Metastable states in the East model and plaquette spin models

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Warwick meeting, Jun 2014

Thanks to:
Juan Garrahan (Nottingham)
Ludovic Berthier (Montpellier)

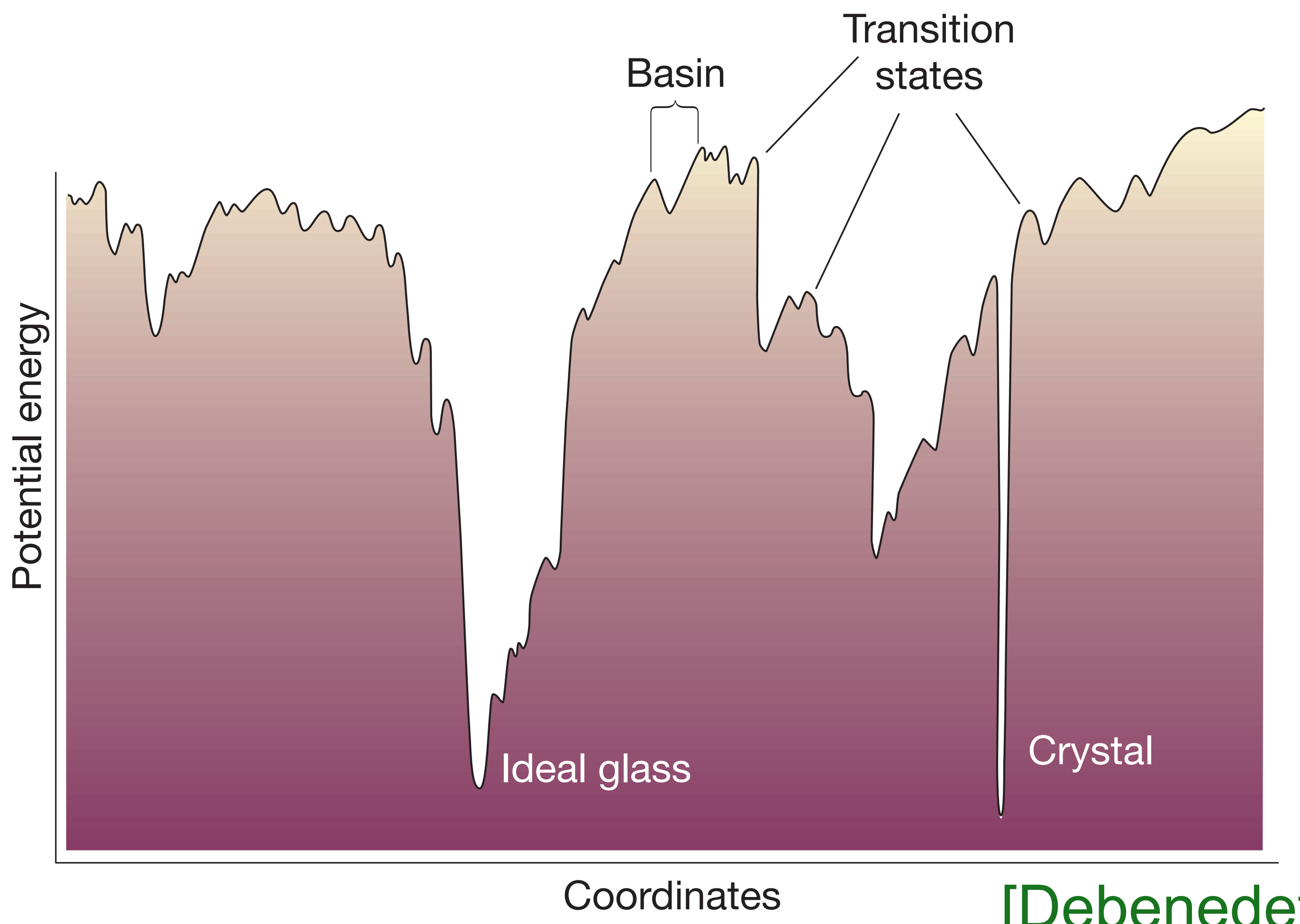
Outline

– Part I : Metastable states in the East model

– Part II : Plaquette models,
Interpreting point-to-set measurements
and overlap fluctuations, using metastable
state arguments

Metastable states

"Basins" / "minima" / "valleys" on a free energy landscape



[Debenedetti and Stillinger, 2001]

Regions of configuration space with *fast* "intra-state" motion and *slow* transitions between states

Counting states

[Kurchan and Levine, J Phys A, 2011]

Regions of configuration space with *fast* "intra-state" motion and *slow* transitions between states

States with lifetime τ, take a time t_{obs} with $1 \ll t_{\mathrm{obs}} \ll \tau$

Averaging over a time period t_{obs}:
same as Boltzmann averaging within the state

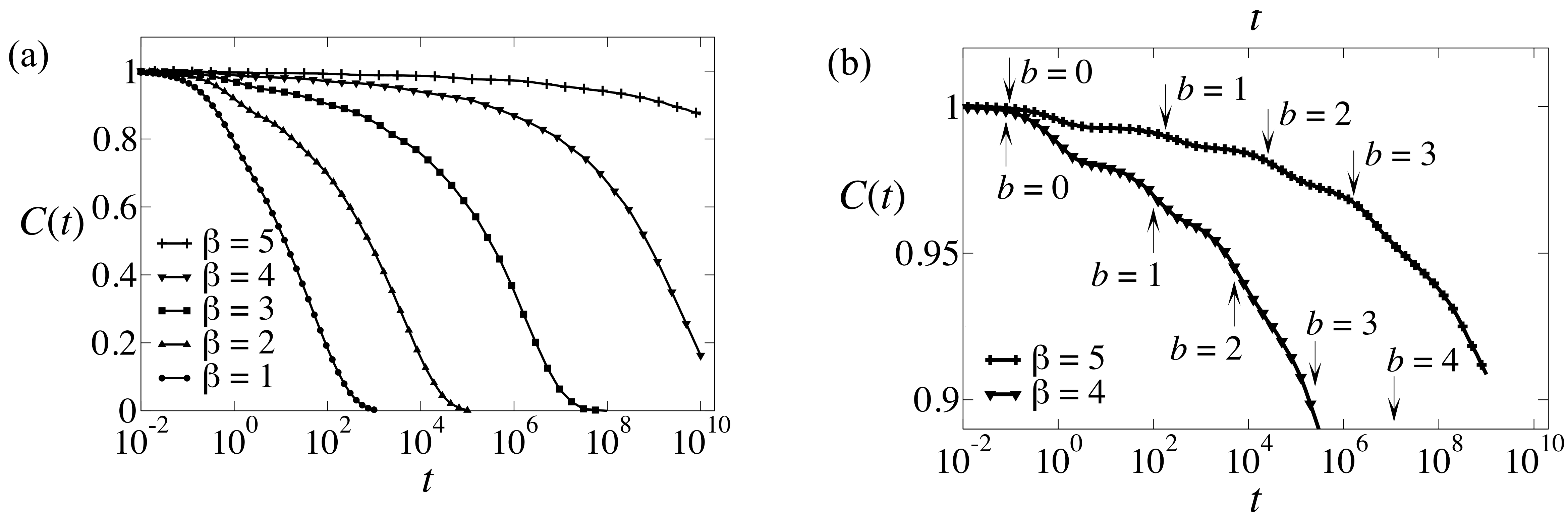
Diversity (entropy) of averaged properties:
… gives number (and properties) of metastable states
… including configurational entropy (complexity)

East model

Spins $n_i = 0, 1$, with $i = 1 \ldots N$.

