Dynamical large deviations and glass transitions

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£ EPSRC The Leverhulme Trust

Dynamics is more than statics

Canonical example → **glass transition problem**

Statistical mechanics of **trajectories** rather than states/configurations

Dynamical **large-deviations** → s-ensemble method ➙ **glasses**

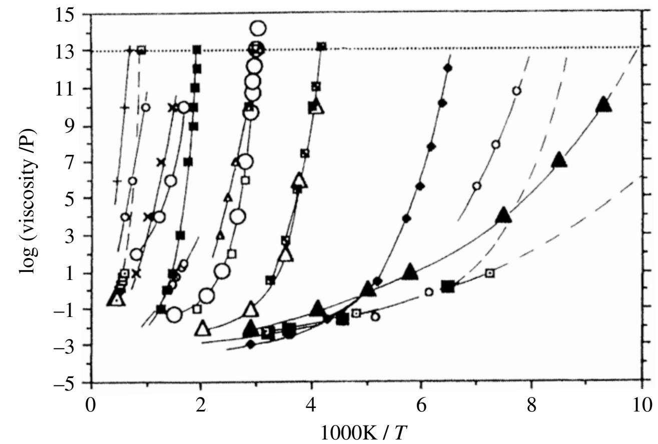
{Ruelle, Derrida, Lebowitz-Spohn, Gartner-Ellis, Donsker-Varadhan, ...}

Applications in **quantum many-body systems?**

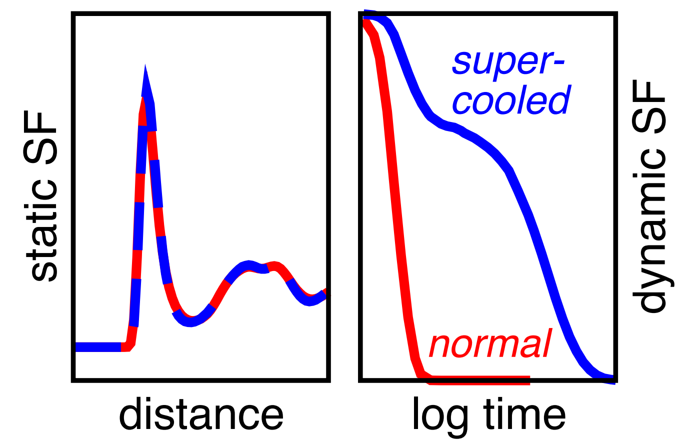
Stylised facts about the glass transition

