Behaviour of the length scale around the higher-order mode-coupling theory critical point

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work done with
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Bangalore, 2014

Mode-Coupling Theory (MCT)

- MCT: formulated in the 80's by Götze and coworkers.
- Gives equation of motion for time-dependent density autocorrelation function: $f_k(t) = \langle \delta\rho_k(t)\delta\rho_{-k}(0)\rangle / S_k$ where $\delta\rho_k(t)$ is the density fluctuation.

$$\frac{\partial^2 f_{\mathbf{k}}(t)}{\partial t^2} + D_L k^2 \frac{\partial f_{\mathbf{k}}(t)}{\partial t} + \frac{k_B T k^2}{S_k} f_{\mathbf{k}}(t) + \int_0^t m_{\mathbf{k}}(t-t') \dot{f}_{\mathbf{k}}(t') dt' = 0,$$

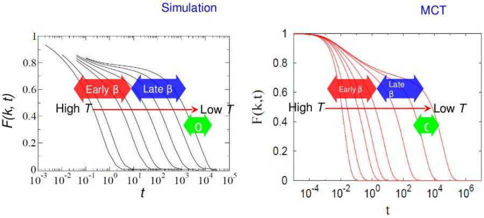
- $m_k(t) \rightarrow$ memory kernel

$$m_k(t) = \frac{k_B T \rho_0}{16\pi^3} \int d\mathbf{q} \left[\hat{k} \cdot (\mathbf{q} c_q + (\mathbf{k} - \mathbf{q}) c_{k-q}) \right]^2 S_q(t) S_{k-q}(t)$$

- Solve it numerically with $S_k = S_k(t = 0)$ as the input.

Pros and cons of MCT

Success:



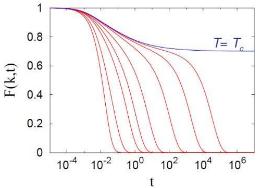
Failures of MCT:

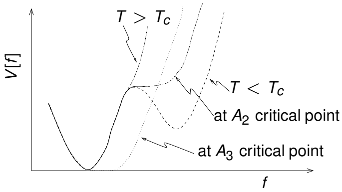
\# Over-estimation of transition point
\# Ergodic to non-ergodic transition
\# Power law predictions break down eventually at low T.

Early β regime: $f(t) \sim t^{-a}$
Late β regime: $f(t) \sim t^{-b}$.

	a	b
Experiment	0.328	0.646
MCT	0.312	0.583

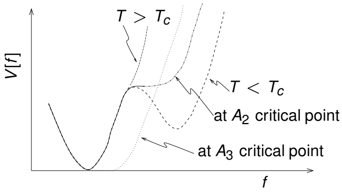
α-regime: $\eta \sim |T - T_{MCT}|^{-\gamma}$
and $\tau_\alpha \sim |T - T_{MCT}|^{-\gamma}$
with $\gamma = \frac{1}{2a} + \frac{1}{2b}$.





- $V[f]$: Landau free energy or the Franz-Parisi potential.
- Impossible (till now) to obtain $V[f]$ for the full k-dependent MCT, but easy for schematic MCT. However, always possible to write down $V'[f]$.

Definitions: A_2 and A_3 critical points:



- Connection with MCT: $V'[f] = \frac{f}{1-f} - \mathcal{F}[f]$
- A_2: $V'[f] = 0$ and $V''[f] = 0$ and $V'''[f] \neq 0$
- A_3: $V'[f] = 0$, $V''[f] = 0$ and $V'''[f] = 0$ and $V^{iv}[f] \neq 0$.
  Need at least two control parameters to reach the A_3 point.

Analysis for the glassy side (only schematic)

Expand $V'[f]$ around the transition point with $f = f_c + \delta f$:

$$V'[f_c] + \frac{\partial V'}{\partial f}\delta f + \frac{\partial^2 V'}{\partial f^2}(\delta f)^2/2 + \frac{1}{3!}\frac{\partial^3 V'}{\partial f^3}(\delta f)^3 + \frac{\partial V'}{\partial \epsilon}\cdot\delta\epsilon + \frac{\partial^2 V'}{\partial f \partial \epsilon}\cdot(\delta f \delta\epsilon)/2 + \ldots = 0, \quad (1)$$

Leading order:

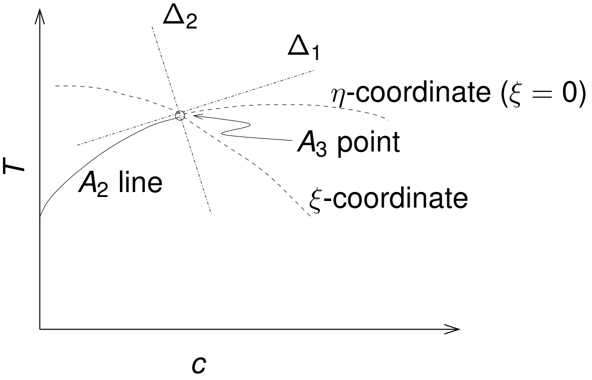
$$\frac{1}{3!}\frac{\partial^3 V'}{\partial f^3}(\delta f)^3 \sim \frac{\partial V'}{\partial \epsilon}\cdot\delta\epsilon \qquad \Rightarrow \delta f \sim (\delta\epsilon)^{1/3} \quad (2)$$

