Lattice glass model in three spatial dimensions: Statics and dynamics at low temperatures

Yoshihiko Nishikawa

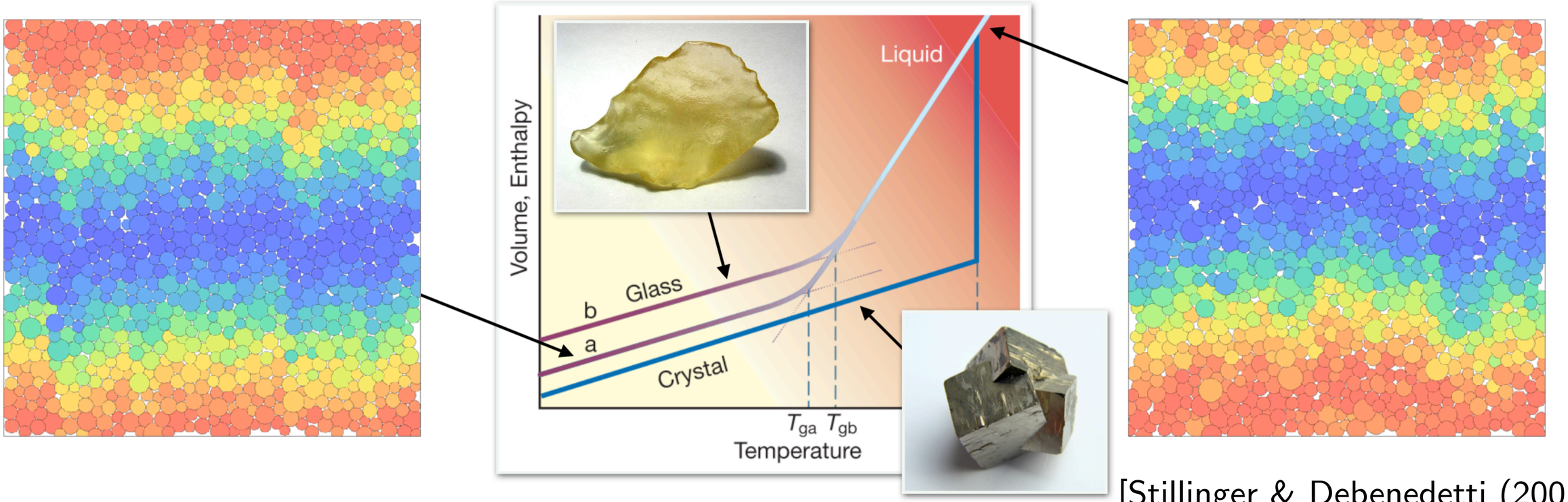
Nagoya University

EAJSSP 2025
15 Oct. 2025

YN and Ludovic Berthier, PRL **132**, 067101 (2024)

YN and Koji Hukushima, PRL **125**, 065501 (2020)

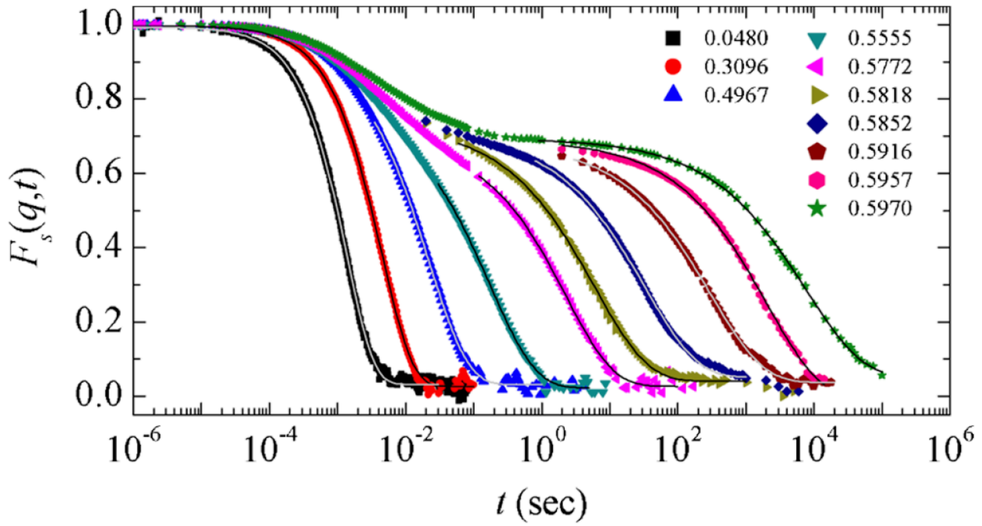
Introduction: The glass transition



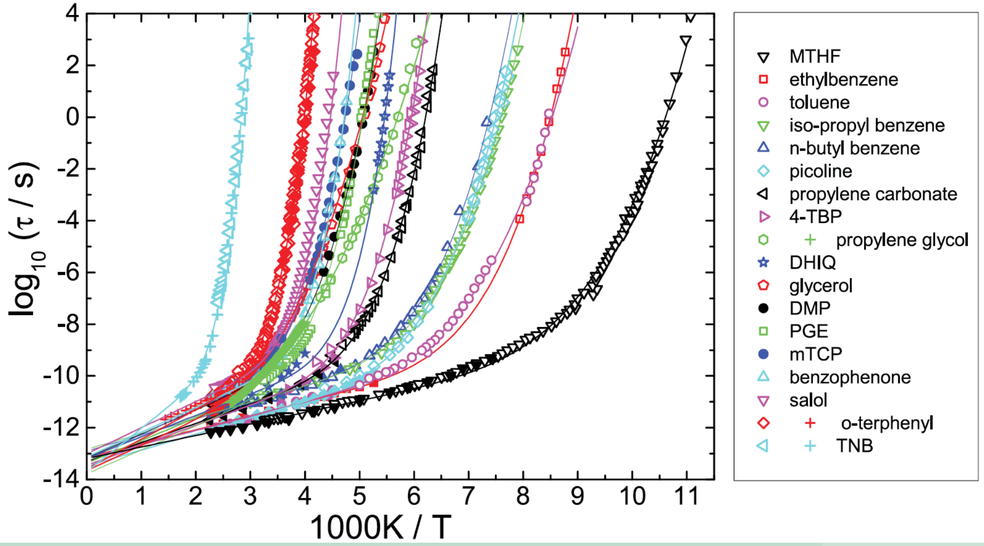
[Stillinger & Debenedetti (2001)]

- Glasses are solid in our timescales, yet have liquid-like, disordered microscopic structures
- Glassy phenomena are universally observed in a wide range of situations/systems
  - Optimization problems, machine-learning models, biological tissues etc...