Spin i can flip only if $n_{i-1} = 1$.

Flip rates c and $1 - c$ gives $\langle n_i \rangle = c = \frac{1}{1+e^{\beta}}$.



$$C(t) = \frac{\langle n_i(t) n_i(0) \rangle - \langle n_i^2 \rangle}{\langle n_i^2 \rangle - \langle n_i \rangle^2}$$

Characteristic times $t_b \approx c^{-(b-\frac{1}{2})}$

[RLJ, Phys Rev E, 2013]

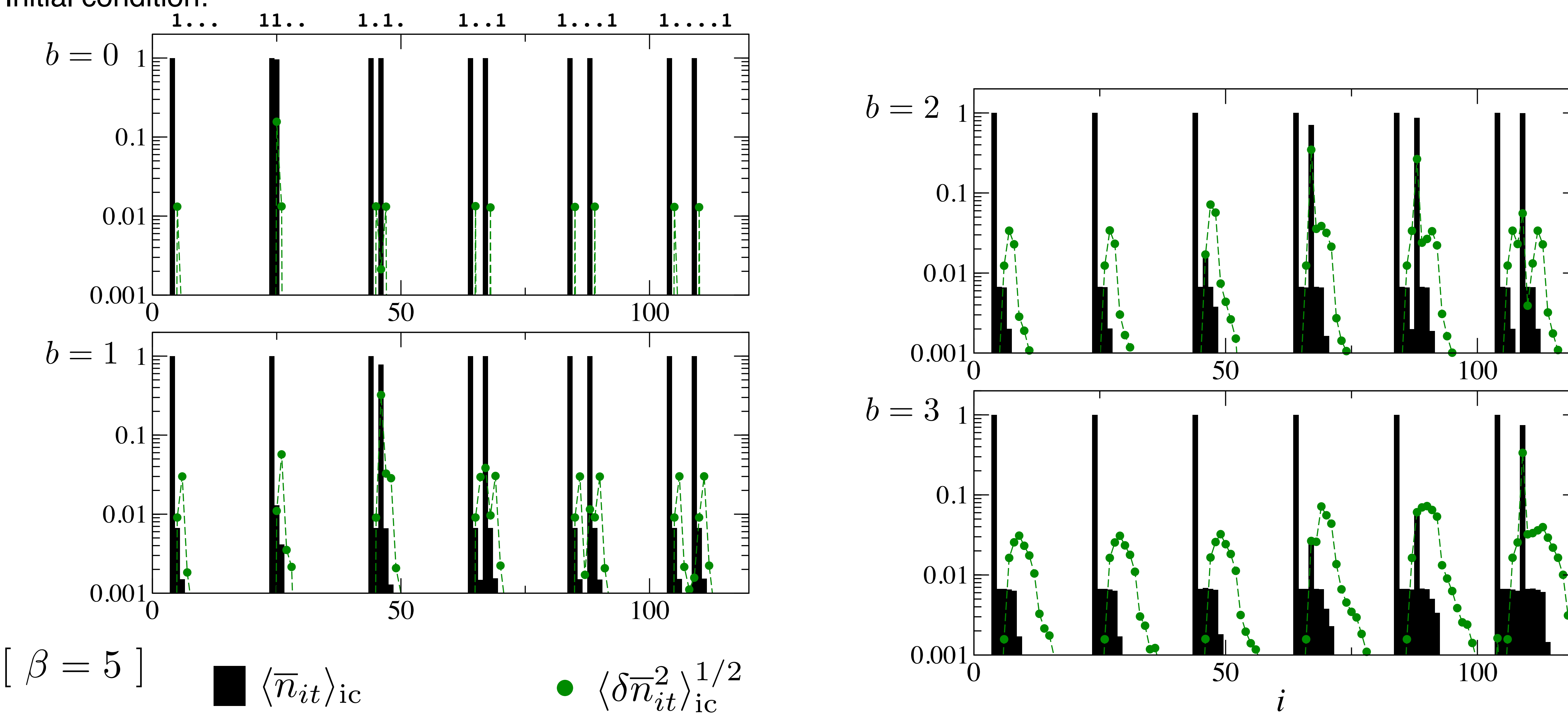
Time averaging…

[RLJ, Phys Rev E, 2013]

$$\overline{n}_{it} = (1/t) \int_0^t \mathrm{d}t' n_i(t'),$$

Characteristic times $t_b \approx c^{-(b-\frac{1}{2})}$

Initial condition:



Time-averages (almost) *determined* by initial condition…

Counting…

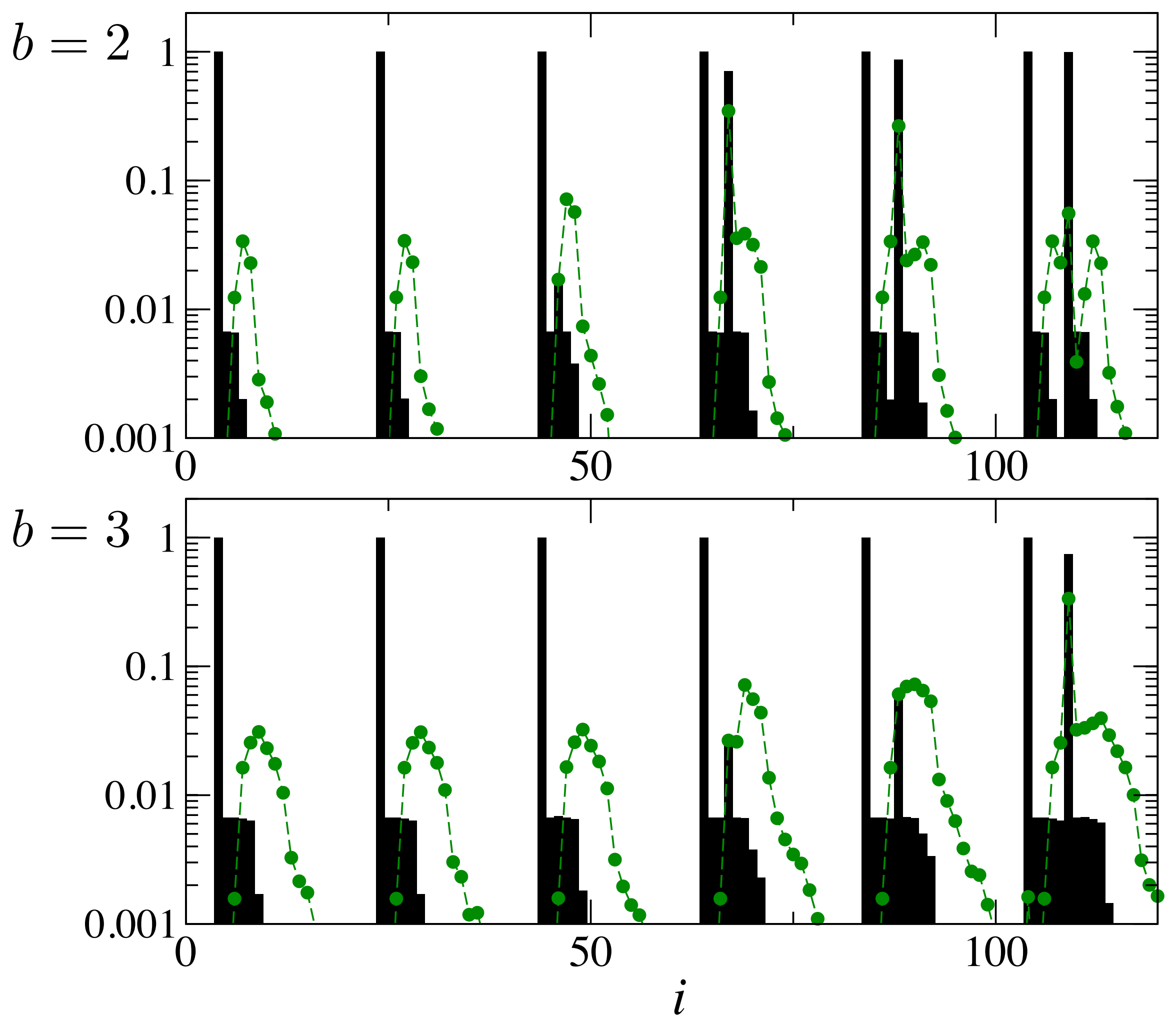
[RLJ, Phys Rev E, 2013]

