Disordered Glassy Models: a Step Beyond Mean FIeld

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Plan

- General considerations about mean-field theories

- Kac models and asymptotic expansions around mean-field

- Mean Field Dysorderd Models for the Glass Transition

- Kac Disordered Models

- Point-to-Set correlations
- Correlation lengths in Kac Glasses

- Power law interactions on hierarchical lattices

Mean-Field Theory in Statistical Physics and Condensed Matter

Simple tool to get qualitative (sometime quantitative) description of complex collective phenomena (phase transition, low temperature ordering…)

- Van der Waals theory of gas-liquid transition
- Curie-Weiss theory of magnetism
- Landau Theory of 2^{nd} order phase transition
- Dynamical Mean Field theory for correlated electrons
- Mode-Coupling Theory of liquids

Based on Neglection of Fluctuations
Exact in models with Long Range Interactions.

Pros

- Qualitative features of phase diagrams
- Description of Phase Transitions

Pathologies

- Non Convex Free-energy functions
- No Phase Separation
- Infinite Life Metastable State
- Phase transition and condensed phases in low D (e.g. D=1)

- Bad description of Fluctuations: Wrong Critical Exponent in Ph. Transitions (RG)

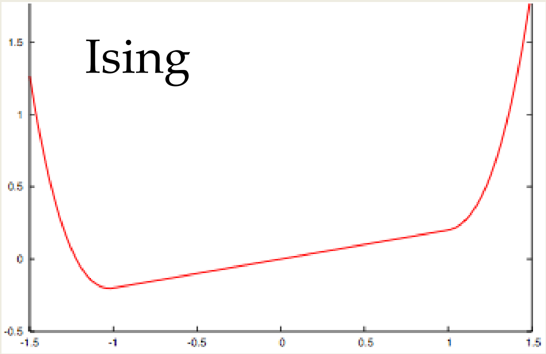
All the known pathologies can be traced in the neglection of finite range character of physical interactions.

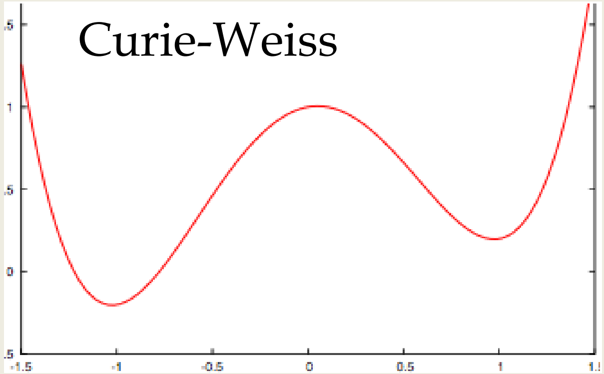
Finite D Ising model vs Curie-Weiss model

$$H = -\sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

$$H = -\frac{1}{N} \sum_{i<j}^{1,N} S_i S_j - h \sum_i S_i$$

$F(m)$ Free-energy for fixed magnetization





Finite D: interfaces → F(m) convex. Nucleation → Relaxation time finite

Recipes:

- Maxwell Construction
- Nucleation Theory

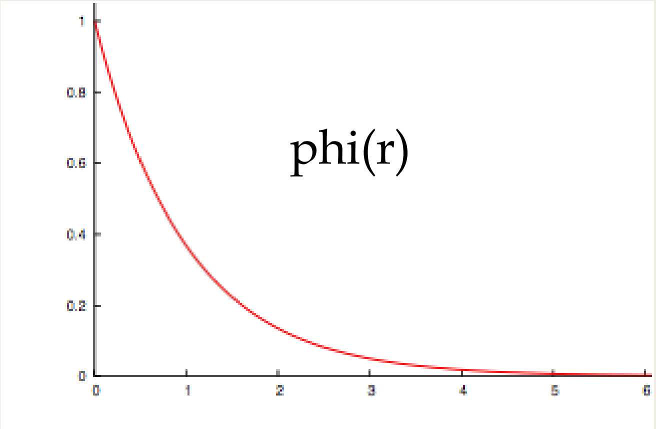
M. Kac 1959

The origin of the pathologies can be traced in the infinite range of the interactions

$$H = -\frac{1}{r_0^d} \sum_{i,j} \phi\left(|i-j|/r_0\right) S_i S_j - h \sum_i S_i$$

r_0 Interaction range

L System size



$r_0 \sim L \to \infty$ Mean Field

$r_0 << L \to \infty$ Finite D behavior

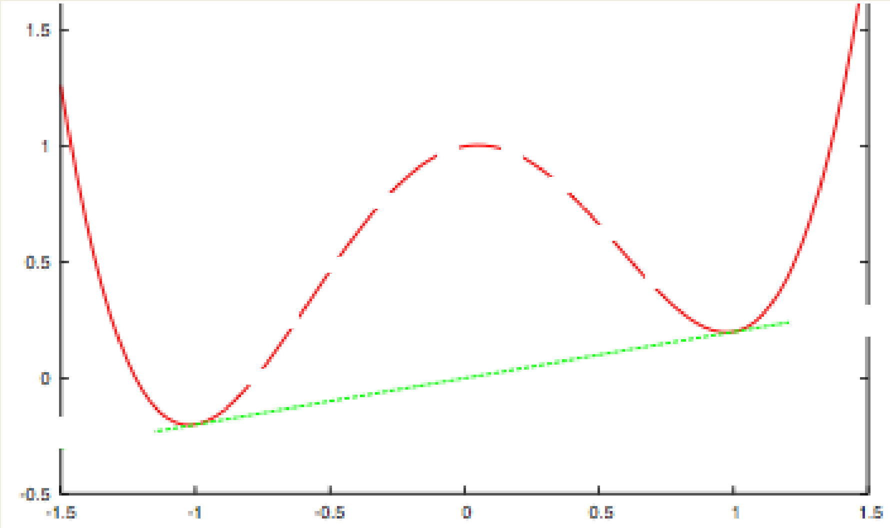
Kac Limit $r_0 \to \infty \quad after \quad L \to \infty$

$$F_{r_0,L}(m) \to F_{MF}(m)|_{Maxwell}$$

Lebowitz-Penrose 1966

- Mean Field in not a singular point
- Kac limit elimitates non-convexity
- It gives interfaces

Interface cost: $\sim r_0 L^{d-1}$



Still phase transition in low D

Rigorous theory of Metastability, i.e. nucleation (Lebowitz-Penrose 1971)

$$\tau_{nucl} \sim \exp(-r_0^d B)$$

Free-energy as a function of the order parameter

$m \longrightarrow m_x$ Local order parameter

x Small volume around i/r_0

Probability of a profile

$$P[m_x] = e^{-r_0^d \Gamma[m_x]}$$

$$\Gamma[m_x] = \beta \frac{1}{2} \int dx\, dy\, m_x \phi(x-y)(m_y - m_x) + \beta \int dx\, F_{MF}[m_x]$$

Starting point for nucleation theory

Inhomogeneous (droplet) solutions of $\frac{\delta \Gamma[m]}{\delta m_x} = 0$

Metastable states: MF construction difficult to define outside MF

Lebowitz-Penrose Metastable States

Regions of configuration space verifying:

1) Time scale separation: Equilibration inside the region is much faster then decay
 from the state.
2) Once abandoned, the time to go back is much larger then the time to get out
3) There is an homogeneous order parameter with a value different from equilibrium (on a coarse graining scale that does not allow phase separation) $m_x \approx m_0$

Describe in terms of constrained equilibrium ensembles

$$I = [m_1, m_2] \qquad \mathcal{R} = \{C \mid m_x(C) \in I \;\; for \;\; all \;\; x\}$$

$$P[C] = \frac{1}{Z_{\mathcal{R}}} e^{-\beta H[C]} \chi(C \in \mathcal{R})$$

Fluctuations within $\mathcal{R}$ are reabsorbed

$$\partial\mathcal{R} = \{C \mid m_x(C) \in I \ \ for \ \ all \ \ x \ \ and \,; m_y(C) = m_1 \ \ for \ \ at \ \ least \ \ one \ \ y\}$$

$$\lambda = \sum_{\mathbf{C}' \notin \mathcal{R} \ \ C \in \mathcal{R}} P(C) W(C \to C')$$

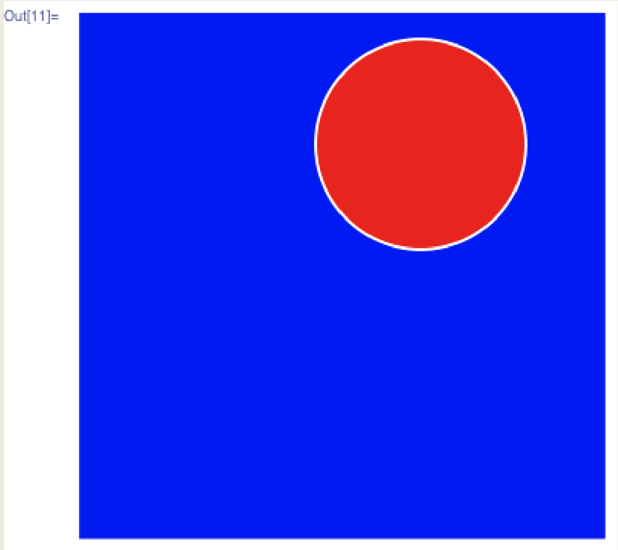
Decay rate of MSS

Local dynamics (No big jumps in configuration space)

$$C \in \mathcal{R} \quad and \quad W \neq 0 \qquad\qquad C \in \partial\mathcal{R}$$

