Kinetically constrained spin models

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Liquid/glass transition: a missing theory

"The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of glass and the glass transition." [Nobel prize P.W. Anderson]

Glasses display properties of both liquids and solids

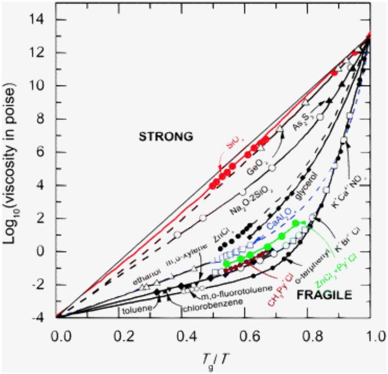
How can you manufacture a glass?

- Take a liquid and cool it rapidly in order to prevent nucleation of the ordered crystal structure;
- relaxation times increase dramatically, the liquid falls out of equilibrium and enters a metastable phase;
- the molecules move slower and slower:
  your liquid is now a thick syrup..
- finally the liquid freezes in a structureless solid:
  here is your glass.

Key features of liquid/glass transition

- huge divergence of timescales;
- no significant structural changes;
- is it purely dynamical phenomenon or is there an underlying thermodynamic transition?
- cooperative relaxation;
- dynamical heterogeneities: non trivial spatio-temporal fluctuations, coexistence of frozen and mobile regions;
- rich phenomenology: anomalous transport properties, aging, rejuvenation, ...
- a similar jamming transition: grains in powders, emulsions, foams, colloidal suspensions, ...

Huge relaxation times



Strong supercooled liquids: *Arrhenius* $\tau \sim \exp(\Delta E/T)$

Fragile supercooled liquids: *superArrhenius* $\tau \sim \exp(c/T^2), \ldots$

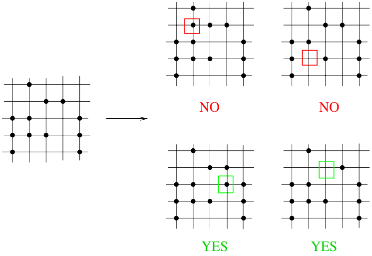
Friedrickson Andersen model on $\mathbb{Z}^2$

Configurations : $\eta = \{\eta_i\}_{i \in \mathbb{Z}^2}$ with $\eta_i \in \{0, 1\}$

Glauber dynamics = Birth and death of particles on $\mathbb{Z}^2$

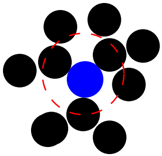
Kinetic constraint = at least 2 empty nearest neighbours

If constraint satisfied: $1 \to 0$ rate q, $0 \to 1$ rate $1 - q$



Ideas behind KCSM

- Liquid/glass transition is a purely dynamical phenomenon;
- free volume shrinks when temperature is lowered;
- molecules should escape the "cage" formed by neighbours.



When density increases:

- motion becomes increasingly cooperative
- blocked structures may percolate → divergence of τ

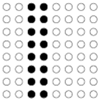
FA model, properties

- Constraint at x does not depend on η_x
  $\rightarrow$ detailed balance w.r.t. product measure

$$\mu(\eta) = \prod_{i \in \mathbb{Z}^2} q^{1-\eta_i}(1-q)^{\eta_i}$$

- μ is not the unique invariant measure

- Blocked clusters, blocked configurations



- Non attractive dynamics $\rightarrow$ failure of coupling arguments and coercive log-Sobolev type inequalities

Blocked clusters

Is there a critical vacancy density $q_c > 0$ below which blocked clusters percolate and relaxation time diverge?

Friedrickson Andersen '84: YES

$$\lim_{t\to\infty} \mu(\eta_x P_t \eta_x) - \mu(\eta_x)\mu(\eta_x) = \begin{cases} 0 & \text{if} \quad q > q_c \\ \neq 0 & \text{if} \quad q \leq q_c \end{cases}$$

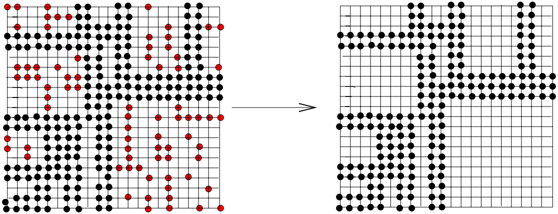
FALSE!

