Random Pinning in Supercooled Liquids
Connection to RFOT theory and Calculation of the Growing Length-scale

Correlation and Disorder in Classical and Quantum Systems
International Centre for Theoretical Sciences

Saurish Chakrabarty
Rajsekhar Das, Smarajit Karmakar and Chandan Dasgupta

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Outline

1. Introduction
   - What is the glass transition?
   - The Random First Order Transition (RFOT) Theory
2. Random pinning results
   - Systems studied & Methods used
   - Random Pinning in Supercooled Liquids
   - Tests of RFOT theory & Results
3. Conclusions

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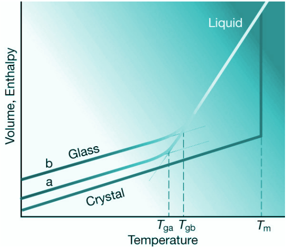
Glass basics



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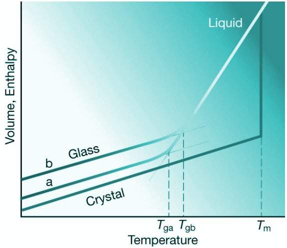

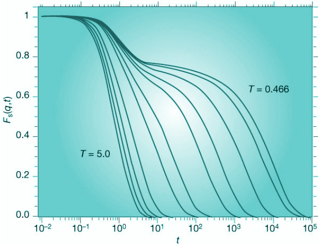

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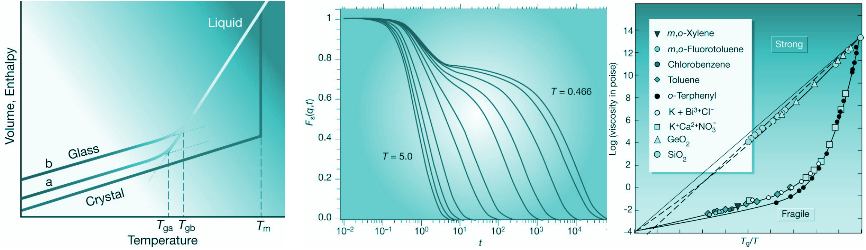

P. G. Debenedetti and F. H. Stillinger, Nature **410**, 259 (2001)

Random First Order Transition (RFOT) Theory

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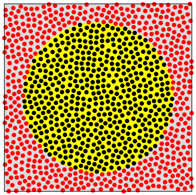
T. R. Kirkpatrick, D. Thirumalai, and P. G. Wolynes, Phys. Rev. A **40**, 1045 (1989)
T. R. Kirkpatrick and D. Thirumalai, Journal of Physics A: Mathematical and General **22**, L149 (1989)
J.-P. Bouchaud and G. Biroli, J. Comp. Phys. **121**, 7347 (2004)

Static length-scales of amorphous order

Point-to-set length-scale



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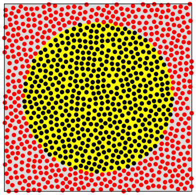

Length-scale from the minimum eigenvalue of the Hessian matrix

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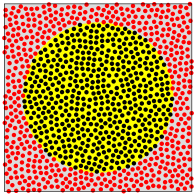

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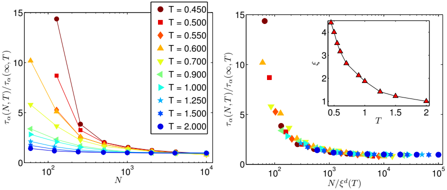

Length-scale from the α-relaxation time

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Systems studied

- 3dKA: Kob-Andersen 80:20 binary Lennard Jones mixture.

  W. Kob and H. C. Andersen, Phys. Rev. E **51**, 4626 (1995)

- 2dmKA: 65:35 binary Lennard Jones mixture with parameters same as 3dKA.

  R. Brüning, D. A. St-Onge, S. Patterson, and W. Kob, J. Phys. Chem. **21**, 035117 (2009)

- 3dR10: 50:50 mixture with $1/r^{10}$ interactions.

  S. Karmakar, A. Lemaître, E. Lerner, and I. Procaccia, PRL **104**, 215502 (2010)

- 2dR10: 50:50 mixture with $1/r^{10}$ interactions.