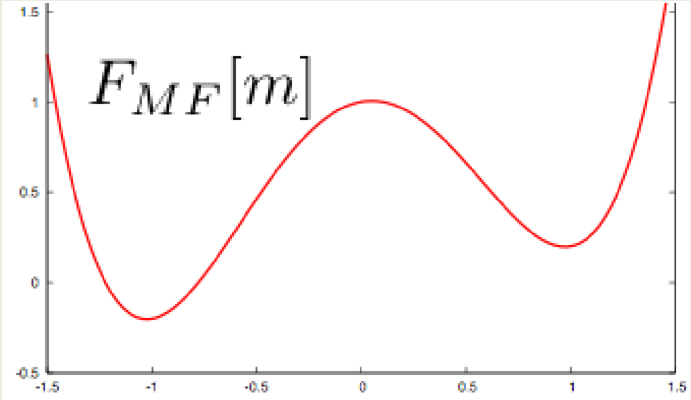
$$\sum_{\mathbf{C}' \notin \mathcal{R}} W(C \to C') \approx 1$$

$$\lambda = \sum_{C \in \, \partial\mathcal{R}} P(C) = \frac{Z_{\partial\mathcal{R}}}{Z_{\mathcal{R}}} = e^{-\beta[F_{\partial\mathcal{R}} - F_{\partial R}]}$$



Kac model

$$P[m_x] = e^{-r_0^d \Gamma[m_x]}$$

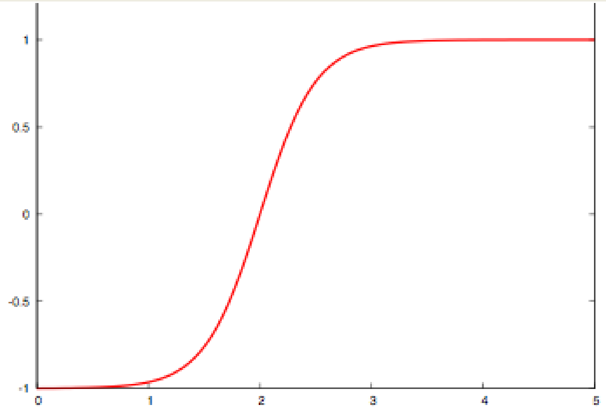


$$\Gamma[m_x] = \beta \frac{1}{2} \int dx\, dy\, m_x \phi(x-y)(m_y - m_x) + \beta \int dx\, F_{MF}[m_x]$$

$$Z_{\mathcal{R}} = \int_I \mathcal{D}m_x\, e^{-r_0^d \Gamma[m_x]} \approx e^{-r_0^d \Gamma[m_0]}$$

$$Z_{\partial\mathcal{R}} = \int_{I; m_{x=0}=m_1} \mathcal{D}m_x\, e^{-r_0^d \Gamma[m_x]} \approx \max_{I; m_{x=0}=m_1} e^{-r_0^d \Gamma[m_x]}$$

Nucleus of the stable phase in the metastable one



The maximizing solution describes a critical nucleus of the stable phase

The relaxation time is exponential in r_0

$$\tau = \frac{1}{\lambda} \approx e^{r_0^d B}$$

Large r0: limit in which relaxation inside the state and MSS decay time are extremely well separated

Nucleation theory becomes exact and relaxation time can be computed with a mean field approximation of an integral.

Mean Field Theory of Disordered Systems

$$H = -\sum_{i,j,k} J_{ijk} S_i S_j S_k \qquad E(J_{ijk}^2) = \frac{1}{N^2}$$

Quenched disorder

p-spin interaction $p \longrightarrow \infty$ REM

KTW Schematic description of glassy phenomenology

- Exact MCT at high T
- Dynamical transition at Td
- Random initial condition → Aging

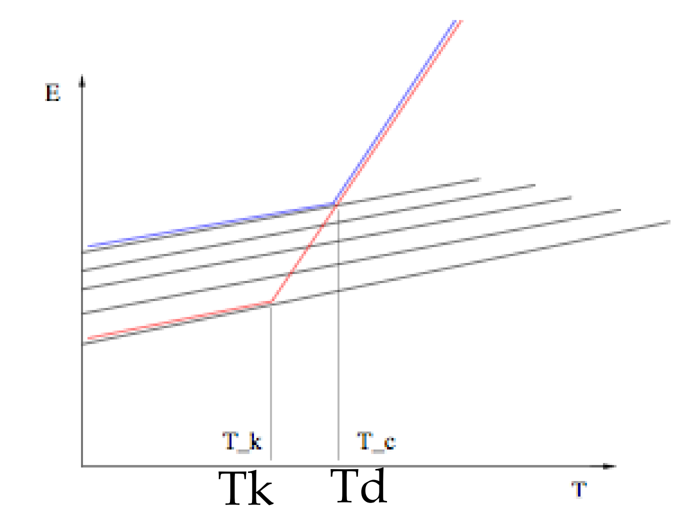
Dynamics

- Extensive log-multiplicity of metastable states below Td (Complexity=configurational entropy)
- Ideal (Kauzmann) transition at Tk

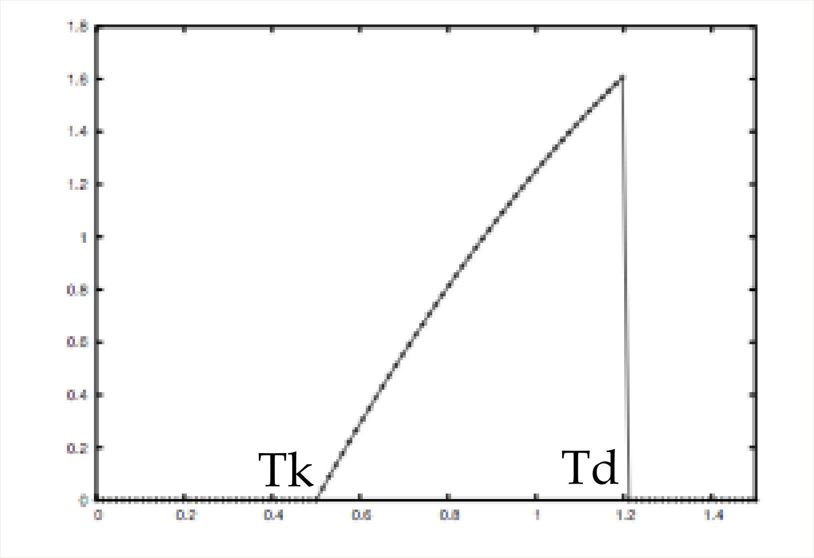
Thermodynamics

Virtue : Show that MCT, Kauzmann etc. are very general phenomena not restricted to supercooled liquids. Unification of different theories and aspects.

Schematic picture of evolution of metastable state energy with temperature. (Iso-complexity lines)



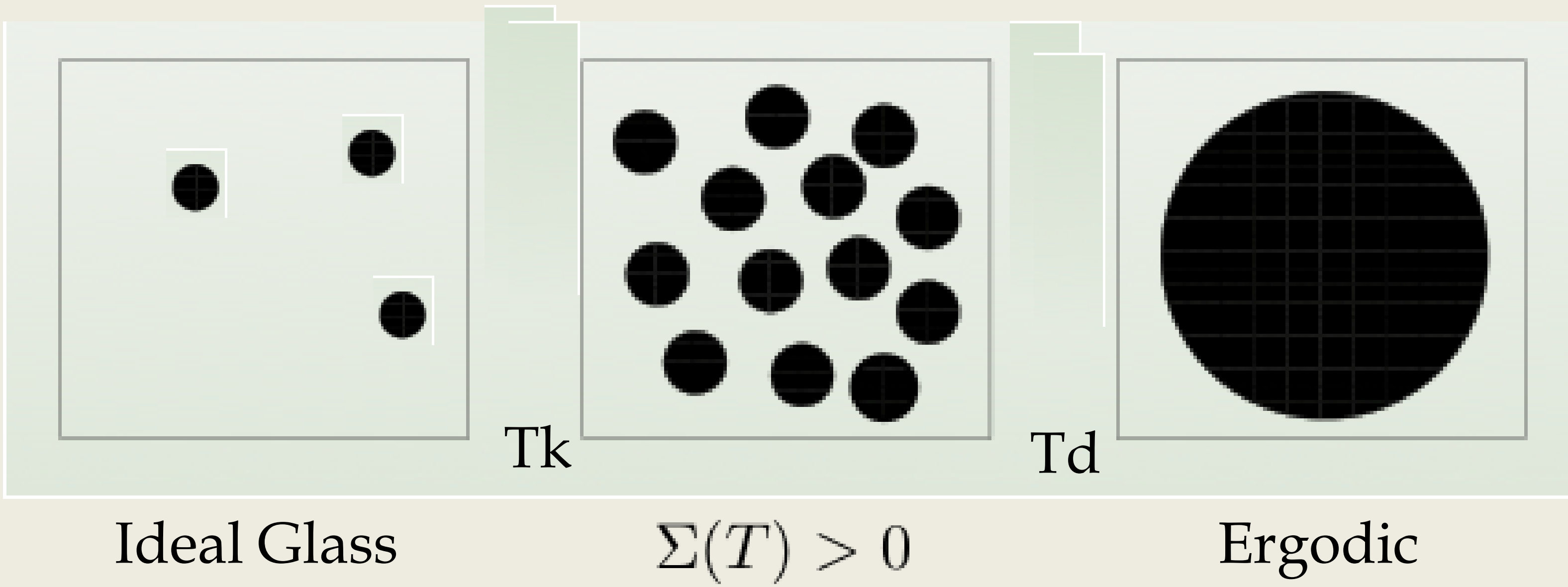
Complexity (configurational entropy) as a function of T