Introduction: Glassy dynamical slowing down in supercooled liquids



[Brambilla *et al.* (2009)]



- Drastic dynamical slowing down toward low temperatures, with two-step relaxation
- For *fragile* supercooled liquids, the structural relaxation time τ_α has a super-Arrhenius growth
  - Empirically following the Vogel-Fulcher-Tammann (VFT) law

$$\tau_\alpha \sim \exp\left[\frac{A}{T - T_0}\right]$$

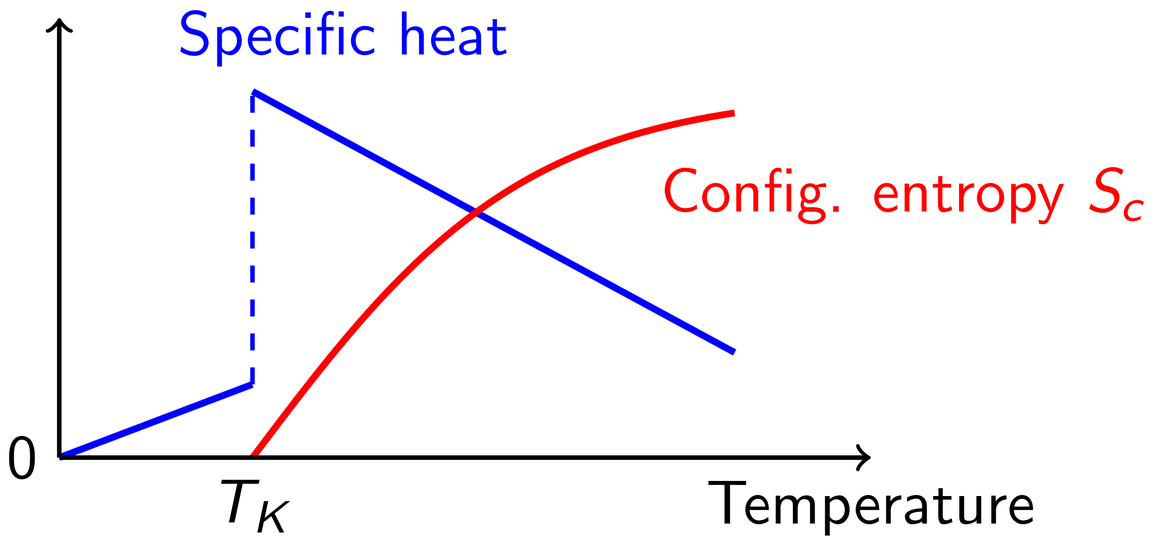
[Schmidtke *et al.* (2013)]

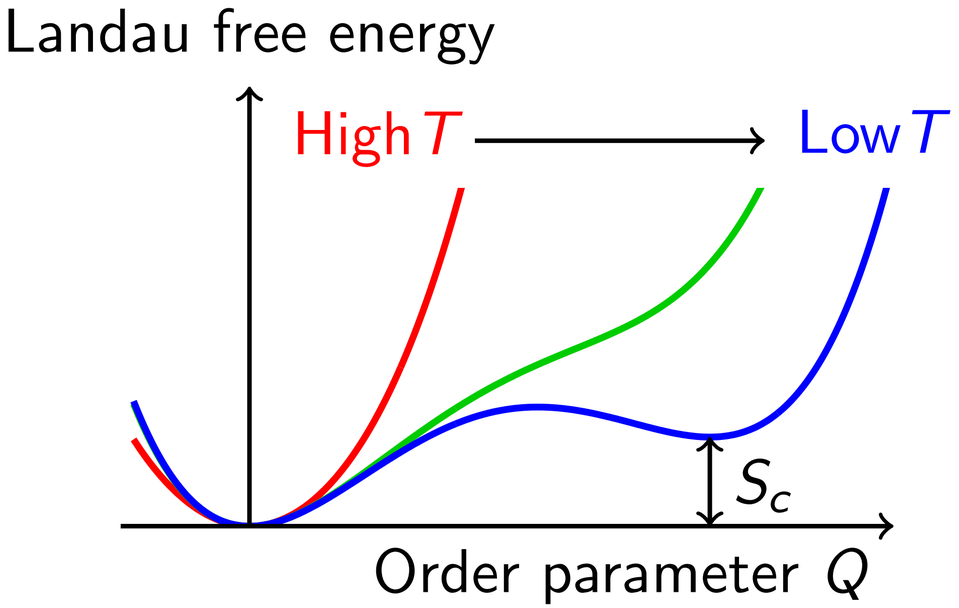
Key question

Why does the relaxation time τ_α grow so rapidly?

- The super-Arrhenius growth usually suggests a growing energy barrier and the collective dynamics
  cf. Critical dynamics at order-disorder transitions
- Yet, static structures of supercooled liquids remain disordered at any temperature
- Does a static *amorphous* order exist?

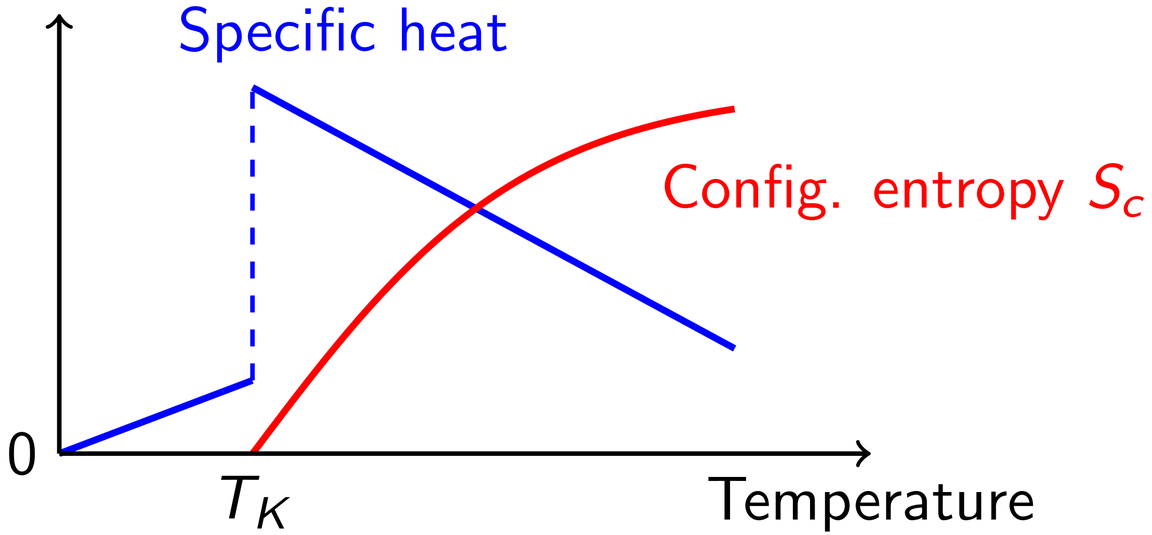
Mean-field scenarios: Random first-order transition [Kirkpatrick,Thirumalai&Wolynes]

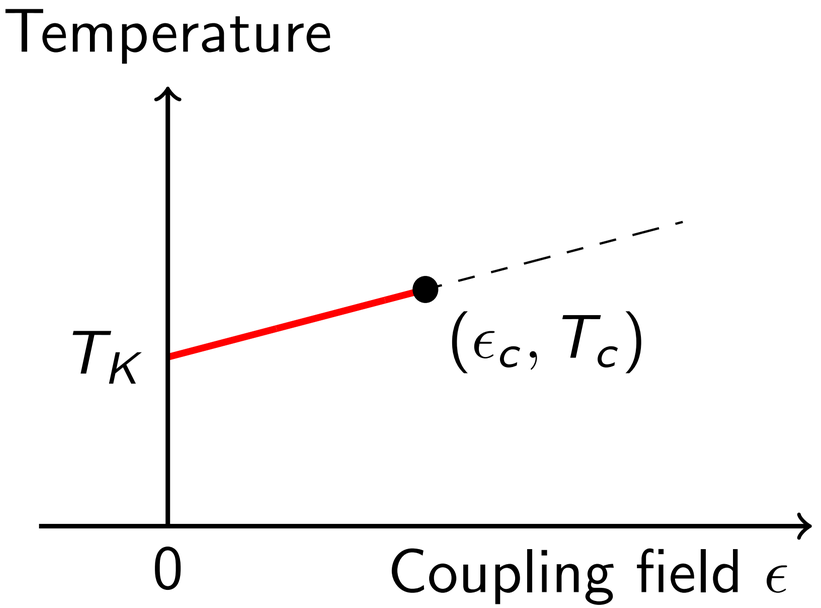




- In the mean-field limit $d \to \infty$, the ideal, static glass transition takes places at $T_K > 0$
  - Configurational entropy S_c goes to zero and specific heat has a finite jump
  - Landau free energy, Franz-Parisi potential, has two minima at low T
  - Phase diagram has a first-order transition line that terminates at a critical point (ϵ_c, T_c)
  - Growing static length scale ξ causes the glassy slowing down

