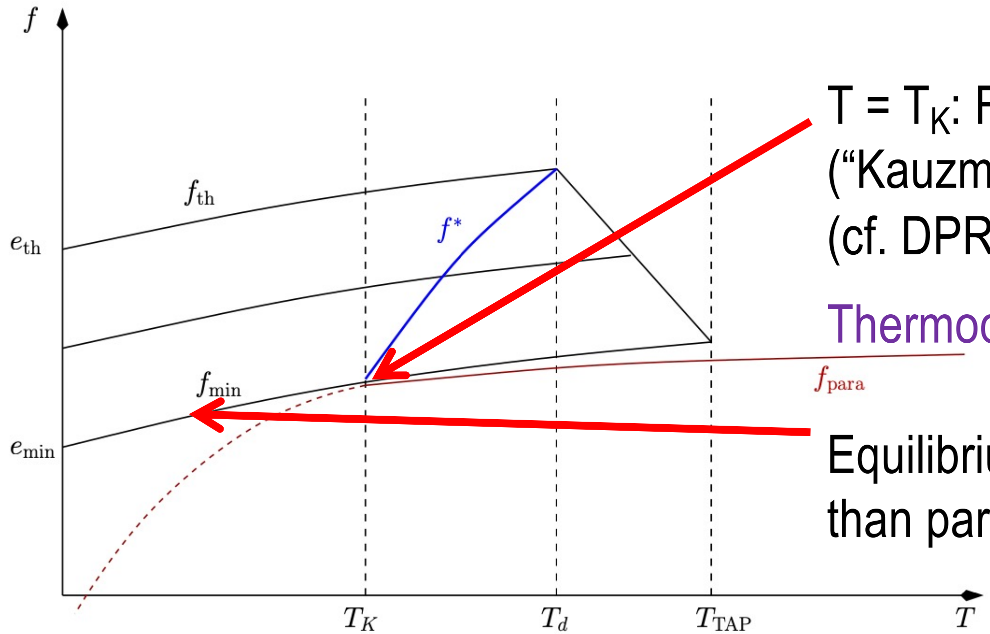

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Equilibrium free energy: Higher than paramagnetic continuation!

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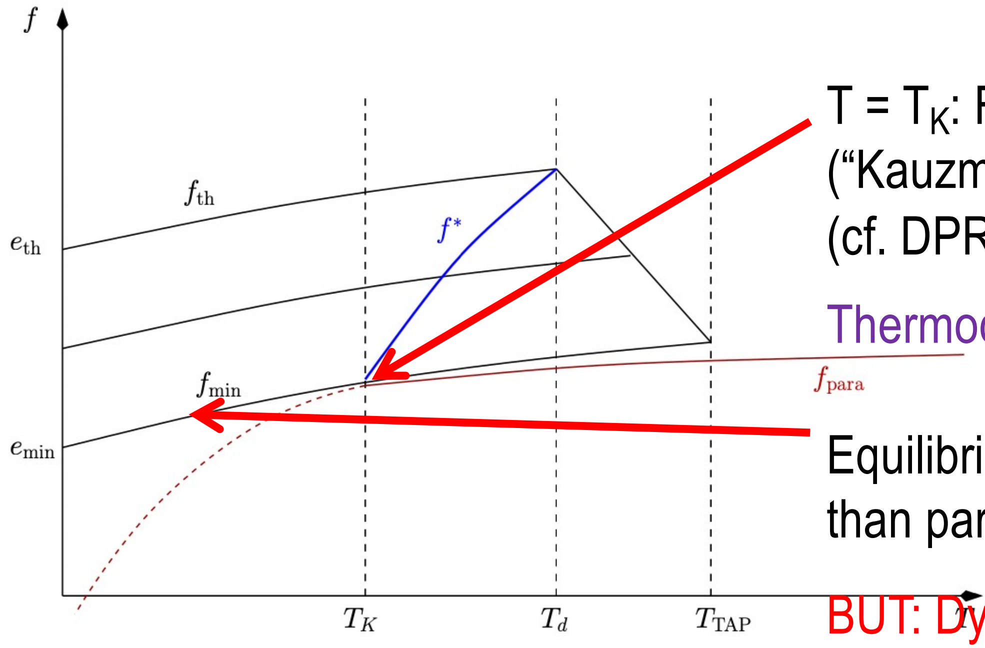

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("Kauzmann temperature"):
(cf. DPRM and REM)

Thermodynamic transition

Equilibrium free energy: Higher than paramagnetic continuation!

BUT: Dynamically inaccessible!

First order nature of the dynamic transition

Important difference to p=2 spin glasses:

Paramagnetic state m = 0 has no instability!

$$\frac{G(\{m_i\})}{N} = -\frac{1}{2\beta}\log(1-q) - \frac{1}{p!N}\sum_{i_1\cdots i_p} J_{i_1\ldots i_p} m_{i_1}\cdots m_{i_p} - \frac{\beta}{4}[1 - pq^{p-1} + q^p(p-1)]$$

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For $p > 2$: intra-state overlap q **jumps** to finite value in the minima!

