The glass transition as a spin glass problem

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Regimes of Liquid/Glass Physics

- Cryogenic anomalies
- Non-Equilibrium State
- Energy Landscape Dominated Transport
- Collisional Transport

Temperature markers:
- $T_D/30$
- $T_D$
- $T_K$
- $T_g$
- $T_m$
- $T_A$
- $T_v$
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 behavior on long lengthscales and timescales

Long lengthscales are probably 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.
Some Glass Phenomenology

- **Vogel-Fulcher law**

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

  In truth just ‘curve-fitting’.

- **Relaxation time(s)** \( \tau \sim \eta \).

- **Kauzmann Paradox**: Configurational entropy per molecule apparently goes to zero at \( T_K \)

  \[ s_c(T) \sim k_B(1 - T_K/T) \sim \Delta C_p(1 - T_K/T) \sim (1 - T_K/T)/D. \]

- 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.

- But at \( T_g \), \( L^*(T) \) is only a few particle diameters.
“Equilibrium” near $T_K$ or $T_0$ cannot be obtained due to freezing into an amorphous solid on experimental time scales.

Consequence: experimental lengthscales cannot be made large and evidence for universality and well-defined power laws will (always?) remain weak.
The thermodynamic transition

- The apparent divergence of $\eta$ 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 the above suggest a transition as $T \to T_0$.

- We will argue the transition is in the universality class of the Ising spin glass in a field $h(T)$ as $h(T) \to 0$.
  (For all $T < T_c$, there is a line of critical points at $h = 0$ when $d < 6$).
- Lengthscales get large when $h(T)$ gets small: $h(T)^2 \sim (T - T_0)$.
- The spin glass transition temperature in zero field $T_c \approx T_A$. 
Glass theories

- Locally geometrically frustrated systems; \( \Rightarrow \) an avoided transition. Explain simply the existence of supercooling.
- Kinetically contrained dynamical models.
- RFOT theory of Wolynes and co-workers. A theory at the level of molecules (a “+”), whose underlying physics related to that of the “p-spin” model in the infinite dimensional limit e.g. use of the “mosaic” picture.
- Mapping to an Ising spin glass in a field. (Not a theory at the level of molecules, (a “−”).

The p-spin model maps to this when treated as a three dimensional system. It allows prediction of the universal exponents \( \psi, \theta, d_s \) etc.

\[
\tau \sim \exp \left[ B_0 L(T)^\psi / k_B T \right], \quad L(T) \sim \left[ \frac{1}{T - T_0} \right]^{\frac{1}{d - 2\theta}}
\]

\( d_s \) is the fractal dimension of the dynamically active regions in \( \alpha \)-relaxation processes.
Effective Potential Formalism

(cf Franz and Parisi, Dzero et al.)

- Define the overlap
  
  \[ p_c(r) = \delta \rho_1(r) \delta \rho_2(r) \]

  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:

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

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

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

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

  \[ \ln Z = \lim_{n \to 0} \left( Z^n - 1 \right) / n. \]
Use an integral representation of the delta function.

\[
\Omega[p_c(r)] = -T \int \prod_{\alpha} \frac{D\lambda_\alpha}{2\pi} \exp \left[ i \sum_\alpha \int d\mathbf{r} \lambda_\alpha(\mathbf{r}) p_c(\mathbf{r}) \right]
\]

\[
\times \left\langle \left\langle \exp \left[ -i \sum_\alpha \int d\mathbf{r} \delta \rho_1^\alpha(\mathbf{r}) \delta \rho_2(\mathbf{r}) \lambda_\alpha(\mathbf{r}) \right] \right\rangle_{\rho_2} \right\rangle_{\rho_1^\alpha}.
\]

Define \( q_{\alpha\beta}(\mathbf{r}) = \lambda_\alpha(\mathbf{r}) \lambda_\beta(\mathbf{r}) \) for \( \alpha \neq \beta \). Trace out the \( \lambda_\alpha, \rho_1^\alpha \) and \( \rho_2 \) fields using cumulant averaging (and further integral representations).

\[
\Omega[p_c] \sim \int \prod_{\alpha<\beta} Dq_{\alpha\beta} \exp[-H[q]].
\]

\( p_c(\mathbf{r}) \) is determined from the condition \( \delta \Omega / \delta p_c = 0 \).

\( H[q_{\alpha\beta}] \) is an even function of \( p_c(\mathbf{r}) \) so \( p_c(\mathbf{r}) = 0 \) is always a solution and this describes the liquid phase. But at the “transition”, \( T = T_0 \), \( \delta \Omega / \delta p_c = 0 \) gives

\[
\lim_{t \to \infty} < \delta \rho(\mathbf{r}, t) \delta \rho(\mathbf{r}, t = 0) > = q_{EA} = p_c.
\]
To cubic order when $p_c(r) = 0$

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

- The coefficients $c$, $\tau$, $w_1$ and $w_2$ will be functions of the temperature $T$ and density of the liquid, with smooth dependence on them.