Special direction in phase space: If $(\partial V'/\partial\epsilon)\cdot\delta\epsilon = 0$:

$$\frac{1}{3!}\frac{\partial^3 V'}{\partial f^3}(\delta f)^3 \sim \frac{\partial^2 V'}{\partial f \partial \epsilon}\cdot(\delta f \delta\epsilon)/2 \qquad \Rightarrow \delta f \sim (\delta\epsilon)^{1/2} \quad (3)$$

Götze and Sjögren, J. Phys.: Condens. Matter **1**, 4203 (1989)

Special direction and choice of parameters



Condition $\frac{\partial V'}{\partial \epsilon} \cdot \delta\epsilon = 0$ is satisfied along the A_2 transition line.
Natural choice for generic control parameters: Δ_1 and Δ_2.
However, for technical reason (convenience of the calculation) we chose η and ξ.
These are equally good choices – why?

Behaviour of length scale (schematic again)

- Perturb the system with external field at wave-vector q_0. Obtain behaviour for a three-point correlator.
- Within schematic formulation: length scale behaves according to the variation of $\delta V''[f] = V''[f] - V''[f_c]$.
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$$V''(f) = V''(f_c) + \frac{\partial V''}{\partial f}\delta f + \frac{1}{2}\frac{\partial^2 V''}{\partial f^2}(\delta f)^2 + \ldots.$$

$$\text{Lowest order: } \delta V''(f) \simeq \frac{1}{2}\frac{\partial^2 V''}{\partial f^2}(\delta f)^2.$$

Due to rotational invariance, for non-zero q_0,
$\delta V''_{q_0}(f) \simeq \frac{1}{2}\frac{\partial^2 V''}{\partial f^2}(\delta f)^2 + q_0^2$.

$$\ell \sim q_0^{-1} \sim \begin{cases} \xi^{-1/3}, & \text{in general ,} \\ \eta^{-1/2}, & \text{if } \xi = 0. \end{cases} \tag{4}$$

Biroli, Bouchaud, Miyazaki and Reichman, PRL **97**, 195701 (2006)

Analysis for the liquid side: Results

- Relaxation times along the two directions:

$$\ln \tau_\beta^{(\xi)} \sim \xi^{-1/6}; \qquad \ln \tau_\beta^{(\eta)} \sim \eta^{-1/4} \tag{5}$$

- Scaling form for the three-point correlator:

$$\chi_{q_0}(\mathbf{q}, t) \simeq \frac{S_q w_q}{\alpha|\xi|^{2/3} + \Gamma q_0^2} \mathcal{G}\left(|\xi|^{1/6} \ln t, q_0/|\xi|^{1/3}\right), \quad \text{in general}, \tag{6}$$

$$\chi_{q_0}(\mathbf{q}, t) \simeq \frac{S_q v_q}{\alpha|\eta| + \Gamma q_0^2} \mathcal{G}\left(|\eta|^{1/4} \ln t, q_0/|\eta|^{1/2}\right), \quad \text{when } \xi = 0, \tag{7}$$

- There exists only β-regime, no α-regime around the A_3 point.

The critical dimension for this theory is 6.

Comparison with numerical solution: the model

- We tested on F_{13} $[= v_1 f(t) + v_3 f(t)^3]$ model.
- Transform v_1 and v_3 in terms of ξ and η.
- Numerically solve the model for both $f(t)$ and $\chi_{q_0}(t)$.

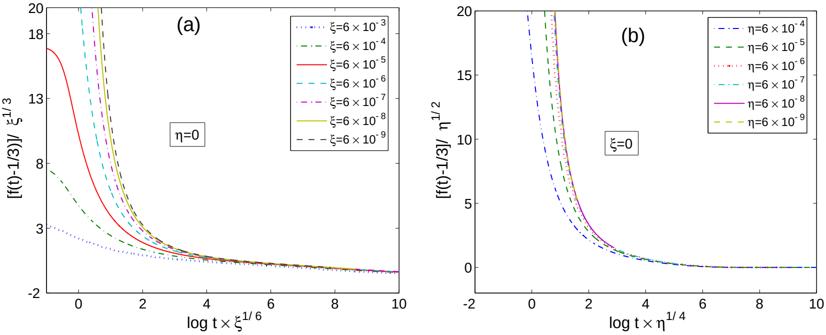

Figure : The scaling tests for two-point correlation function: (a) The logarithm of the relaxation time varies as $\xi^{-1/6}$ when $\eta = 0$ and $(f - f_c) \sim \xi^{1/3} p_I(\ln t/\ln\tau)$. The data collapse ensures that the scaling relations are valid. (b) Same as in (a) now along the η-line where $\xi = 0$. Here $\ln\tau \sim \eta^{-1/4}$ and $(f - f_c) \sim \eta^{1/2} p_{II}(\ln t/\ln\tau)$.

