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!

Free enery landscape

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!

Simple model for 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 disorder!)

The spherical p-spin model

Hamiltonian

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

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

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

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:

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

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

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

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

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

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

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

The spherical p-spin model

Hamiltonian

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

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

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

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

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

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

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

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

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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)

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

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Pure states = Minima of G !

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

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

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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 $w_\alpha \propto \exp(-\beta N f_\alpha)$

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

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

Hamiltonian

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Pure states = Minima of G !

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

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

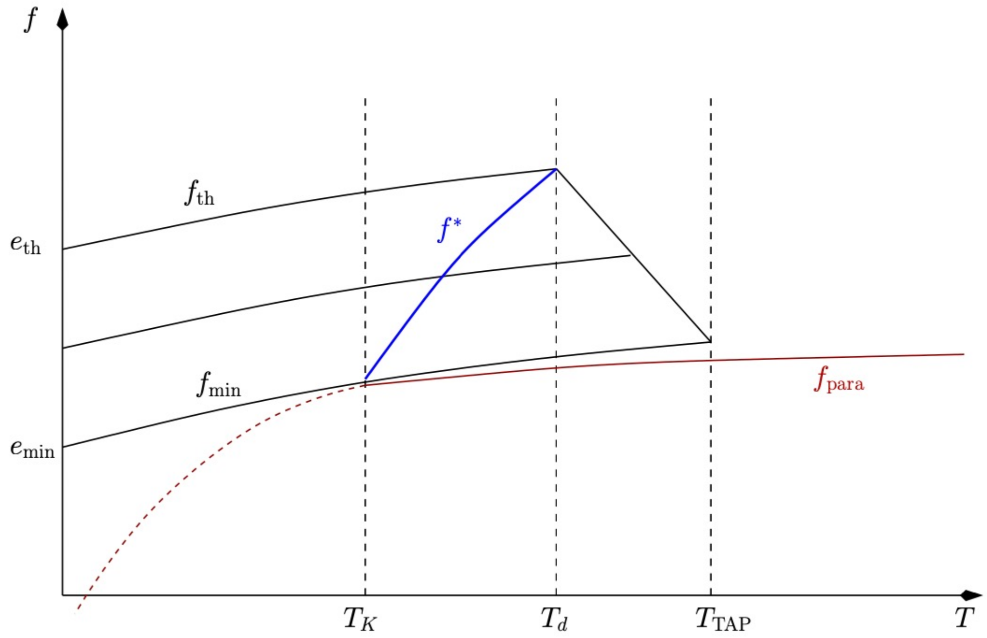
Solutions to the angular equations:

T = 0 :

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

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

threshold →



The spherical p-spin model

Solutions to the angular equations:

T = 0 :

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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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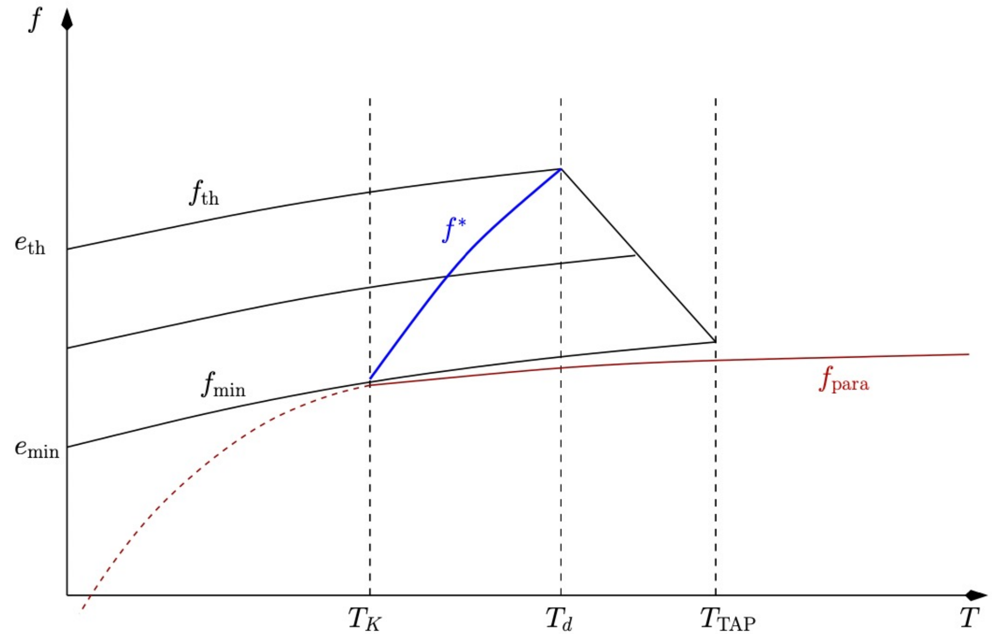

