III) Interesting lattice models for glasses

Justification: RFOT in mean field, complex in $d=\infty$
and not obvious it survives.

→ Lattice models with glassy behavior provide additional insights, or different viewpoints on how glassy dynamics emerges in many body systems.

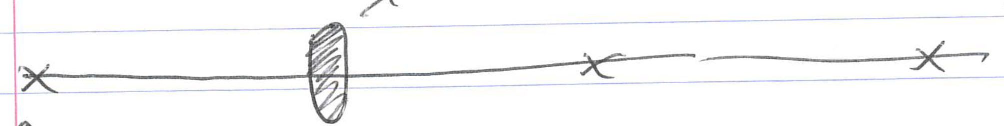
a) Defect models

(Glarum 1960, JCP)

Goal: Show that the influence of rare diffusing defects leads to broad distrib° of relaxation times / stretched exp.

1d model

molecule $\phi_0(t) = e^{-t/\tau_{rot}}$ if no defect



diffusing defects D

× If hit by defect → relax

$$\Rightarrow \phi(t) = \phi_0(t)\,[1 - I(t)] \qquad (1)$$

probability be hit by defect

25

1 defect at distance ℓ at $t=0$

$$\frac{dP}{dt}(\ell,t) = \frac{\ell}{\sqrt{4\pi D}} \frac{1}{t^{3/2}} e^{-\ell^2/4Dt} \quad \text{RW}$$

$\rho(\ell)$ = distrib° of distances.

$$\frac{dP}{dt}(t) = \int_0^\infty d\ell' \, \rho(\ell') \frac{dP}{dt'}(\ell',t) \qquad (2)$$

(1)+(2) solved in Laplace domain

→ $\Phi(t)$ stretched exp with

$$\beta = \frac{\alpha}{1+\alpha} \quad \text{with} \quad \alpha = \sqrt{\frac{\ell_0^2/D}{t_{rot}}}$$

(ratio of rot° and diff° timescales.)

Conclusion sparse defects → dyn. heterogeneity.

b) Fredrickson Andersen model (FA, PRL '84)

Sparse defects ~ ideal gas

$$H = J \sum_{i=1}^{N} n_i \qquad n_i = 0 \text{ no def} \qquad = 1 \text{ def}$$

$$\langle n_i \rangle = c(T) = \frac{1}{1+e^{J/T}} \approx e^{-J/T}$$

rare at low $T \ll J$

<u>Dynamics</u> $\frac{dP}{dt}(\{n\},t) = \sum_{n'} W_{n'n} P(n',t) - \sum_{n'} W_{nn'} P(n,t)$

(master eq)

× Single spin flips $W(n_i \to 1-n_i)$?

× unconstrained dynamics $W_0(\Delta E) = \frac{1}{1+e^{\beta\Delta E}}$

(Glauber Dynamics)

$n_i = 0 \underset{1-c}{\overset{c}{\rightleftarrows}} n_i = 1$

Satisfies detailed balance

$\frac{W_{nn'}}{W_{nn'}} = \frac{P^{eq}(n')}{P^{eq}(n)}$

× constrained dynamics

$n_i = 0 \underset{(1-c)f_i}{\overset{cf_i}{\rightleftarrows}} n_i = 1$

$f_i = 0$ for certain transitions

Equilibrium is ok if appears in both sides!

<u>Leads to Family of models</u> (f,d) FA models

f — constraint parameter

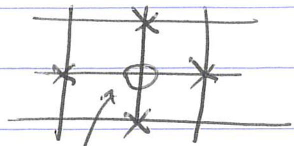
d — dimension

$f_i = 1$ if # up spins $\geq f$

$= 0$ otherwise

- <u>Initial FA papers ('84–'86)</u>

(2,2) FA model $\begin{cases} d=2 \\ f=2 \end{cases}$



can flip if at least 2 defects among 4 neighbors

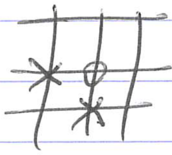
- Directed version (Jäckle 1991)

East model ($d=1$) North East ($d=2$)

North East Front ($d=3$)

etc.

Only look in 1 direction



North East model

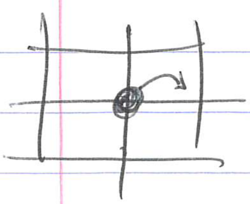
<u>Rem</u> defects are not conserved ("non conservative")

but mobility cannot appear spontaneously in vacuum ($f \neq 0$)

- <u>Conservative models – Lattice gases</u>

$n_i = 0, 1$ are now occupation numbers on the lattice

particle can hop to nearest neighbor if



+ site is empty
+ # neighbor before/after move $\underbrace{\leq m}$

constraint if $m < 4$ in $d=2$

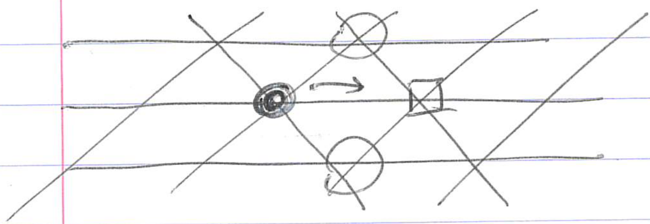
Kob-Andersen model '93

$d=3$; $m=3$

× Sites with low density act as defects

× more physical: motion if not too crowded!