{Biroli-JPG, **JCP Pespective: The Glass Transition 2013**}

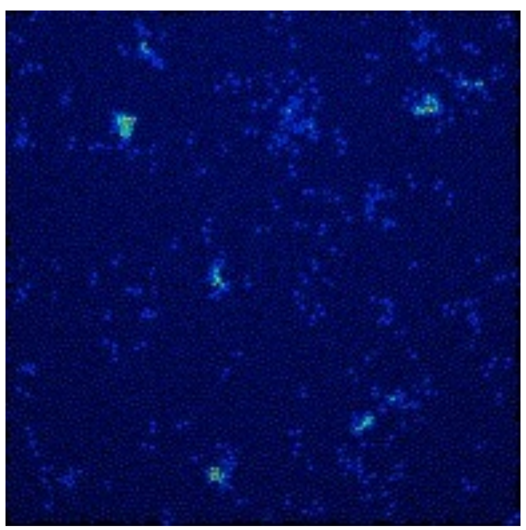
#1: Slowdown w/o structural change



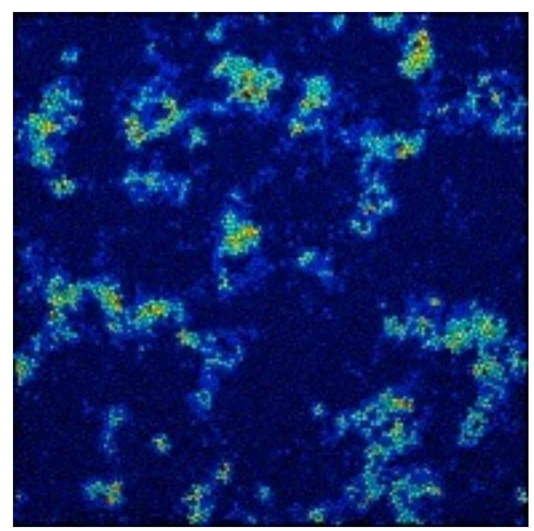
{Angell 1995}



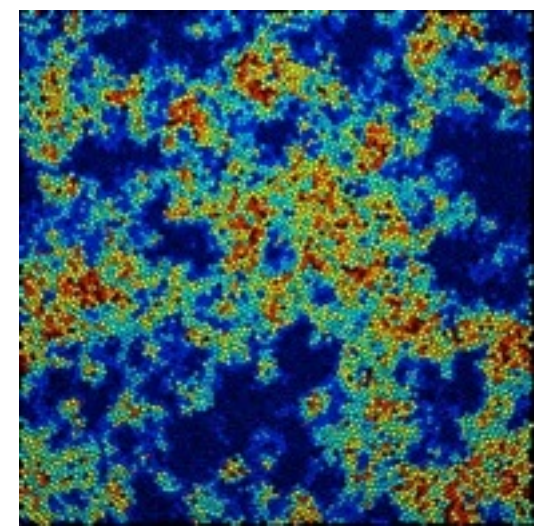
$t \ll \tau_\alpha$



$t \approx \tau_\alpha$



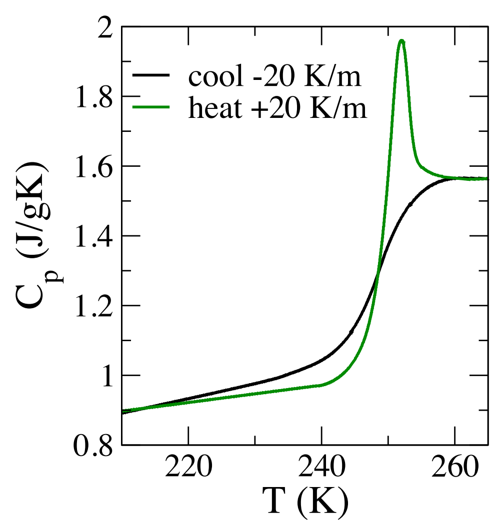
$t \gg \tau_\alpha$

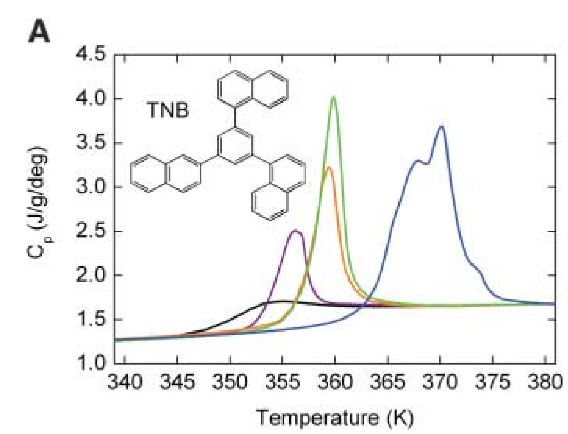


e.g.
50:50 L-J mixture
{Hedges 2009}

#2: Dynamical heterogeneity