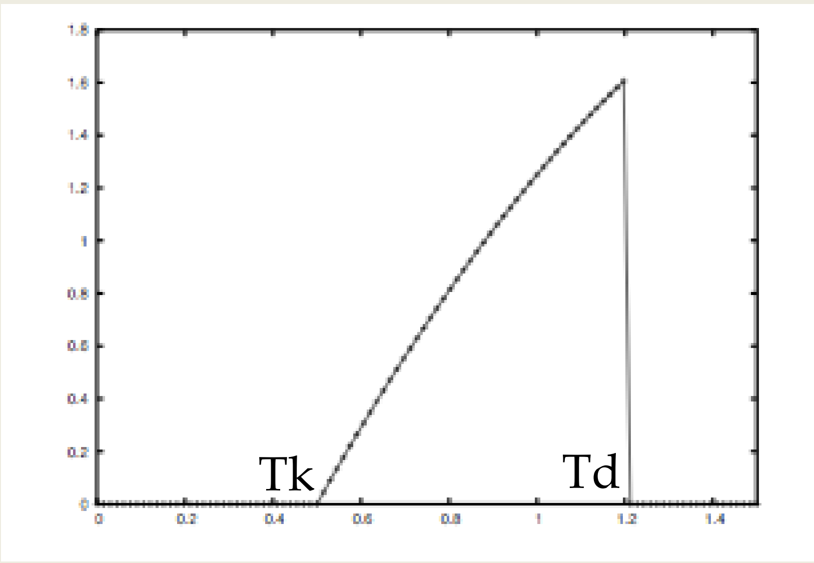


Multiplicity of equilibium states

First Objection : Quenched disorder + geometrical aspects

Mean-Field like approx. for liquids give the same picture (cf Mezard)





The picture is common with Optimization problems, Random Constraint Satisfaction Neural Networks. “Unifying Picture of Glassy Physics (and more)”

Second Objection: Pathologies and limits related to the infinite character of the interaction range

- It does not allow to study possible growth (and nature) of correlation lengths
- Infinite life metastable states
- "Spurious" MCT dynamical transition
- It lacks "activated processes"

The pathologies disappear as soon as a finite interaction range (no matter how large) is introduced

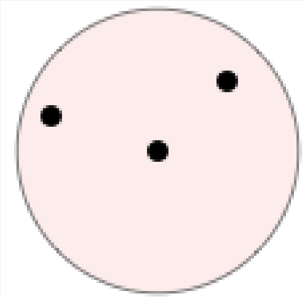
Natural choice Kac model with range r0

- Analytic computations possible in the asymptotic limit $r_0 >> 1$
- Locally Mean-Field Behavior
- Natural Test-Ground for RFOrT which assumes local MF.

….If then the description applies to systems with $r_0 \sim 1$ is a different problem

Kac models for the Glass transition

i, j, k Points of the d dimensional square lattice



$$H = -\sum_{i,j,k} J_{ijk} S_i S_j S_k$$

$$E(J_{ijk}^2) = \frac{1}{r_0^{3d}} \sum_l \psi\left(|i-l|r_0^{-1}\right) \psi\left(|j-l|r_0^{-1}\right) \psi\left(|k-l|r_0^{-1}\right)$$

1) Detail the relation with the MF model
2) Test of RFOT ideas: study of correlation lengths (dynamical + mosaic)
3) Study of Metastability and Activated processes.

Kac limit

Convergence of free-energy and local correlations

$$\lim_{r_0 \to \infty} \lim_{L \to \infty} F_L(r_0) = F_{MF}$$

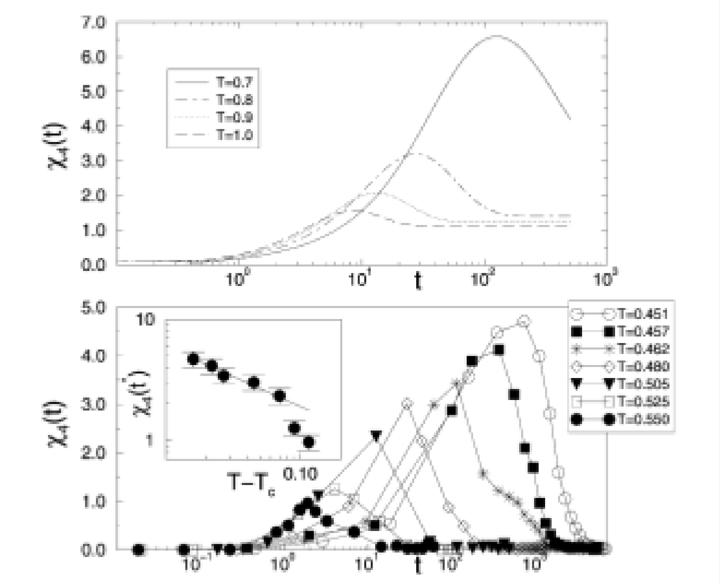
$$E(\langle S_{i_1} \ldots S_{i_r} \rangle^2)_{Kac} \rightarrow E(\langle S_{i_1} \ldots S_{i_r} \rangle^2)_{MF}$$
$$|i_l - i_m| \sim r_0$$

MF models are not singular points

Study finite D phenomena (growing correlation lengths + activated dynamics) in asymptotic expansions around $r_0 \to \infty$

$\tau \sim e^{r_0^d B}$ MSS neatly defined

What correlation length(s) on approaching the glass transition ?



Dynamic heterogeneities view (MCT, Kinetically constrained models,…)
Purely dynamical length (typical size of correlated motion)

Thermodynamic view (Mosaic-RFOrT picture)

Locally Mean Field structure competing with Entropic Pressure (Bulk/Surface competition)

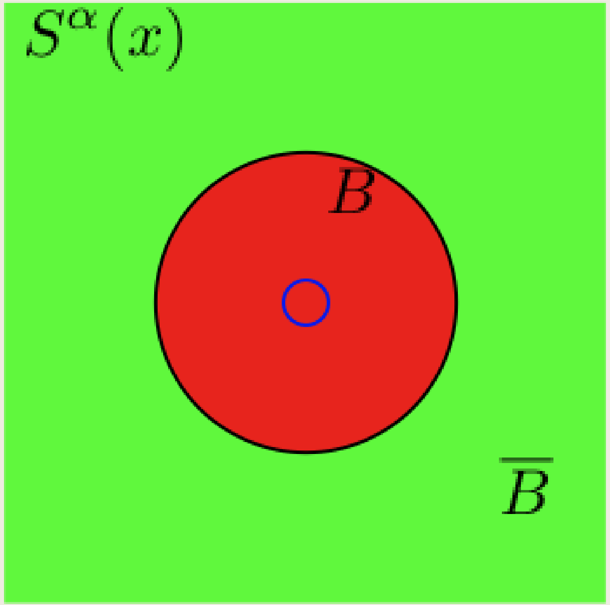
Purely Thermodynamic length

…but typical spatial extension of activated processes

Point-to-Set correlation function

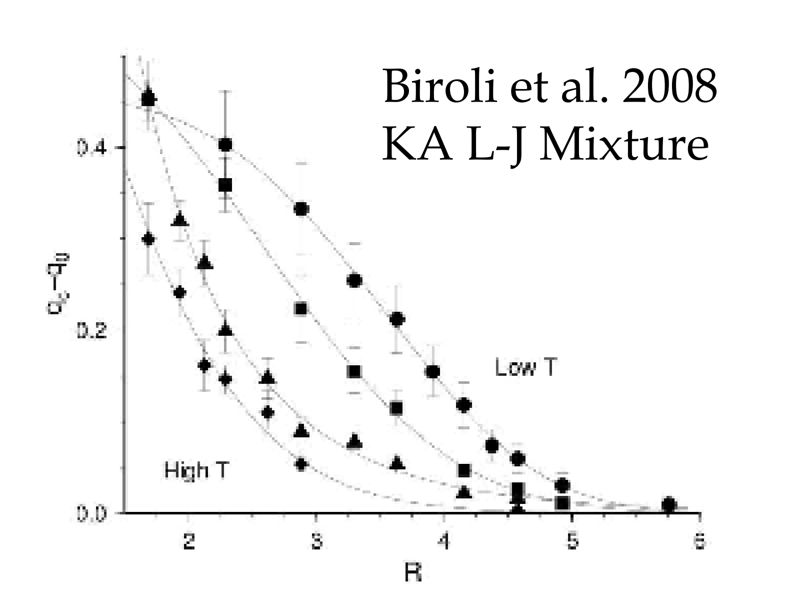
$$P(S_\alpha) = \frac{1}{Z} e^{-\beta H[S_\alpha]}$$

$$P(S_B | S_{\overline{B}} = S_{\alpha;\overline{B}}) = \frac{1}{Z[S_{\alpha;\overline{B}}]} e^{-\beta H[S_B, S_{\alpha;\overline{B}}]}$$

