

The glass transition as a spin glass problem

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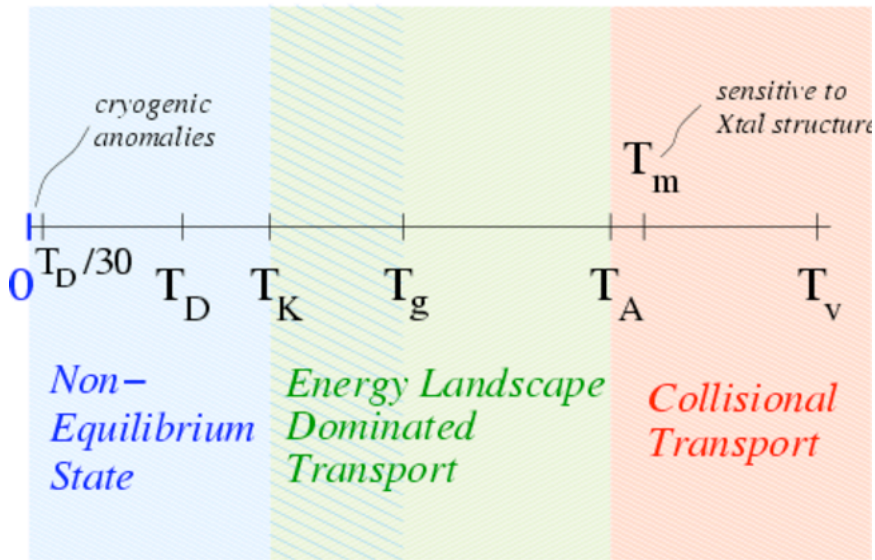
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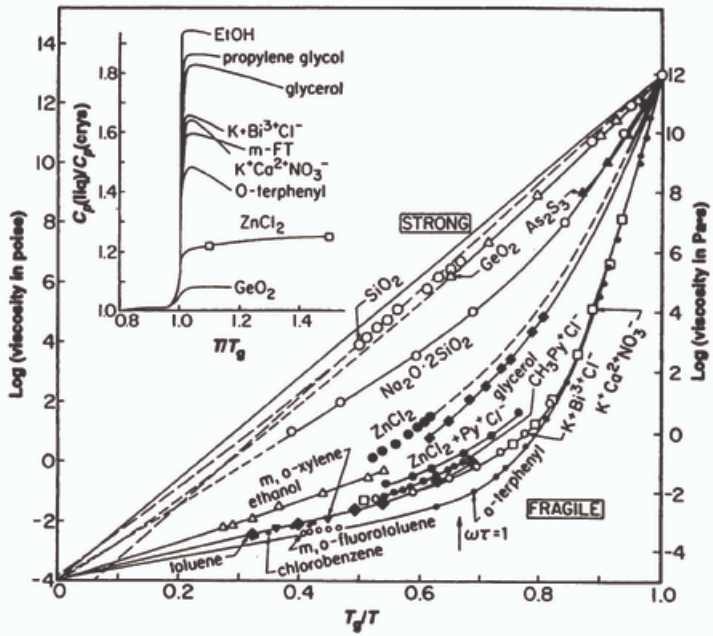
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Regimes of Liquid/Glass Physics





Plan of Talk

- Glass phenomenology
- Formalism — to show that the supercooled liquid (**with no disorder**) near its glass transition is in the universality class of the **Ising spin glass in a field** (**with quenched disorder**)
- Droplet scaling ideas: predicts behaviour on **long lengthscales and timescales**
- Long lengthscales are not being reached in experiments, glasses are in a **pre-asymptotic regime** — numerical work on Ising spin glass in a field indicates that it mimics conventional glass phenomenology when lengthscales are modest

Why might there be a thermodynamic glass transition?

- Vogel-Fulcher law

$$\eta \sim \exp[DT_0/(T - T_0)].$$

(But no data near T_0 so no evidence of a real transition at T_0).