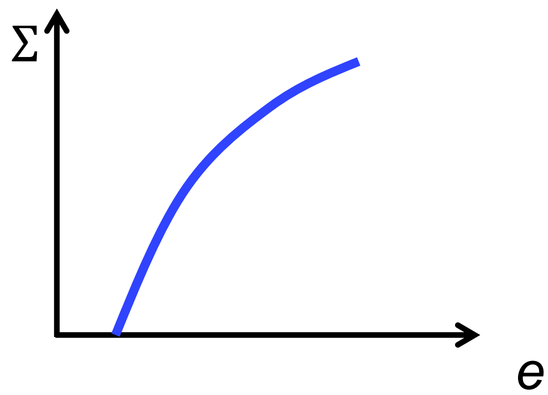

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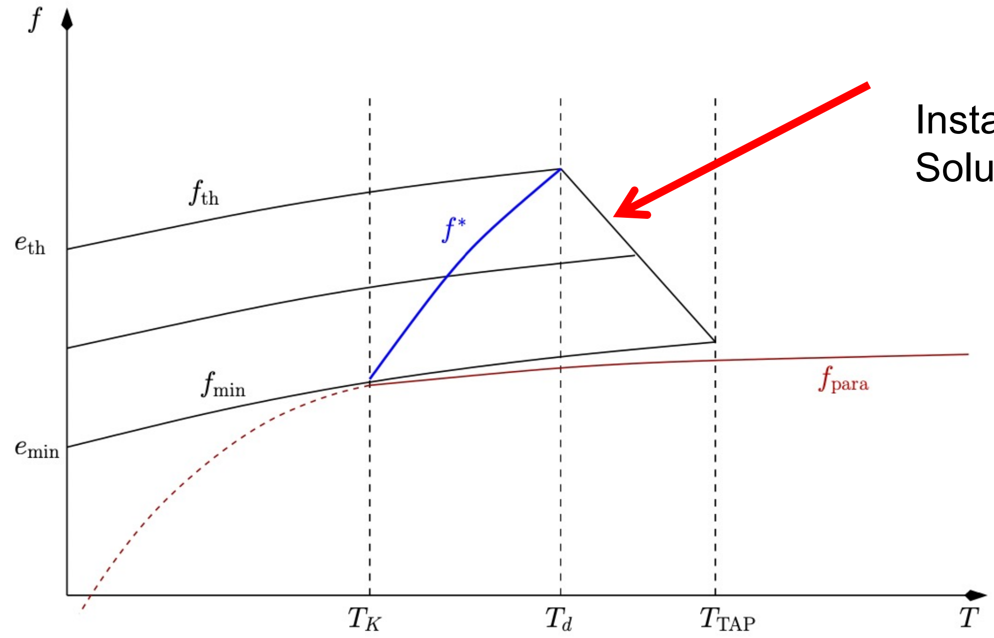