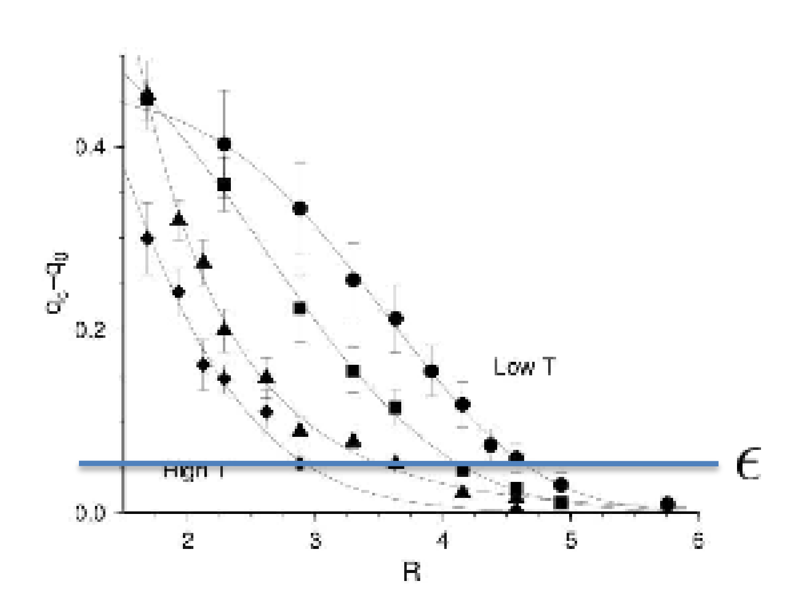


R Cavity Radius

$$Q(R) = \langle q_0(S_\alpha, S) \rangle$$



Semerjian-Montanari Theorem



R_ϵ Cavity size beyond which the PS Correlation is smaller then ϵ

τ_ϵ Relaxation time

$$Const_1 \times R_\epsilon < \tau_\epsilon < e^{Const_2 \times R_\epsilon^d}$$

discrete variable systems with local Monte Carlo dynamics

The growth of relaxation time and PS length are related

Kac models : the two possible regimes can be sharply separated

Biroli-Bouchaud Argument (RFOrT – Mosaic)

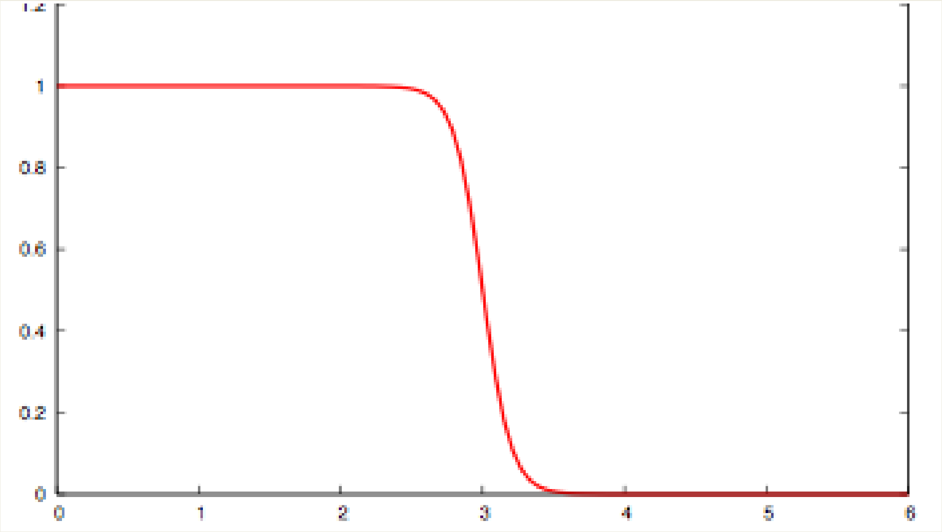
$$Z_R = e^{-\beta f R^d}[1 + e^{\Sigma R^d - Y R^\theta}]$$

All available states have the same internal free-energy

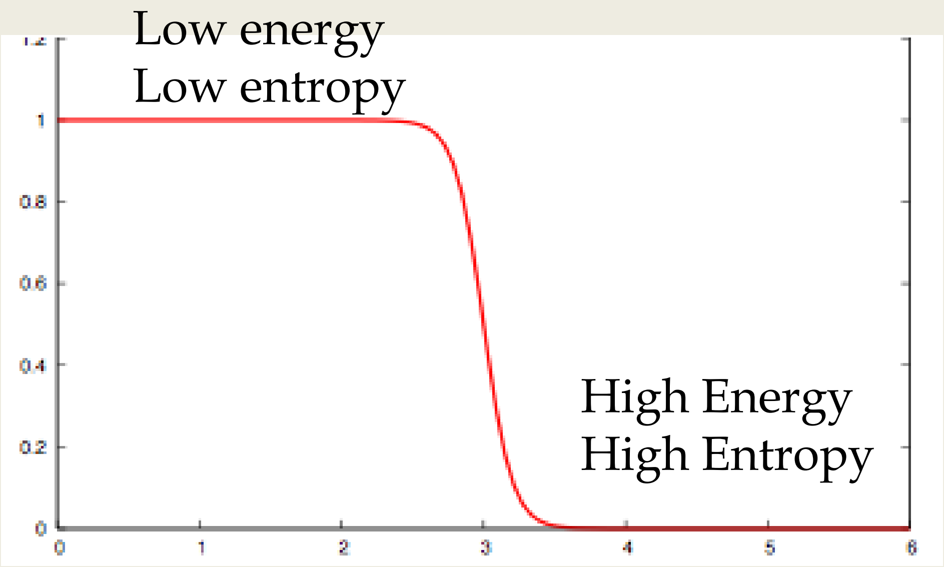
First order-like jump

Σ Bulk configurational entropy Y Interface free-energy

Consequence: Sharp cross-over $\xi_{mos} \sim (Y/\Sigma)^{1/(d-\theta)}$



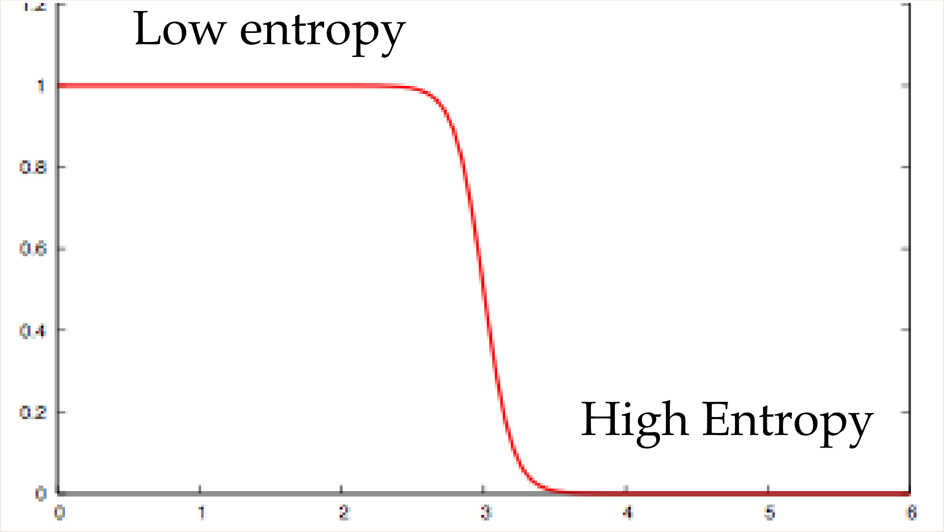
If Y is interpreted as a surface energy



Easy to prove that $U(R)/V_R$ is independent of R

Spatial energy fluctuations

Y could be interpreted as an interface reduction of entropy



Low R: The system remains correlated because of Lack of states

High R: The system has many states at its disposal and decorrelates

Field Theoretical Study of PS function

$$W[q_x] = -T\,\overline{\log Z[q_x, S^\alpha]}$$

$$Z[q_x, S^\alpha] = \sum_S e^{-\beta H[S]} \prod_x \delta(Q_x(S, S^\alpha) - q_x)$$

Landau free-energy functional for glassy systems

Order Parameter : Similarity with a reference eq. configuration

« New Replicas » Cf. Mezard lecture

$$\overline{Log Z[q_x, S^\alpha]} \rightarrow (\overline{Z[q_x, S^\alpha]^n} - 1)/n$$

Possible in principle to use Mezard's liquid theory approach

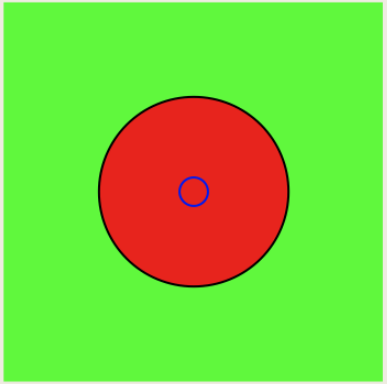
Different route: Kac limit of disordered models

