INSTITUT D'ÉTUDES SCIENTIFIQUES DE CARGÈSE

# Glass transitions, and cooperative length scales

**Chiara Cammarota**

*26. 8. 2014 Cargèse*

## Questions on glass transition still to be answered

Critical properties of the glass transition

The glass transition does really exist?

Does the static approach explain the mechanism for glass formation?

## Issues about the glass transition

Relaxation time diverges exponentially at the transition

Slow growth of the correlation length: the universal behavior is not within reach

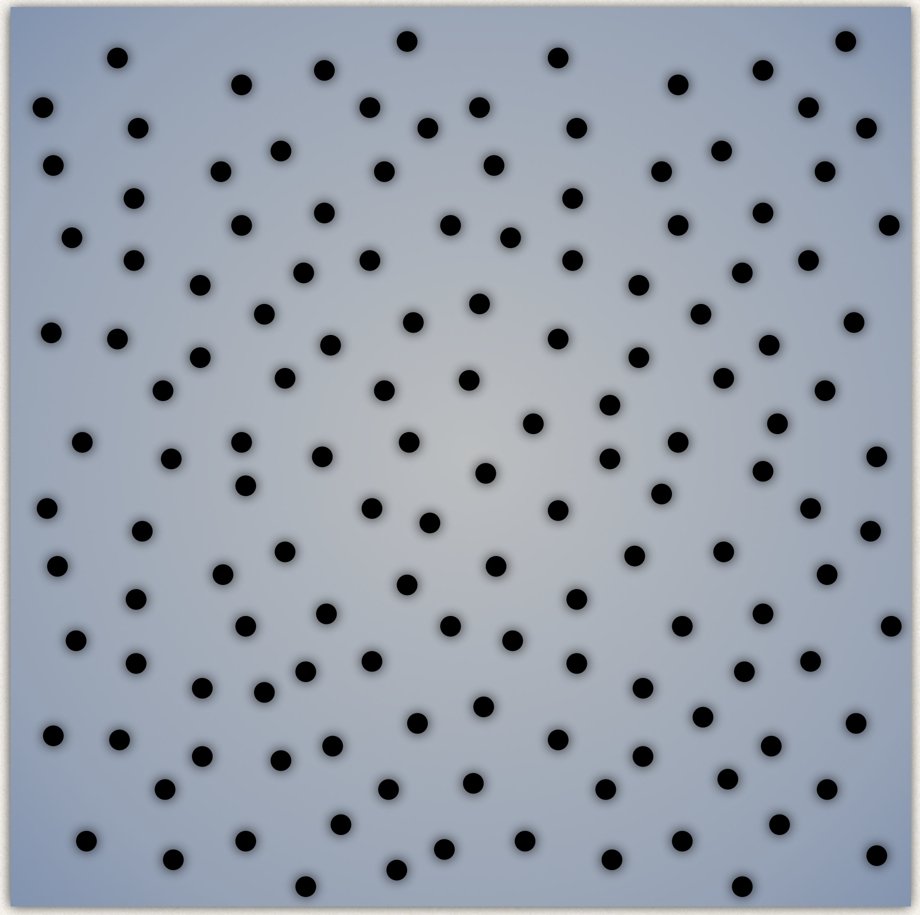
The low temperature phase is not known


**Time and length scales *"pleasure and pain"* of the glass transition**

# A new glass transition

# The ideal glass transition (the old one)

An equilibrium configuration at temperature $T$.



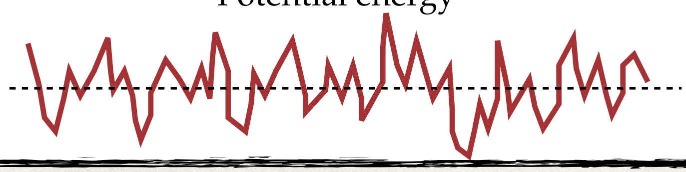
**The RFOT theory:**

*T.R. Kirkpatrick, D. Thirumalai, and P.G. Wolynes, Phys. Rev. A 40, 1045 (1989)*

$$\mathcal{N}(f) = \exp(l^d s_c(f)) \longrightarrow T s_c(T) l^d \;\; vs \;\; \Upsilon l^\theta$$

$$\Delta F_I = \Upsilon l^\theta$$

$$l_s = \left(\frac{\Upsilon}{T s_c}\right)^{1/(d-\theta)}$$

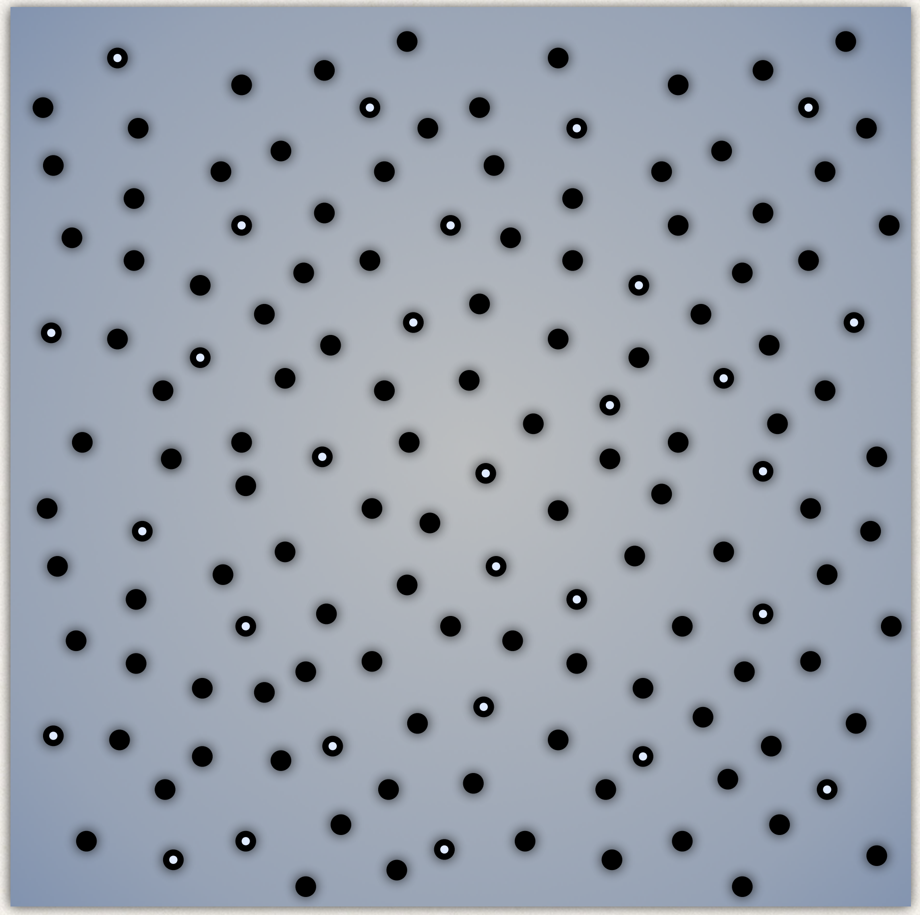



$$\tau = \tau_0 \exp\left(A l_s^\psi / T\right)$$

# Glass transition by random pinning

*C.C. and G.Biroli, PNAS 109 8850 (2012)*

We freeze a fraction $c$ of particles randomly chosen in an equilibrium configuration at temperature $T$.