How can we identify blocked structures?

- Erase all particles which have the constraint satisfied;
- Iterate until no particle is left or until reaching a backbone of particles that are all blocked by the constraints.

$\Rightarrow$ Blocked backbone = blocked structures for KCSM dynamics

$\Rightarrow$ Deterministic algorithm = Bootstrap Percolation (BP)



Bootstrap percolation: key results

- blocked clusters do not percolate [Van Enter '87]:

$$\mu(\text{origin empty at the end of bootstrap}) = 1 \quad \forall q > 0$$

- crossover length L_c
  $L \times L$ box with periodic b.c., take joint limit $L \to \infty$ $q \to 0$
  $\mu(\exists\text{blocked cluster}) \to 0$ if $L \gg L_c$
  $\mu(\exists\text{blocked cluster}) \to 1$ if $L \ll L_c$

$$L_c \sim \exp(\frac{\pi^2}{18q})$$

[Aizenmann, Lebowitz '88, Holroyd '02, ...]

$\to L_c =$ linear size of internally blocked clusters

FA model: Ergodicity

μ is ergodic $\forall q > 0$ [Cancrini, Martinelli, Roberto, C.T. '08]:

$\mathcal{L}f = 0 \to f$ constant a.s. w.r.t. μ

$\to \lim_{t\to\infty} \mu(f P_t g) - \mu(f)\mu(g) = 0 \quad \forall f, g$

Key ingredients:

- path arguments
- bootstrap results

Relaxation to equilibrium

- How fast do we converge to μ? Exponentially
  [Cancrini, Martinelli, Roberto, C.T. '08]

$$\mu(f P_t g) - \mu(f)\mu(g) \leq C_{f,g} \exp(-t/\tau(q)), \quad \forall f, g$$

$$\tau(q) < \infty \quad \forall q > 0$$

- Which scaling for τ (=inverse of spectral gap) as $q \downarrow 0$?
  [Martinelli, C.T. '16]

$$e^{c/q} = L_c \leq \tau(q) \leq e^{c|\log q|/q}$$

A generic KCSM on $\mathbb{Z}^d$

The influence classes:
choose $C_1, \ldots, C_m$ finite subsets of $\mathbb{Z}^d$ with $0 \notin \cup_{i=1}^m C_i$.

Constraint at x:
at least one of the m translated sets $C_i + x$ is completely empty.

Ex.1 Friedrickson Andersen k-facilitated models (FA-kf) on Z^d: $m = \binom{2d}{k}$ and $C_1, \ldots C_{\binom{2d}{k}}$ are all the k-uples of nearest neighbours, i.e. at least k empty neighbours, $k \in [1, d]$

Ex.2 East on $\mathbb{Z}^d$: $m = d$ and $C_1 = -\vec{e}_1, \ldots C_d = -\vec{e}_d$, e.g. $d = 2$ constraint $x =$ *at least one* empty site in $x - \vec{e}_1 \cup x - \vec{e}_2$

Ex. 3 North East on $\mathbb{Z}^2$: $m = 1$ and $C_1 = (\vec{e}_1, \vec{e}_2)$, i.e. top and right neighbours both empty.

Properties

- μ is a reversible invariant measure
- blocked clusters and blocked configurations;
- blocked clusters $\leftrightarrow$ occupied sites in the final configuration for the correspondent monotone cellular automata
- critical density
  $q_c = \inf\{q \in [0,1] : \mu_q(\text{cellular automata empties } 0) = 1\}$
- East and FA-kf : $q_c = 0$
- North-East: $q_c \in (0,1)$ = critical density of oriented perc.
- $\tau(q) < \infty \quad \forall q > q_c \quad , \tau(q) = \infty$ for $q \leq q_c$
- $L_c \leq \tau \leq e^{L_c^d}$ [Cancrini, Martinelli, Roberto, C.T. '08]

FA1f and East : Arrhenius vs superArrhenius

Is τ determined only by L_c? NO

FA1f and East: both $L_c = \left(\frac{1}{q}\right)^{1/d}$ yet very different τ

FA-1f: $\tau(q) \sim L_c^{\alpha}$ [Cancrini, Martinelli,Roberto, C.T. '08]

East: $\tau(q) \sim L_c^{d \log L_c/(2\log 2)}$ [Aldous, Diaconis '02, Cancrini, Martinelli, Roberto, C.T.'08, Chleboun, Faggionato, Martinelli'15]

