Ginzburg criterion for the dynamical glass transition

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Outline

1. The random first order transition framework
2. Landau theory and gradient expansion
3. Ginzburg criterion
4. Numerical results and discussion

A path towards a theory of the glass transition

Theory of second order PT (gas-liquid)

- Qualitative MFT (Landau, 1937)
  Spontaneous Z_2 symmetry breaking
  Scalar order parameter
  Critical slowing down

- Quantitative MFT (exact for $d \to \infty$)
  Liquid-gas: $\beta p/\rho = 1/(1-\rho b) - \beta a \rho$
  (Van der Waals 1873)
  Magnetic: $m = \tanh(\beta J m)$
  (Curie-Weiss 1907)

- Quantitative theory in finite d (1950s)
  (approximate, far from the critical point)
  Hypernetted Chain (HNC)
  Percus-Yevick (PY)

- Corrections around MFT
  Ginzburg criterion, $d_u = 4$ (1960)
  Renormalization group (1970s)
  Nucleation theory (Langer, 1960)

Theory of the liquid-glass transition

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  Spontaneous replica symmetry breaking
  Order parameter: overlap matrix q_{ab}
  Dynamical transition "à la MCT"

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  Kirkpatrick and Wolynes 1987
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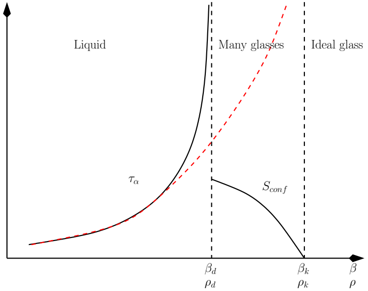
Qualitative MFT of the glass transition



Free energy functional $F[\rho(x)]$ – to be minimized

Three temperature regimes (Kirkpatrick-Thirumalai-Wolynes, 1987-1989)

1. $T > T_d$: one single minimum with $\rho(x) = \rho$, the liquid state – finite $\tau_\alpha \sim (T - T_d)^{-\gamma}$
2. $T_k < T < T_d$: $S_{conf} > 0$, an exponential number of states – infinite τ_α
   The superposition of all glasses is the liquid: no phase transition
3. $T < T_k$: $S_{conf} = 0$, infinite τ_α
   A thermodynamic transition to the ideal glass happens at T_k

The dynamical (Mode-Coupling) transition

The mean-field dynamical transition is characterized by strong ergodicity breaking and infinite barriers

- Apparent divergence $\tau \sim (T - T_d)^{-\gamma}$ and associated MCT phenomenology
- Finite configurational entropy below T_d
- Diverging dynamical susceptibility χ_4 around T_d, associated to a large dynamical correlation length ξ_4 (dynamical heterogeneities)
- Similar to a spinodal: $f = f_c + \sqrt{T - T_d}$ (jump + power law)

Not in finite dimensions: barriers must be finite and can be crossed by thermal activation

- The dynamical transition becomes a crossover, where dynamics slows down but without complete arrest (again, similar to a spinodal)
- The transition is still clearly visible in high enough dimensions ($d \geq 4$)
- In $d = 2, 3$ ergodicity breaking is much more mixed with activation: ambiguity in the identification of the mean-field regime
- Several “remnants” of the mean-field transition are observed in low dimensions, in particular a strongly increasing χ_4 and ξ_4 around T_d
- The value of the exponents associated to the four-point susceptibility is debated

Our aim is to study the critical properties of the dynamical transition *as if it were a true transition*, **hence neglecting activation**