Mean-field scenarios: Random first-order transition [Kirkpatrick,Thirumalai&Wolynes]

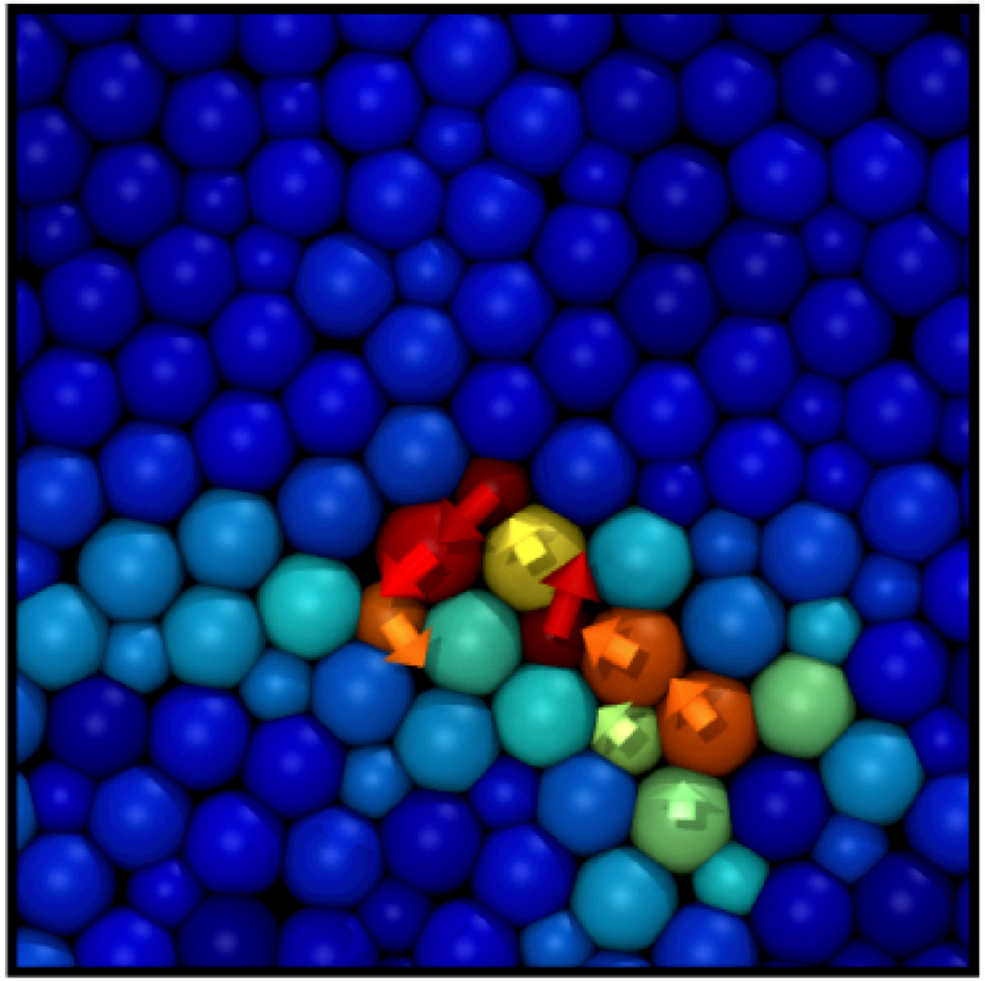




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Dynamical facilitation picture

[Chandler & Garrahan]

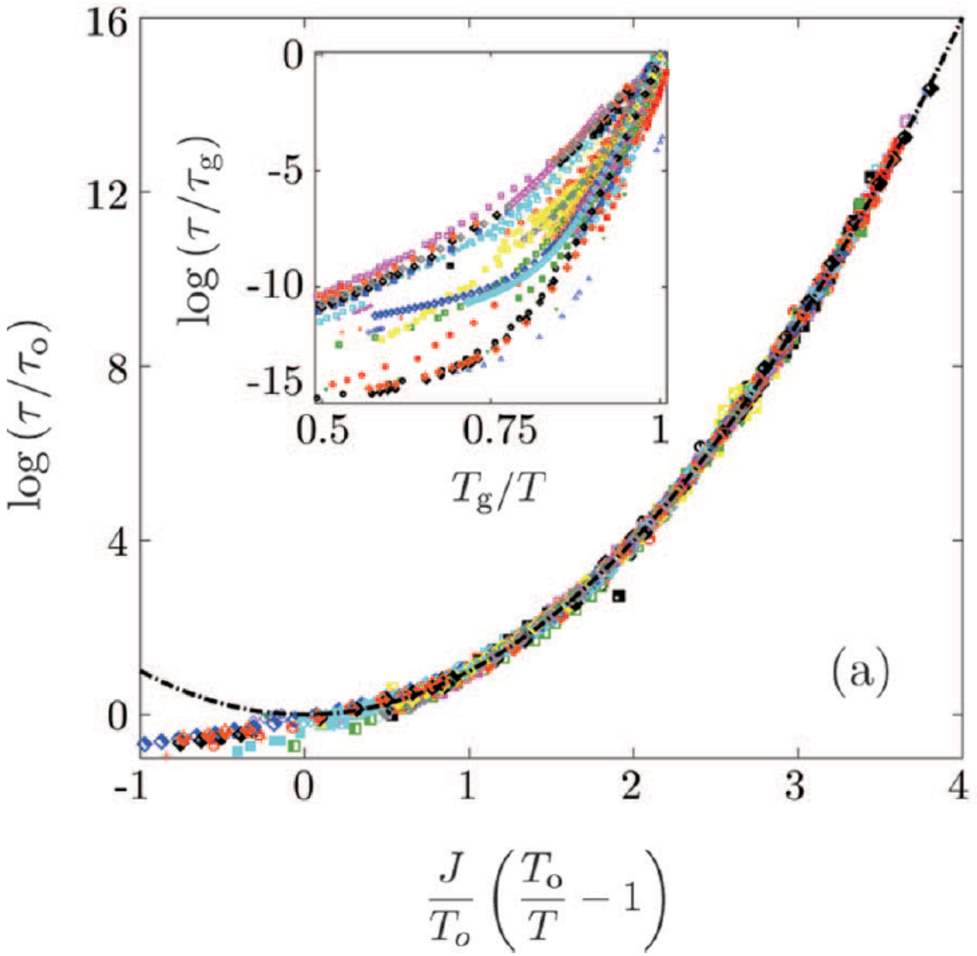


[Keys *et al.* (2011)]

- Emergent *dynamical defects* induce chains of displacements in real space: Dynamical Facilitation
- Relaxation of glasses are triggered by these defects
- No growing static length scale is needed
  cf. Kinetically constrained models (KCMs) with trivial thermodynamics show glassy dynamics

Dynamical facilitation picture

[Chandler & Garrahan]



[Elmatad *et al.* (2009)]

- Density of dynamical defects becomes small at low $T \rightarrow$ Glassy slowing down
- The parabolic law for the relaxation time τ:

$$\log\left(\frac{\tau}{\tau_o}\right) \sim \left(\frac{T_o}{T}-1\right)^2$$

- Recent numerical studies on atomistic models have confirmed the DF process appears at low T
  [PRL 117, 145701 (2016)] [PRX 12, 041024 (2022)] etc...