$$\overline{n}_{it} = (1/t)\int_0^t \mathrm{d}t' n_i(t'),$$

Characteristic times $t_b \approx c^{-(b-\frac{1}{2})}$

$$\tilde{n}_i = \Theta(\overline{n}_i - \tfrac{1}{2}) = 0, 1$$

Measure *entropy* of $\tilde{n}_i$
by pattern-counting at length ℓ



$$S_\ell = \sum_{\mathcal{B}_\ell} p(\mathcal{B}_\ell)\ln(1/p(\mathcal{B}_\ell))$$

$\mathcal{B}_\ell$: state of $(\tilde{n}_i, \ldots, \tilde{n}_{i+\ell-1})$

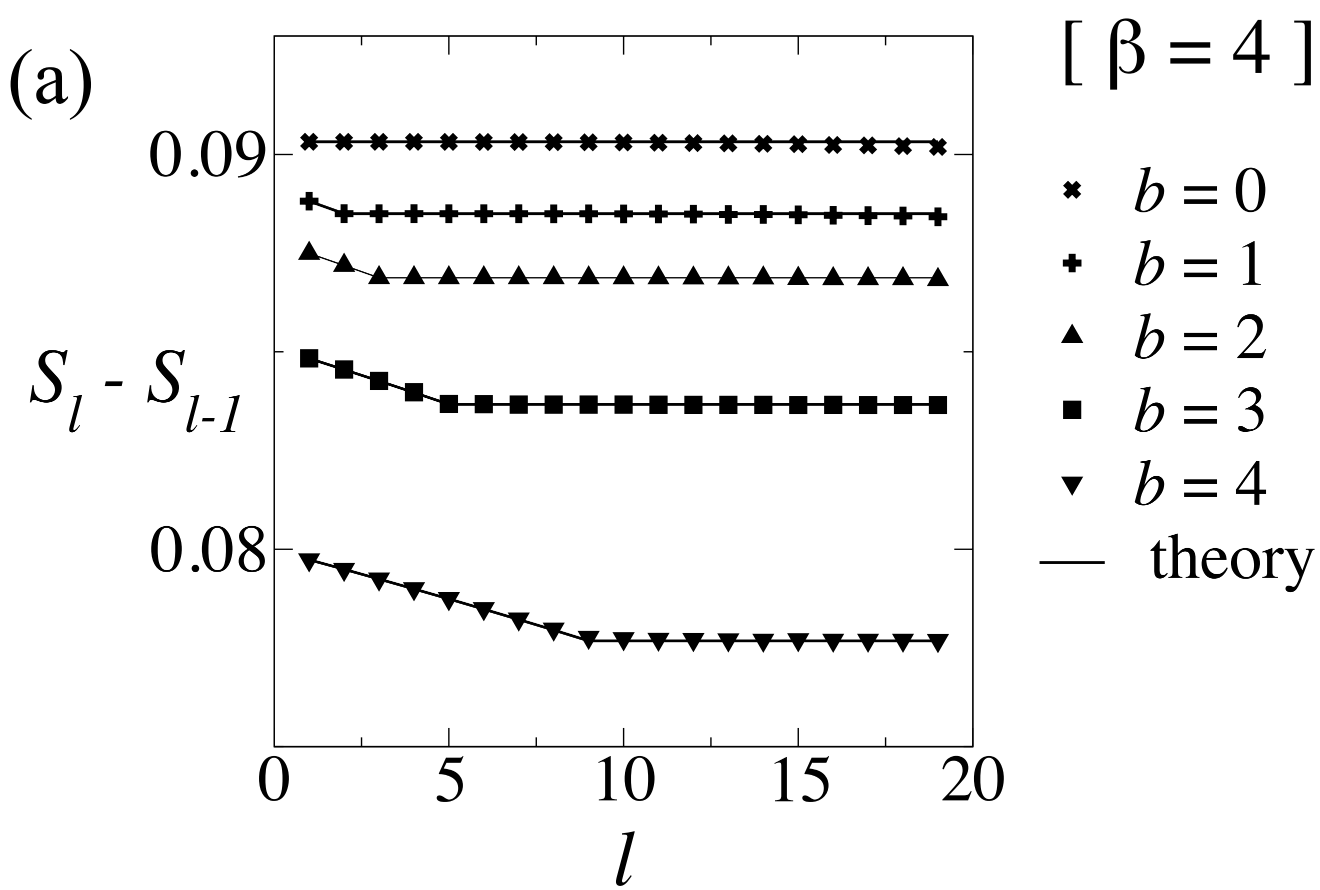
E.g., $\mathcal{B}_{\ell=4} = (1,0,1,0)$ almost never occurs for $b \geq 2$

Counting...

[RLJ, Phys Rev E, 2013]