  S. Chakrabarty, R. Das, S. Karmakar, and C. Dasgupta, J. Comp. Phys. **145**, 034507 (2016)

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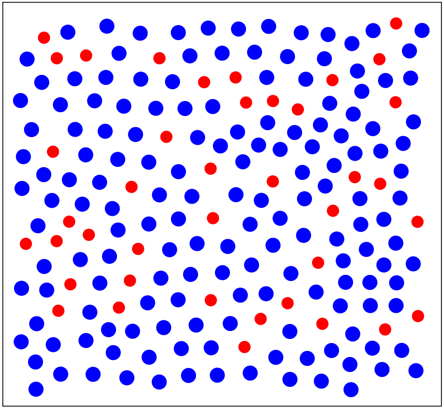
Random Pinning



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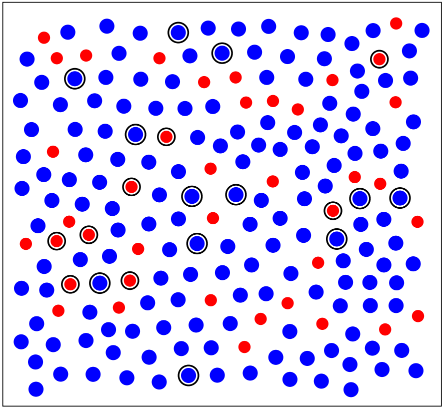

The overlap correlation function

$$Q(t) = \overline{\left\langle \frac{1}{N} \sum_i w(|\vec{r}_i(t) - \vec{r}_i(0)|) \right\rangle_0}$$

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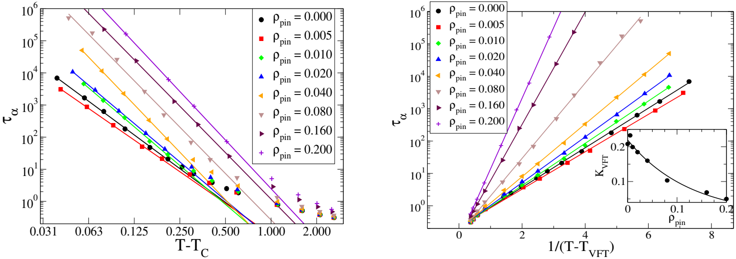
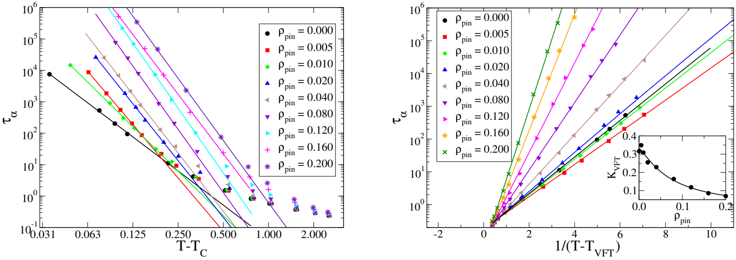
Extraction of T_c and T_{VFT}

3dKA



3dR10



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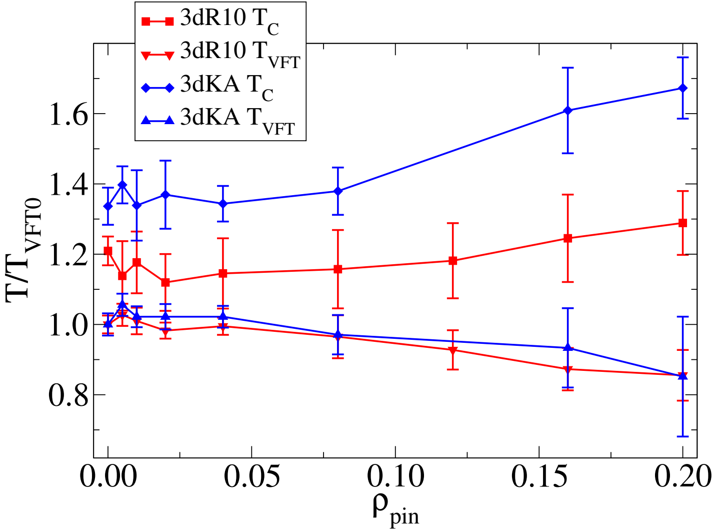
The phase diagram