- If one knows the correlation functions of the liquid, then in principle one could determine these parameters.

- The transition is usually driven by $\tau$ changing sign as a function of temperature. Here the growing lengthscale will arise from $w_2$ going to zero: $w_2 \sim (T - T_0)$ in the ‘low-temperature’ regime $\tau < 0$.

- The $w_2$ term breaks time-reversal invariance.

- The physical significance of $q_{\alpha\beta} = \lambda_\alpha \lambda_\beta$ is not simple!
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 $p_c(r)$ becomes non-zero).

![Temperature Scale]

- 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 length scales. (All visible at mean-field level).
- When $w_2/w_1 < 1$ a continuous transition to a glass state with full RSB exists at mean-field level. Moore and Drossel (2003), Moore and Yeo (2006) showed that this transition was in the same universality class as that of an Ising spin glass in a field.

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij}S_iS_j - h \sum_i S_i, \quad w_2 \sim h(T)^2$$
Ising spin glass in a field

- 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 AT transition for $d < 6$ (Moore 2005) where the loop expansion around the mean-field theory fails.
- For $d < 6$, a transition arises only if $h(T) \to 0$. The whole line $T < T_c$ is critical i.e. the correlation length is infinite.
Droplet scaling

- The lengthscale $L(T)$ is the size of a compact region, (containing $\sim L^d$ spins) in which the spins flip to lower their magnetic energy.
- Domain wall energy $\sim L^\theta$, $\theta \approx 0.2$ when $d = 3$.
- Magnetic field energy gained $\sim h(T)L^{d/2}$
- Equating these two energies – the Imry-Ma argument

$$L(T) \sim \left[ \frac{1}{h(T)^2} \right]^{\frac{1}{d-2\theta}} \sim \left[ \frac{1}{T - T_0} \right]^{\frac{1}{d-2\theta}} \sim \left[ \frac{1}{T - T_0} \right]^{0.4}$$

- Contrast with the mosaic picture: $\gamma(T)L(T)^{d-1} \sim s_c(T)L^d$.
- Barrier against flipping $B(T) \sim B_0L(T)^\psi$, $\psi$ not yet determined.
- From Arrhenius

$$\tau \sim \tau_0 \exp \left[ \frac{B(T)}{k_B T} \right] \sim \tau_0 \exp \left[ \frac{DT_0}{T - T_0} \right]^{0.4\psi}$$
The broken symmetry of the glass transition

The transition arises from taking the field $h(T)$ to zero as $T \to T_0$. At $h = 0$, the Ising spin glass Hamiltonian has time-reversal invariance (up-down symmetry).

At the level of molecules the transition is driven by $w_2$ going to zero at $T_0$. There must be an extra symmetry in the system at this temperature.

What is it? Particle-hole symmetry?

Notice that $\langle q_{\alpha\beta} \rangle = \langle \lambda_{\alpha} \lambda_{\beta} \rangle$ is non-zero at all $T$. 
The p-spin version of the RFOT and the Ising spin glass in a field have the same starting functional.

The mapping to the Ising spin glass in a field applies when the loop corrections destroy the mean-field character of the transition.

The RFOT and mosaic pictures will be OK in a regime not too close to $T_0$ where loop corrections might be small.

The existence of such a regime would seem to require the existence of “long-range” interactions.

This does not imply that the intermolecular interactions have to be long-ranged, but just that the parameters $c, \tau, w_1, w_2$ in the functional are such as to make loop corrections small and $w_2/w_1 > 1$ when $T \approx T_A$.

‘Success’ of MCT and RFOT theories suggest that this might be the case! Then only as $T \rightarrow T_0$ would the crossover to Ising spin glass behaviour in a field emerge.
Numerical Studies of Ising Spin Glass in a Field

3d spin glasses in a field are being studied by Peter Young. One-dimensional Ising spin glass – useful illustration of some points:

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

In \( d = 1 \) there is no spin glass phase. \( h(T) \) was kept temperature independent, (so entropies are too low to be “realistic”). Glass-like features emerge because of a growing lengthscale as \( T \) is reduced. Size of domains saturates at a lengthscale: \( \xi \) 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 $\tau$: $\langle S_i(t_W)S_i(t + t_W) \rangle_c \sim \exp(-(t/\tau)^\beta)$

- **Vogel-Fulcher fit** $\tau = \tau_0 \exp[A/(T - T_0)]$ with $T_0$ similar to $T_K$ works!
- **Stretched exponential exponential exponent** $\beta$ arises because there is a range of relaxation times.
Conclusions

- 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 as the temperature decreases, 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) may ‘work’ in this pre-asymptotic region as well as (possibly) RFOT ideas.