

The Thermodynamic Glass Transition

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Introduction and motivation

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- 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 as $T \rightarrow T_0$.

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- We shall produce a formalism which maps onto the Ising spin glass in a field and then use the **droplet model of spin glasses** to understand the properties of structural glasses.

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between two configurations of density variations $\delta\rho = \rho - \langle\rho\rangle$ in **two copies** of the liquid.

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Use an integral representation of the delta function.

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

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

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

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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

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

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

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

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

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All these coefficients are in principle calculable from liquid state theory. Finally we trace out the $u_{\alpha\beta}$ to get an effective Hamiltonian $H[q_{\alpha\beta}]$.

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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.

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- Outside mean-field theory no true dynamical transition anyway exists as true metastable states do not exist in finite dimensions.
- 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).

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$J_{ij}^{(1)}$ etc. are quenched random couplings between nearest-neighbour sites on which two kinds of Ising spins σ_i and τ_i sit.

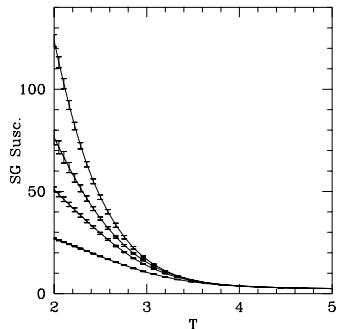
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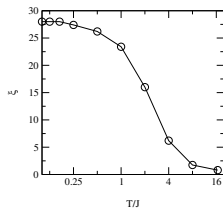
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- This Hamiltonian has the **same** effective replicated functional as we derived for liquids, with $w_2/w_1 < 1$.

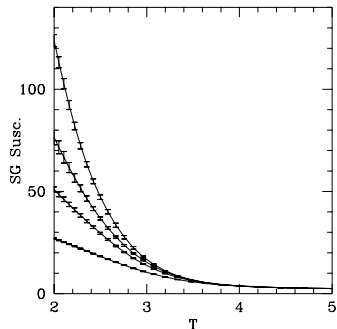
Simulations ($d = 4$)
(Parisi et al.)



MK approximation (for $d = 3$)
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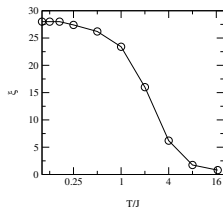


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$L = 3, 4, 5, 6$

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Infinite system

Reduction to Ising spin glass in a field

- $\langle q_{\alpha\beta} \rangle$ is non-zero **even in the liquid state** because of the term in w_2 in $H[q]$.

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- Outside the mean-field limit the low temperature state has full RSB. (The one step RSB is associated with the first-order transition which arises when $w_2/w_1 > 1$.)
- 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**.

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

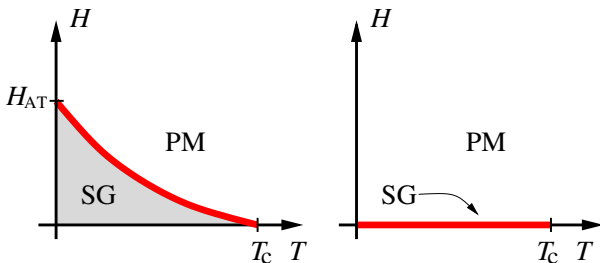
- For $h = 0$ there is a transition at temperature T_c at least for $d \geq 3$.

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

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

Use of Droplet Scaling Ideas

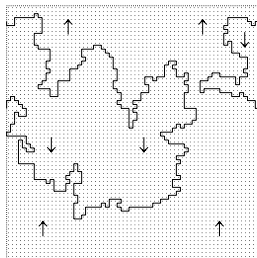
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(From Hartmann and Young. NB Droplet surfaces are fractal.)

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- Then $\frac{L^*}{\xi(T)} \sim \frac{1}{h^{\frac{2}{d-2\theta}}}$ is large if h is small.

- Since $w_2 \approx h^2$ and as we expect w_2 to be a function of the temperature T (and density) of the liquid, a simple form for h^2 is

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- Time scale to create a droplet of size L^* is of Arrhenius form:

$$\tau \sim \tau_0 \exp[B(L^*)/T].$$

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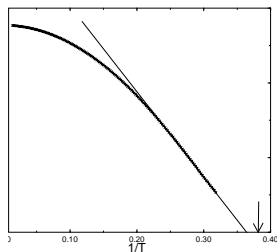
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- Its form could be probed by studies of the four-point density correlation functions at different times.

The Configurational Entropy



(Parisi et al. – the 4d p-spin model)

The droplet picture can also be used to obtain the configurational entropy.

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- The calculation explains the apparent coincidence of the Kauzmann temperature T_K at which the entropy vanishes, and the Vogel-Fulcher temperature T_0 .