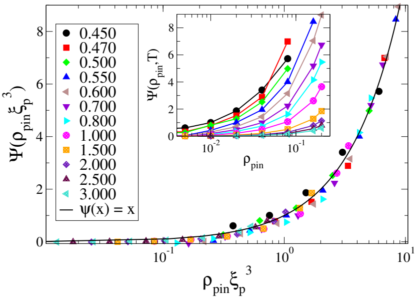


The static length-scale from pinning

Data Collapse:

$$\Psi(\rho_{pin}, T) \equiv \ln\left[\frac{\tau_\alpha(\rho_{pin}, T)}{\tau_\alpha(0, T)}\right] = Cf(\rho_{pin}\xi_p^d(T))$$

3dKA



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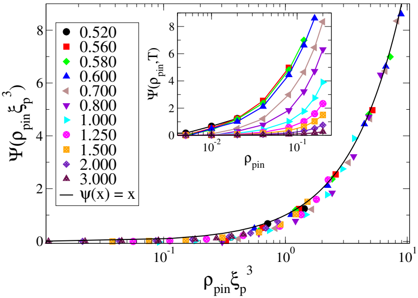

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Some relations obtained from RFOT theory

- RFOT $\Longrightarrow$ modified Adam-Gibbs relation

$$\tau_\alpha(T) = \tau_\infty \exp\left(\frac{B}{Ts_c^\alpha}\right), \qquad \alpha = \frac{\psi}{d-\theta}$$

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- Assume $s_c(\rho_{pin}, T) = F(\rho_{pin}) s_c(0, T) \implies$

$$T\xi_p^d(T) = \frac{1}{s_c^\alpha(0, T)} \propto \xi_s^\psi(0, T).$$

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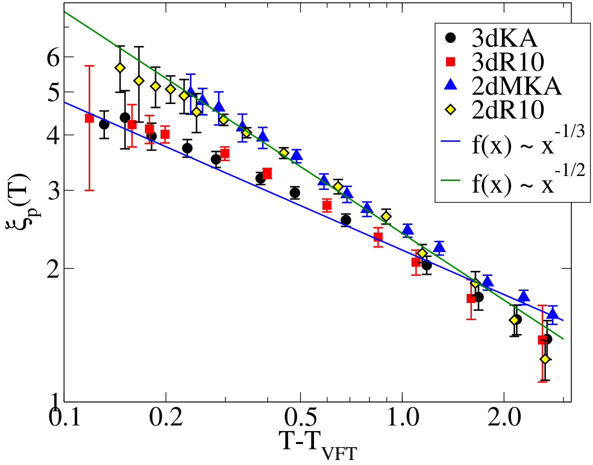
Divergence of the pinning length-scale

Growing length-scale: $\xi_p(T) = [1/(Ts_c^{\alpha}(0,T))]^{1/d} \propto [1/(T - T_{VFT})]^{1/d}$