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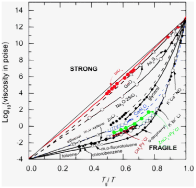


$q \leftrightarrow (1 + \exp(1/T))^{-1}$

) for FA1f: *Arrhenius*

^{2}) for East: *superArrhenius*

Intuition behind the $1/q^{\Theta(1)}$ scaling for FA-1f

- An isolated vacancy cannot disappear
- A vacancy can create a vacancy nearby at rate q
- A vacancy with a nearby vacancy disappears at rate $1-q$

At low q : a vacancy moves to a nearest neighbour at rate q

Ex. $d=1$:
$\tau \sim 1/q^3 =$ time to cover equilibrium intervacancy distance $1/q$

Intuition behind the $1/q^{\Theta(\log(1/q))}$ scaling for East

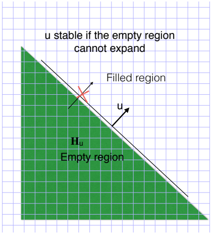
The model has logarithmic energy barriers

Ex. d=1

- combinatorial result [Chung, Diaconis, Graham]:
  if 0 is empty and the next vacancy to the right is at ℓ, filling 0 requires creating at least $\log_2(\ell)$ simultaneous vacancies in $(0, \ell)$
- Equilibrium distance among 0's is $1/q$
- physicists $\rightarrow \tau = \frac{1}{q}^{|\log_2 q|}$ (Evans, Sollich '03)
- Correct result accounting for entropy contributions
  $\rightarrow \tau = \frac{1}{q}^{|\log_2 q|/2}$
  (Cancrini, Martinelli, Roberto, C.T. '08)

A universality result for cellular automata in $\mathbb{Z}^2$

Take $u \in S^1$, let $H_u := \{x \in \mathbb{Z}^2 :< x, u >< 0\}$.
u is a stable direction if starting from η empty on H_u and filled on $\mathbb{Z}^2 \setminus H_u$ no other site can be emptied.



- supercritical if $\exists$ open semicircle without stable directions;
- critical if every open semicircle has a stable direction and $\exists$ a semicircle with a finite number of stable directions
- subcritical otherwise

A universality result for cellular automata in $\mathbb{Z}^2$

Theorem [Bollobas, Smith, Uzzell '15]

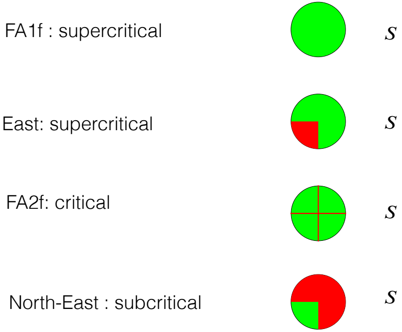
- Supercritical models: $q_c = 0$ and $L_c = 1/q^{\Theta(1)}$
- Critical models: $q_c = 0$ and $\exists \alpha > 0$ s.t. $L_c = \Theta(\exp(1/q^{\alpha}))$
- Subcritical models: $q_c > 0$

$L_c(q)$ is determined by the action of the cellular automata on discrete half planes

For supercritical models there is a finite empty cluster, the droplet from which we can empty an infinite region.

Our examples

Red= stable direction; Green= unstable direction



A single empty site is a droplet both for East and FA1f

Supecritical KCSM on $\mathbb{Z}^2$

Theorem [Martinelli, C.T. '16]

A refined classification : a supercritical model is rooted if there are two non opposite stable directions. It is unrooted otherwise.

- for all supercritical unrooted models $\tau \sim 1/q^{\Theta(1)}$
- for all supercritical rooted models $\tau \sim 1/q^{\Theta(\log(1/q))} \gg L_c$

Namely

- unrooted models: $\tau \leftrightarrow L_c$, Arrhenius behavior
- rooted models: $\tau \gg L_c$, superArrhenius behavior

In particular: FA1f is unrooted, East is rooted

Intuition behind the rooted/unrooted result

- Unrooted models
  - there is an *empty droplet* that can be *shifted* along a line
  - empty droplet plays the role of the vacancy of FA1f
  - scaling proven via renormalization to FA1f model

- Rooted models
  - there is not an *empty droplet* that can be *shifted*
  - from any finite empty region we can empty only a cone. Ex. East with vacancy at 0: we empty the positive quadrant
  - a combinatorial argument gives logarithmic energy barriers