Relaxation time $\tau \sim \eta$. D is the 'fragility'

“Strong” glasses: simple Arrhenius (i.e. $T_0 = 0$)

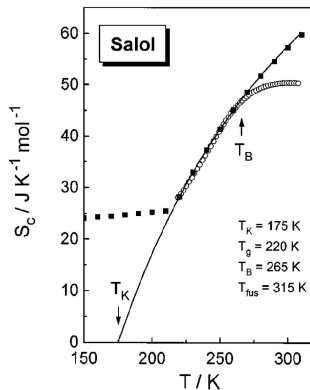
- Kauzmann Paradox: Configurational entropy per molecule apparently goes to zero at T_K

$$s_c(T) \sim k_B(T - T_K)/T_K \sim \Delta C_p(T/T_K - 1)$$

(But no data right up to the Kauzmann temperature T_K).

- The ratio T_K/T_0 lies between 0.9-1.1 for many glass formers for which T_K ranges from 50 K to 1000 K.
- Simulations (and experiment) support existence of a growing lengthscale $L^*(T)$; increasingly large regions have to move simultaneously for the liquid to flow. At T_g , $L^*(T)$ only about 6 particle diameters.

$$\tau \sim \tau_0 \exp[A/Ts_c(T)]$$



$$s_c(T) \zeta^*(T)^d \sim k_B \ln 2$$

- The apparent divergence of η at T_0
- The apparent vanishing of $s_c(T)$ at T_K
- The closeness of T_0 and T_K for many glasses
- A growing lengthscale $L^*(T)$

All suggest a thermodynamic glass transition as $T \rightarrow T_0$.

- We believe that for $d < 6$ no actual transition exists.
- But in fragile glasses transition may be avoided i.e.

$$L^*(T_0) \gg \text{interparticle distance.}$$

(Alas, probably not \gg in reality!)

- In strong glasses

$$L^*(T_0) \sim \text{interparticle distance}$$

and hence not even an avoided transition.

Effective Potential Formalism

(cf Franz and Parisi, Dzero et al.) Define the overlap

$$\rho_c(\mathbf{r}) = \delta\rho_1(\mathbf{r})\delta\rho_2(\mathbf{r})$$

between two configurations of density variations $\delta\rho = \rho - \langle\rho\rangle$ in **two copies** of the liquid. Compute the **constrained** partition function by averaging over the density configurations in the first copy:

$$Z[\rho_c(\mathbf{r}), \delta\rho_2(\mathbf{r})] = \langle \delta(\rho_c(\mathbf{r}) - \delta\rho_1(\mathbf{r})\delta\rho_2(\mathbf{r})) \rangle_{\rho_1}.$$

The effective potential is given by averaging the **free energy** with respect to the density configurations in the **first copy**

$$\Omega[\rho_c(\mathbf{r})] = -T \langle \ln Z[\rho_c, \delta\rho_2] \rangle_{\rho_2}.$$

Use the **replica trick** to average the logarithm

$$\ln Z = \lim_{n \rightarrow 0} (Z^n - 1)/n.$$

Use an integral representation of the delta function.

$$\Omega[\rho_c(\mathbf{r})] = -T \int \prod_{\alpha} \frac{\mathcal{D}\lambda_{\alpha}}{2\pi} \exp \left[i \sum_{\alpha} \int d\mathbf{r} \lambda_{\alpha}(\mathbf{r}) \rho_c(\mathbf{r}) \right] \\ \times \left\langle \left\langle \exp \left[-i \sum_{\alpha} \int d\mathbf{r} \delta\rho_1^{\alpha}(\mathbf{r}) \delta\rho_2(\mathbf{r}) \lambda_{\alpha}(\mathbf{r}) \right] \right\rangle \right\rangle_{\rho_2, \rho_1^{\alpha}} .$$

Average over ρ_1^{α} and ρ_2 by cumulant expansions.