Convenient to plot $S_\ell - S_{\ell-1}$

... converges for large ℓ to entropy per site



Length scale $\ell^* \approx 2^{b-1}$

For $b = 0$, expect $\tilde{n} = n$, 'static' result

Well-defined complexity

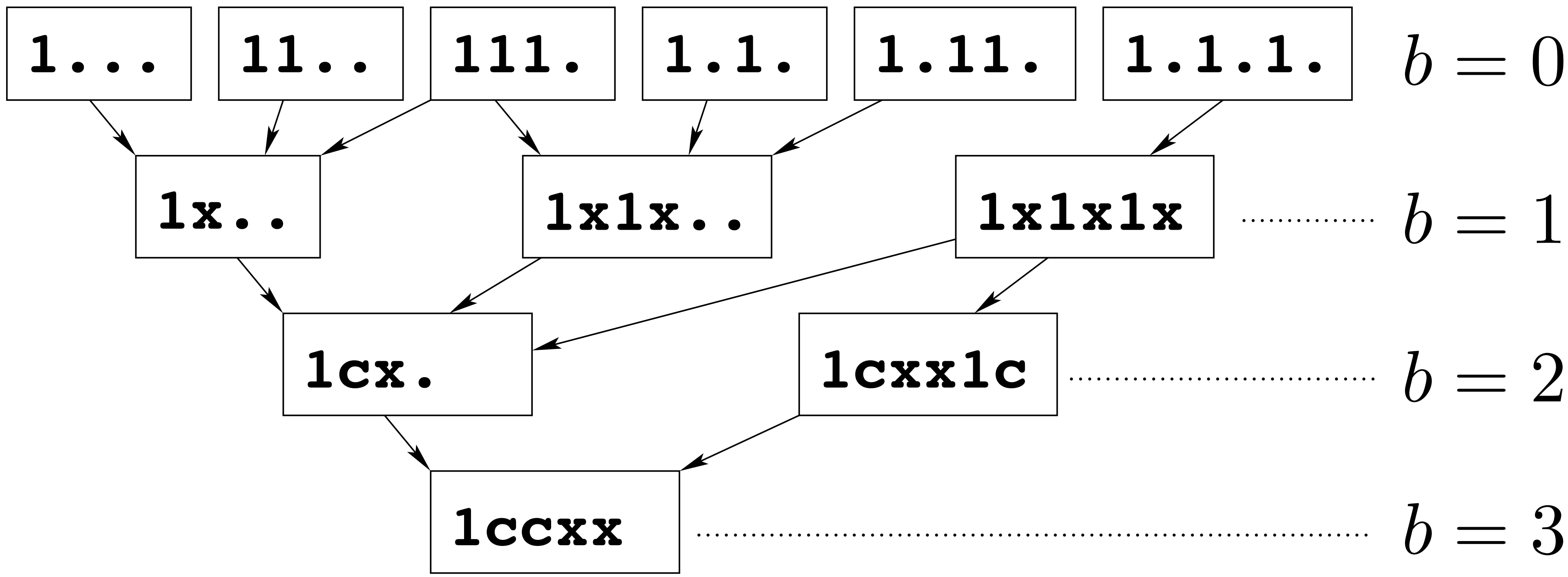
. . . for states of lifetime t_b

Theory: up spins are never closer than ℓ^*, otherwise randomly distributed. . .

. . . "hard rods"

Hard rod states

[RLJ, Phys Rev E, 2013]



$\texttt{1} : \overline{n}_i \approx 1$

$\texttt{0} : \overline{n}_i \approx 0$

$\texttt{c} : \overline{n}_i \approx c \pm \mathcal{O}(c^{3/2})$

$\texttt{x} : \overline{n}_i \approx c \pm \mathcal{O}(c^{1/2})$

Evolution to "longer rods", some deterministic and some stochastic steps…

Part I summary

Time scale separation means metastable states are well-defined…

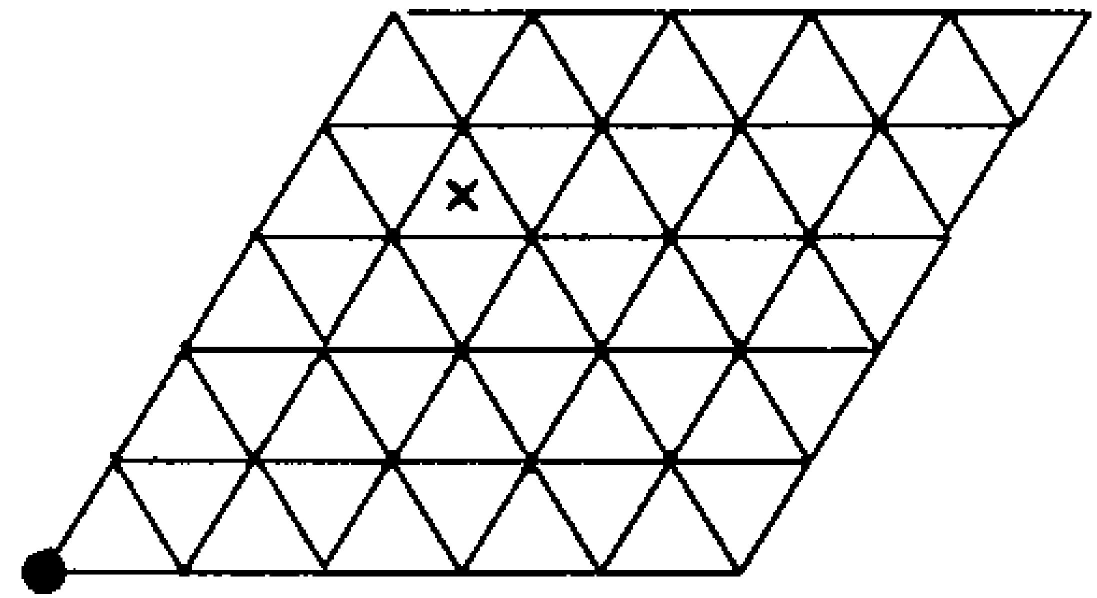
Kurchan-Levine method allows counting of metastable states (of given lifetime)… [Kurchan and Levine, J Phys A, 2011]

In the East model, these states correspond with those of "hard rod" systems…
... at least for times $t_{\mathrm{obs}} \ll \tau_\alpha$ (that is, $\ell^* \ll 1/c$)
… diverging length scale coupled with diverging time scale

[RLJ, Phys Rev E, 2013]

Triangular Plaquette Model

[Newman and Moore 1999, Garrahan and Newman 2000, Garrahan 2002]



Ising spins $s_i = \pm 1$
on vertices of triangular lattice

Energy

$$E = -\frac{1}{2} \sum_{\triangle} s_1 s_2 s_3 = \frac{N}{2} - \sum_{\mu} n_\mu$$

μ labels "plaquettes", $n_\mu = \frac{1}{2}(1 - s_1 s_2 s_3) = 0, 1$

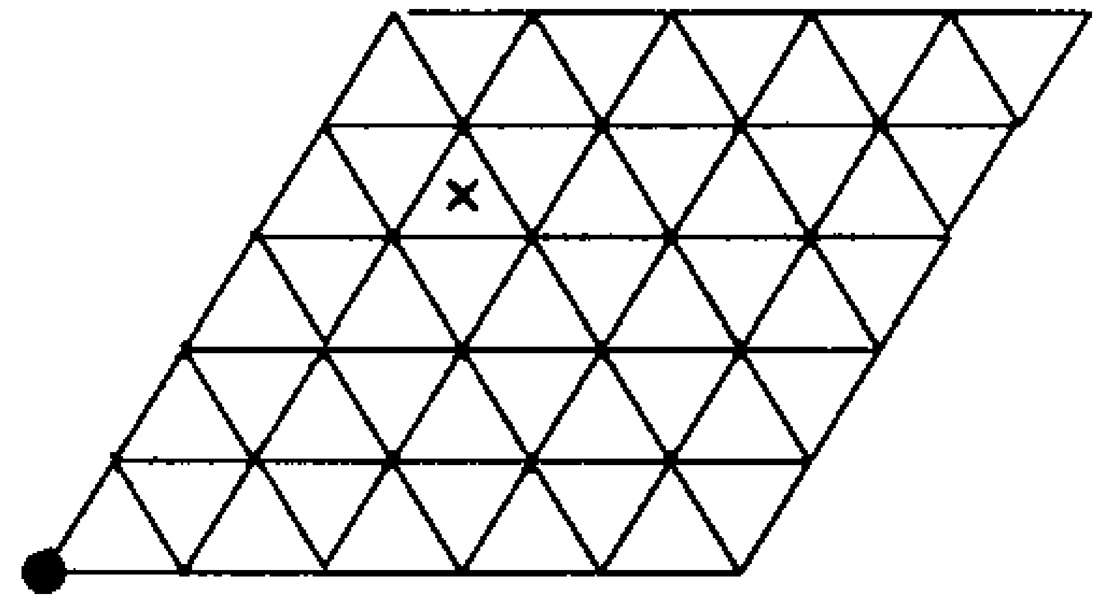
At equilibrium, n_μ are uncorrelated (as in KCMs)

Glauber dynamics (single spin flips)...
Relaxation time $\tau \sim \mathrm{e}^{c/T^2}$, as in East model

TPM: spin correlations

[Newman and Moore 1999, Garrahan and Newman 2000, Garrahan 2002]

Ising spins $s_i = \pm 1$
on vertices of triangular lattice



$\langle s_i \rangle = 0, \qquad \langle s_i s_j \rangle = 0$

Selected three-point and higher correlations are non-zero,
Correlation length $\xi \sim c^{-\log 2 / \log 3}$

Many metastable states...
Assuming complexity $\approx$ simple entropy,
$S_\ell \approx \ell^2 c \ln c + 2\ell \ln 2$

[Cammarota and Biroli, EPL, 2012]

KCM or mosaic?