Disordered Kac models

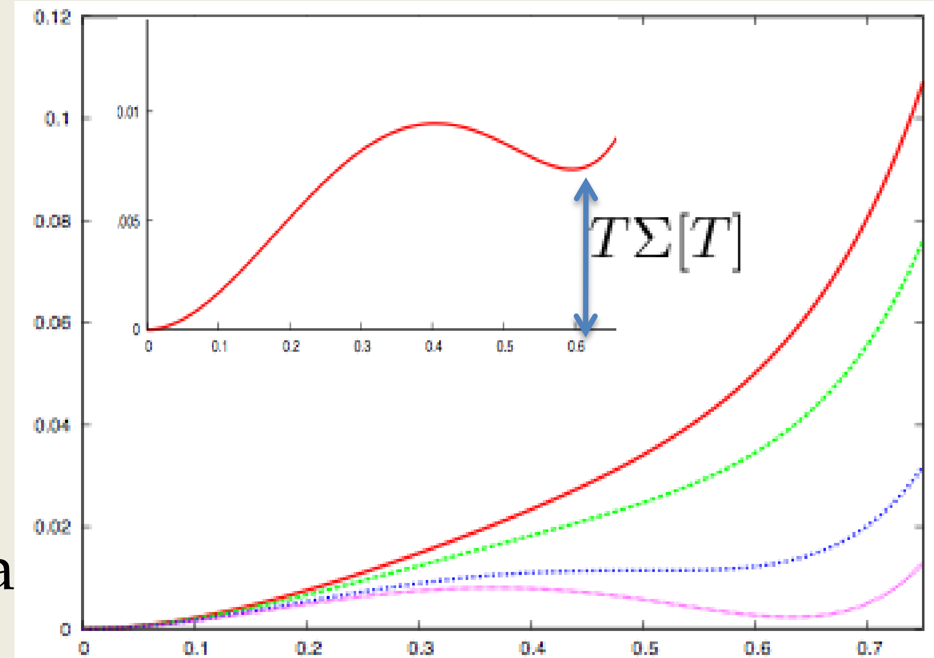
For large r_0, Equilibrium profiles are obtained by the functional minimization of

$$W[q(x)] = r_0^d \int d^d x \; \left(\frac{1}{2} c (\nabla q_x)^2 + V_{MF}[q_x] \right)$$

PS function: fix $q_x = 1$ for $x > R/r_0 = \ell$

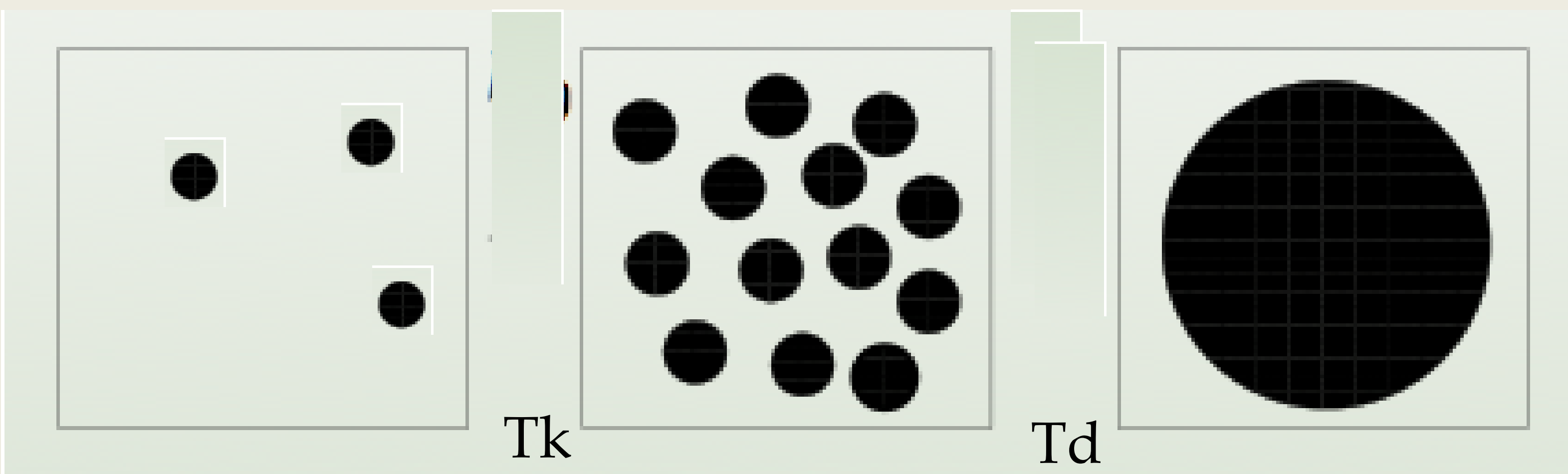


Shape of the function $V_{MF}[q]$



High T	Convex
$T < T^*$	Non-Convex
$T < T_d$	Two Minima
$T < T_K$	Degenerate Minima

Free energy cost for imposing a given overlap for



Ideal Glass $\Sigma(T) > 0$ Ergodic

Kac Model

$$W[q(x)] = r_0^d \int d^d x \ \left(\frac{1}{2} c (\nabla q_x)^2 + V_{MF}[q_x] \right)$$

Length measured in unities of r_0

Scaling limit

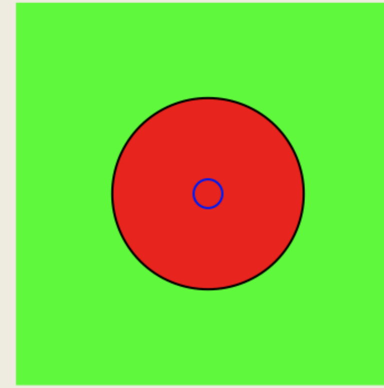
$$r_0 \to \infty, \quad R \to \infty \qquad R/r_0 = \ell$$

Solve

$$\frac{\delta W}{\delta q_x} = 0 \quad \to \quad c \Delta q_x = \frac{d V_{MF}(q_x)}{d q_x} \qquad\qquad q_x = q(|x|) \quad q(\ell) = 1$$