Pin particles at fixed $T$: $c \uparrow \longrightarrow s_c \downarrow \quad l_s^p \uparrow\uparrow \quad \tau^p \uparrow\uparrow$

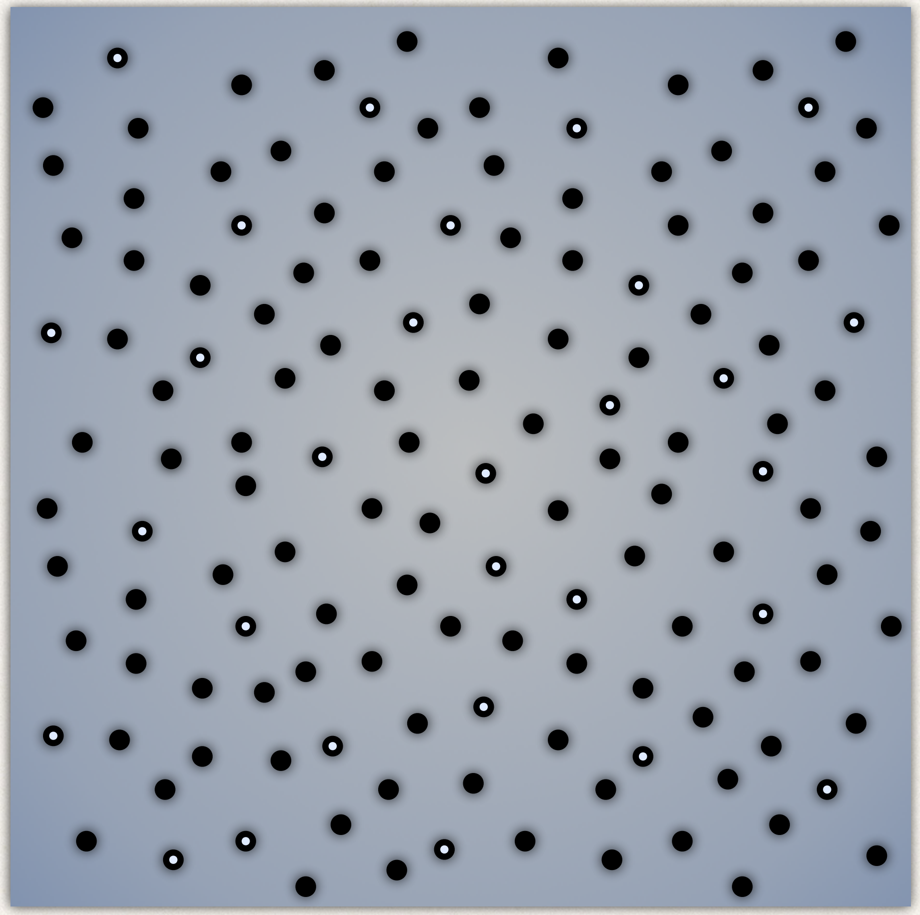
# Glass transition by random pinning

*C.C. and G.Biroli, PNAS 109 8850 (2012)*

$c, T:$

$$s_c^P(T,c) \simeq s_c(T) - cY(T)$$
$$c_K(T) = s_c(T)/Y(T)$$

$$\Upsilon^P(T,c) \sim \Upsilon(T)$$



**Entropy vanishing transition induced by pinning!**

↓

**The RFOT theory reloaded:**

$$l_s^P = \left(\frac{\Upsilon^P}{T s_c^P}\right)^{1/(d-\theta)} = \left(\frac{\Upsilon}{T(s_c - cY)}\right)^{1/(d-\theta)} \gg l_s$$

$$\tau^p \sim \exp\left[A(l_s^p)^\psi/T\right]$$

# Glass transition by random pinning

An indirect study of the glass transition and of metastability in glass-formers.

*S.Franz and G.Parisi, Phys. Rev. Lett. 79, 2486 (1997)*

An induced glass transition with favourable features:

For $c < c_K$, the same glass phenomenology and critical properties as $T > T_K$ .

The configuration chosen to pin particles is always a typical equilibrium configuration.

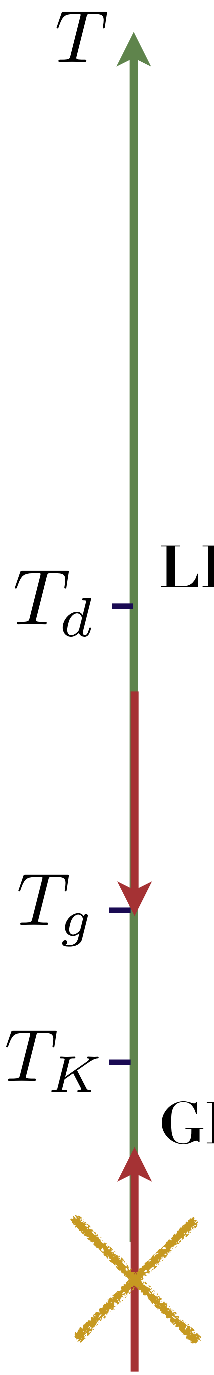
Equilibrium can be observed in the glassy phase.

Study of the glass transition not left to doubtful extrapolations.

The large amount of predictions: a stringent test for theories of glassiness (i.e. RFOT theory).


**$c$ , a second control parameter for the liquid-glass phase diagram**

# The liquid-glass phase diagram




*V.Krakoviack, PRE 84, 050501(R) (2011)*
*G.Szamel and E.Flenner EPL 101 66005 (2013)*
*S.Nandi et al., arXiv:1401.3253 (2014)*

*W.Kob and L.Berthier, PRE 85 011102 (2012)*
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*F.Krzakala et al., Phys. Rev. X 2, 021005 (2012)*
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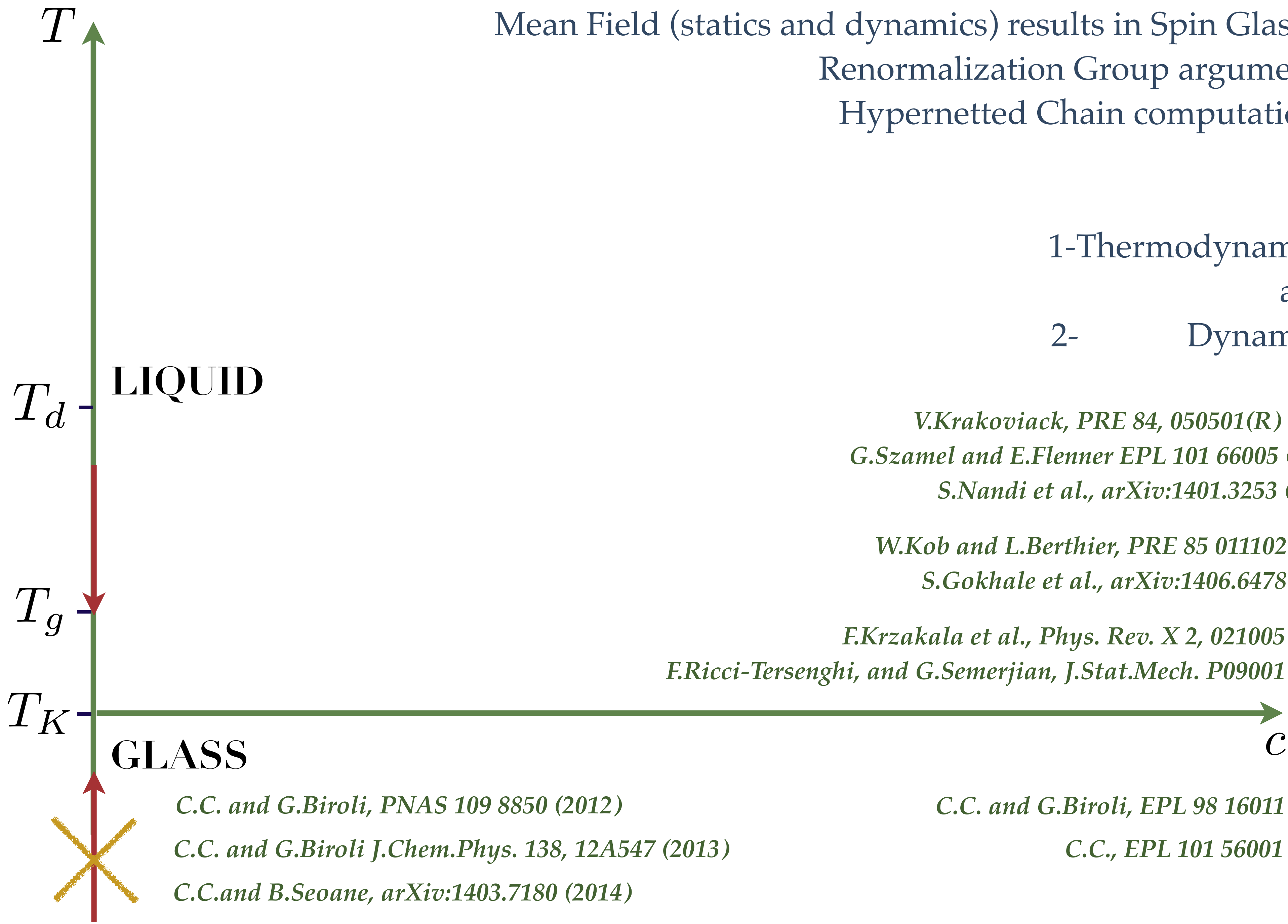