Instability: *T*=T*(e)*
Solutions disappear at too high T

The spherical p-spin model

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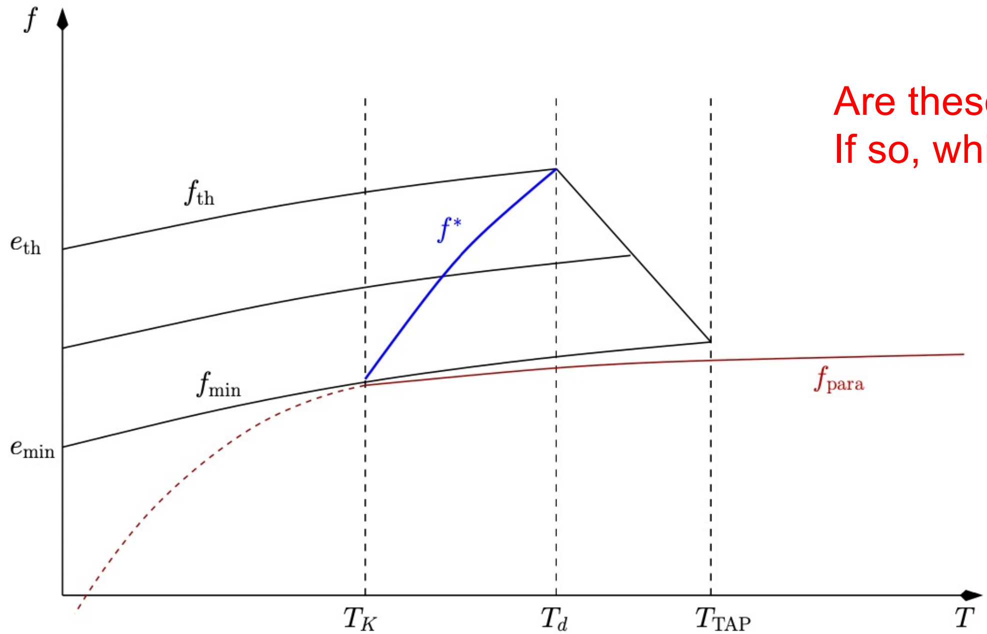

Are these minima relevant?
If so, which ones?

The spherical p-spin model

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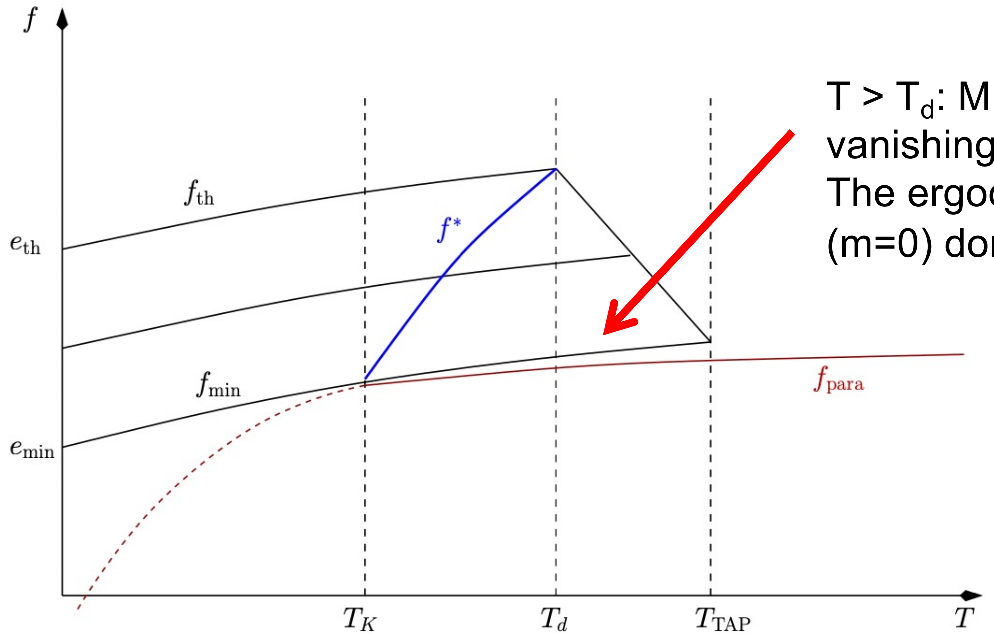

T > T_d: Minima exist, but occupy a vanishing corner of phase space. The ergodic paramagnetic solution (m=0) dominates