Theoretical scenarios for the glass transition

- Experiments and numerical simulations cannot discriminate those scenarios easily
  - The both theories (and others) seem to be correct to some extent at accessible low T
  - Reaching temperatures near the putative T_K is needed
- Whether a growing static length scale exists at low T is the key to disentangle the situation
  - Kinetic theories such the DF theory do not refer to a complex landscape
  - Static theories including RFOT predict a non-trivial temperature evolution of the free-energy landscape and a diverging static length scale at T_K
  - Drastic growth of a time scale hinders a direct access to very low-T glasses...
- Simpler *toy* models and new numerical techniques are essential to address the origin of the glassy dynamics

Why toy models?: Roles of toy models in stat mech

- Toy models do not give a detailed, quantitative explanation, but provide *scenarios*
  - Often oversimplified and microscopically unrealistic
  - Yet, those would solve technical difficulties in *realistic* models and suggest new observations
    e.g. Random energy model (REM) by B. Derrida
  - The RFOT theory is built on toy models of spin glasses

- The glassy dynamics is universally observed not only in molecular liquids and realistic models, but also in "toy" models
  - Graph coloring, k-SAT, etc
  - Kinetically constrained models, Lattice glass models

- The *universal* theory for the glass transition (if it exists) must explain the glassy dynamics of these toy models as well

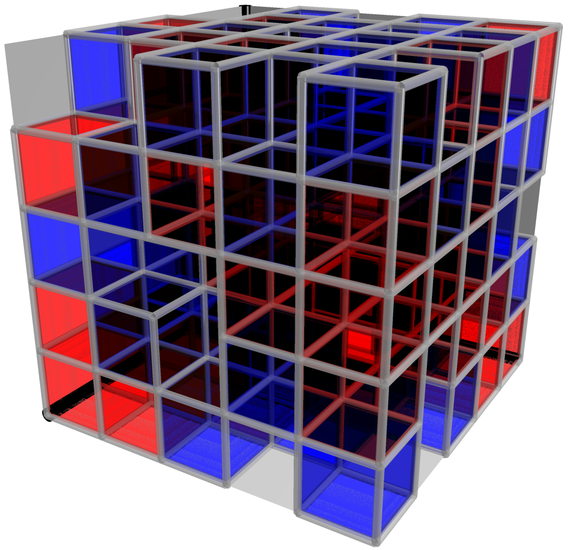
Lattice glass model in 3d

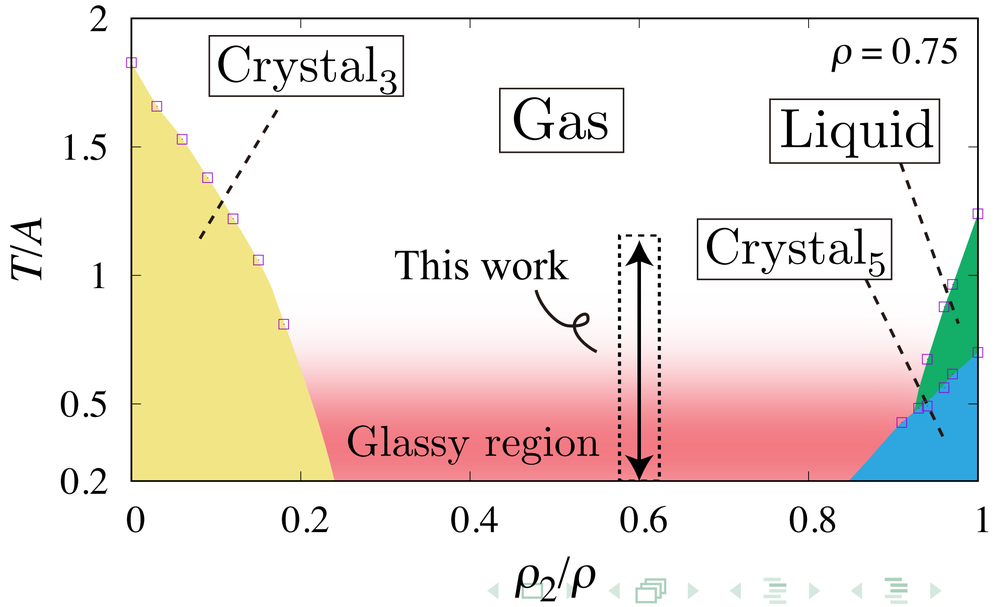
[YN&Hukushima, PRL **125**, 065501 (2020)]

- N particles on a periodic cubic lattice with linear dimension L:

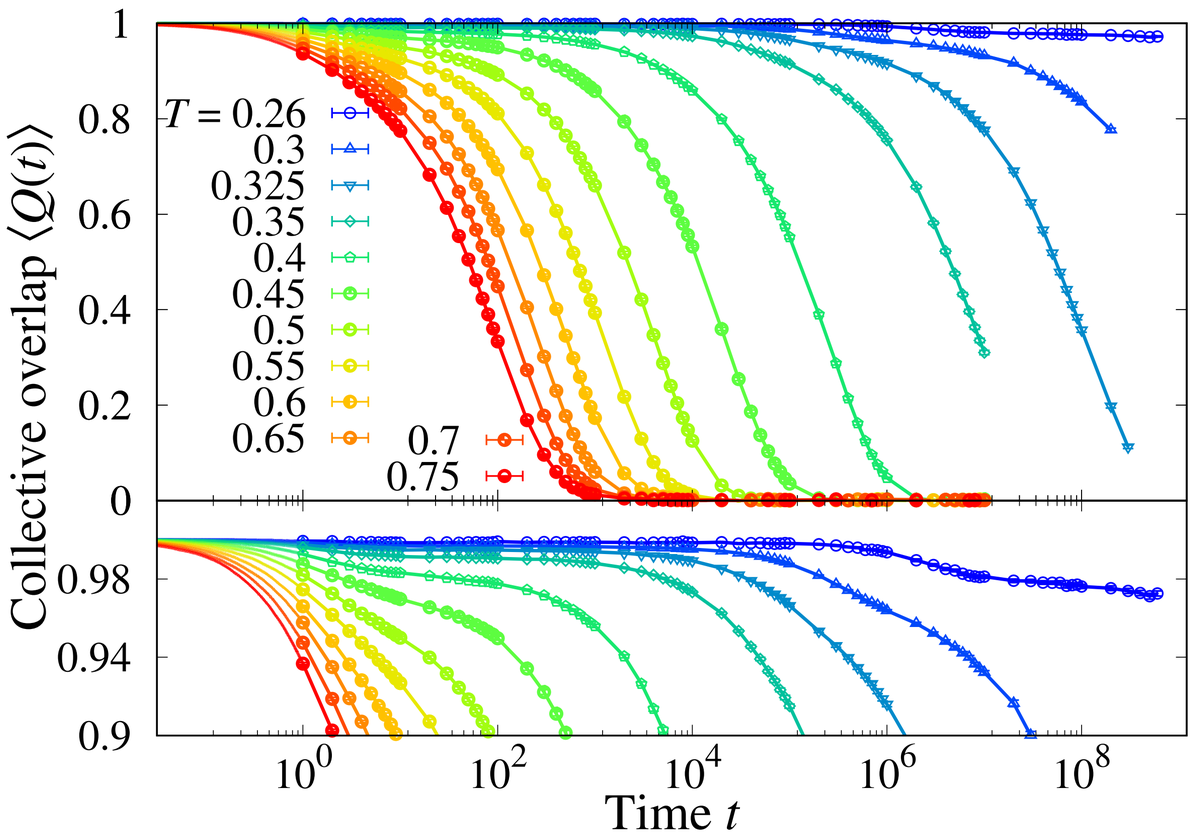
$$H/A = \sum_{i}^{N} \Big(\underbrace{\sum_{j} \delta_{|\boldsymbol{r}_i - \boldsymbol{r}_j|,1}}_{\#\text{ of neighbors}} - \ell_{\sigma_i} \Big)^2, \quad A > 0$$