Mean Field (statics and dynamics) results in Spin Glasses
Renormalization Group arguments
Hypernetted Chain computations

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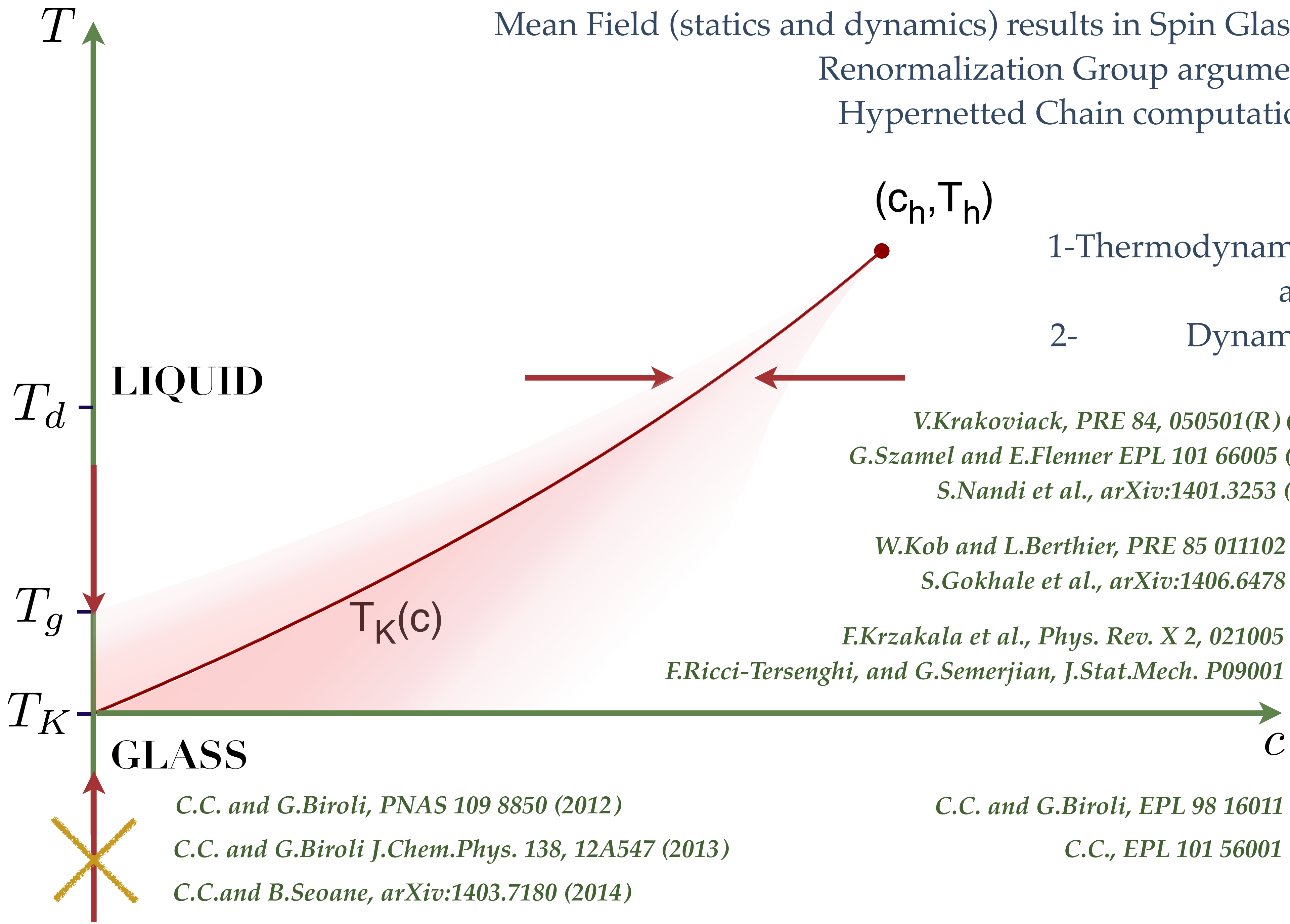


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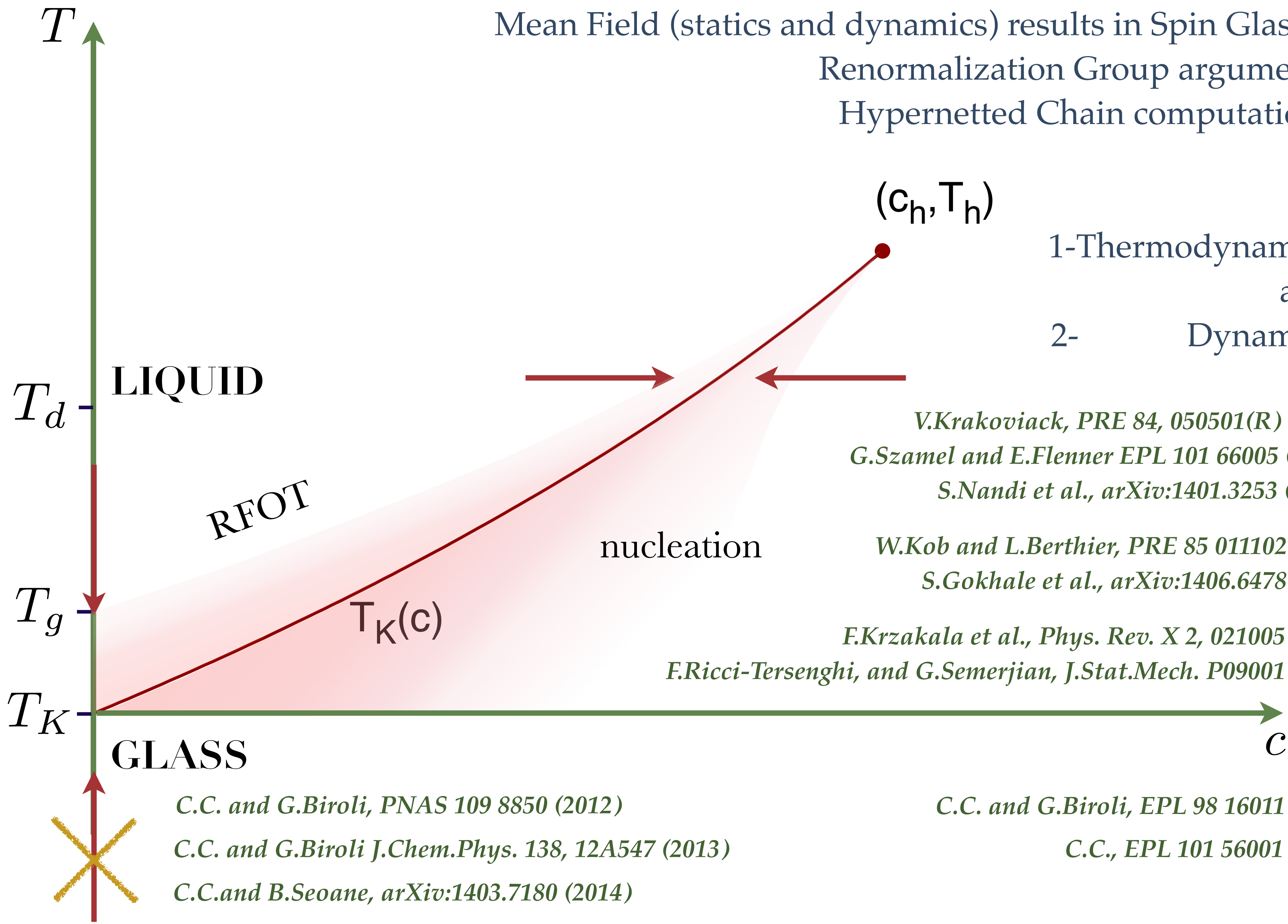