The spherical p-spin model

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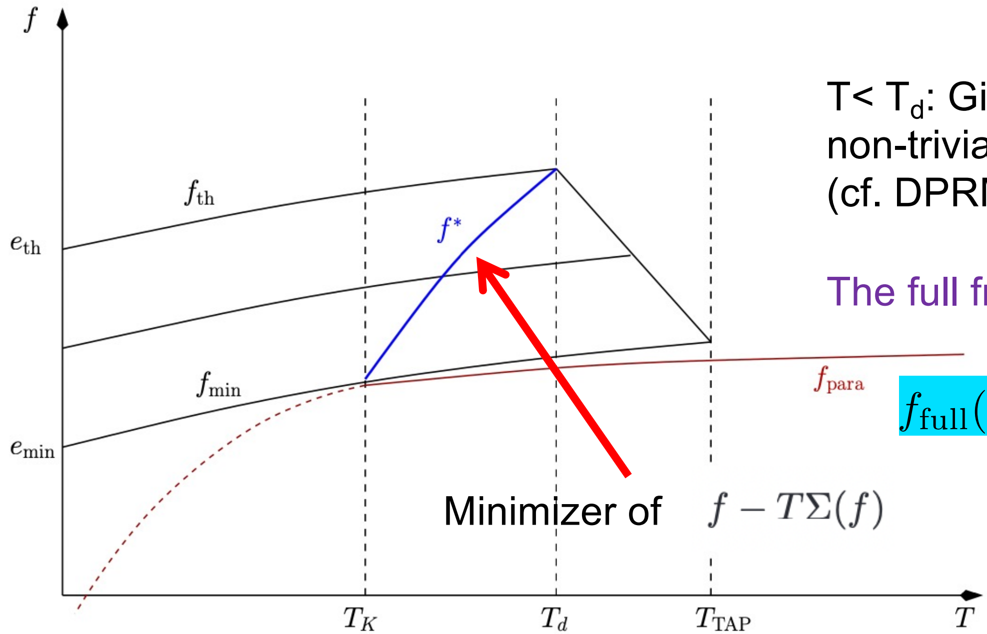

T< T_d: Gibbs weight is dominated by non-trivial minima f* (cf. DPRM and REM)

The full free energy remains analytic:

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

The spherical p-spin model

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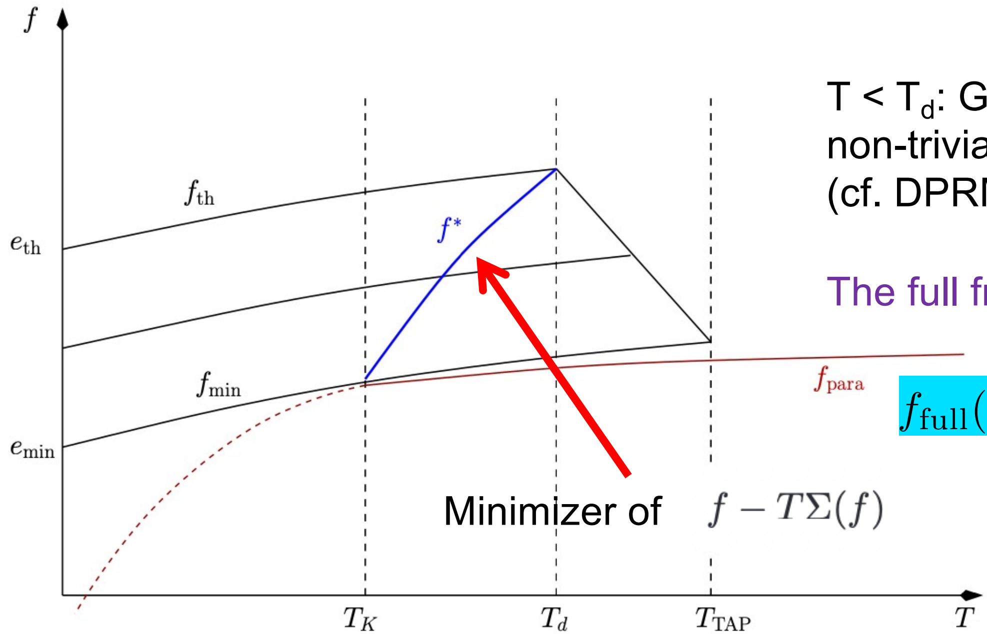

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BUT: dynamics gets stuck in pure states → non-ergodic