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Landau theory – ferromagnet

Landau theory can be derived from the high temperature expansion

- d-dimensional ferromagnet: $H = -\frac{1}{2d} \sum_{\langle i,j \rangle} S_i S_j$
- Order parameter: $m_i = \langle S_i \rangle$
- The free energy $F[m]$ can be computed by a small β expansion (Georges-Yedidia 1991):
  $$-\beta F[m] = -\sum_i \left(\frac{1+m_i}{2} \log \frac{1+m_i}{2} + \frac{1-m_i}{2} \log \frac{1-m_i}{2} \right) + \frac{\beta}{2d} \sum_{\langle i,j \rangle} J_{ij} m_i m_j + \frac{\beta^2}{8d^2} \sum_{\langle i,j \rangle} (1-m_i^2)(1-m_j^2) + \dots$$
- Note: the series in β is actually a series in β/d, and mean field theory is obtained *by truncating this series at any finite order*
- Expansion at weakly non-uniform and small m_i gives
  $$-\beta F[m] \sim \sum_i (\epsilon m_i^2 + g m_i^4) + \sum_{\langle i,j \rangle} \sigma (m_i - m_j)^2 + \cdots \sim \int dxdy\, m(x) M(x-y) m(y) + g \int dx m(x)^4$$
  ϵ, g, σ can be computed as series in β
- From $\epsilon \sim (T - T_c)$ and $g \sim 1$ we obtain $\langle m \rangle \sim |\epsilon|^{1/2}$
- The correlation function is $\langle S_i S_j \rangle = \left[\frac{d^2 F}{dm_i dm_j} \right]^{-1} \sim \langle m(x) m(y) \rangle = M^{-1}(x-y)$

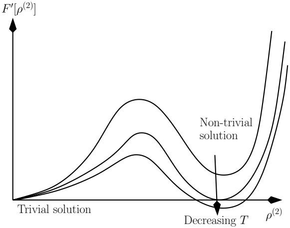
  Gradient expansion $M(p) \sim \epsilon + \sigma p^2 + \cdots$, hence $M^{-1}(p) = \frac{1}{\epsilon + \sigma p^2} = \frac{1/\epsilon}{1 + \sigma (p/\sqrt{\epsilon})^2}$
  - Correlation: $\langle S_i S_j \rangle = M^{-1}(x-y) \sim e^{-|x-y|/\xi}$ with $\xi \sim |\epsilon|^{-1/2}$
  - Susceptibility: $\chi = \frac{dm}{dh} = M^{-1}(p=0) = 1/\epsilon$

Landau theory – glass

Landau theory can be derived from the high temperature/low density (virial) expansion

- Particle system: $H = \sum_{ij} v(r_i - r_j)$
- No obvious static order parameter
  Consider m replicas and take the correlation between two replicas as the order parameter
  $\rho_a(x)$ density of replica a – $\rho^{(2)}_{ab}(x,y)$ correlation between replicas a and b
- Morita and Hiroike 1961: $F[\rho,\rho^{(2)}] = F_{\rm id}[\rho,\rho^{(2)}] + F_{\rm ring}[\rho,\rho^{(2)}] + F_{\rm 2PI}[\rho,\rho^{(2)}]$
  $F_{\rm id}[\rho,\rho^{(2)}]$ and $F_{\rm ring}[\rho,\rho^{(2)}]$ can be written explicitly
  $F_{\rm 2PI}$ is the sum of all two-particle irreducible diagrams
- Instead of truncating at a finite order here we drop $F_{\rm 2PI}$: HNC approximation
  Note that what follows remains true for any other approximation scheme that gives the correct mean-field phenomenology

At the mean-field level:
• above T_d, $\rho^{(2)} = \rho^2$, no correlation;
• below T_d, a non-trivial $\rho^{(2)}$ is found ;
The transition is a bifurcation at finite $\rho^{(2)}$, akin to a spinodal, hence
$\rho^{(2)}(x,y) = \rho^{(2)}_c(x,y) + 2\rho^2\kappa\sqrt{\epsilon}k_0(x,y)$
$\epsilon = T - T_d$