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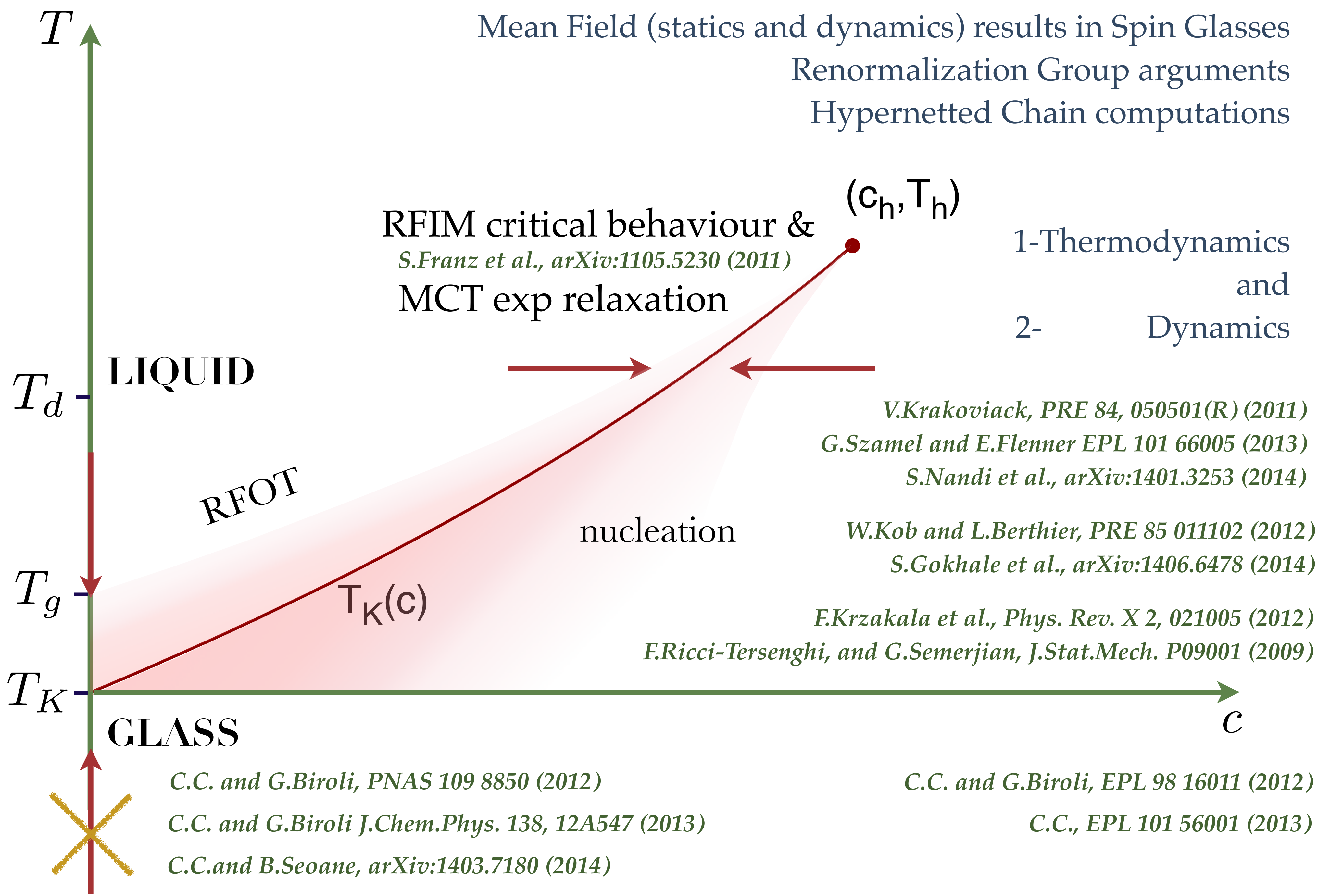

# Cooperative length scales

# A first correlation length-scale from random pinning

*C.C. and B.Seoane, arXiv: 1403.7180 (2014)*

Amorphous order reconstructed by at least $Nc_K(\phi)$ **pinned particles**.
First principle computation of a cooperative length scale

$$\xi_c(\phi) = 1/c_K^{1/d} \quad \text{with} \quad c_K \sim s_c(\phi) \quad \text{such that} \quad s_c^P(c_K, \phi) = 0$$

*S.Karmakar, and I.Procaccia, arXiv:1105.4053 (2011)*

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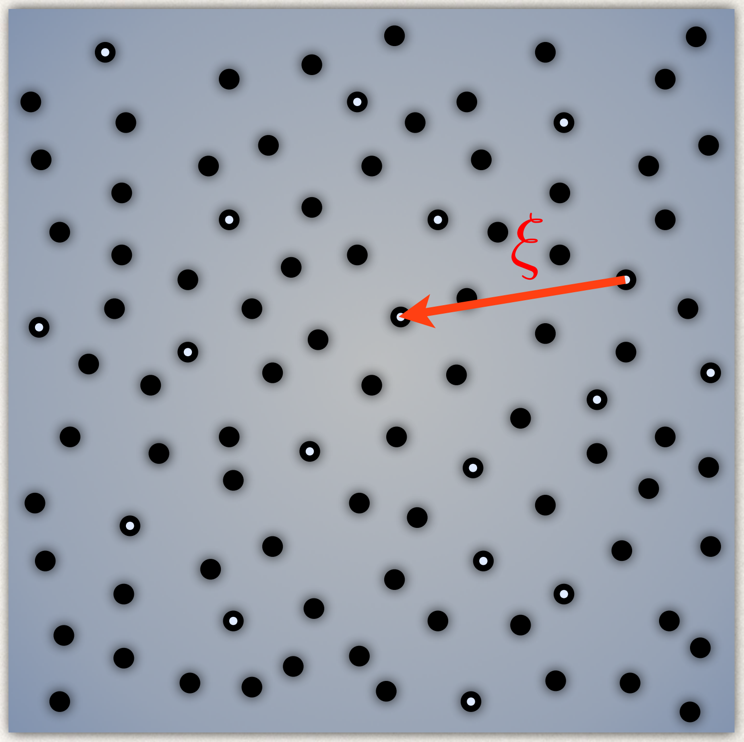
*B.Charbonneau et al., Phys. Rev. Lett. 108, 035701 (2012)*