Can think of TPM as a kinetically-constrained model

… or as a “mosaic” made up of metastable states

BUT:
No domain walls,
No surface tension between states

“Nucleation” dynamics among states:
barrier scales with $\log \ell$
(not ℓ^p as in CNT)

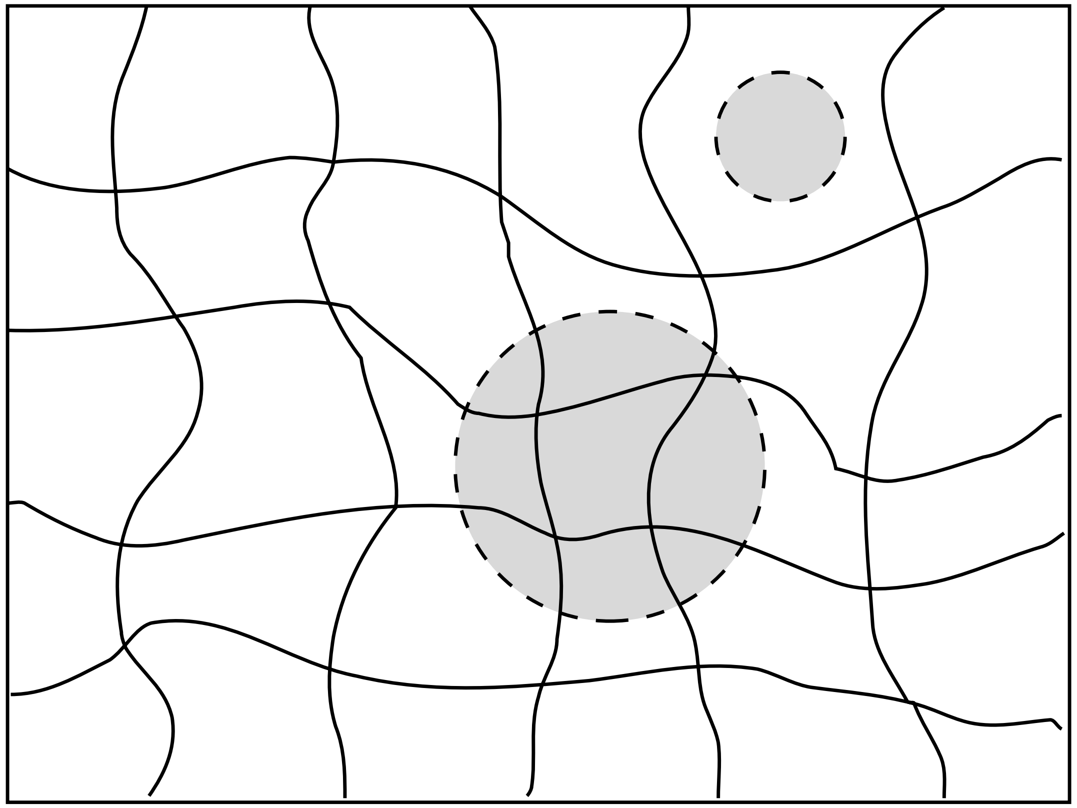


FIG. 1. An illustration of the “mosaic structure” of super-cooled liquids. The mosaic pieces are not necessarily the same

[Xia and Wolynes, PRL 2001]

[RLJ and Garrahan, JCP, 2005]

“Cavity” point-to-set

To measure “mosaic” tile size…

Immobilise system outside a “cavity” of size ℓ

What is the smallest ℓ
for which the cavity has more than 1 state available?

[Bouchaud and Biroli, J Chem Phys, 2004]

For the TPM: this size is $\xi_{\mathrm{mos}} \sim c^{-\log 2/\log 3}$

[RLJ and Garrahan, J Chem Phys, 2005]

Relaxation on length scale ξ_{mos}
determines bulk relaxation time
(consistent with rigorous bound)

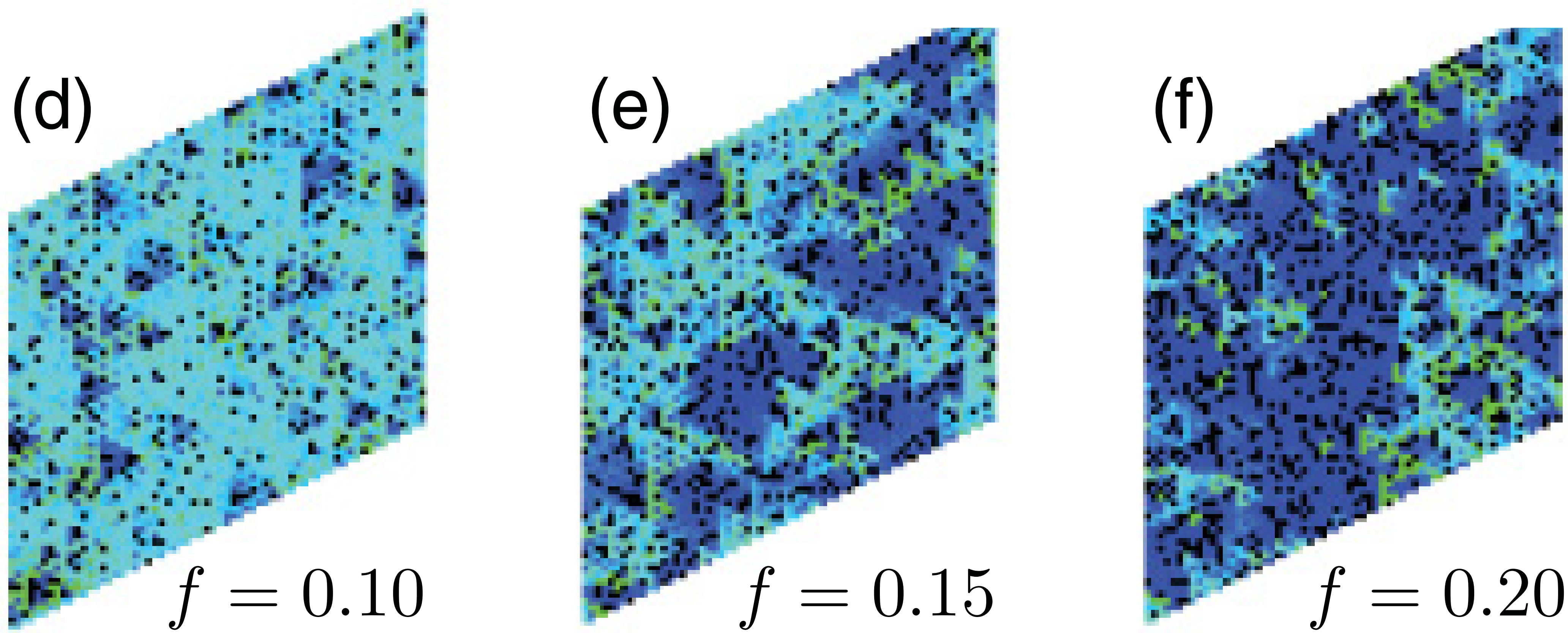
[Montanari and Semerjian, J Stat Phys, 2006]

Random pinning

Random pinning: from an equilibrium configuration $\mathcal{C}_0$, 'pin' (immobilise) each spin w/prob f