Landau theory – the mass matrix and the zero mode

- The order parameter is not a one-point function $m(x)$, but a *two-point function* $\rho^{(2)}_{ab}(x,y)$.
- The inverse correlation is *a four-point function*
  $M_{ab;cd}(x_1,x_2;x_3,x_4) = \left. \frac{\delta^2 F[\rho,\rho^{(2)}]}{\delta\rho^{(2)}_{ab}(x_1,x_2)\delta\rho^{(2)}_{cd}(x_3,x_4)} \right|_{\overline{\rho}_{ab}}$
  and because of replica symmetry it has the form
  $M_{ab;cd} = M_1\left(\frac{\delta_{ac}\delta_{bd}+\delta_{ad}\delta_{bc}}{2}\right) + M_2\left(\frac{\delta_{ac}+\delta_{ad}+\delta_{bc}+\delta_{bd}}{4}\right) + M_3$
- Crucial property: k_0 is a *zero mode* of M_1 :
  $\int dx_3 dx_4\, M_1(x_1,x_2;x_3,x_4) k_0(x_3-x_4) = \mu\sqrt{\epsilon} k_0(x_1-x_2)$
  Remark: the operators M_2 and M_3 do not have zero modes.
- k_0 is translationally invariant. We can define
  $\Delta\rho^{(2)}_{ab}(p,q) = \int dx_1 dx_2\, e^{ip\left(\frac{x_1+x_2}{2}\right)+iq(x_1-x_2)}\Delta\rho^{(2)}_{ab}(x_1,x_2)$
  such that the translationally invariant sector corresponds to $p=0$.
- The quadratic part of the action becomes
  $\Delta_2 F = \frac{1}{2}\sum_{a\neq b\ c\neq d}\int\frac{dp\,dq\,dk}{(2\pi)^{3D}}\Delta\rho^{(2)}_{ab}(p,q) M^{(p)}_{ab;cd}(-q,-k)\Delta\rho^{(2)}_{cd}(p,k)$
  and in fact shows that different p sectors are uncorrelated.

Landau theory – gradient expansion

- $\Delta_2 F = \frac{1}{2}\sum_{a\neq b\ c\neq d}\int \frac{dp\,dq\,dk}{(2\pi)^{3D}} \Delta\rho^{(2)}_{ab}(p,q) M^{(p)}_{ab;cd}(-q,-k)\Delta\rho^{(2)}_{cd}(p,k)$
- Small p and small ϵ expansion of the operator $M^{(p)}_{ab;cd}(-q,-k)$:
  $\left[M_1^{(p)}\right]^{-1}(q,k) \simeq \frac{1}{\mu\sqrt{\epsilon}+\sigma p^2} k_0(q) k_0(k)$
- The correlation function is
  $G^{(p)}_{ab;cd}(q,k) = [M^{(p)}_{ab;cd}(-q,-k)]^{-1} = FT[\langle \Delta\rho^{(2)}_{ab}(x_1,x_2)\Delta\rho^{(2)}_{cd}(x_3,x_4)\rangle]$
  and its component have the critical behavior:
  $G_1^{(p)} = \left[M_1^{(p)}\right]^{-1}$
  $G_2^{(p)} \sim 2\left[M_1^{(p)}\right]^{-1}$
  $G_3^{(p)} \sim \left[M_1^{(p)}\right]^{-1} \otimes \left\{M_2^{(p)} - M_3^{(p)}\right\} \otimes \left[M_1^{(p)}\right]^{-1}$
  and because M_2 and M_3 are not critical, the critical behavior is dominated by M_1.
  Note the double pole in G_3.
- In experiments one always "smooths" the density field with some function $f(x)$:
  $G^{(f)}_{ab;cd}(p) = \int \frac{dq\,dk}{(2\pi)^{2D}} f(-q) f(-k) G^{(p)}_{ab;cd}(q,k)$
  Popular examples are a box function in real space, or a delta function in Fourier space, with k equal to the maximum of $S(k)$.