  - Binary mixture: $\sigma_i \in \{1, 2\}$, $\ell_1 = 3$, and $\ell_2 = 5$
  - Fixed densities: $\rho = N/L^3 = 0.75$, $\rho_1 = N_1/N = 0.4$, and $\rho_2 = N_2/N = 0.6$
  - No quenched disorder





Glassy dynamics: Time correlation and relaxation time

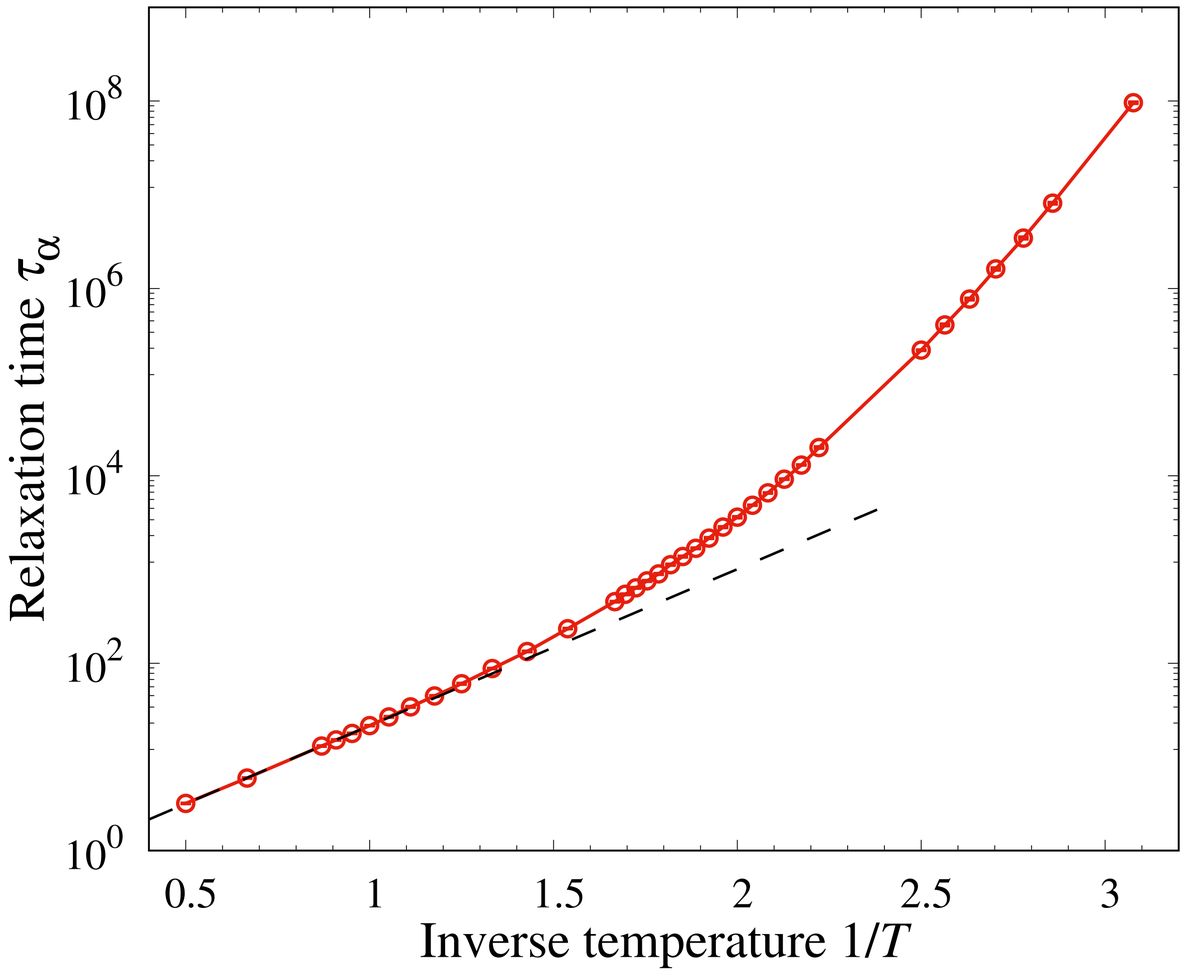


- Local swap dynamics: A randomly-chosen pair of neighboring sites are swapped with the Metropolis probability
  - No kinetic constraint at all
- Equilibrated at very low T using efficient non-local swap algorithm
- Time correlation

$$\langle Q(t) \rangle = \frac{1}{1 - Q_0} \left\langle \frac{1}{N} \sum_i q_i(t) - Q_0 \right\rangle$$

has two-step relaxation at $T \lesssim 0.55$

Glassy dynamics: Time correlation and relaxation time



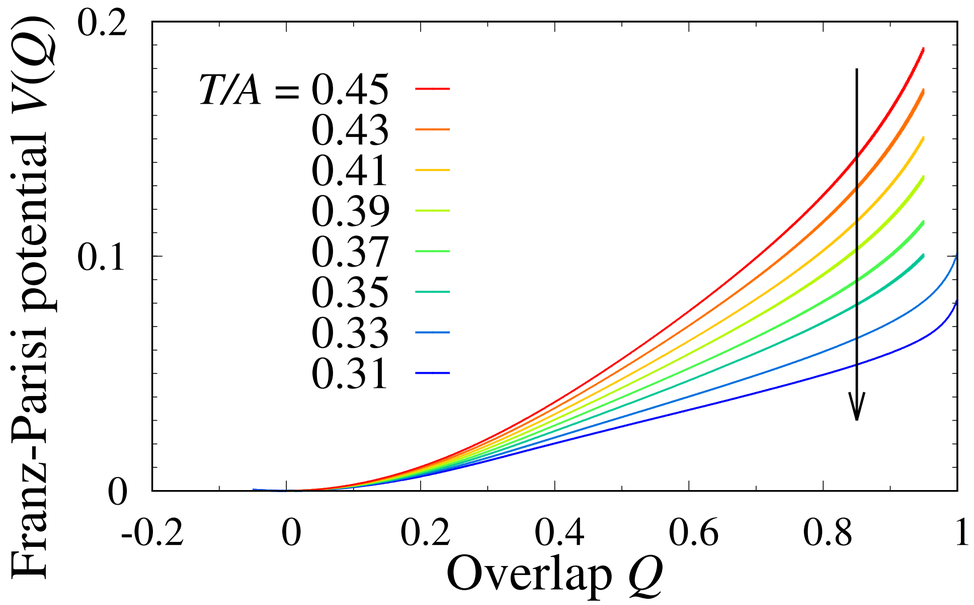
- Local swap dynamics: A randomly-chosen pair of neighboring sites are swapped with the Metropolis probability
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- The relaxation time τ_α grows rapidly, faster than the Arrhenius law