## HNC computations in an Hard Sphere system



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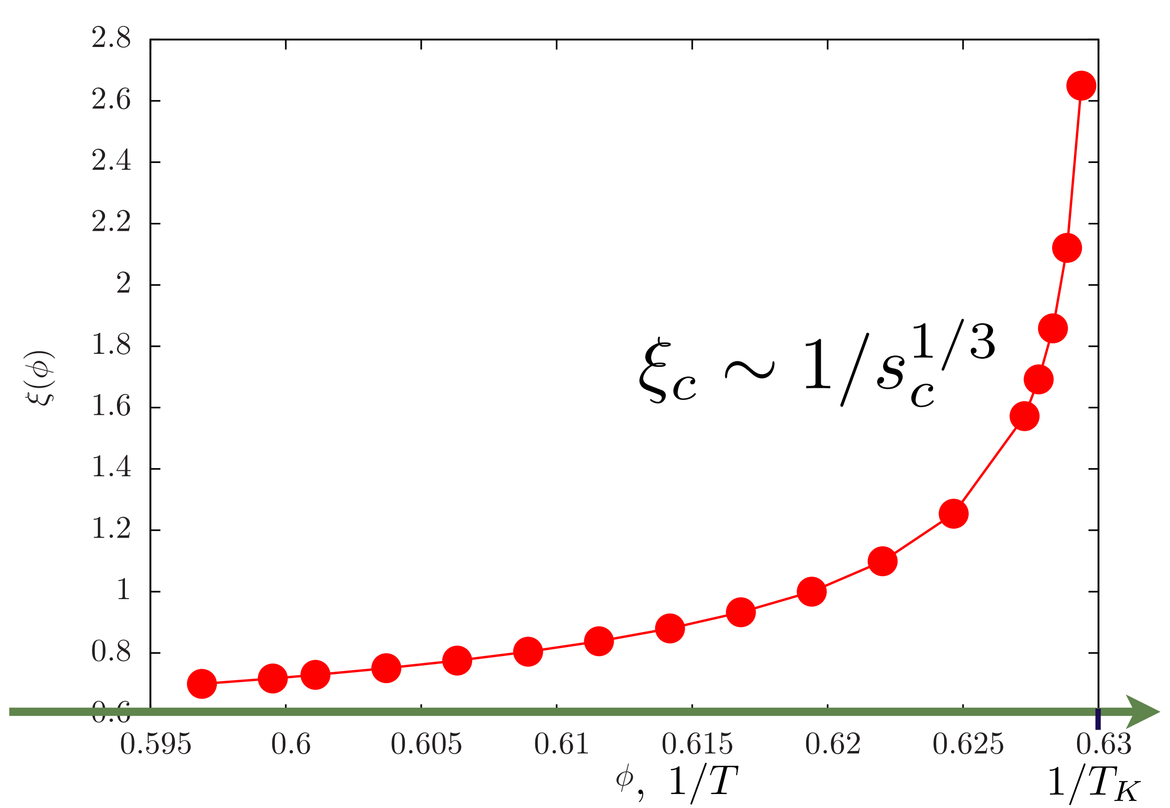


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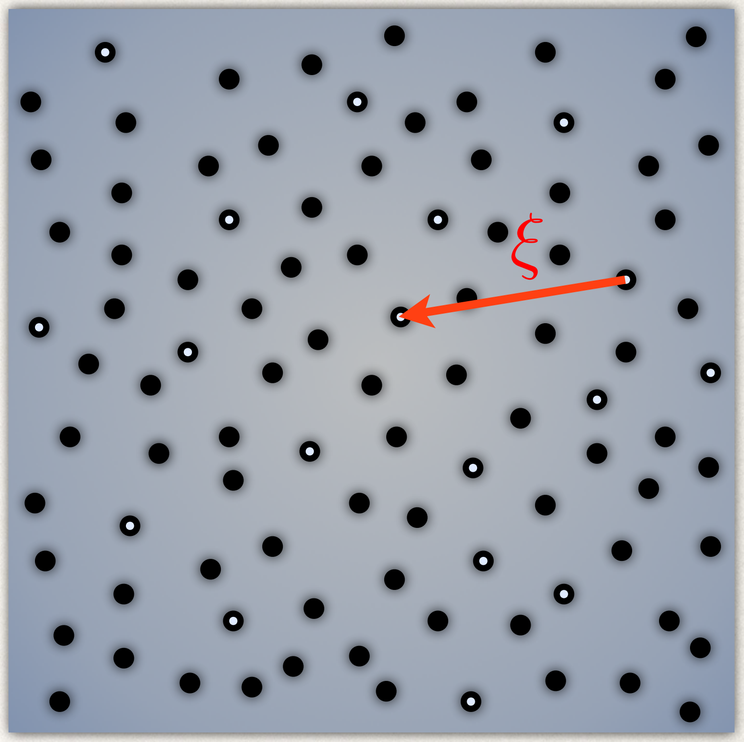


Quite a slowly divergent length-scale!
Irrelevant in the experimentally/numerically accessible region

# More than one correlation length scale!

C.C. and B.Seoane, arXiv: 1403.7180 (2014)

$$s_c(\phi, R) \simeq s_c(\phi) R^d - Y(\phi) R^{d-1}$$

S.Franz, and A.Montanari, J.Phys.A 40 F251 (2007)
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G.M.Hocky, T.E.Markland, D.R.Reichman, PRL 108 225506 (2012)
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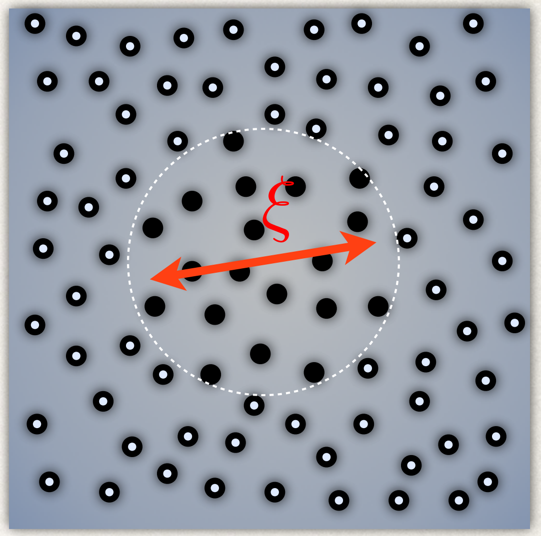
$$s_c^P(\phi, c) \simeq s_c(\phi) - cY(\phi)$$

When does the boundary select the **cavity** configuration?