Landau theory – physical correlations

Connection replicas-physics:

- Local two-point correlation $\hat{C}(r,t) = \int dx\, f(x)\hat{\rho}\left(r+\frac{x}{2},t\right)\hat{\rho}\left(r-\frac{x}{2},0\right)$
- Two averages: $\langle \bullet \rangle$ over the dynamics, $\mathbf{E}$ over the initial condition
- Standard four-point function $G_4(r,t) = \mathbf{E}[\langle \hat{C}(r,t)\hat{C}(0,t)\rangle] - \mathbf{E}[\langle \hat{C}(r,t)\rangle]\mathbf{E}[\langle \hat{C}(0,t)\rangle]$
- Iso-configurational four-point function $G_{th}(r,t) = \mathbf{E}\left[\langle \hat{C}(r,t)\hat{C}(0,t)\rangle - \langle \hat{C}(r,t)\rangle\langle \hat{C}(0,t)\rangle\right]$
- In the glass phase (or in the β-regime), using replicas they correspond to
  $G_4(p,t\to\infty) = G^{(f)}_{ab;ab}(p) = [G^{(f)}_1(p) + G^{(f)}_2(p)]/2 + G^{(f)}_3(p)$
  $G_{th}(p,t\to\infty) = G^{(f)}_{ab;ab}(p) - G^{(f)}_{ab;ac}(p) = G^{(f)}_1(p)/2 + G^{(f)}_2(p)/4$
- We obtain:
  $G_{th}(p) \sim \frac{(f\star k_0)^2}{\mu\sqrt{\epsilon}+\sigma p^2} = \frac{G_0\epsilon^{-1/2}}{1+\xi^2 p^2}$
  $G_4(p) \sim \frac{A}{(\mu\sqrt{\epsilon}+\sigma p^2)^2} = \frac{G_0'\epsilon^{-1}}{(1+\xi^2p^2)^2}$
- Therefore

  $$\xi = \sqrt{\frac{\sigma}{\mu}}\epsilon^{-1/4} \qquad \chi_{th} \sim G_0\epsilon^{-1/2} \qquad \chi_4 \sim G_0'\epsilon^{-1}$$

  All the coefficients depend on the matrix M and the zero mode: they can be computed explicitly from the microscopic potential!

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Reminder of the Ginzburg criterion

- Bare (mean field) action: $S[\varphi] = \frac{1}{2}\int \mathrm{d}x\, \varphi(x)(\epsilon - \nabla^2)\varphi(x) + \frac{g}{4!}\int \mathrm{d}x \varphi^4(x)$
- At the mean field level $G_0(p) = \frac{1}{\epsilon + p^2}$ and $\chi = G_0(p=0) = \frac{1}{\epsilon} = \xi^2$
- With 1-loop corrections $\chi^{-1} = \epsilon + \frac{g}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{q^2+\chi^{-1}}$
- Critical point: $\chi^{-1} = 0 \quad \Rightarrow \quad \epsilon = -\frac{g}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{q^2} \quad \Rightarrow \quad \epsilon_{1L} = \epsilon + \frac{g}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{q^2}$
- Then $\epsilon_{1L} = \chi^{-1}\left(1 - \frac{g}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{q^2(q^2+\chi^{-1})}\right)$
- We want to impose that $\epsilon_{1L} \sim \chi^{-1}$ and the correction is small
- If $d < 4$, integral UV convergent, $\Lambda \to \infty$:
  $\epsilon_{1L} = \chi^{-1} - \frac{g}{2}\chi^{(2-d)/2}\frac{\Omega_d}{(2\pi)^d}\int_0^\infty \mathrm{d}x\, x^{d-1}\frac{1}{x^2(x^2+1)} = \chi^{-1} - g\, C_d\, \chi^{(2-d)/2}$
  The Ginzburg criterion is $\chi^{(4-d)/2} \ll 1/(gC_d)$ or $\xi^{4-d} \ll 1/(gC_d)$ and is *universal*
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  Mean field always qualitatively correct. For *quantitative* agreement the condition is
  $1 \gg \frac{g}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{q^2(q^2+\chi^{-1})}$
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Ginzburg criterion – glass