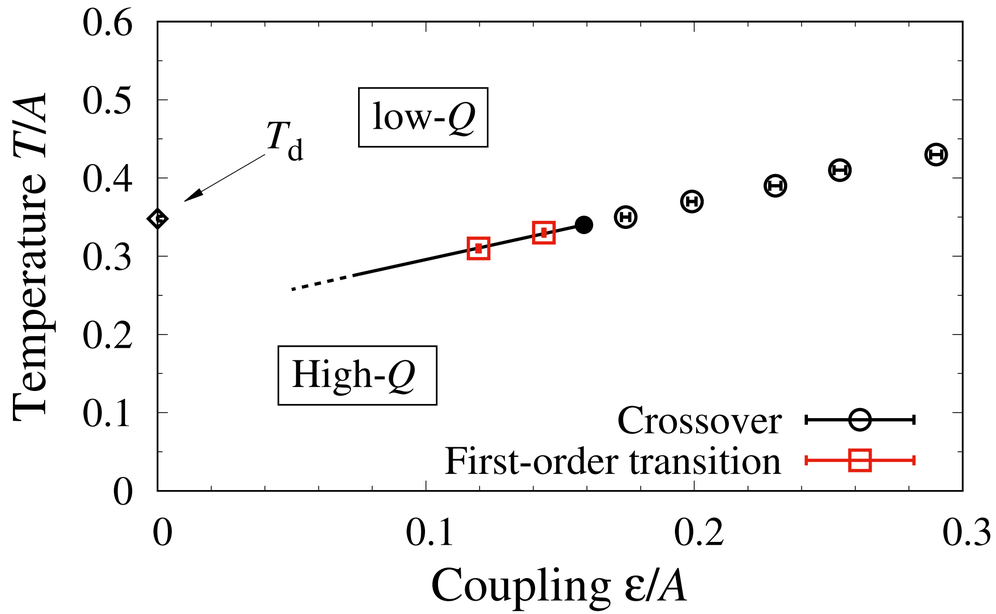
  $\rightarrow$ Fragile-glass-like bulk dynamics

Testing RFOT: Franz–Parisi potential

[YN+Hukushima (2020)]

- The Franz–Parisi potential $V(Q)$ indicates large fluctuations of the overlap at low T: Decreasing configurational entropy
- At $T \lesssim 0.34$, a first-order transition at finite coupling ε: RFOT-like phase diagram

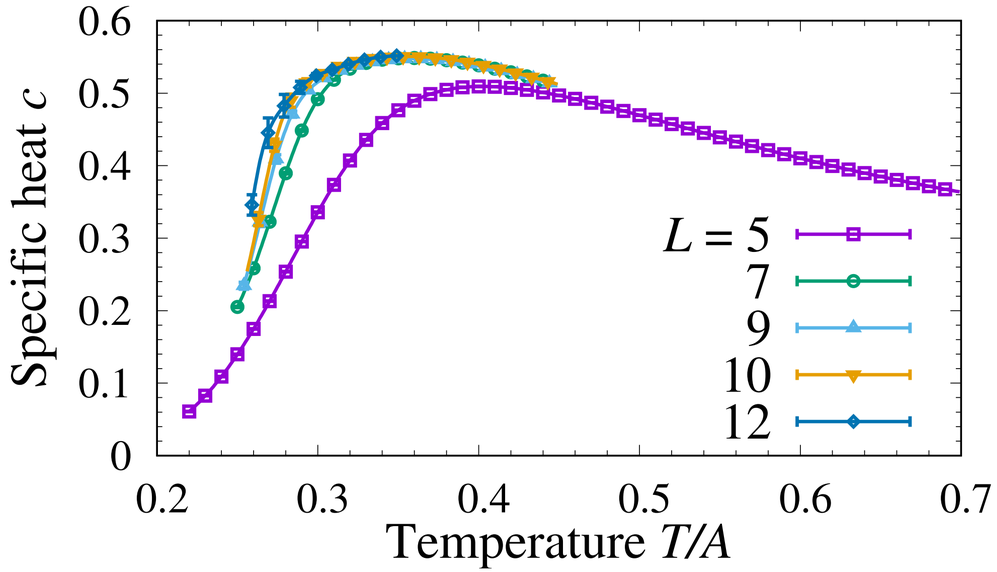


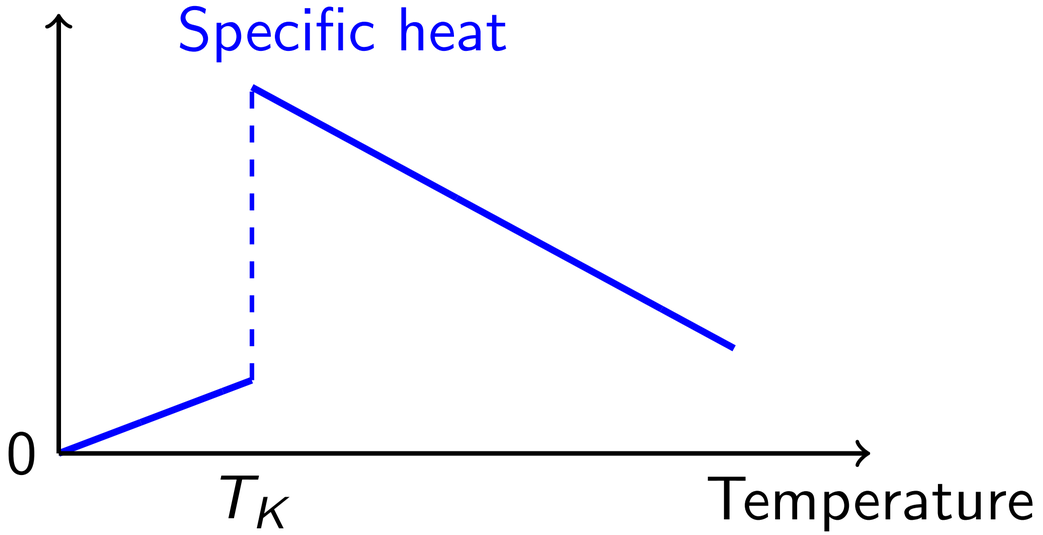


Testing RFOT: Specific heat

[YN+Hukushima (2020)]

- RFOT theory predicts a finite jump in the specific heat
  - Critical exponents $\alpha = 0$ and $\nu = 2/d$ [Kirkpatrick, Thirumalai & Wolynes]
- The specific heat of the LG model has a rapid drop at $T \simeq 0.24$
  - $(\partial c/\partial T)^* \sim L^\theta$ with $\theta = (1+\alpha)/\nu$, $\alpha = 2 - d\nu$ (hyperscaling) $\rightarrow \nu = 3/(\theta + d)$
  - $\alpha = -0.03(3)$ and $\nu = 0.68(1)$: Consistent with RFOT so far
  - Very efficient non-local swap algorithm allows a direct access at $T \simeq T_K$