$$\xi_{PS} \sim Y(\phi)/S_c(\phi)$$

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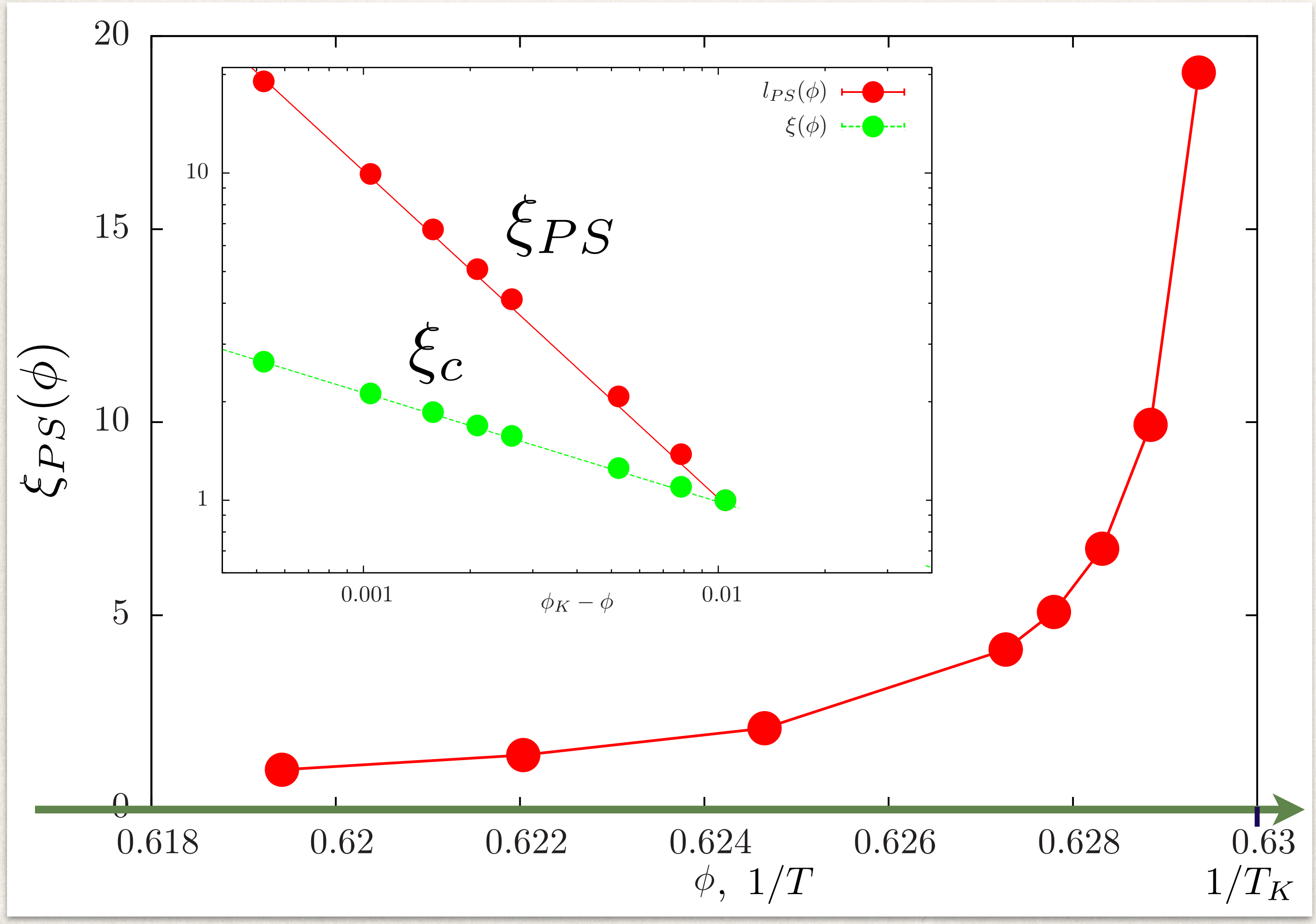
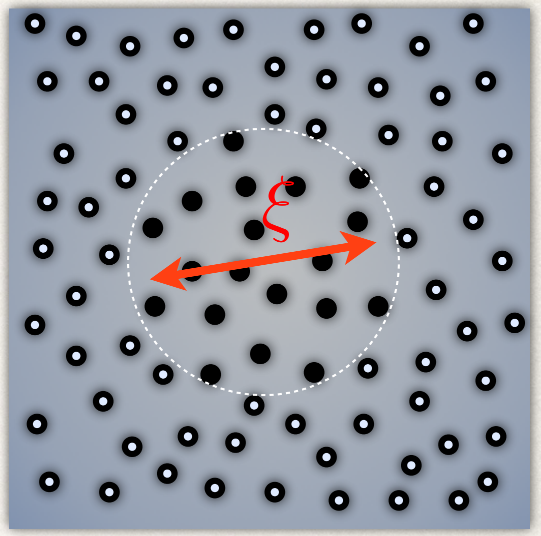



$$\xi_{PS} \sim Y(\phi)/S_c(\phi)$$

A faster divergence!

A way to test the RFOT theory

# More than two correlation length scales…

*P.Scheidler, W.Kob, K.Binder, and G.Parisi, Phil.Mag.B 82 283 (2002)*

*W.Kob, S. Roldán-Vargas, and L.Berthier, Nat.Phys. 8, 164-167 (2012)*

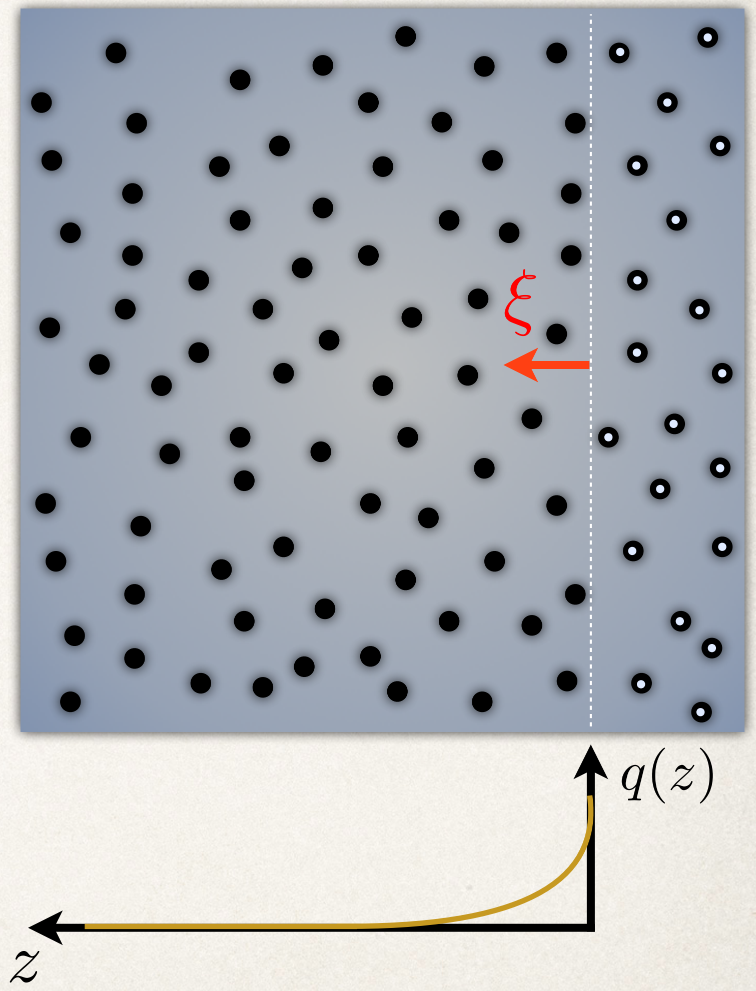
*G.Gradenigo et al., J. Chem. Phys. 138, 12A509 (2013)*

How far the **wall** selects the left-side configuration?

The high/low-$q$ interface behaves like an elastic manifold in a random field environment!

*G.Biroli and C.C., to appear*

*An effect of the self induced disorder encoded in the wall configurations*



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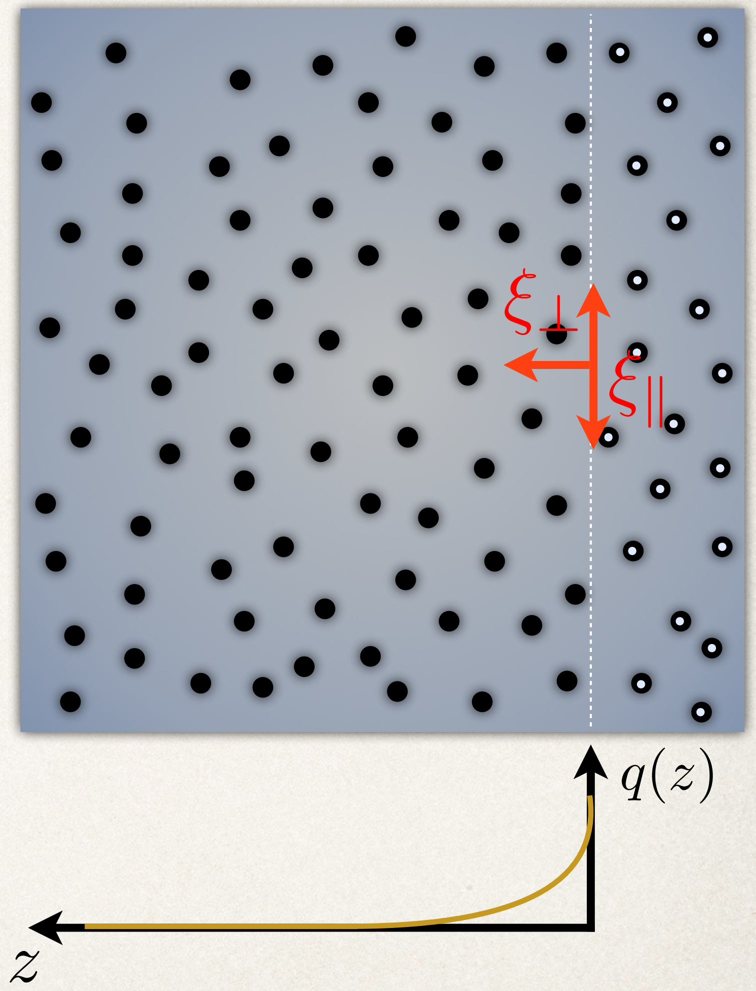
$$\Delta F_W \sim \frac{\mathcal{S}}{\xi_\parallel^{d-1}} \left( s_c(T)\xi_\perp \xi_\parallel^{d-1} - B\xi_\perp^{2-2/\zeta}\xi_\parallel^{d-1} + \sigma\xi_\parallel^{d-1} \right)$$