The spherical p-spin model

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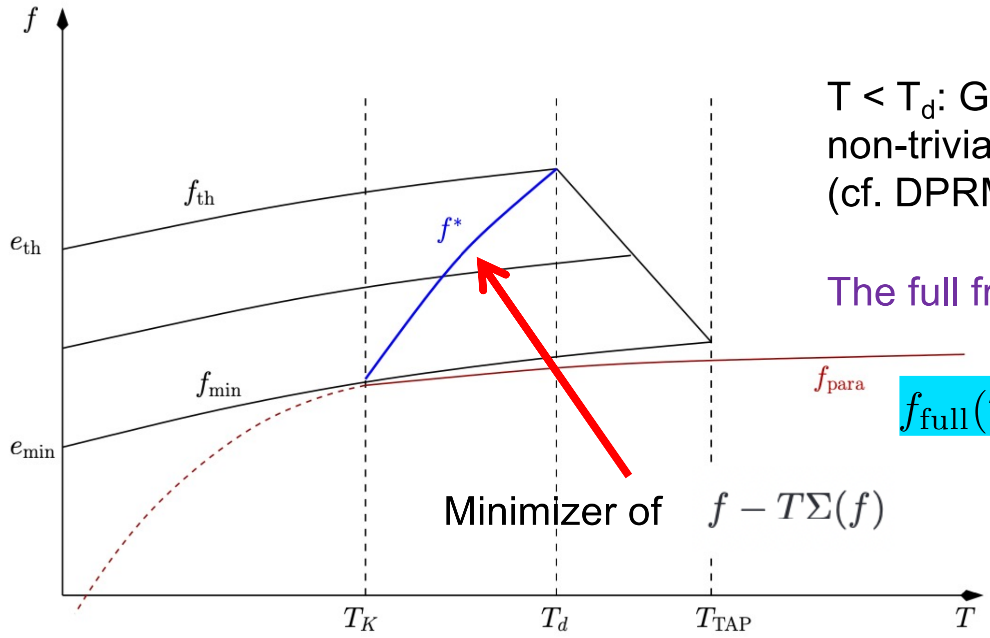

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$$f_{\text{full}}(T) = f^* - T\Sigma(f^*) \stackrel{!}{=} f_{\text{para}}(T)$$

BUT: dynamics gets stuck in pure states $\rightarrow$ non-ergodic
Beyond mean field: onset of activated dynamics across (finite barriers)

The spherical p-spin model

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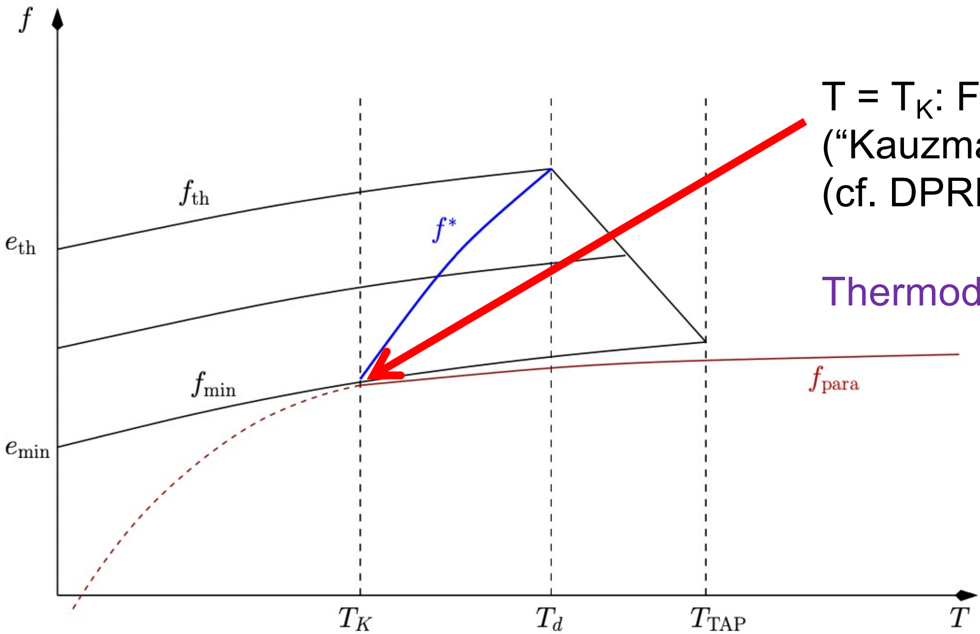