Allow model to relax to configuration $\mathcal{C}$, measure overlap $\langle q(\mathcal{C},\mathcal{C}_0)\rangle = \langle s_i s_i^0 \rangle$

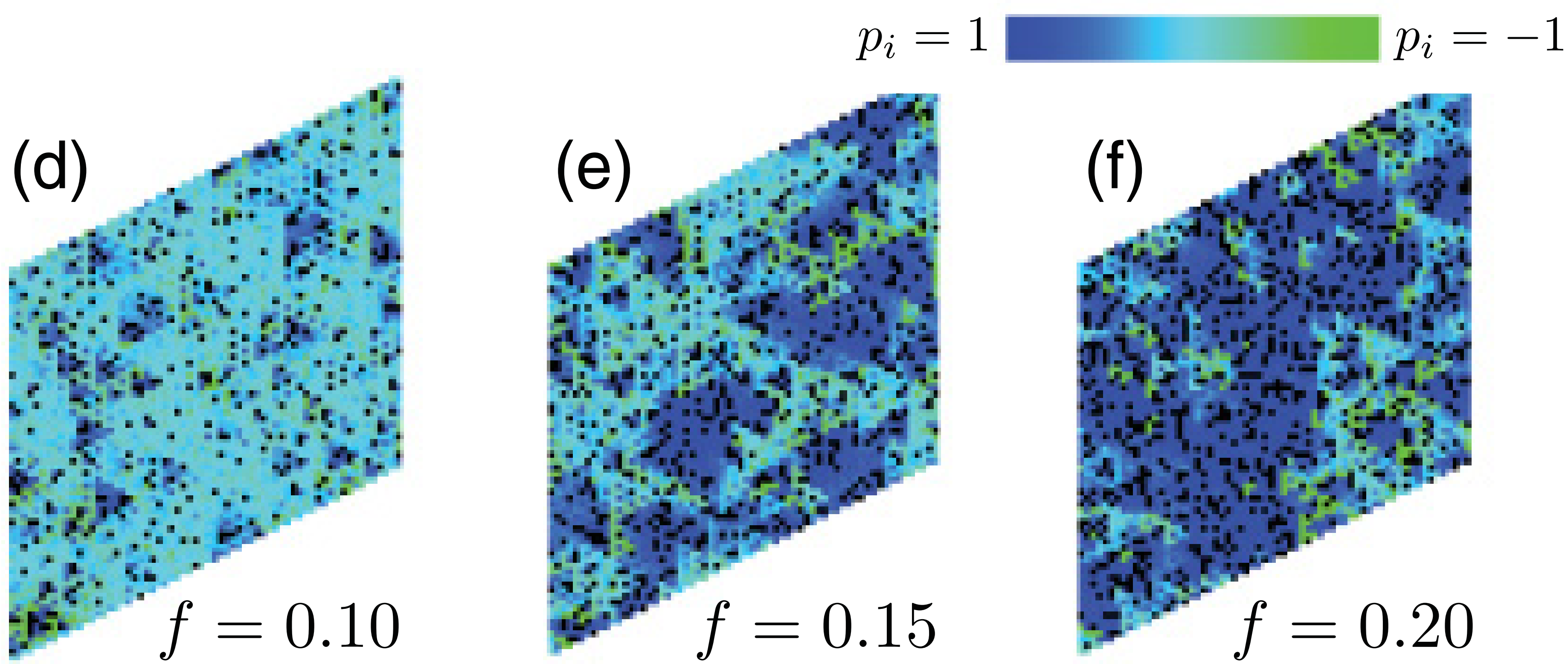
Also, measure $p_i = \langle s_i s_i^0 \rangle_{\mathcal{C}}$



Finite length scale $\xi \sim (1/c)$

[RLJ and Berthier, PRE 2012]

TPM "mosaic"



[RLJ and Berthier, PRE 2012]

Finite length scale $\xi \sim (1/c)$ (from numerics)

Natural mosaic length scale $\xi_{\mathrm{mos}} \sim (1/c)^{\log 2/\log 3}$

Mean-field idea: pinning reduces number of available states, with fixed surface tension: diverging length scale (at fixed *c*)

[Cammarota and Biroli, EPL 2012]

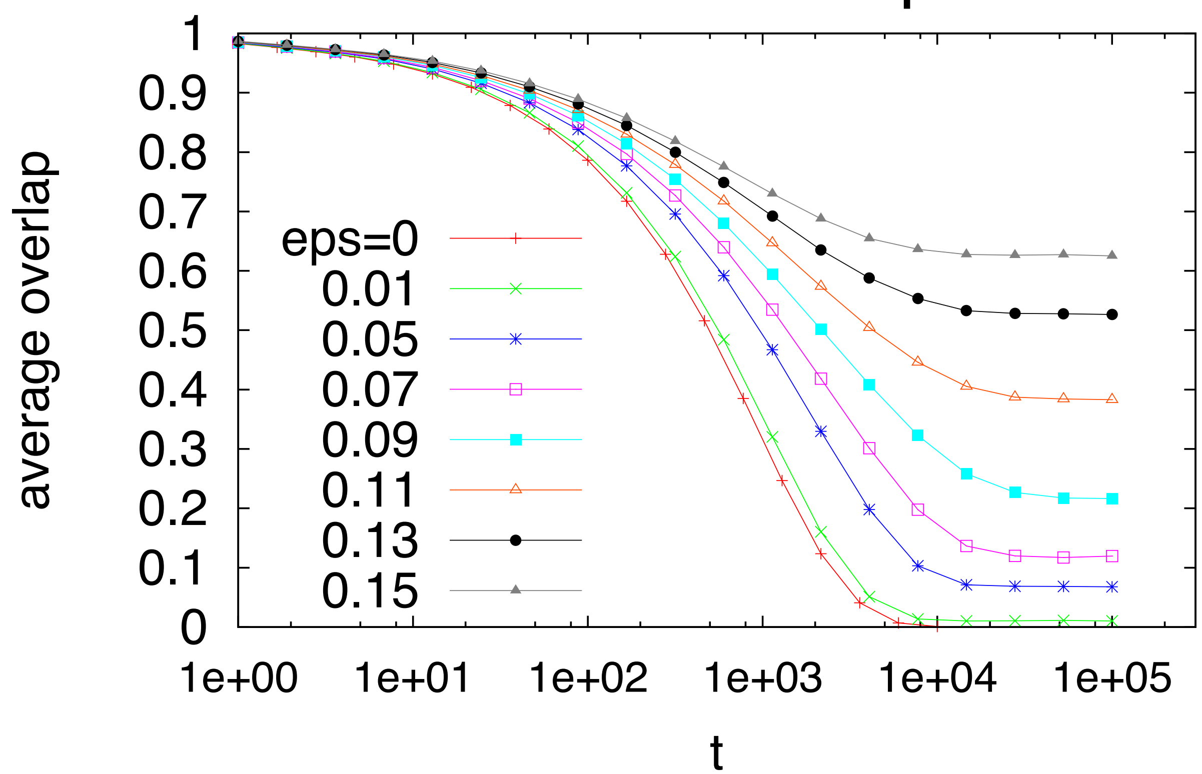
Coupling between spatial domains too weak for this, in TPM ??