Numerical test: three-point function

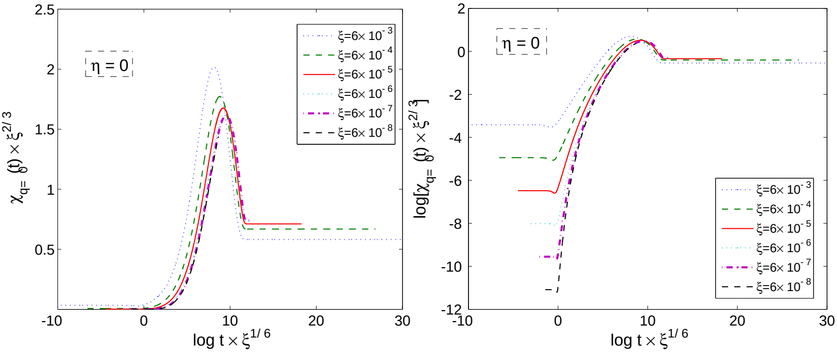

Figure : At $q_0 = 0$, if we plot $\chi_{q_0=0}(t)\xi^{2/3}$ as a function of $\xi^{1/6}$ ln t, the curves for different ξ should follow a master curve close to the critical point where ξ is very small. The figure in right is the same as in left with the y-axis being in logarithmic scale.

Numerical test: three-point function

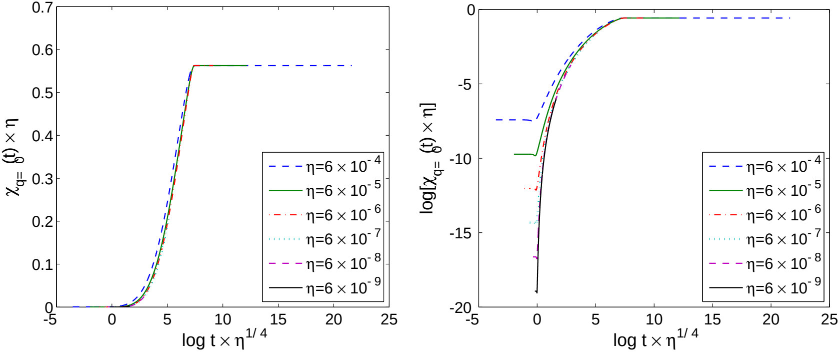

Figure : The scaling function of $\chi_{q_0=0}$ along the η-coordinate. The figure in the right is the same as in the left with the y-axis being in logarithmic scale.

Numerical test: non-zero q_0

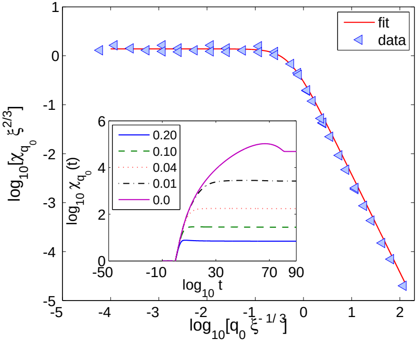

Figure : Length $\ell \sim \xi^{-1/3}$

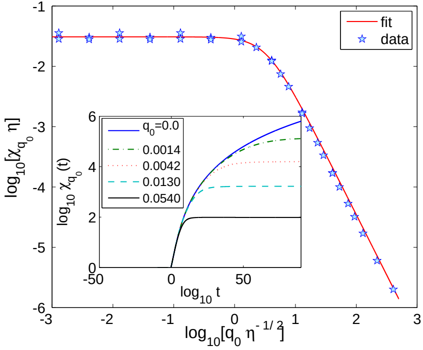

Figure : Length $\ell \sim \eta^{-1/2}$

Discussion

- At A_3 point: dynamic and thermodynamic transitions take place at the same time. If MCT is the correct mean-field theory, it must work better here.
  [Seems to be the case: R. Jack and C. J. Fullerton, PRE (2013)]
- Power law near A_2 point vs activated relaxation laws around A_3 point:
  MCT near A_2 line: $\tau \sim \xi^{\#}$.
  For activated dynamics: $\ln \tau \sim \xi^{\#}$
  Interesting point: MCT near A_3 point predicts activated relaxation laws.

Analogy with the phase diagram of RFIM

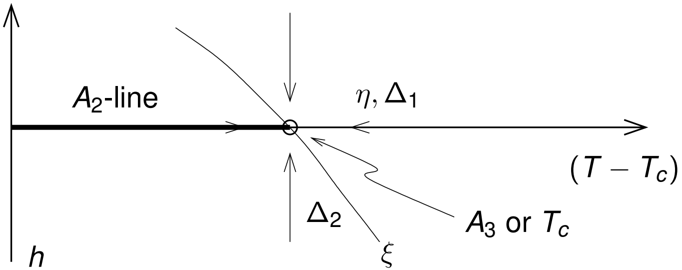

Figure : Analogy of the phase diagram of a glassy system around the A_3 critical point with that of an Ising model in an external field. η or Δ_1 directions are parallel to the A_2 transition line and Δ_2 is the perpendicular direction. We considered a different direction ξ although the critical exponents along the Δ_2 and ξ directions will be same.