T = T_K: Freezing transition ("Kauzmann temperature"): (cf. DPRM and REM)

Thermodynamic transition

The spherical p-spin model

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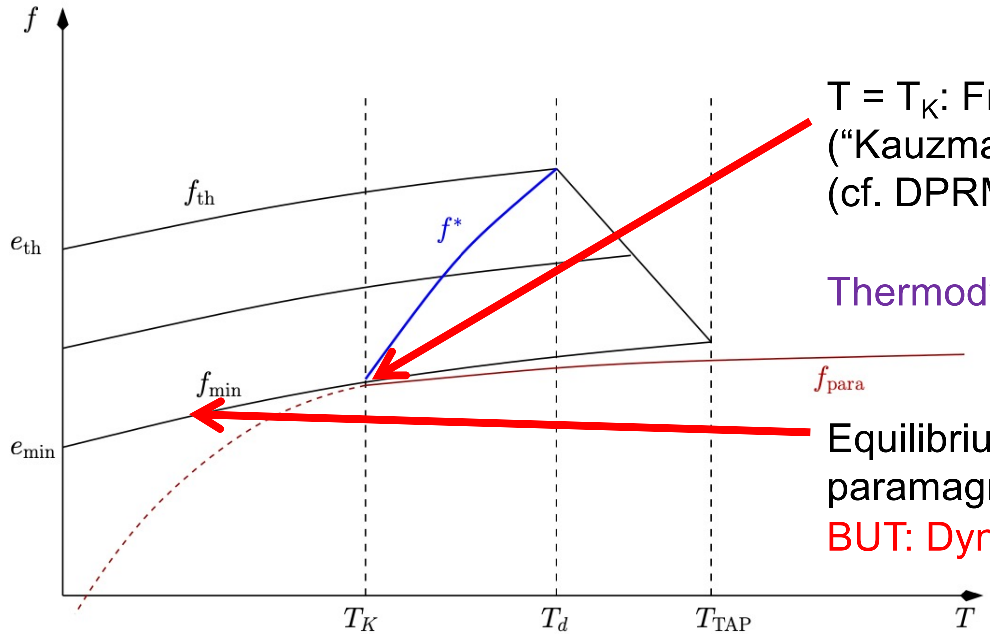

T = T_K: Freezing transition ("Kauzmann temperature"): (cf. DPRM and REM)

Thermodynamic transition

Equilibrium free energy: Higher than paramagnetic continuation!

BUT: Dynamically this is 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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Energy-entropy balance of freezing:

Energy gain: $O(m^p)$ $\overset{p>2,\, m\ll 1}{\ll}$ Entropic cost: $O(m^2)$

Continuously emerging minima with very small m are possible only for p=2!

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Energy-entropy balance of freezing:

$p > 2, m \ll 1$

Energy gain: $O(m^p)$ $\ll$ Entropic cost: $O(m^2)$

Continuously emerging minima with very small m are possible only for $p=2$!

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

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

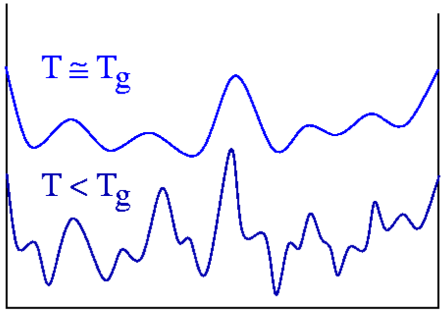
Spin glass universality classes

Two different types of (mean field) spin glasses

Continuous

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

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

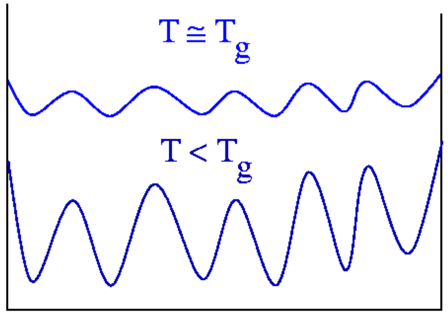


Discontinuous

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

$p \geq 3$

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



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

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