Configurational entropy cost (volume)

Free-energy gain due to roughness



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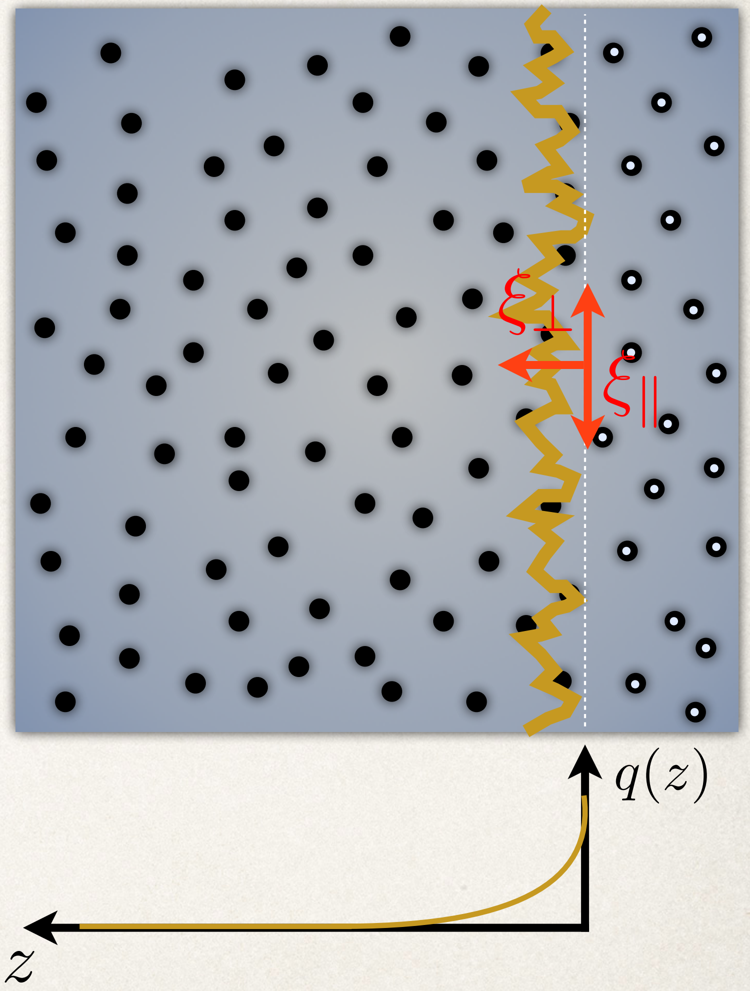


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Configurational entropy cost (volume) — Free-energy gain due to roughness

$$d = 3 \qquad \zeta = 2/3$$

$$\xi_\perp \sim s_c(T)^{-1/2}$$

$$\xi_c \ll \xi_\perp \ll \xi_{PS}$$

# Other static correlation length scales!

*C.C. et al., PRL 111 107801 (2013)*

*M.Mosayebi et al., PRL 104 205704 (2010)*

*G.Biroli, S.Karmakar, and I.Procaccia, PRL 111, 165701 (2013)*

*J.Kurchan and D.Levine, J.Phys.A 4 035001 (2011)*

*C.C. and G.Biroli, Europhys. Lett. 98 36005 (2012)*

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# A refined Random First Order Transition theory

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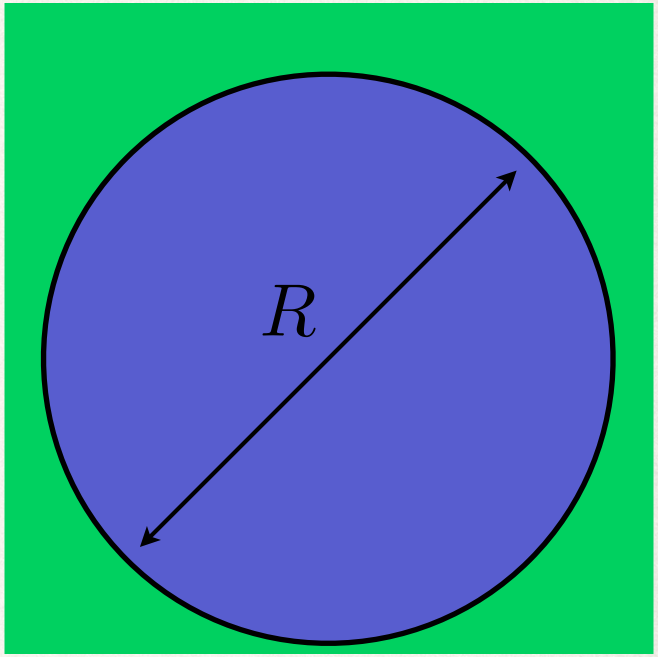
$$\Delta F(R) = \Delta F_s(R) - s_c R^d \;\Rightarrow\; \xi_{PS}$$



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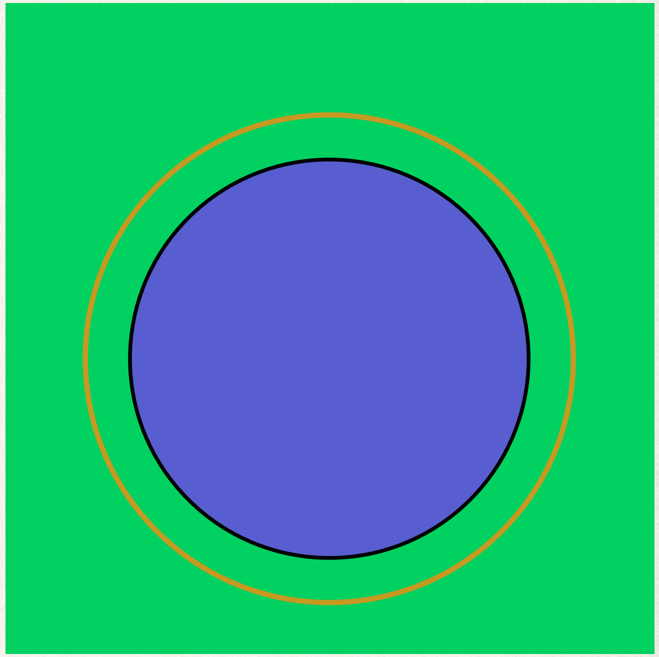