$$\Omega[p_c(\mathbf{r})] = -T \int \prod_{\alpha} \frac{\mathcal{D}\lambda_{\alpha}}{2\pi} \exp \left[i \sum_{\alpha} \int d\mathbf{r} \lambda_{\alpha}(\mathbf{r}) p_c(\mathbf{r}) \right] \\ \times \left\langle \left\langle \exp \left[-i \sum_{\alpha} \int d\mathbf{r} \delta\rho_1^{\alpha}(\mathbf{r}) \delta\rho_2(\mathbf{r}) \lambda_{\alpha}(\mathbf{r}) \right] \right\rangle \right\rangle_{\rho_2, \rho_1^{\alpha}}.$$

Average over ρ_1^{α} and ρ_2 by cumulant expansions. The integrals can be expressed in terms of liquid-state correlation functions like

$$G(\mathbf{r}_1, \mathbf{r}_2) = \langle \delta\rho(\mathbf{r}_1) \delta\rho(\mathbf{r}_2) \rangle, \quad G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \langle \delta\rho(\mathbf{r}_1) \delta\rho(\mathbf{r}_2) \delta\rho(\mathbf{r}_3) \rangle.$$

$$\Omega[p_c(\mathbf{r})] \simeq -T \int \prod_{\alpha} \frac{\mathcal{D}\lambda_{\alpha}}{2\pi} \exp \left[i \sum_{\alpha} \int d\mathbf{r} \lambda_{\alpha}(\mathbf{r}) p_c(\mathbf{r}) \right] \\ \times \exp \left[-\frac{1}{2} \int d1 d2 G^2(1, 2) \sum_{\alpha} \lambda_{\alpha}(1) \lambda_{\alpha}(2) \right] \\ \times \exp \left[\frac{i}{6} \int d1 d2 d3 G^2(1, 2, 3) \sum_{\alpha} \lambda_{\alpha}(1) \lambda_{\alpha}(2) \lambda_{\alpha}(3) \right]$$

Define $q_{\alpha\beta}(\mathbf{r}) = \lambda_{\alpha}(\mathbf{r})\lambda_{\beta}(\mathbf{r})$ for $\alpha \neq \beta$. Insert into the expression for Ω the identity

$$1 = \int \prod_{\alpha < \beta} \mathcal{D}q_{\alpha\beta} \int \prod_{\alpha < \beta} \frac{\mathcal{D}u_{\alpha\beta}}{2\pi} \exp[i \sum_{\alpha < \beta} \int d\mathbf{r} u_{\alpha\beta}(\mathbf{r}) (q_{\alpha\beta}(\mathbf{r}) - \lambda_{\alpha}(\mathbf{r})\lambda_{\beta}(\mathbf{r}))]$$

Trace out the λ_{α} fields. To cubic order in $u_{\alpha\beta}$,

$$\begin{aligned} \Omega[p_c(\mathbf{r})] &\sim -T \int \prod_{\alpha < \beta} \mathcal{D}q_{\alpha\beta} \int \prod_{\alpha < \beta} \frac{\mathcal{D}u_{\alpha\beta}}{2\pi} \exp[i \sum_{\alpha < \beta} \int d\mathbf{r} u_{\alpha\beta}(\mathbf{r}) q_{\alpha\beta}(\mathbf{r})] \\ &\times \exp\left[\frac{i}{2} \sum_{\alpha < \beta} \int d1d2d3 A(1, 2, 3) u_{\alpha\beta}(1) p_c(2) p_c(3)\right] \\ &\times \exp\left[-\frac{1}{2} \sum_{\alpha < \beta} \int d1d2 B(1, 2) u_{\alpha\beta}(1) u_{\alpha\beta}(2)\right] \\ &\times \exp\left[\frac{i}{6} \sum_{(\alpha, \beta, \gamma)} \int d1d2d3 C(1, 2, 3) u_{\alpha\beta}(1) u_{\beta\gamma}(2) u_{\gamma\alpha}(3)\right] \\ &\times \exp\left[\frac{i}{6} \sum_{\alpha < \beta} \int d1d2d3 D(1, 2, 3) u_{\alpha\beta}(1) u_{\alpha\beta}(2) u_{\alpha\beta}(3)\right]. \end{aligned}$$