Overlap fluctuations

For fixed (quenched) $\mathcal{C}_0$, bias $\mathcal{C}$ to lie near $\mathcal{C}_0$, with biasing probability $\mathrm{e}^{\epsilon N q(\mathcal{C},\mathcal{C}_0)}$

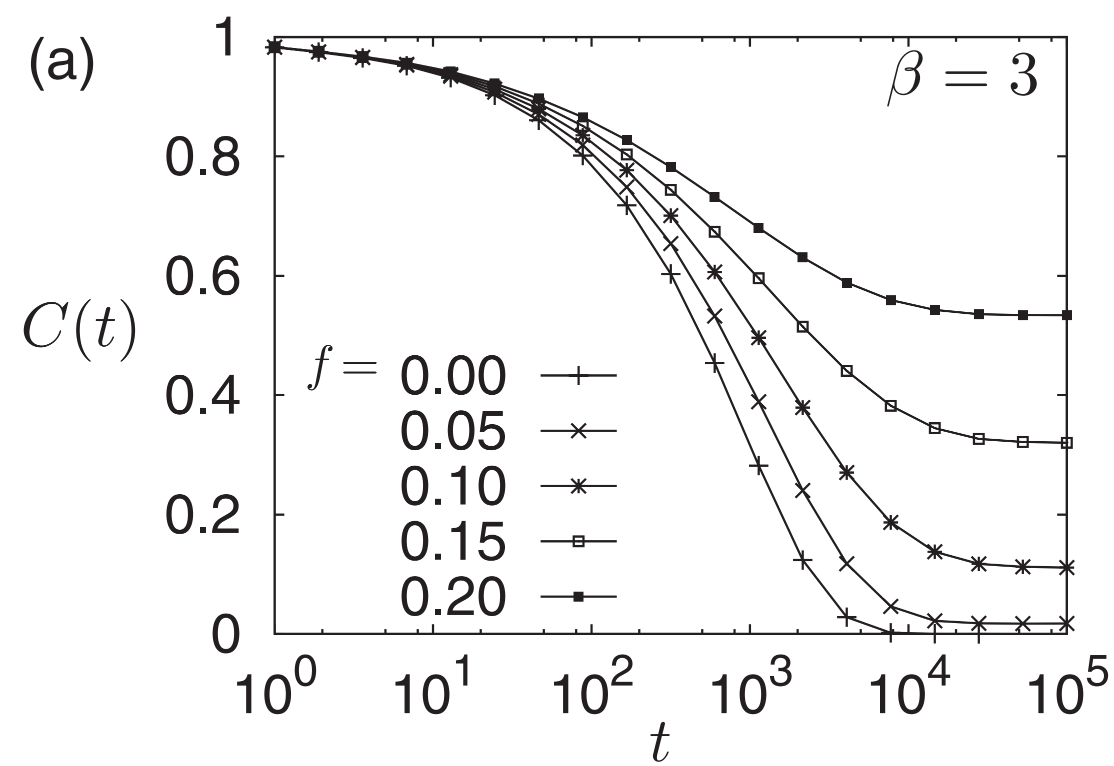
Allow model to relax to configuration $\mathcal{C}$, measure overlap $\langle q(\mathcal{C},\mathcal{C}_0)\rangle = \langle s_i s_i^0 \rangle$

biased overlap…



[RLJ and Garrahan, unpublished]

random pinning…

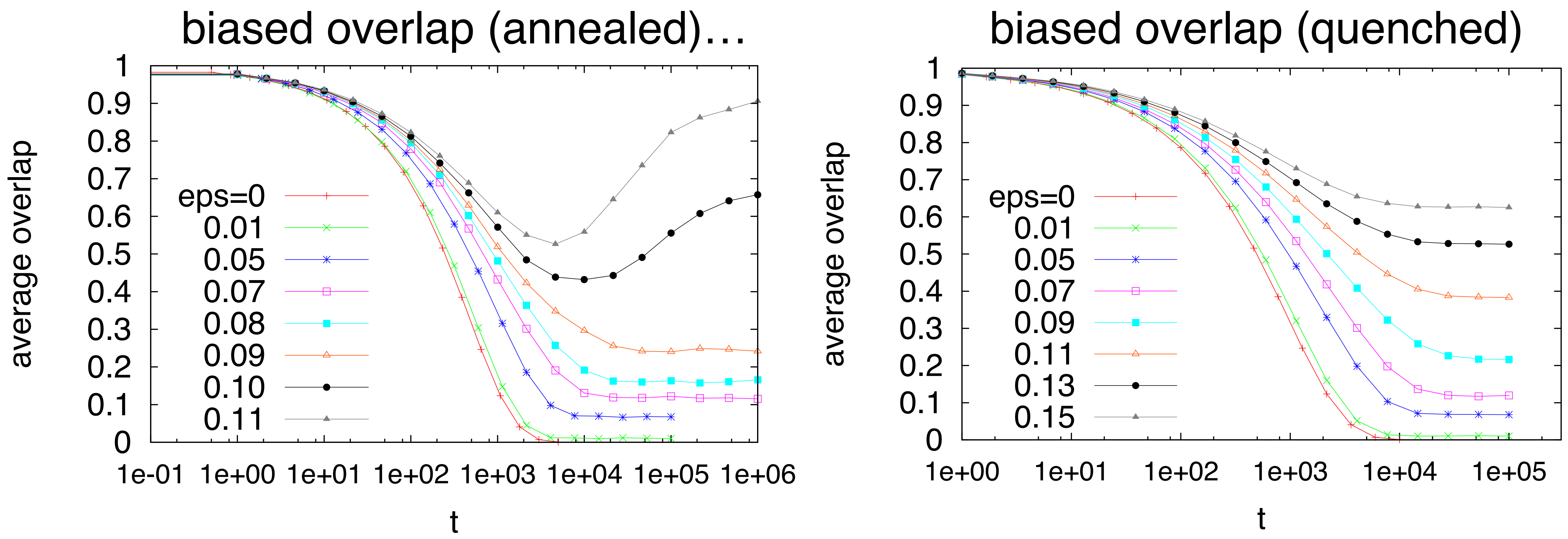


[RLJ and Berthier, PRE 2012]

Overlap fluctuations

For two configurations $\mathcal{C}, \mathcal{C}_0$, bias $\mathcal{C}$ to lie near $\mathcal{C}_0$, with biasing probability $\mathrm{e}^{\epsilon N q(\mathcal{C},\mathcal{C}_0)}$ (annealed case)

First order phase transition at non-zero ϵ^*



[Garrahan PRE 2014, RLJ and Garrahan, unpublished]