Triangular Lattice Gas (Jäckle '94)



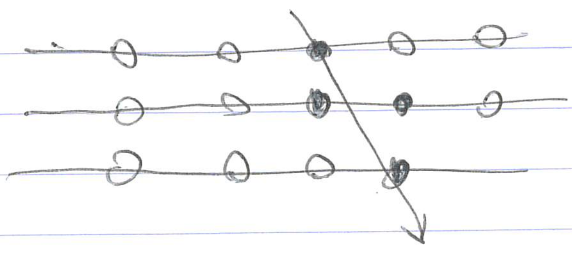
Jump allowed if
- site is empty □
→ ○ and ○ are empty
2TLG
→ either ○ or ○ is empty
1TLG

even more physical?

All these models are called
→ Kinetically Constrained Models (KCM)

c) Basic physics of KCM

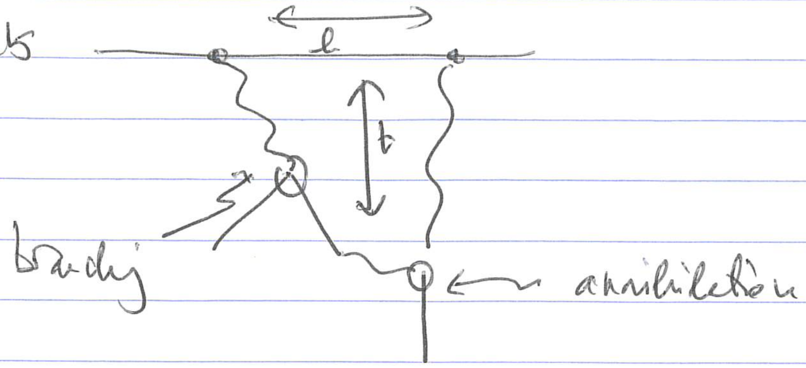
1d FA model



proba $c \ll 1$
$p \sim 1-c \sim 1$

rare defects diffuse with $D \sim c(T) \sim e^{-1/T}$

2 defects



$l \sim 1/c$

$\tau(T) \sim l^2/D \sim \frac{1}{c^2} \times \frac{1}{c} \sim e^{3/T} =$

$\phi(t) = \exp\left(-\left(\frac{t}{\tau(T)}\right)^{1/2}\right)$ (similar to glasses)

Growing τ, l, stretched exponential even in simplest model

For $d > 1$ = exponential decay

(diffusion-limited aggregation model)

Rem $t \sim l^z$ with $z = 2$ (defects diffuse)

East Model

1 0 0 0 1
1 1 0 0 1
1 1 1 0 1
1 0 1 0 1
1 0 1 1 1
1 0 1 1 0
1 0 1 0 0
1 1 1 0 0
1 1 0 0 0
1 0 0 0 0

naive 3 bits; in reality 2

If d bits; $E(d) \sim d$ (naive)

more efficient $E(d) = \log d$.

$E(l_{eq} = \frac{1}{c}) = -\log c = \frac{1}{T}$

$\tau(T) = \exp\left(\frac{E}{T}\right) = \exp\left(\frac{A}{T^2}\right)$

+ super Arrhenius (Bässler)
+ dyn. het
+ stretched exp
+ $\tau \sim e^{-z(T)}$ with $z(T) \sim \frac{1}{T}$

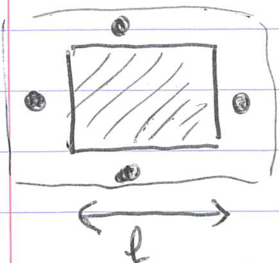
subdiffusive growth

+ In fact very realistic behavior!

• Cooperative models

(2,2) AA to predict $\tau(T)$ find a possible path to relax

$$\tau(T) \leq \tau_{path}$$



$$p(\ell) = [1 - \underbrace{(1-c)^{\ell}}_{\text{proba to have no vacancy on each side}}]^4$$

$$I = \prod_{\ell=0}^{\infty} [1-(1-c)^{\ell}]^4 \sim e^{-4\exp(1/T)}$$

$$\tau(T) \simeq \exp\left(4 \exp\left(\frac{1}{T}\right)\right)$$

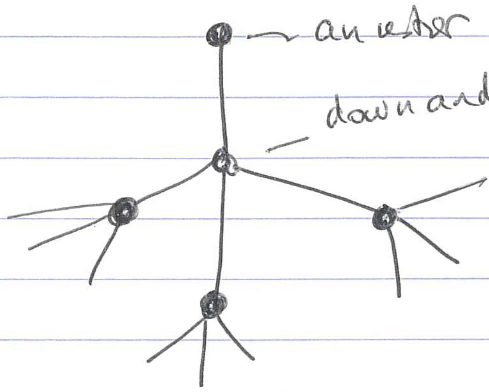
+ very fragile behavior
+ het., stretched, etc.
+ picture: diffusion of "super defects" of size $\xi \sim -\log(1-c)$