Ginzburg criterion for the glass transition

- We restrict to low-energy fluctuations along the zero mode: $\Delta\rho^{(2)}_{ab}(p,q) = \phi_{ab}(p)k_0(q)$
- We obtain an action for the field ϕ_{ab} whose coefficients can be computed microscopically
- Crucial result: the most divergent loop corrections are the same as those of a non-replicated cubic theory in random field
  $S(\varphi) = \frac{1}{2}\int \mathrm{d}x\, \varphi(x)(-\nabla^2 + m_0^2)\varphi(x) + \frac{g}{6}\int \mathrm{d}x \varphi^3(x) + \int \mathrm{d}x(h_0(x) + \delta h(g,\Delta))\varphi(x)$
  [Franz, Parisi, Ricci-Tersenghi, Rizzo, Eur. Phys. J. E. (2011)]
- Note: cubic theory because it is a spinodal point
  Random field encodes the "disorder" due to the initial condition
- Repeating the previous calculation for this theory we get
  $\epsilon_{1L} = \chi^{-1}\left(1 - 3\frac{\Delta g^2}{2}\int^\Lambda \frac{\mathrm{d}q}{(2\pi)^d}\frac{1}{(q^2+\chi^{-1})^4}\right)$
- The upper critical dimension is $d = 8$ and for $d < 8$ the Ginzburg criterion is
  $\mathrm{Gi}\,\xi^{8-D} \ll 1$ $\quad\quad\quad$ $\mathrm{Gi} = \frac{g^2\Delta}{4(4\pi)^{D/2}}\Gamma\left(4 - \frac{D}{2}\right)$
  and Gi can be computed microscopically.

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Numerical results in $d = 3$

Potential $v(r) = \varepsilon f(r/r_0)$
Lengths are given in units of r_0 and energies in units of ε, with $k_B = 1$.
Data at fixed temperature, with $\epsilon = \rho_{\rm d} - \rho$.

$$G_{th}(p) \sim \frac{G_0 \epsilon^{-1/2}}{1+\xi^2 p^2} \qquad \xi = \xi_0 \epsilon^{-1/4} \qquad \chi_{th} \sim G_0 \epsilon^{-1/2} \qquad \mathrm{Gi}\, \xi^{8-D} \ll 1$$

System	T	$\rho_{\rm d}$	λ	ξ_0	G_0	Gi
r^{-6}	1	6.691	0.348	0.601	224	0.0267
r^{-9}	1	2.912	0.353	0.548	34.3	0.0125
r^{-12}	1	2.057	0.354	0.498	14.2	0.0118
LJ	0.7	1.407	0.355	0.489	6.00	0.00833
HarmS	10^{-3}	1.336	0.359	0.315	2.82	0.0434
HarmS	10^{-4}	1.196	0.378	0.274	1.69	0.0632
HarmS	10^{-5}	1.170	0.382	0.278	1.66	0.0635
HS	–	1.169	0.381	0.280	1.67	0.0639

The Ginzburg criterion is $\xi \ll (1/\mathrm{Gi})^{1/5} \sim 2$, deviations from mean field should be observable
Quantitative results from replicated HNC are not very good (e.g. λ is off by a factor of 2)
We need to develop better approximation schemes (in progress)

Summary and discussion

- Landau theory and Ginzburg criterion of the dynamical (Mode-Coupling) transition, neglecting activation
- Diverging correlation length associated to dynamical heterogeneities, $\xi = \xi_0 \epsilon^{-1/4}$
- Singular four point correlations G_{th} and G_4 *with different critical behavior*
- Upper critical dimension $d_u = 8$
- Results consistent with the inhomogeneous Mode-Coupling theory (Biroli-Bouchaud-Miyazaki-Reichman) and with the results of Biroli-Bouchaud on the upper critical dimension
- The static (replica) formulation is convenient because it can be systematically improved
- To be tested numerically (in progress, with P.Charbonneau)

Thank you for your attention!