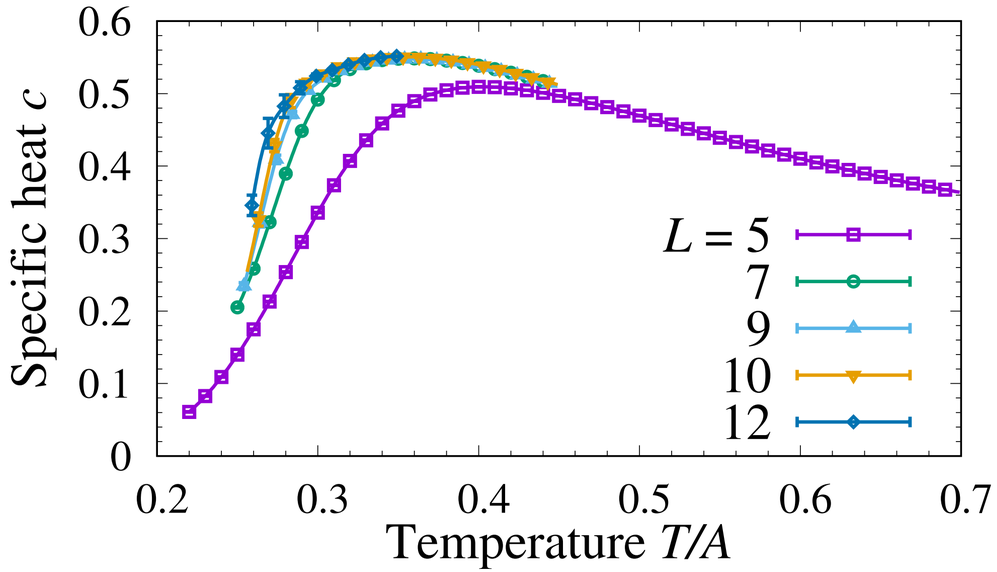


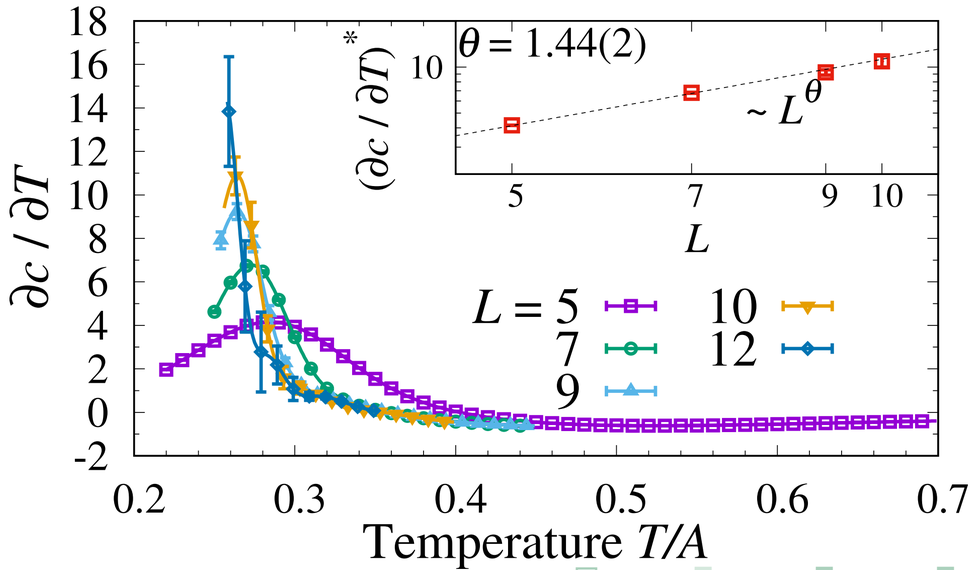


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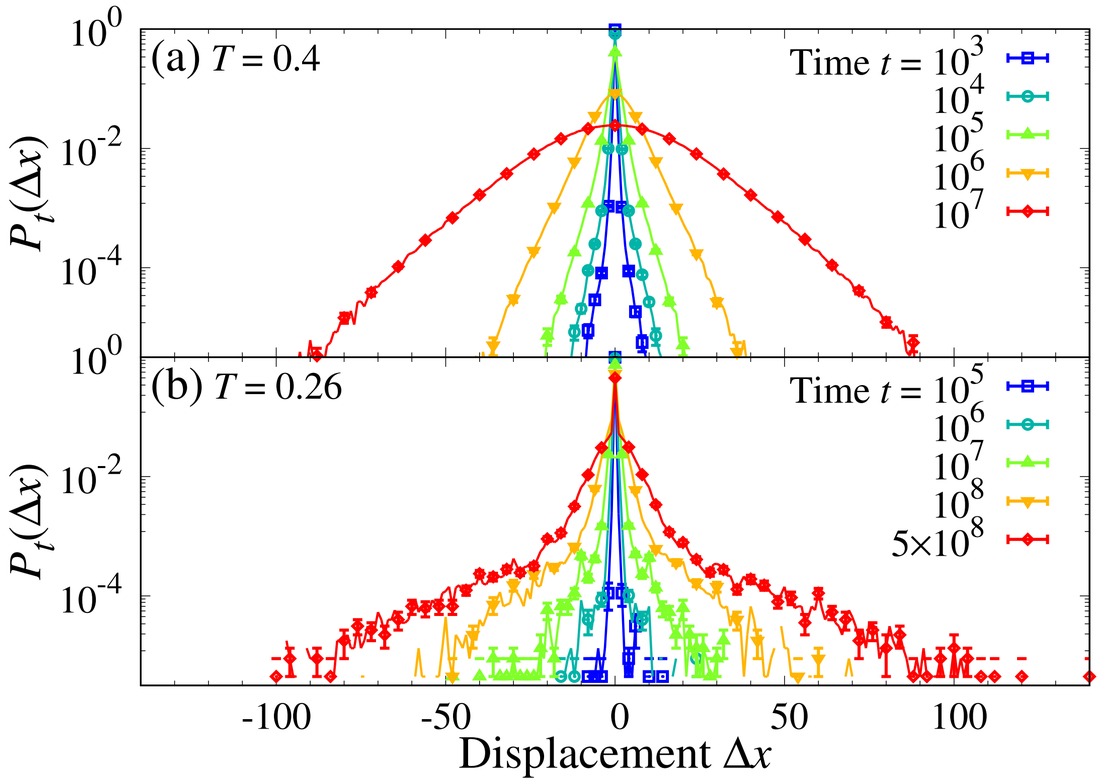




Some questions for further testing the RFOT theory

- RFOT seems correct for static behaviors in the LG model
  - First-order transition in the coupled system
  - Decreasing configurational entropy towards low T
  - Rapid drop in the specific heat with critical exponents $\alpha \approx 0$ and $\nu \approx 2/d$
- What drives the (microscopic) relaxation dynamics near at low T?
- Does the growing static length scale control the slow glassy dynamics?
- Does the RFOT-type activated dynamics really matter?

Highly heterogeneous dynamics



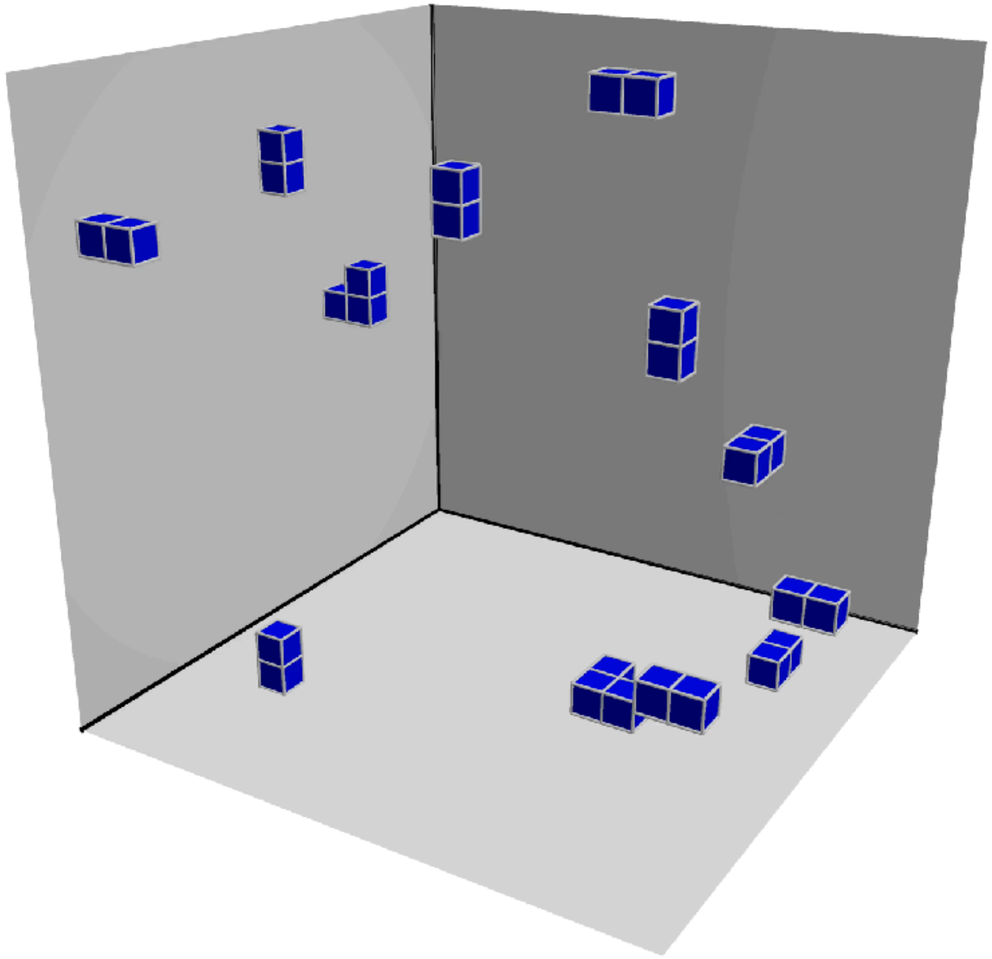
The van Hove distribution

$$P_t(\Delta x) = \left\langle \frac{1}{3N} \sum_{i,\alpha} \delta\big(\Delta x - (r_{i,\alpha}(t) - r_{i,\alpha}(0))\big) \right\rangle$$