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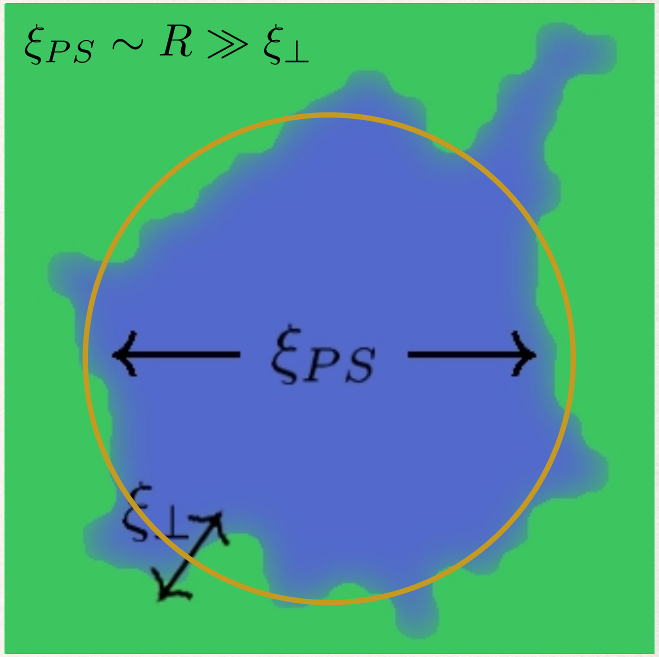
$$\Delta F(R) = \Delta F_s(R) - s_c R^d \;\Rightarrow\; \xi_{PS}$$

$$\Delta F_s(R) \sim R^{d-1}(\sigma - D\xi_\perp^{2-2/\zeta}) \quad \text{with} \quad \xi_\perp \sim s_c(T)^{-1/2} \quad \text{and} \quad 2 - 2/\zeta < 0$$

*C.C. et al, J.Chem.Phys. 131, 194901 (2009)*



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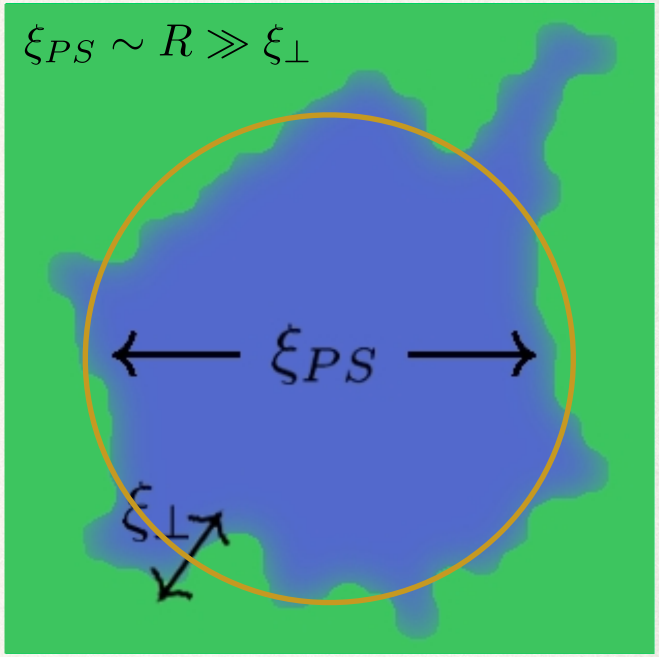
Near $T_K$

$$\Delta F_s(R) \sim R^{d-1}\sigma \quad \text{and} \quad \xi_{PS} \sim s_c(T)^{-1}$$



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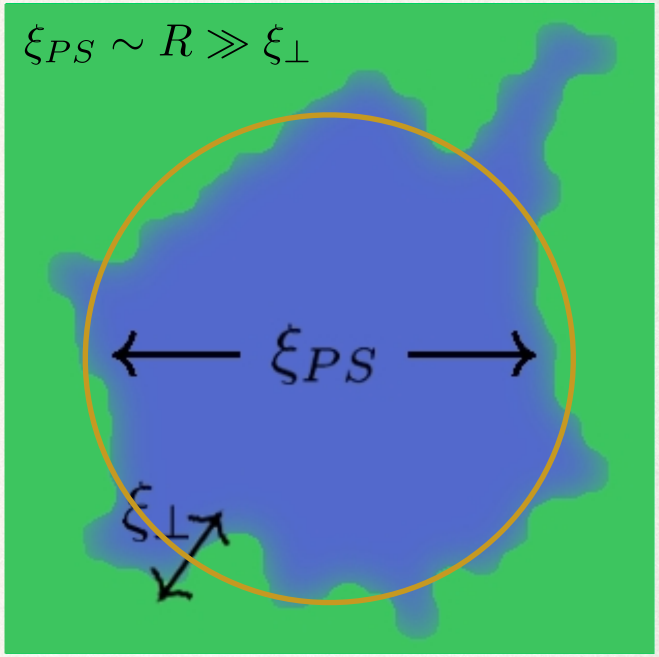


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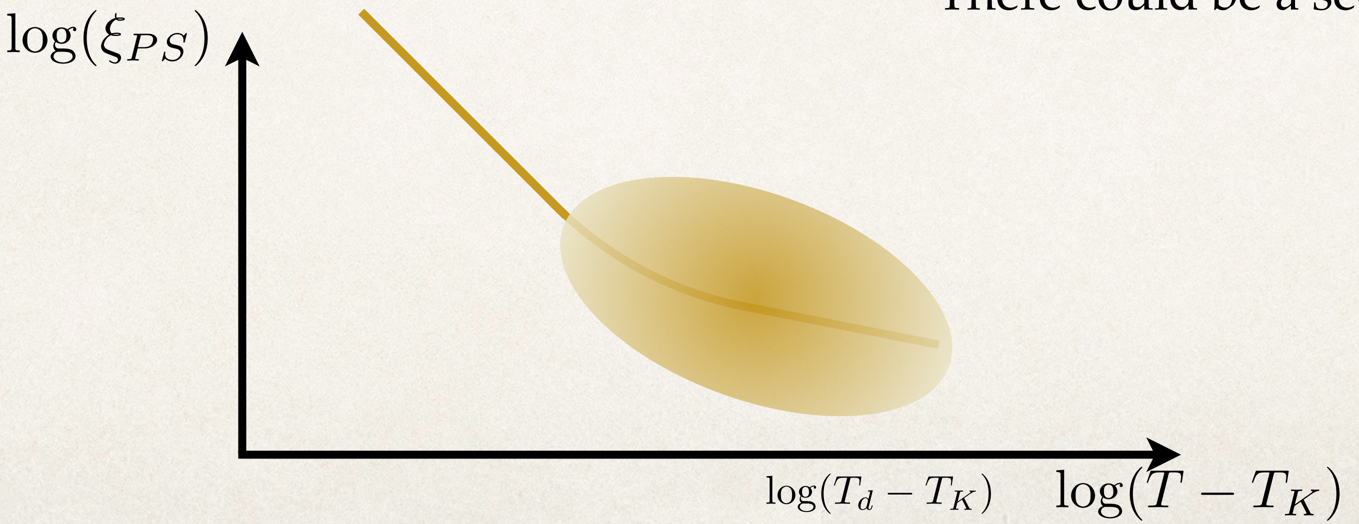
Near $T_K$

$$\Delta F_s(R) \sim R^{d-1}\sigma \quad \text{and} \quad \xi_{PS} \sim s_c(T)^{-1}$$

For $T \lesssim T_d$, $\sigma$ small, $s_c$ finite

There could be a second regime!



# Conclusions and perspectives

- Static cooperative length scale, the cornerstone of the RFOT theory
  - Nowadays many *length scales* have been found, explained, putted in mutual relation
  - among them $\xi_{PS} \sim s_c^{-1}$ give information on the size of rearranging regions
  - and $\xi_{\perp} \sim s_c^{-1/2}$ can be used to refine the RFOT picture

- In the meanwhile the challenge for the study of the ideal glass transition and its critical properties pushed to approach the problem from a promising new perspective through <u>the random pinning procedure</u>

What is left?

- tests for the validity of the liquid-glass phase diagram
- ..and of the refined thermodynamic picture of the glass formation
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