- **Discontinuous (first-order-like) onset of frozen magnetization**
- **No instability** of paramagnetic state

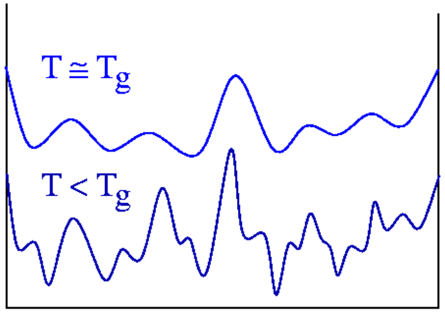
Spin glass universality classes

Two different types of (mean field) spin glasses

Continuous

SK-model $H = \sum_{i<j} J_{ij} s_i s_j$

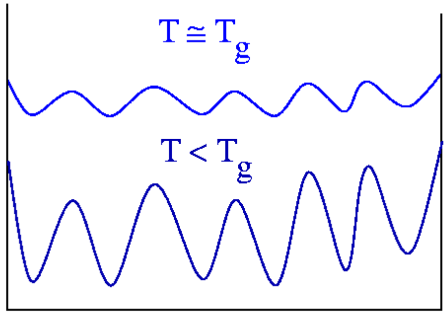
$$q_{EA} = \frac{1}{N}\sum_i \langle s_i \rangle^2 \underset{T \to T_g}{\to} 0$$



Discontinuous

p-spin models $H = \sum_{i_1<\ldots<i_p} J_{i_1\ldots i_p} s_{i_1} \cdots s_{i_p}$
$p \geq 3$

$$q_{EA} \underset{T \to T_g}{\to} q_c > 0$$



Next time: "Full replica symmetry breaking" | "One step replica symmetry breaking"

MF-Model for real spin glasses | MF-analogon for structural glasses

Given these metastable states, how does the spin dynamics sense them?

Dynamics

T. Castellani and A. Cavagna
Spin-Glass Theory for Pedestrians, cond-mat/0505032

Langevin equation

$$\partial_t \sigma_i(t) = -\frac{\partial H}{\partial \sigma_i} - \mu(t)\sigma_i(t) + \eta_i(t) \quad \text{with} \quad \langle \eta(t)\eta(t') \rangle = 2T\delta(t-t')$$

Enforces the spherical constraint

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Correlation and response

$$C(t,t') = \frac{1}{N}\sum_i \langle \sigma_i(t)\sigma_i(t')\rangle \qquad R(t,t') = \frac{1}{N}\sum_i \langle \frac{\partial \sigma_i(t)}{\partial h_i(t')}\rangle$$

Disorder averaged dynamics: C and R are the same as for a single spin with memory and modified noise:

$$\partial_t \sigma(t) = -\mu(t)\sigma(t) + \frac{1}{2}p(p-1)\int dt'' R(t,t'')C(t,t'')^{p-2}\sigma(t'') + \xi(t)$$

$$\langle \xi(t)\xi(t')\rangle = 2T\delta(t-t') + \frac{p}{2}C(t,t')^{p-1}$$

... → ... Closed self-consistent equations $\quad \partial_t C = f_C[C(t'),R(t')] \quad \partial_t R = f_R[C(t'),R(t')]$

Dynamics

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In an ergodic regime:

Expect: time translational invariance (TTI)

$$\text{TTI:} \begin{cases} C(t_1, t_2) = C(t_1 - t_2) \equiv C(\tau) \\ R(t_1, t_2) = R(t_1 - t_2) \equiv R(\tau) \end{cases} \qquad (\tau \equiv t_1 - t_2)$$

Fluctuation dissipation relation: response function (dissipation) and correlation function (fluctuation) are linked [time-differential version of: $\chi_{ij} = \langle \frac{\partial s_i}{\partial h_j} \rangle = \frac{1}{T} \langle s_i s_j \rangle$]

$$\text{FDT:} \qquad R(\tau) = -\frac{1}{T} \frac{dC(\tau)}{d\tau}$$

$\longrightarrow$ Equation for $C(\tau)$

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→ Self-consistent evolution equation for average the spin –spin correlator C only:

$$\dot{C}(\tau) = -TC(\tau) - \frac{p}{2T} \int_0^\tau du \; C^{p-1}(\tau - u) \dot{C}(u)$$

Diffusion under thermal noise

Counteracted ($\dot{C} < 0!$) by memory: caging effect! Strong at low T.

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At T_d: get stuck ($\dot{C} = 0$) in the threshold states: at C= q_{th} !

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P-spin models vs structural glasses?

Why should p-spin models be reasonable models for supercooled liquids (structural glasses) without disorder?

Compare dynamics!

A simple model for supercooled liquids

Kirkpatrick, Thirumalai, Wolynes

Simple liquid Hamiltonian $$H = \frac{\mu(t)}{2}\phi^2 + \frac{g}{p!}\phi^p$$ $\phi(r)$: local density

Langevin equation $$\frac{\partial \phi}{\partial t} = -\mu(t)\phi - \frac{g}{(p-1)!}\phi^{p-1} + \eta$$

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- Field theory for dynamics (perturbative expansion in g)
- Approximately resum diagrammatics ("no vertex corrections")

  "Mode coupling theory" (exact for large number of field components)
- Compare with Langevin dynamics for spherical spins with p-spin interactions:

→ Identical dynamical equations for response and correlation functions!

(even though there is no disorder in the liquid Hamiltonian!!)

Conjecture / Belief: **Glass transition and structure of glass phase of p-spin models with p>2 capture the essence of the physics of structural glasses!**