- At $T = 0.4$, $P_t(\Delta x)$ has exponential tails and becomes Gaussian at $t \to \infty$
- At $T = 0.26$, $P_t(\Delta x)$ has a large peak at $\Delta x = 0$ and long, extended tails

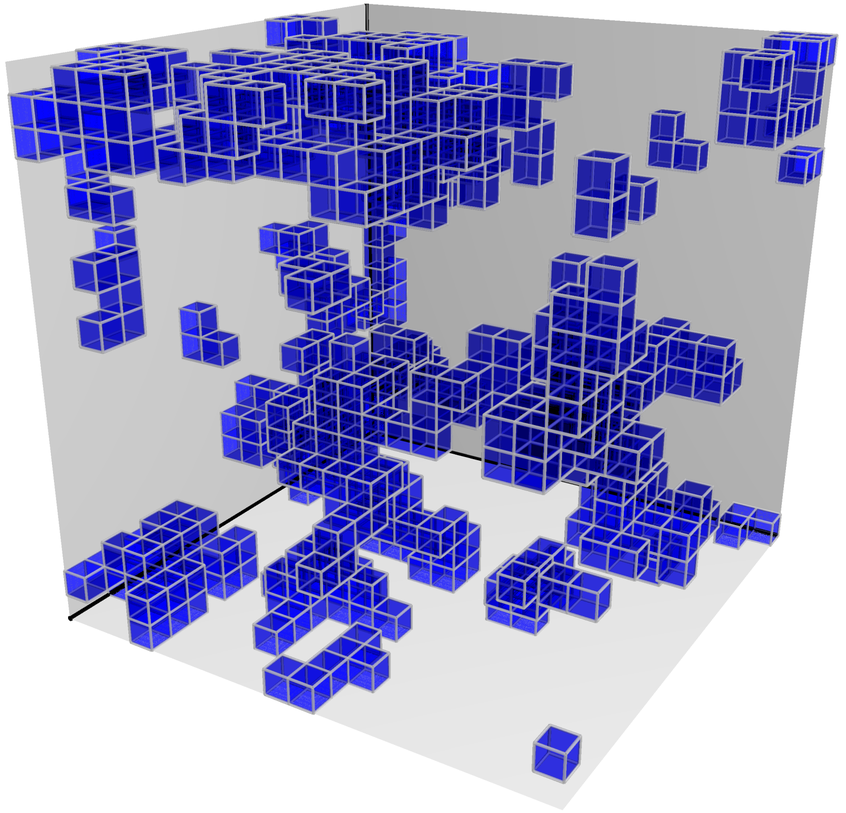
The dynamics is highly heterogeneous at the particle level

Emergent quasiparticles as dynamical defects



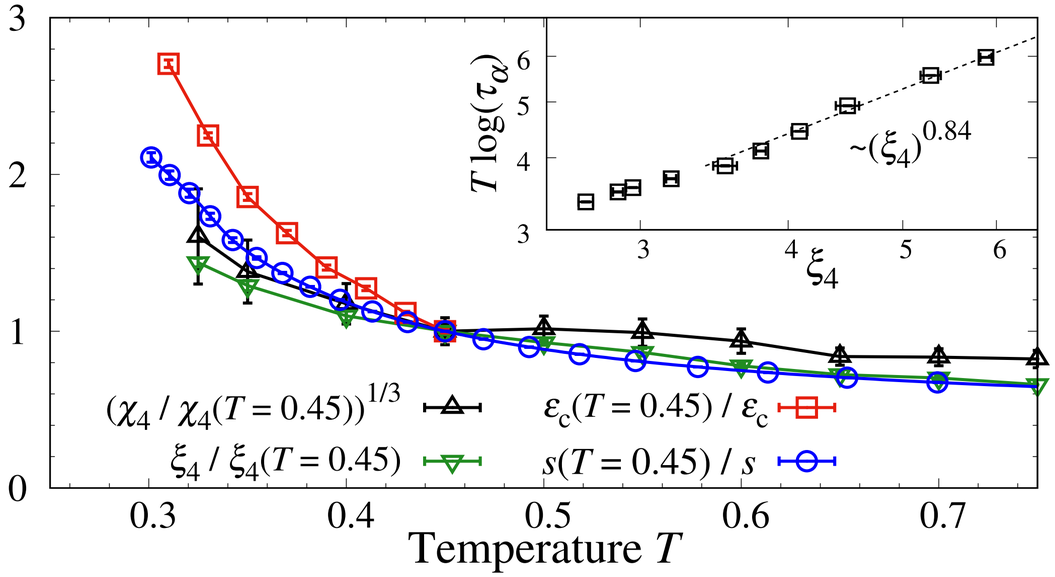
- Most of lattice sites with local energy barrier $\Delta e/T \leq 0$ are very stable with time $\rightarrow$ Local vibrations of particles
- From time to time, a cluster composed of ~ 4 sites appears and runs rapidly in the system $\rightarrow$ Emergent *quasiparticles*
- Those quasiparticles facilitate particle motions and gradually relax the system $\rightarrow$ Dynamic facilitation

Narrow mobile channels in space



- Quasiparticles can rapidly move only in a limited region in space
- A (large) rigid cluster that quasiparticles cannot invade
  $\rightarrow$ Quasiparticles slowly melt the cluster from its surface
- Coexistence of super slow and fast regions in space
  $\rightarrow$ Spatially heterogeneous dynamical facilitation

Growing dynamic/static length scales



- ε_c^{-1} and s^{-1} as static length scales
- The dynamic and static length scales grow towards low T as well
  $\rightarrow$ Strong coupling between statics and dynamics
- $\log \tau_\alpha \sim (\xi_4)^\psi / T$ with $\psi \approx 0.84$
  - $\psi = d/2$ or $d-1$ for simple activated dynamics as discussed in RFOT
  - $\psi < 1$ from experiments on molecular liquids [Capaccioli *et al.* (2008)]

Possible *reconciliation* between DF and RFOT:
Static length scales control the slow dynamics, but not in the way the RFOT theory assumes

Summary

- A new $3d$ LG model with the typical fragile-glass dynamics is proposed
  - Thermodynamic properties are fully consistent with RFOT
- Numerical simulations have revealed facilitated and collective dynamics at low T
  - Particles move collectively by spontaneously forming *quasiparticles*, inducing dynamical facilitation
  - Yet, dynamic and static length scales are strongly coupled, suggesting a thermodynamic origin of the slow glassy dynamics
- The dynamics does not exactly follow the RFOT scenario
  - Dynamical facilitation becomes more relevant at low T
  - $\log \tau_\alpha \sim (\xi_4)^\psi / T$ with $\psi \approx 0.84$, largely different from the RFOT value $\psi = d/2$ and $d-1$ for activated dynamics at low T, but consistent with an experimental estimate $\psi < 1$ [Capaccioli *et al.*]
- Testing this new scenario in realistic models will be the focus of future work

Thank you for your attention