#3: Anomalous response if driven out-of-equilibrium

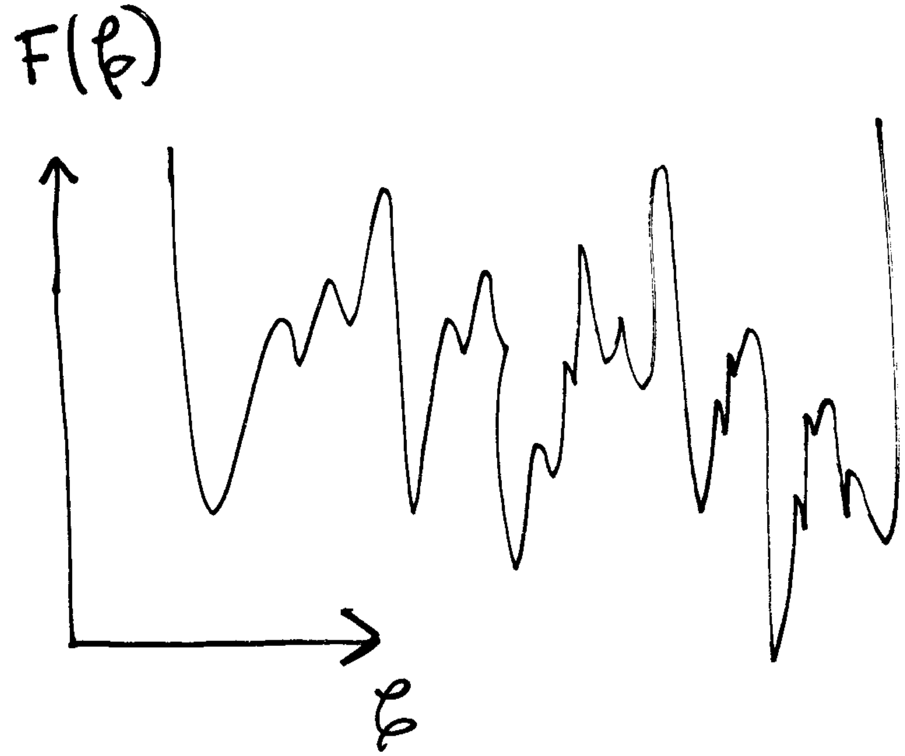




{Swallen+ 2007}

Perspectives on glass transition

Thermodynamic



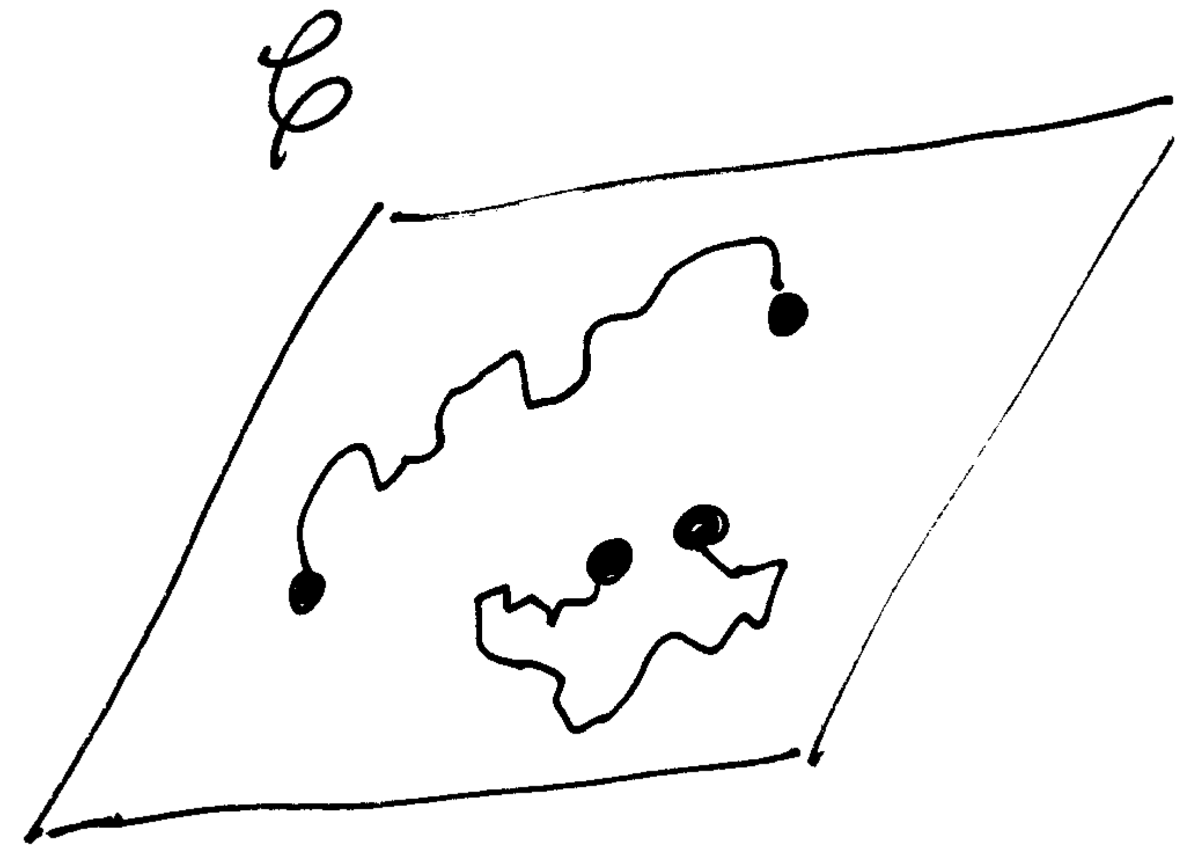
Statics ⇒ Dynamics

eg. **RFOT**

{Parisi+Wolynes+many others}

ideal models e.g. **p-spin spin glass**

Dynamic



Statics **does not** ⇒ Dynamics

metric → Dynamic facilitation

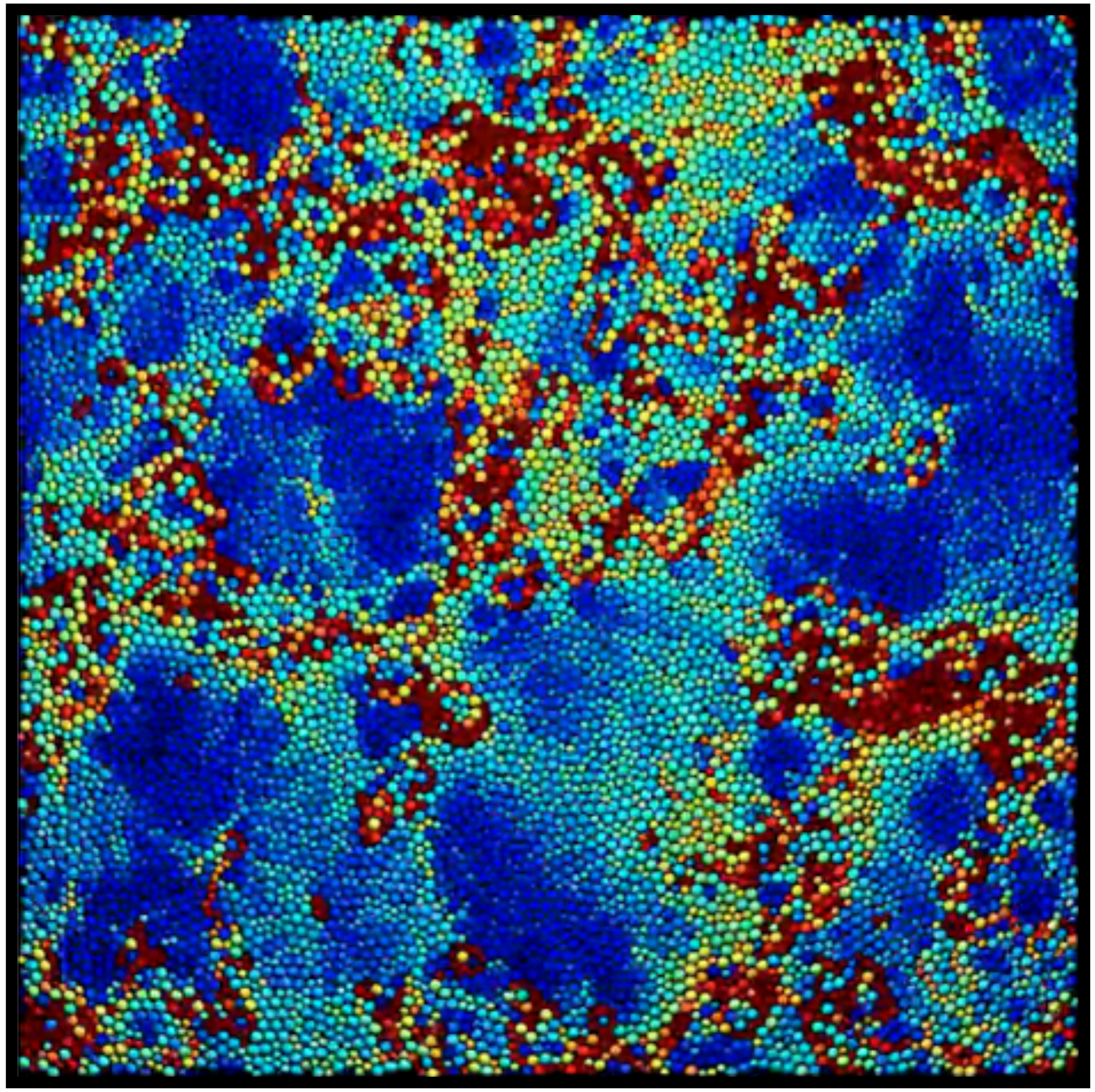
ideal models **KCMs**

{Anderson+Andersen+Jackle+many others}