Out of equilibrium

What happens if we start from an initial measure $\nu \neq \mu$?
Do we converge to μ?
Blocked configurations $\longrightarrow$ convergence to equilibrium cannot be uniform on all initial configurations

Conjecture

If $q, q' > q_c$ and ν is Bernoulli-q' measure

$$\lim_{t \to \infty} \int d\nu(\mu)\mathbb{E}_\eta(f(\eta_t)) = \mu(f) \quad \forall f \text{ local}$$

Main difficulties:

- non attractive $\longrightarrow$ failure of coupling arguments
- failure of classic coercive inequalities
- log Sobolev constant diverges with the volume

Out of equilibrium: East model

Theorem [Cancrini, Martinelli, Schonmann, C.T.'10], [Chlebloun, Faggionato, Martinelli'15]

$$|\lim_{t\to\infty}\int d\nu(\mu)\mathbb{E}_\eta(f(\eta_t))-\mu(f)| \le c(f)\begin{cases}\exp(-t\,\mathrm{gap}) & \text{if} \quad d=1\\ \exp(-t^{1/2d}c) & \text{if} \quad d\ge 2\end{cases}$$

Key ingredients (d=1):

Oriented constraints: evolution at x is influenced by evolution only on $y > x$ and influences evolution only on $y < x$

- start with x empty and let t_1 be the time of its first update;
- at t_1: η_x is distributed with μ and $x + 1$ is empty;
- let $t_2 > t_1$ be time of the first updated at $x + 1$;
- at t_2: η_{x+1}, η_x are distributed with μ and $x + 2$ is empty ...
- equilibrium is preserved and extended

Out of equilibrium: FA1f

Theorem [Blondel, Cancrini, Martinelli, Roberto, C.T. '12]

$\exists \bar{q} < 1/2$ s.t. if $q > \bar{q}$ and ν is Bernoulli-q' with $q' > 0$

$$|\lim_{t\to\infty} \int d\nu(\mu)\mathbb{E}_\eta(f(\eta_t)) - \mu(f)| \le c(f)\exp(-t^{1/d}/c)$$

Key ingredients:

- starting from a single zero we can unblock any region
- prove that $\forall \epsilon > 0$ with high probability a completely filled region of $> \epsilon t$ sites does not occur in $[0, t]$
- $\rightarrow$ effective Sobolev constant is ϵt $\rightarrow$ use hypercontractivity

Out of equilibrium: (many) open issues

- extend FA1f result to the whole regime $q > 0$
- extend to more complicate constraints, e.g. FA-2f
- what happens if $q' > q_c$ and $q < q_c$? coarsening of blocked structures..

Summary

- KCSM are stochastic models for liquid/glass and jamming transitions
- intimate relation to monotone cellular automata (e.g. bootstrap percolation)
- the ergodic regime corresponds to the non percolating regime for the cellular automata
- $\tau = 1/\text{gap} < \infty$ in the ergodic regime
- the critical scaling can be $\gg$ then the critical length of the cellular automata $\rightarrow$ energy barriers

Open

- scaling of τ as $q \downarrow q_c$ for a generic KCSM;
- out of equilibrium = evolution after a density quench
- prove the emergence of a non random limiting shape

East model: why a log barrier?

Start with a single vacancy at the origin
$\mathcal{S}$= configs reacheable via paths with $\leq n$ simultaneous 0's;
$L(n)$= distance from the origin of leftmost 0 maximized on $\mathcal{S}$

$\mathcal{S}_1$= configurations in $\mathcal{S}$ *and* with only one vacancy in $[-\infty, -1]$;
$L_1(n)$= distance from the origin of leftmost 0 maximized on $\mathcal{S}_1$

- optimal path proceeds via *stepping-stones*: create isolated vacancy at $-L_1(n)$; restart from it to create an isolated vacancy at $-L_1(n) - L_1(n-1)$; etc..

$$L(n) = L_1(n) + L_1(n-1) + \ldots L_1(1)$$

- to put an isolated 0 at $-L_1(n)$ we should have a 0 at $-L_1(n) + 1$ and remove it using at most $n-1$ vacancies

$$L_1(n) = L(n-1) + 1$$

$$\Rightarrow L(n) = 2^n - 1$$