The coefficients A, B, C and D are given, to the lowest order, by

$$A(1, 2, 3) \simeq K(1, 3)K(2, 3),$$

$$B(1, 2) \simeq K^2(1, 2),$$

$$C(1, 2, 3) \simeq K(1, 2)K(2, 3)K(3, 1),$$

$$D(1, 2, 3) \simeq - \int \prod_{i=4}^9 dr_i G^2(4, 5, 6)G^2(7, 8, 9) \\ \times K(1, 4)K(1, 7)K(2, 5)K(2, 8)K(3, 6)K(3, 9).$$

K is defined via

$$\int d3K(1, 3) [G^2(3, 2)] = \delta(12).$$

All these coefficients are in principle calculable from liquid state theory.

Finally we trace out the $u_{\alpha\beta}$ to get an effective Hamiltonian $H[q_{\alpha\beta}]$.

The Glass Transition Functional

$$\Omega[p_c] \sim \int \prod_{\alpha < \beta} \mathcal{D}q_{\alpha\beta} \exp[-H[q]].$$

There are terms in $H[q_{\alpha\beta}]$ like $p_c^{2k} q_{\alpha\beta}^{k'}$ with integers k and k' i.e. H is an **even** function of $p_c(\mathbf{r})$. $p_c(\mathbf{r})$ is determined from the condition

$$\delta\Omega/\delta p_c = 0,$$

so $p_c(\mathbf{r}) = 0$ is always a solution and holds in the **liquid phase**. Then to cubic order

$$H[q] = \int d\mathbf{r} \left\{ \frac{c}{2} \sum_{\alpha < \beta} (\nabla q_{\alpha\beta}(\mathbf{r}))^2 + \frac{t}{2} \sum_{\alpha < \beta} q_{\alpha\beta}^2(\mathbf{r}) - \frac{w_1}{6} \text{Tr} q^3(\mathbf{r}) - \frac{w_2}{3} \sum_{\alpha < \beta} q_{\alpha\beta}^3(\mathbf{r}) \right\}.$$

The coefficients c , t , w_1 and w_2 will be functions of the temperature and density of the liquid, with smooth dependence on them.

Properties of the Functional

- The **same** replica functional arises in studies of the p-spin model (and also Potts models).
- If $w_2/w_1 > 1$ there are two transitions at mean-field level, a dynamic transition at T_A and a **first-order** thermodynamic glass transition at T_K (below which $p_c(\mathbf{r})$ becomes non-zero).

0----- T_K ----- T_A -----

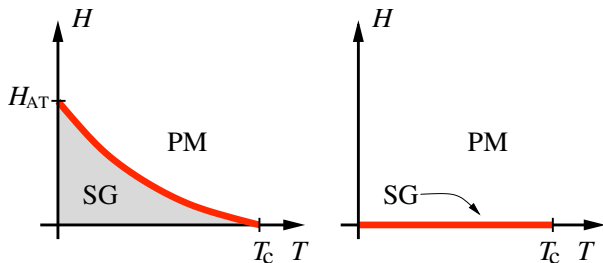
- Glass phase ($T < T_K$) has one-step replica symmetry breaking (1RSB) order.
- Above T_A , dynamics parallels that in mode-coupling theory.

Beyond the mean-field approximation

- Outside mean-field theory no true dynamical transition T_A exists as true metastable states do not exist in finite dimensions.
- Outside mean-field theory **the 1RSB phase below T_K does not exist.** It is destroyed by thermal excitation of large droplets: the free energy cost of a droplet of linear extent L falls as $\exp(-L/\xi)$.
- Numerical studies of the 10-state Potts models in three dimensions: no sign of MCT like effects or a glass transition or growing lengthscales. (All visible at mean-field level).
- When $w_2/w_1 < 1$ a continuous transition to a glass state with full RSB can exist at least if $d \geq 6$.
Moore and Drossel showed that this transition (if any) was in the **same universality class as that of an Ising spin glass in a field.**

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} S_i S_j - h \sum_i S_i.$$

- de Almeida-Thouless (AT) line at which there is a continuous ‘replica symmetry breaking transition’. Exists at mean-field level and possibly for all $d > 6$?
- No transition for $d < 6$ (Moore 2005) – based on perturbative analysis of diagrams.
- Bray and Roberts (1981) failed to find a fixed point in an ϵ expansion in $6 - \epsilon$ dimensions – no transition when $d < 6$?