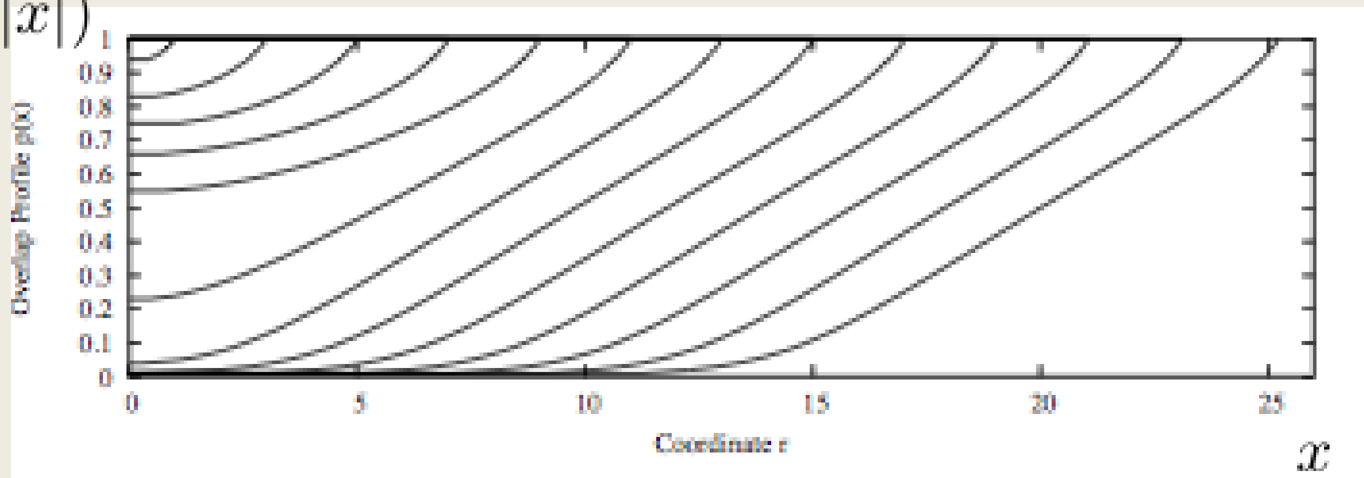
$Q(\ell) = q(0)|_\ell$ PS correlation

$q(|x|)$ Overlap profile



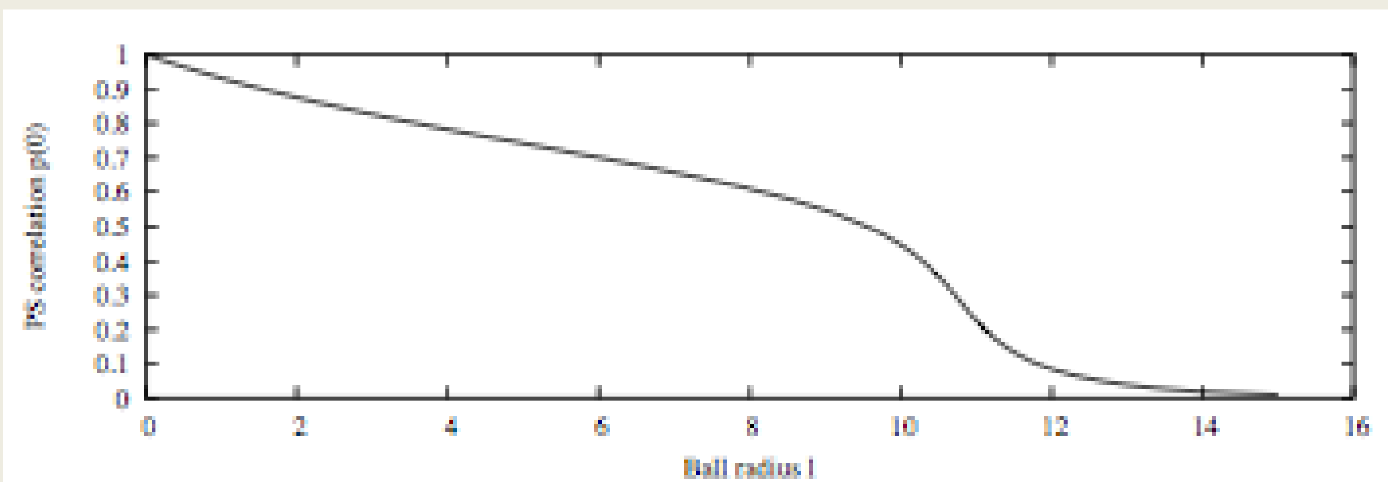
$T > T^*$

$q(|x|)$



x

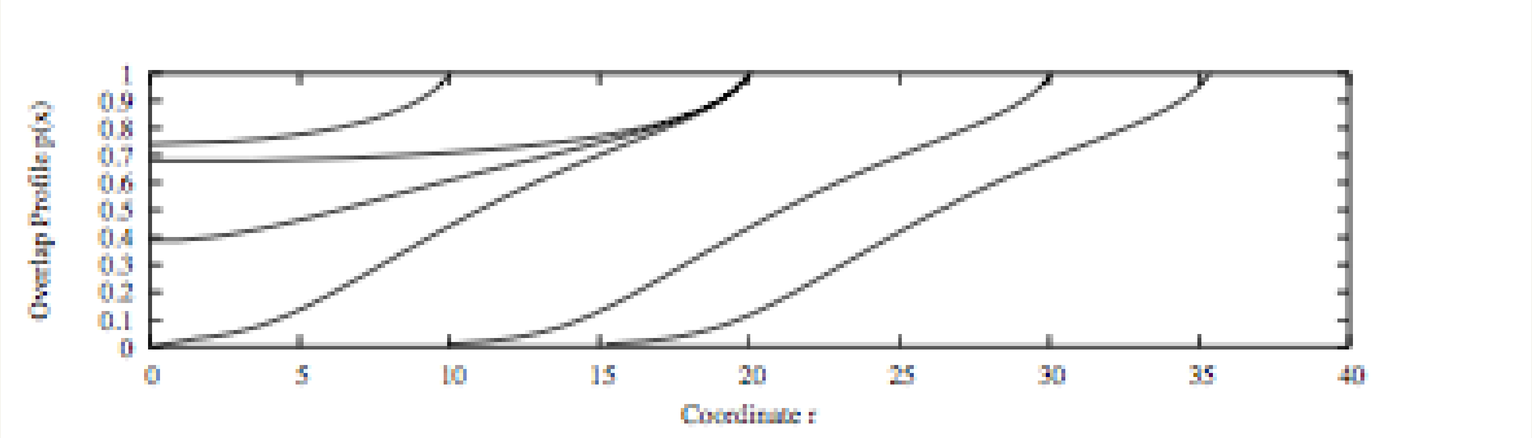
$Q(\ell)$



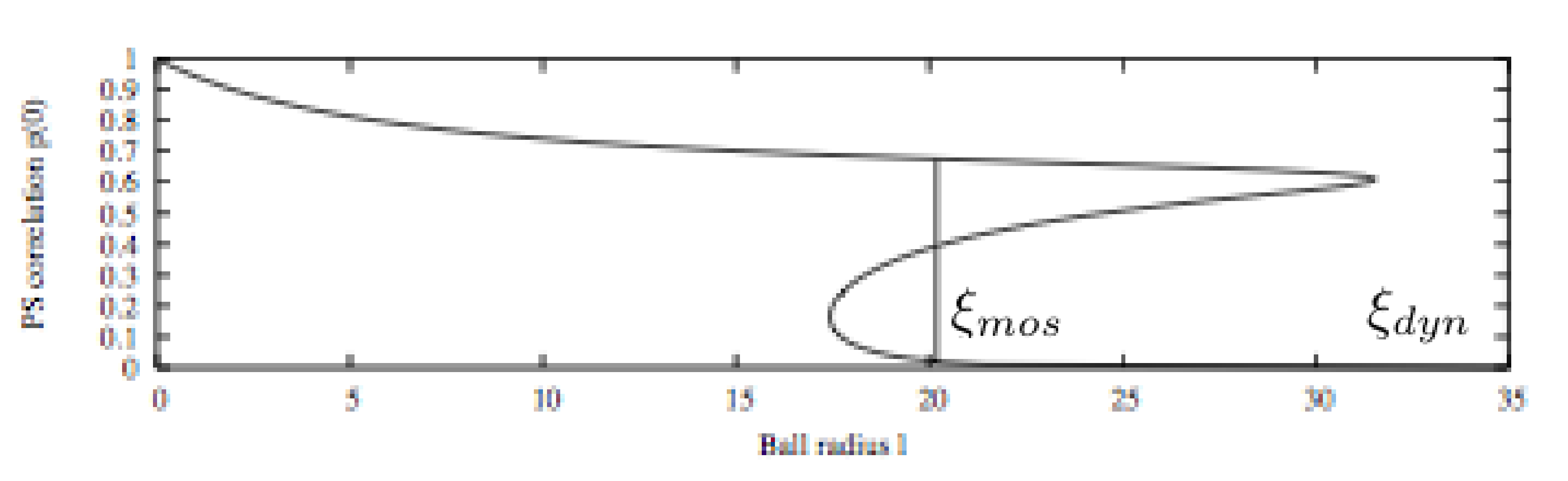
ℓ

$T_d < T < T^*$

$q(|x|)$

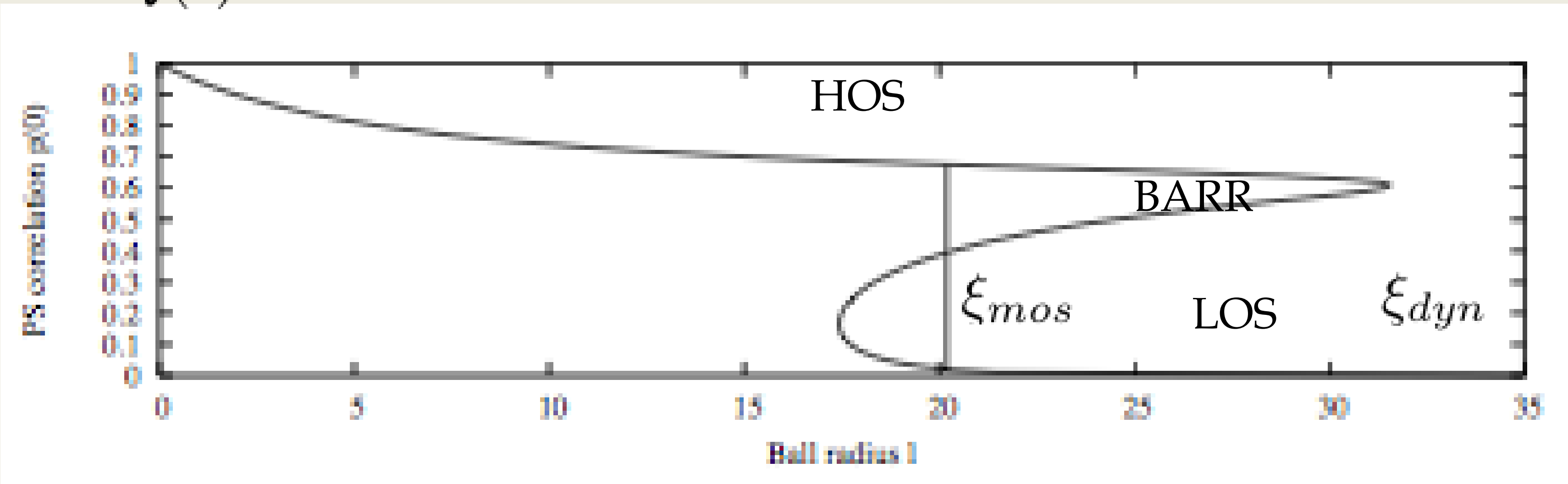


$Q(\ell)$



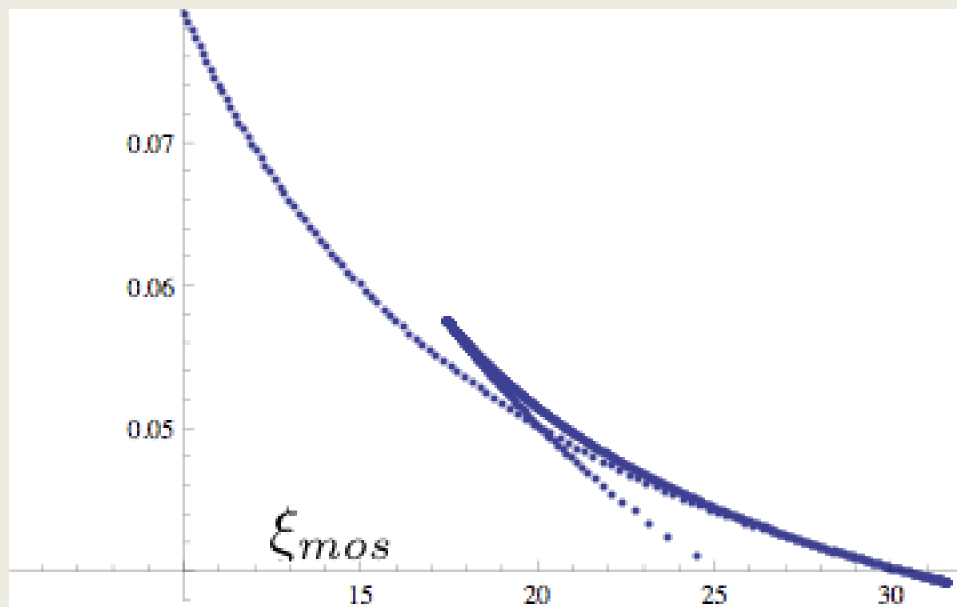
ξ_{mos} Defined well above Td

$Q(\ell)$

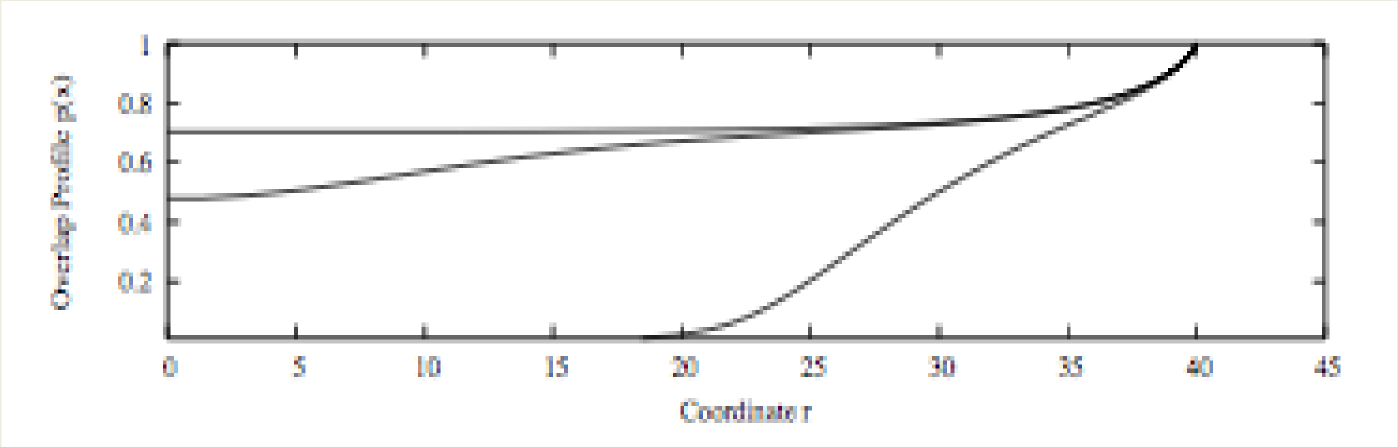


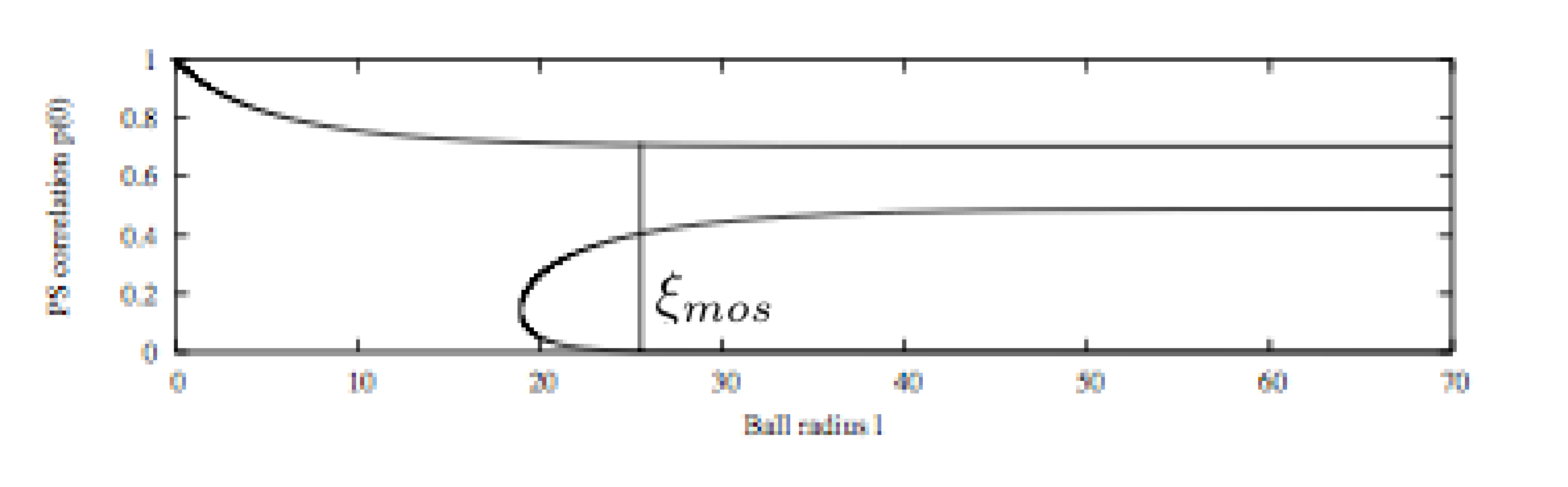
Free-energy

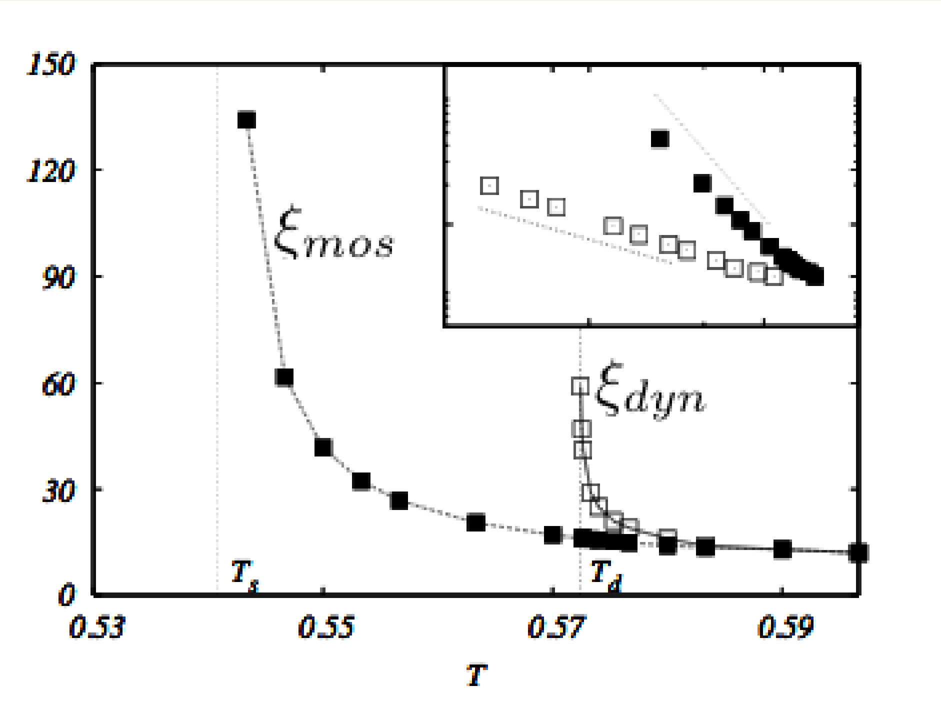
$$\ell < \xi_{mos} \quad F_{HOS} < F_{LOS}$$