#2: Dynamical heterogeneity

Cold/dense Lennard-Jones mixture
{L. Hedges}

$N_A = N_B = 10^4 \quad (1:1.4)$
$T = 1.1 < T_{\text{onset}}$

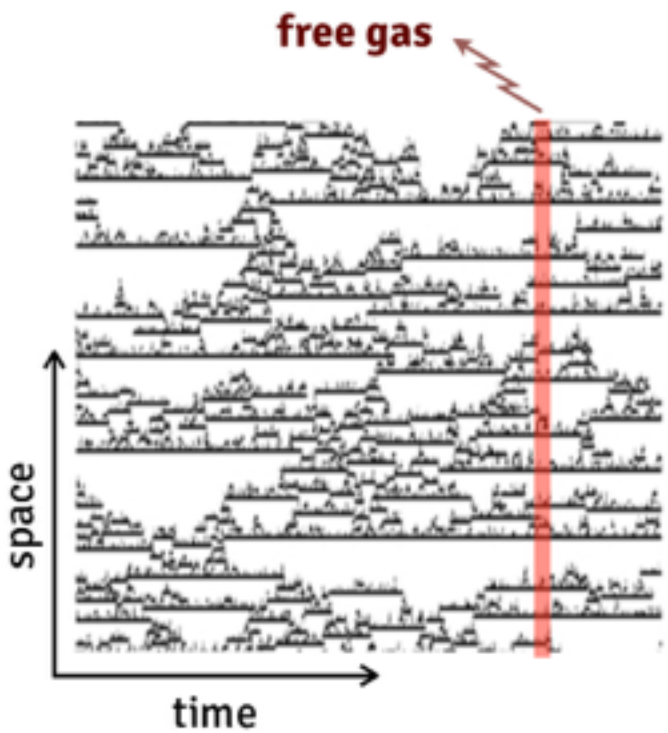


Motion begets motion ➙ **dynamical facilitation**

Effective excitations are **localised** {Keys-et-al, **PRX 2011**}

Interesting structure in trajectories not in configurations/states

Dynamic facilitation → kinetically constrained models



East model
{Jackle 1991}

FA model
{Fredrickson-Andersen 1984}