• Models with phase transition at $T > 0$

very specific rules ("spiral model")

or Bethe Lattice ("mean field")

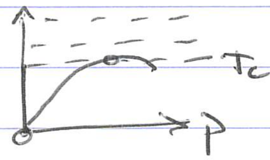
2 spin facilitated model



P = proba down and blocked if ancestor down and blocked

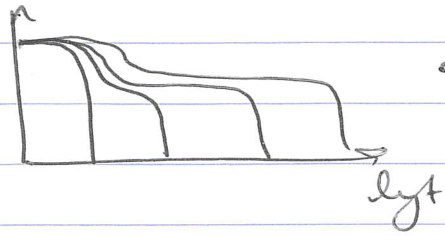
$$P = \underbrace{(1-c)}_{\text{down}}\underbrace{\Big[\underbrace{P^3}_{\text{all three daughters}} + \underbrace{3(1-P)P^2}_{\text{2 daughters | 1 not down/blocked}}\Big]}_{\text{blocked}}$$

$\Leftrightarrow$ $$1 + e^{-1/T} = P(3-2P) \equiv f(P)$$



$\hookrightarrow$ $$P = P(T_c) + \alpha\sqrt{T_c - T}$$

discontinuous emergence of frozen backbone



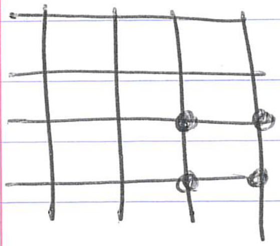
$\tau \sim |T - T_c|^{-\gamma}$

similar to MCT!

d) Plaquette models

Family of interacting models where rare defects and facilitation emerge spontaneously

example Square plaquette model



$$S_i = \pm 1$$

$$H = -J \sum_{i,j=1}^{L} S_{ij}\, S_{i+1\,j}\, S_{i\,j+1}\, S_{i+1\,j+1}$$

4-spin interactions around plaquettes

Define $p_{ij} = S\,S\,S\,S = \pm 1$

$$H = -J \sum_{ij} p_{ij}$$ dual representation

$\Downarrow$

trivial thermodynamics

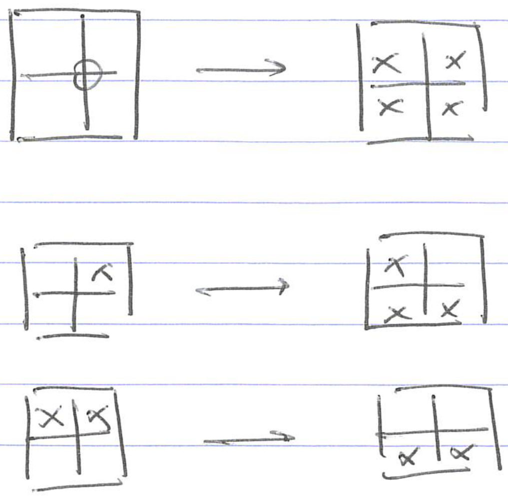
$$\langle p_{ij} \rangle = c = \frac{1}{1+e^{1/T}} \sim e^{-1/T}$$

Few plaquettes are excited at low T

<u>dynamics</u>

Single spin flip

no excitation



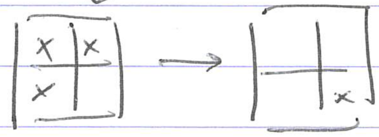
4!

$\Delta E = 4$

$\Delta E = 3$

$\Delta E = 0$

pairs of defects move fast!



annihilation.

$\tau \sim c^{-2} \times c$ as in FA model

↳ strong glass

Mirage excited plaquettes are sources of mobility

→ dynamic facilitation.

As in FA models but here is <u>emergent properties</u>

Models with more fragile behavior also exist

(analog of East model = Triangular Plaquette model)

e) Lattice glass models

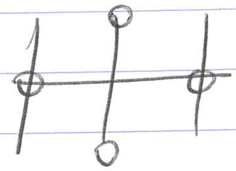
Biroli Mézard PRL 2002

Inspired initially by KA model lattice gases

$n_i = 0, 1$: occupation number on the lattice

~~$H = \sum_i \theta(n_i < \ell)$~~

ℓ_i = # of neighbors of i



Configurations with $\ell_i \geq \ell$ are forbidden
All other configs have $E = 0$

Here the constraint is on the thermodynamics!

Soft version $H = \sum_i \left(\sum_j \delta(|r_i - r_j|, 1) - \ell \right)^2$

On the Bethe lattice (ie mean field)
exact realisations of RFOT,
just like p-spin or $d = \infty$ liquids

* Glassy dynamics in $d < \infty$ not yet known!