$$\ell > \xi_{mos} \quad F_{HOS} > F_{LOS}$$



$T_K < T < T_D$


Overlap Profile p(x)
Coordinate r


PS correlation p(0)
Ball radius l
ξ_{mos}



Physical meaning of lengths

ξ_{dyn} Typical size of MCT relaxation processes

Below that scale Relaxation requires activation

$$\xi_{dyn} \sim \frac{1}{(T - T_{dyn})^{1/4}} \sim \xi_4^{MCT}$$

$$T_{dyn}(\ell) = T_{dyn} + \ell^{-4}$$

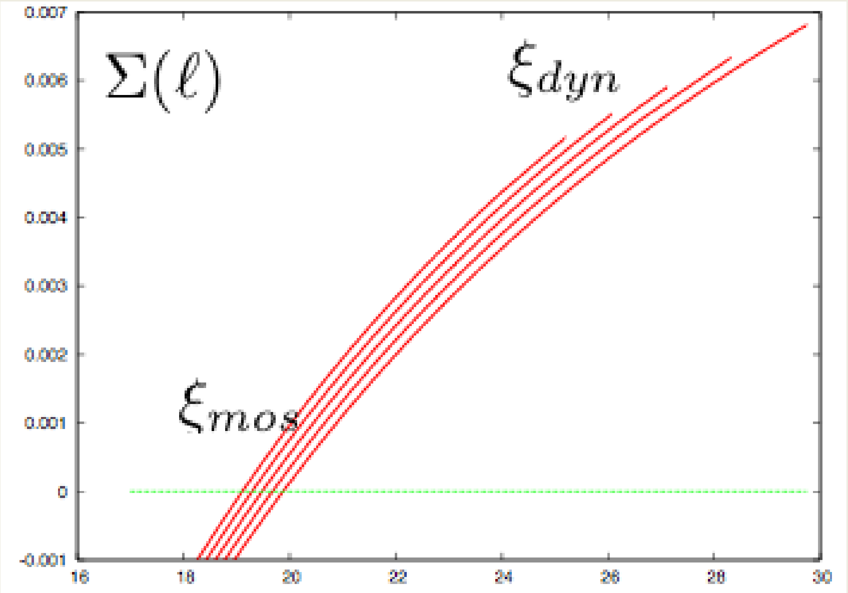
$$\xi_{mos} \sim \frac{1}{(T - T_K)}$$

$$T_K(\ell) = T_K + \ell^{-1}$$

Smaller systems have higher glassy temperature

What kind of picture for the dynamic and static transitions ?