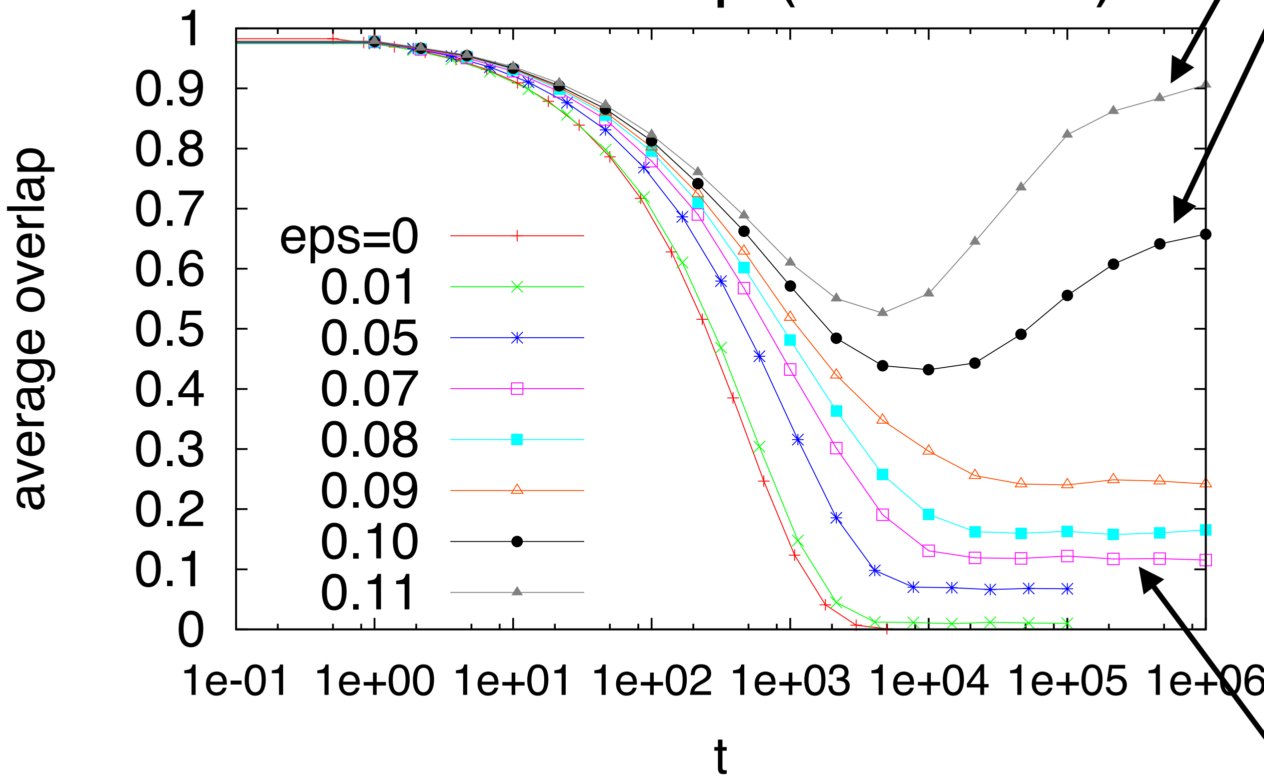
Overlap fluctuations

[RLJ and Garrahan, unpublished]

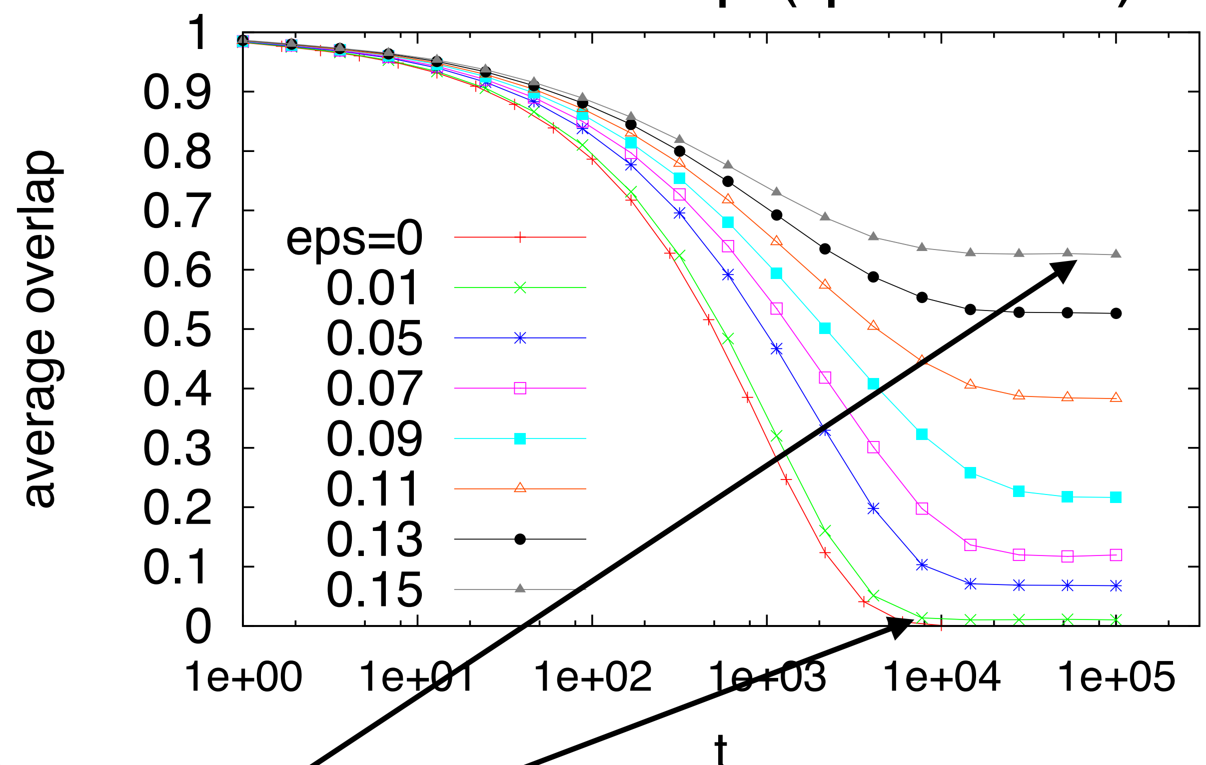
Why are the quenched/annealed cases so different?

Defect density $\langle n_\mu \rangle \approx c^2$

biased overlap (annealed)…



biased overlap (quenched)



Defect density $\langle n_\mu \rangle \approx c$

Annealed case: system is sampling *non-typical* metastable states

Dimensionality?

[RLJ and Garrahan, unpublished]

Are two-dimensional models special?

If *surface tension* between metastable states exists,
can relate pinned systems to random-field Ising magnets…
(hence no phase transitions in 2d)

In TPM, no surface tension, so this argument does not apply…

preliminary results for 3d generalisation of TPM
… consistent with 1st order transition with annealed coupling,
no transition for quenched coupling,
(as in 2d)

Dynamics and metastability

Alternate probe of non-typical metastable states:
bias trajectories of a system using time-integrated quantities

Let $\mathcal{C}$ be a "configuration".
Consider trajectories $\mathcal{C}(t)$ of length t_{obs} (sample paths)

Bias probabilities as:

$$\mathrm{Prob}[\mathcal{C}(t); s] = \mathrm{Prob}[\mathcal{C}(t); 0] \frac{\mathrm{e}^{-s t_{\mathrm{obs}} \overline{k}[\mathcal{C}(t)]}}{Z(s)}$$

$\overline{k}[\mathcal{C}(t)]$: time-averaged measurement along trajectory

[Ruelle, Gallavotti-Cohen, Evans, Derrida, Lebowitz, Gaspard, Maes, etc]

Dynamics and metastability

Bias probabilities as:

$$\mathrm{Prob}[\mathcal{C}(t); s] = \mathrm{Prob}[\mathcal{C}(t); 0] \frac{\mathrm{e}^{-s t_{\mathrm{obs}} \overline{k}[\mathcal{C}(t)]}}{Z(s)}$$

Effect of field s is to enhance probabilities of long-lived states with small $\overline{k}$

This can lead to "dynamical phase transitions": singular responses to field s

[Garrahan *et al* 2007, Hedges *et al* 2009, …]

System arrives in non-typical metastable states…
(cf annealed overlap calculation)

Summary

KCMs (and the TPM) have well-defined metastable states (with a range of lifetimes…)

Random pinning and quenched overlap calculations reveal correlations among “mosaic tiles” but (apparently) no phase transitions…

No evidence for surface tension between states in TPM, [Relevant for “nucleation” arguments about dynamics, could be a scenario for atomistic systems(?)]

Annealed overlap and *s*-ensemble calculations probe *non-typical* metastable states and do lead to phase transitions in KCMs, TPM, …