- Replicated spin glass functional in a field:

$$H[q] = \int d\mathbf{r} \left\{ \frac{c}{2} \sum_{\alpha < \beta} (\nabla \tilde{q}_{\alpha\beta}(\mathbf{r}))^2 + \frac{t}{2} \sum_{\alpha < \beta} \tilde{q}_{\alpha\beta}^2(\mathbf{r}) - \frac{w_1}{6} \text{Tr} \tilde{q}^3(\mathbf{r}) - h^2 \sum_{\alpha < \beta} \tilde{q}_{\alpha\beta}(\mathbf{r}) \right\}.$$

- The Edwards-Anderson order parameter is $\tilde{q} = \sum_i \langle S_i \rangle^2 / N$ and is always non-zero when $h \neq 0$.
- We will take $T \approx T_0 \ll T_c$, so \tilde{q} is ≈ 1 .
- Then the term in the glass functional

$$\frac{w_2}{3} \sum_{\alpha < \beta} q_{\alpha\beta}^3 \approx \frac{w_2}{3} \sum_{\alpha < \beta} \langle q_{\alpha\beta}^2 \rangle q_{\alpha\beta} \approx h^2 \sum_{\alpha < \beta} q_{\alpha\beta}.$$

so

$$h^2 \sim \frac{w_2}{3} \langle q_{\alpha\beta}^2 \rangle \sim w_2$$

as when $T \approx T_0 \ll T_c$, $\langle q_{\alpha\beta}^2 \rangle \sim \text{constant}$, independent of α and β .

Numerical Studies of Ising Spin Glass in a Field

Lengthscales in real glasses have not become **large enough** to apply droplet scaling ideas.

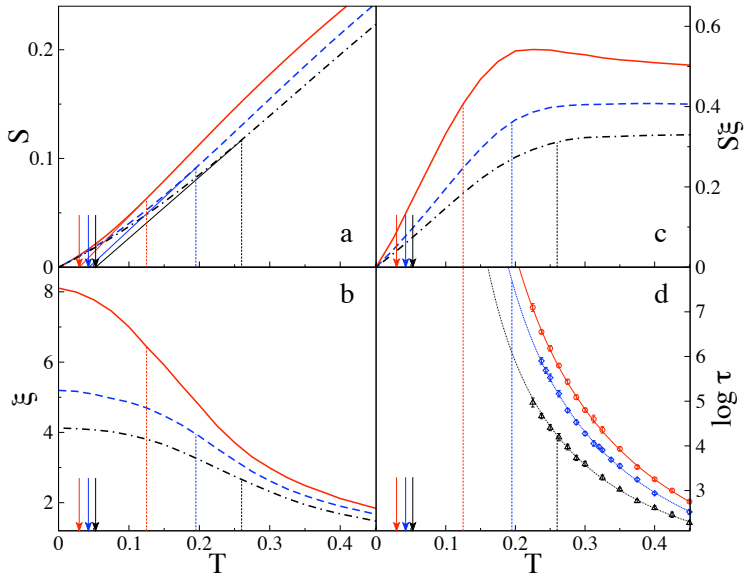
One-dimensional Ising spin glass – useful illustration:

$$\mathcal{H} = - \sum_i J_i S_i S_{i+1} - h \sum_i S_i.$$

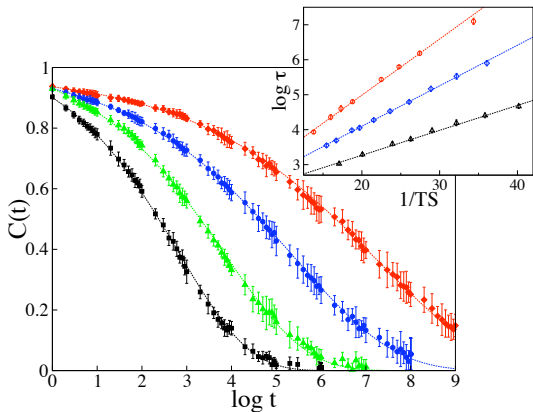
Size of domains (droplet scaling): ξ at $T = 0$: $J\xi^\theta \sim h\xi^{d/2}$

For $d = 1$, $\theta = -1$, so $\xi \sim h^{-2/3}$

$\xi(T)$ and S can be **exactly** calculated by RG decimation.



Relaxation time τ : $\langle S_i(t_W)S_i(t + t_W) \rangle_c \sim \exp(-(t/\tau)^\beta)$

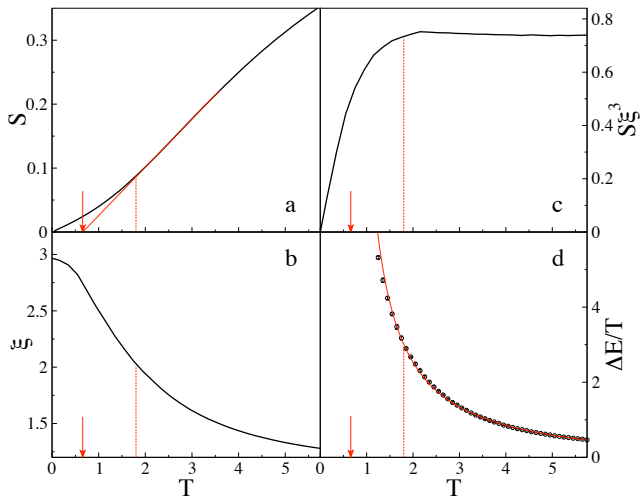


Vogel-Fulcher fit: $\tau = \tau_0 \exp[A/(T - T_0)]$

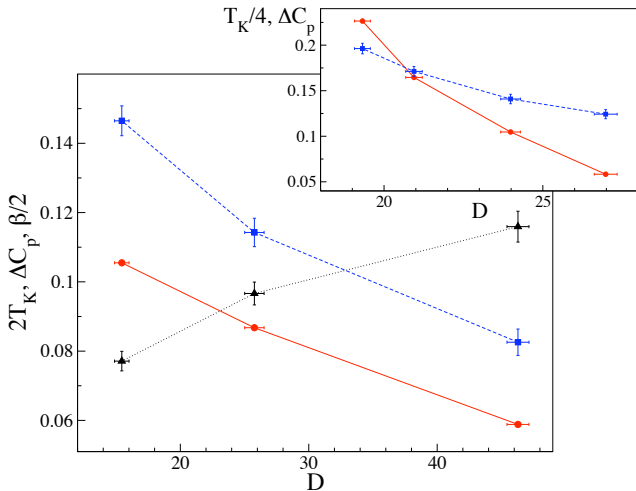
- T_0 is similar to T_K .
- **But all this is curve-fitting!**

There will be no singularity at T_0 .

Three dimensions: Midgal-Kadanoff approximation



β , ΔC_p , T_K versus fragility D in $d = 1$ and $d = 3$.



$\Delta C_p \sim 1/D$ experimentally.

- A functional can be derived from liquid state theory which maps the glass transition problem onto the Ising spin glass problem in a field
- Droplet arguments predict that lengthscales should increase up to some maximum as the temperature decreases in fragile glasses, but at T_g lengthscales may not be large enough for asymptotic droplet scaling formulae to be appropriate.
- Conventional fits, (Vogel-Fulcher, Kauzmann, Adams-Gibbs) 'work' in this pre-asymptotic region