cf Bulk – interface competition of RFOrT



Compute $F_{HOS}(\ell) - F_{LOS}(\ell)$

and $\Sigma(\ell)$

$$F_{HOS}(\ell) - F_{LOS}(\ell) = T\Sigma(\ell)$$

Purely entropic Random First Order Transition

$T_{dyn}(\ell)$ Dynamical transition line (Activated processes appear)

$T_K(\ell)$ Kauzmann transition (Complexity vanishes)

Below T_{dyn} $$\Sigma(\ell) \to \Sigma_\infty \sim \frac{1}{T - T_K}$$

$\ell^d \Sigma(\ell) = \ell^d \Sigma_\infty - Y \ell^{d-1}$ Reduction of entropy due to boundary

$\theta = 2$ Interface exponent

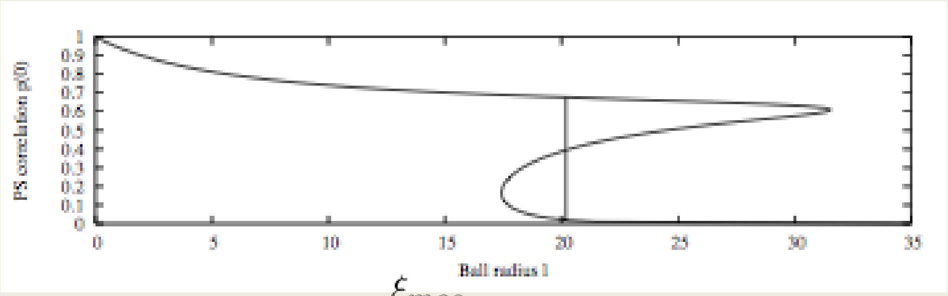
$$\xi_{mos} \sim \frac{Y}{\Sigma_\infty} \sim \frac{1}{T - T_K}$$

Barriers and dynamical length

Estimate:

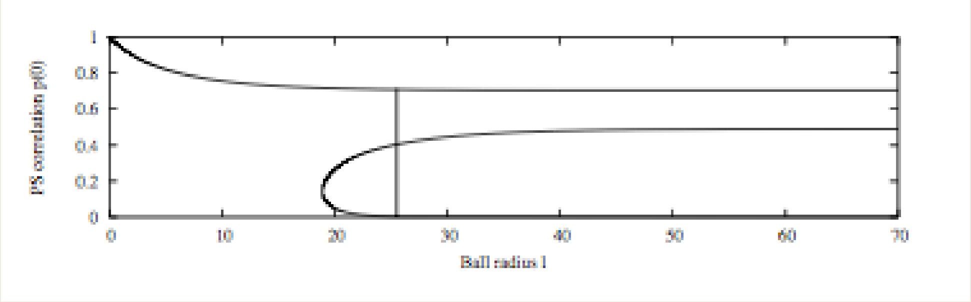
$$\tau(\ell) = \tau_0(\ell) \times e^{-r_0^d B(\ell)}$$

$$B(\ell) = F_{BARR} - F_{HOS}$$



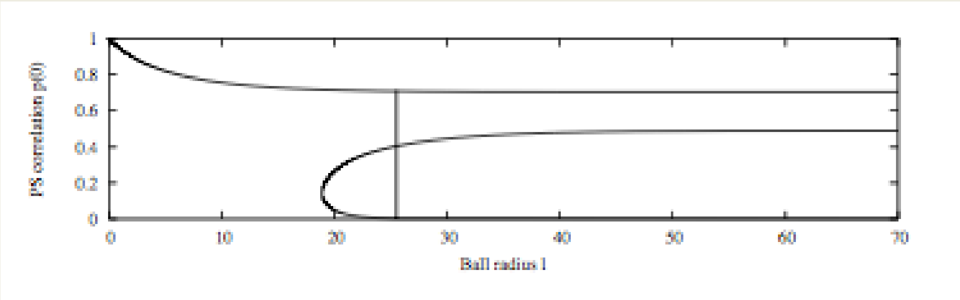
ξ_{mos}

$$B(\ell) \to 0 \quad \ell \to \xi_d \quad T > T_d$$



$$B(\ell) \to B_\infty \quad \ell \to \infty \quad T < T_{dyn}$$

B_∞ Bulk relaxation barrier



$$B(\ell) = F_{BARR} - F_{HOS}$$ It converges on scales $\ell \sim \xi_{mos}$

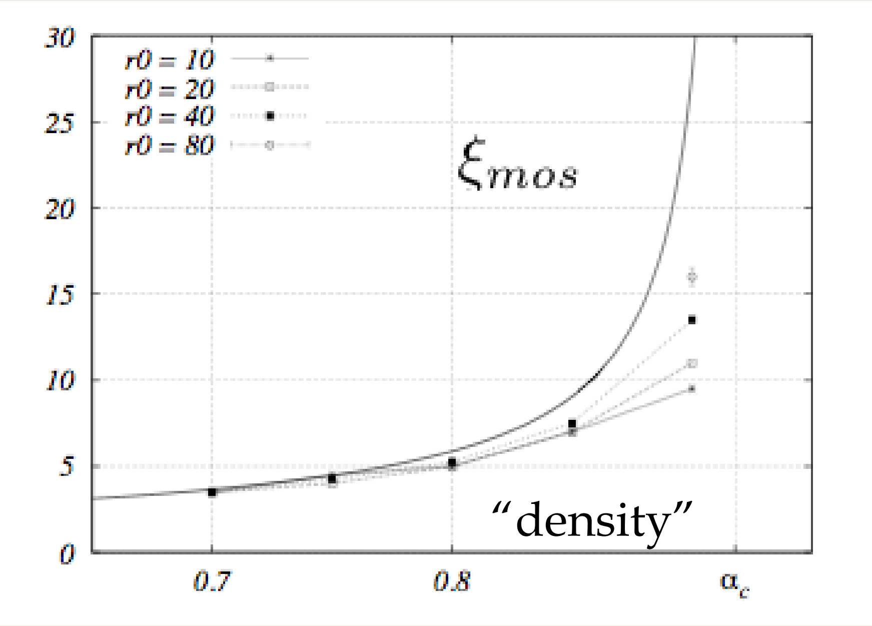
$$B_\infty \sim \xi_{mos}^{d-1} \sim \left(\frac{Y}{\Sigma}\right)^{d-1} \sim \frac{1}{(T-T_K)^{d-1}}$$

$$\psi = d-1$$

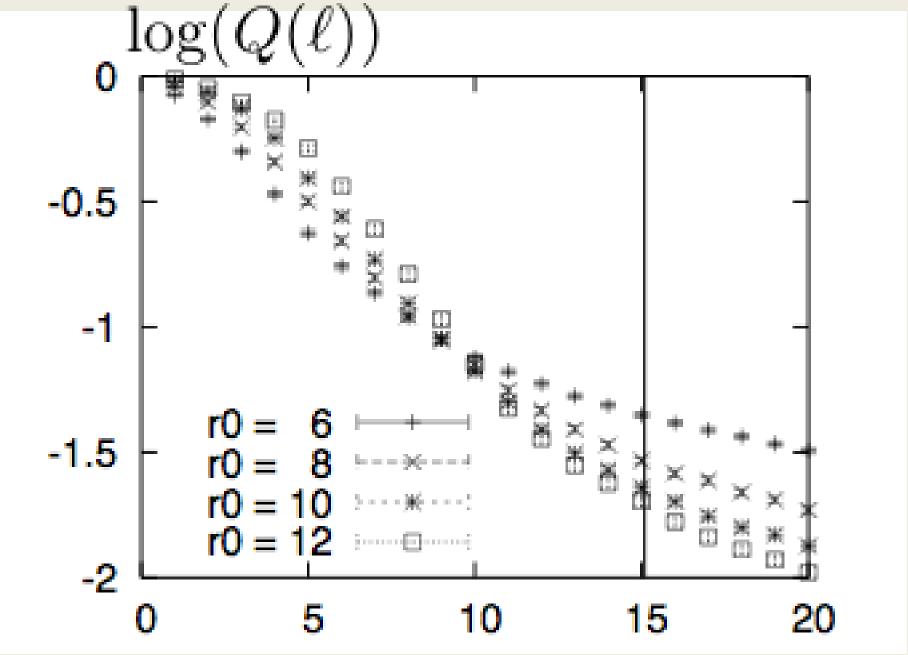
The theory has a built it mechanism to evoid the dynamical transition

It does not suggest a mechanism destroying the Kauzmann transition

1 D Kac models for finite r_0



Slow approach to the Kac limit results



Summary

- Two correlation length scenario of the glass transition
- Dynamical length * possibility of relaxation w/out activation
- Mosaic Length * Entropic cross-over to liquid behavior
- They set the scale of dynamical processes dominating above and below T_{dyn} respectively
- Purely entropic transition mechanism
- Barrier : trivial exponents
- No mechanism to avoid Ideal Glass Transition

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