Spatial structures and dynamics of kinetically constrained models of glasses

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The Glass Transition

- Dramatic increasing of the structural relaxation timescale
- Super-Arrhenius dependence
- Non exponential relaxation
- Dynamical heterogeneity
- ….

Kinetically constrained lattice gases

- Simple statistical mechanics model for glassy relaxation.
- Basic assumption: the glass transition is caused by geometrical constraints on dynamical rearrangements with static correlations playing no role.

Kob-Andersen Model

- Kinetically constrained lattice system
- At each time step a particle *a* and one of its neighbours j is chosen at random. *a* is moved to j if:
  - j is not occupied.
  - the number of occupied neighbors of *a* is less than z-s before and after the move

Vacancies move only if the initial and final sites have at least s neighbor vacancies

✓Consequence: the stationary distribution is uniform (H=0)

Previous results on the 3D s=2 KA

- Slow dynamics at high density. Dynamical phase transition at density 0.881 in 3D (s=2)? (Kob, Andersen)
- Off-equilibrium and aging (Kurchan, Peliti, Sellitto)
- Test of the Edwards hypothesis and/or the mean field scenario for the off equilibrium dynamics (Barrat, Kurchan, Loreto, Sellitto)
- Dynamical heterogeneous at high density (Franz, Mulet, Parisi)

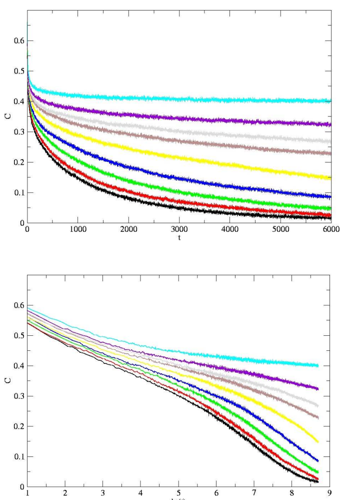
Dynamical Transition on a Bethe Lattice

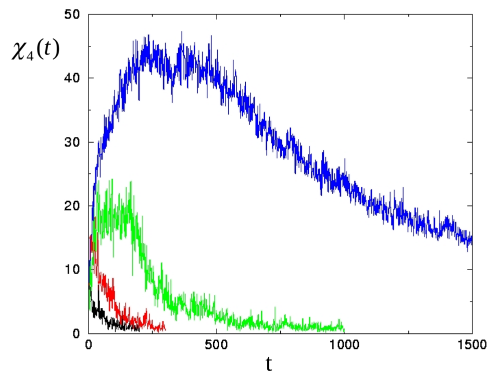
- Iterative equation on the probability (A) that vacancies can be rearranged within a branch so that the bottom site and and at least s of its neighboring sites are vacant
- Transition at a density less than one for s different from 0 and k
- First order: the fraction of sites belonging to the infinite cluster is discontinuous at the transition (except s=k-1)
- Marginality: A has a square root singularity at the critical density. There is a diverging dynamical correlation length at the transition!
- The configurational entropy jumps discontinuously from zero at the critical density.

Alternative Procedure

- KA Bootstrap Percolation: take away all the particles that can move under the KA rules
- Transition at a density less than one.
- First order: the fraction of sites belonging to the infinite cluster is discontinuous at the transition
- Marginality: the fraction of sites belonging to the infinite cluster has a square root singularity at the transition

Simulations on the Bethe lattice





Remarks

- The dynamical transition of KA on the Bethe lattice is physically analogous to the one of mean field glassy systems (1RSB)
- These basic features hold even including finite size loops at any finite order
- The case s=0,k correspond to normal diffusive behavior (s=0) and to always frozen dynamics (s=k)

Ergodicity, Absence of transition and crossover length in finite D

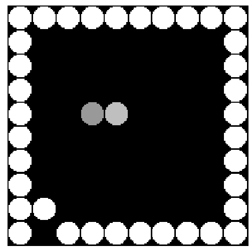
Strategy:

- Identify an ergodic component A
- Show that A covers all the configuration space at any density less than one

Let's focus on 2D s=1

Remark I: framed configurations with the same density belong to the same ergodic component

Proof:

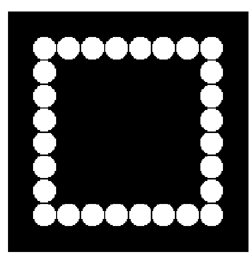


Remark II: all frameable configurations with the same density belong to the same ergodic component A

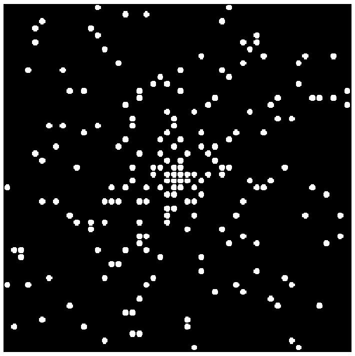
Iterative procedure to construct frameable configurations

Remark III:A framed L by L configuration can be reduced to a L+2 by L+2 framed configuration if it has two vacancies adjacent to each side of the L by L square

Proof:



Use the previous procedure starting from the origin



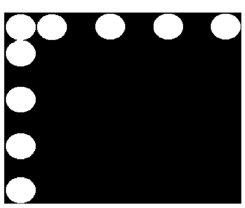
$$P_L(\rho) = (1-\rho)^4 \prod_{l=2}^{L/2} (1-\rho^{2l} - 2l(1-\rho)\rho^{2l-1})^4 \cong$$

$$\cong \exp\left(\frac{-c}{1-\rho}\right) \qquad L > \xi(\rho) \approx \frac{-\log(1-\rho)}{1-\rho}$$

$$\frac{L_c^2}{\xi^2} P_{L_c}(\rho) \approx O(1) \qquad L_c(\rho) \approx \exp\left(\frac{c}{2(1-\rho)}\right)$$

- When $L >> \exp\left(\frac{c}{2(1-\rho)}\right)$ A covers almost all the configuration space.
- From bootstrap percolation results (Aizenman, Lebowitz) the configuration space is broken up in many pieces for $L << \exp\left(\frac{c'}{2(1-\rho)}\right)$

Optimal framing in 2D



- A framed square is expandable if there is a vacancy in either the line segment next to any of its edge or the line segment next to that.

•When $L >> \exp\left(\frac{c}{2(1-\rho)}\right)$ A covers almost all the configuration space.

•From recent bootstrap percolation results* the configuration space is broken up in many pieces for $L << \exp\left(\frac{c}{2(1-\rho)}\right)$

With the same $c = \frac{\pi^2}{9}$!

*A.E. Holroyd, Probab. Theory Rel 125 (2003) 195

General results for hypercubic lattices and any value of s

0<s<D $\quad L_c \cong \exp^{\otimes s}\left(\frac{c}{(1-\rho)^{\frac{1}{D-s}}} \right)$

e.g. 3D s=2 (original KA) $\quad L \cong \exp\exp\left(\frac{c}{1-\rho} \right)$

s=0 is the usual non interacting lattice gas

s>D-1 is non ergodic at any density

Dynamical behavior

- The self diffusion coefficient is strictly positive at density less than one
- There is no transition in the equilibrium dynamics
- Apparent or avoided transition (focus on 2D s=1)

  A group of 3 vacancies can move along a vacancy network that is linked no more weakly than via third nearest neighbors

  At the percolation transition a crossover takes place in the dynamics from single vacancy motion to collective motion

Collective motion at high density

•At very high density only the cores (of size ξ) of frameable regions can move

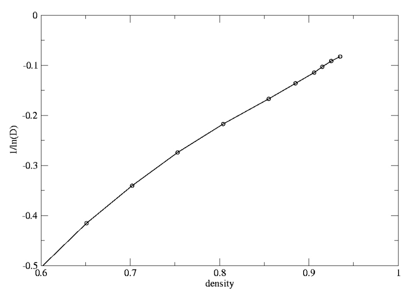
•Their density is $n_M(\rho) \approx \frac{1}{L_c^D(\rho)}$

•Their typical timescale is $\tau(\rho) << L_c^D(\rho)$

$$\frac{1}{D_S} \approx \frac{\tau}{n_M} \approx L_c^D \approx \exp^{\otimes S}\left(\frac{c}{(1-\rho)^{\frac{1}{D-s}}}\right)$$

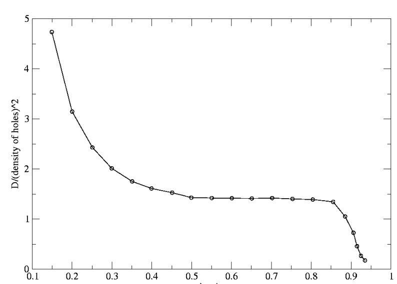
Other possible cases: (1) normal diffusion with $D_S \approx (1-\rho)^q$ (e.g. s=0 on hypercubic lattice or s=1 for a triangular lattice), (2) always frozen at any finite density (e.g. s>D-1 for hypercubic lattices)

Self Diffusion coefficient by 2D simulations



Good fit with a and c close to one

$$\exp\left(\frac{c}{(1-\rho)^a}\right)$$



The scaling behavior pointed out by Dawson et al. is verified in a large regime of densities but it eventually crosses over to a more rapid decreasing

Stretched exponential relaxation

- Mechanism à la Griffiths (preliminary):

With a very low probability ($\exp(-cL^D)$) one can have an usual high density ρ' on a L by L region

If $L << L_c(\rho')$ the region is blocked and it can unblock only thanks to the environment. Thus its relaxation timescales has to scale with L (indeed $\tau \propto L^2$)

At long times this mechanism gives rise to a stretched exponential relaxation with exponent D/(D+2)

Conclusions

- Dynamical transition 1RSB-like on the Bethe lattice
- The ergodicity is restored in finite D above a critical length…
- …and the mean-field like transition is replaced by a crossover
- The relaxation at high density is due to collective vacancy motion. The length and time sclaes increases very rapidly in a super-Arrhenius way
- Dynamical heterogeneity and stretched exponential relaxation