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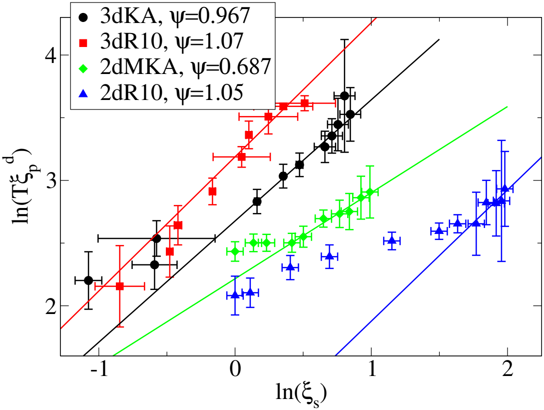
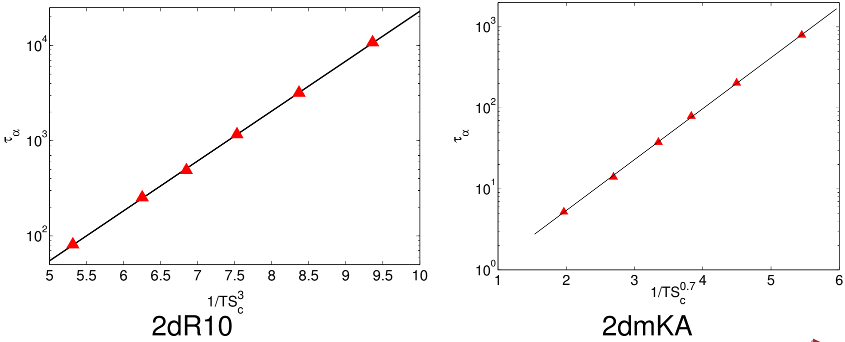
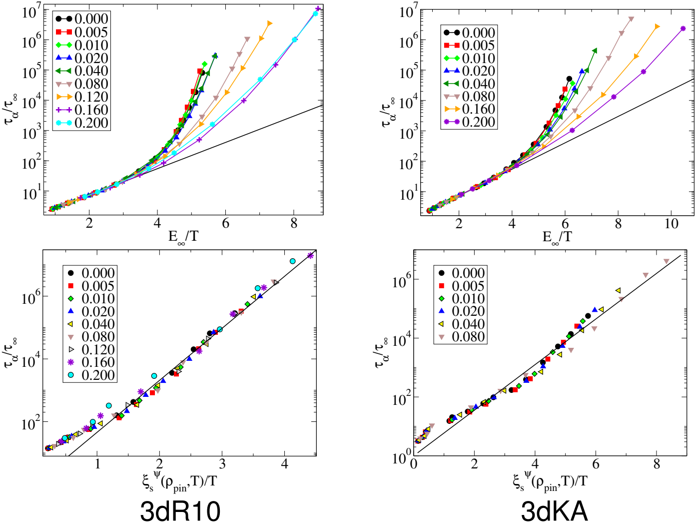
The exponent ψ



The modified Adam Gibbs relation in two dimensions



Fragility & the static length-scale



The surface tension exponent, θ

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RFOT may not be valid for 2dR10

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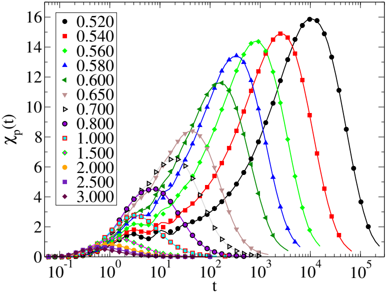

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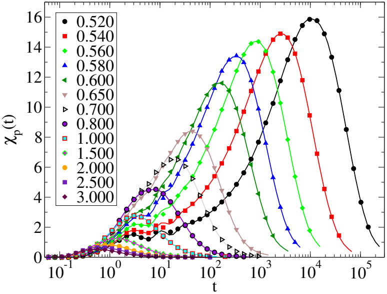

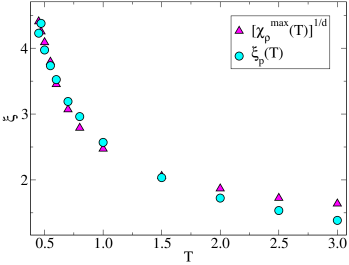

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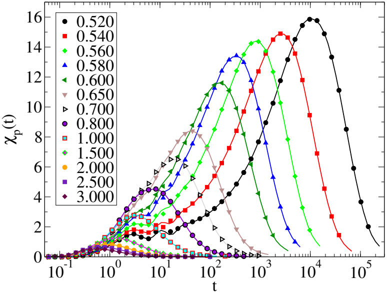

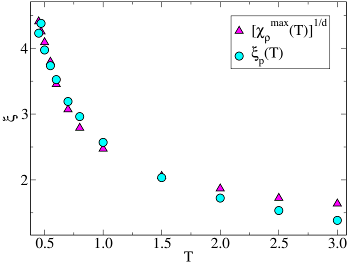

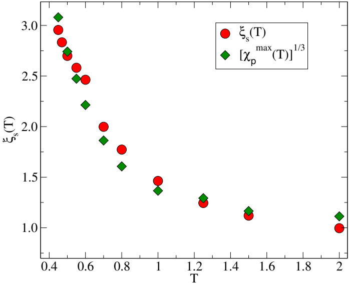

Thank You