$$\partial_t |P\rangle = \mathbb{W}|P\rangle \quad \rightarrow \quad \mathbb{W} = \sum_i (n_{i-1} + \delta)\left[\epsilon\sigma_i^+ + \sigma_i^- - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1)$$

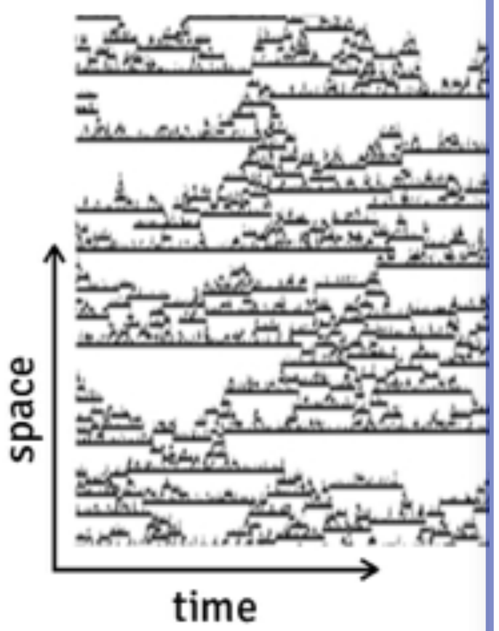
constraint = operator valued rate

Trivial statics but **heterogeneous & hierarchical dynamics**

East model $\quad \tau_{\mathrm{relax}} \approx \tau_0 \exp\left(\frac{A}{T^2} + \frac{B}{T}\right)$ {Sollich-Evans 1999}

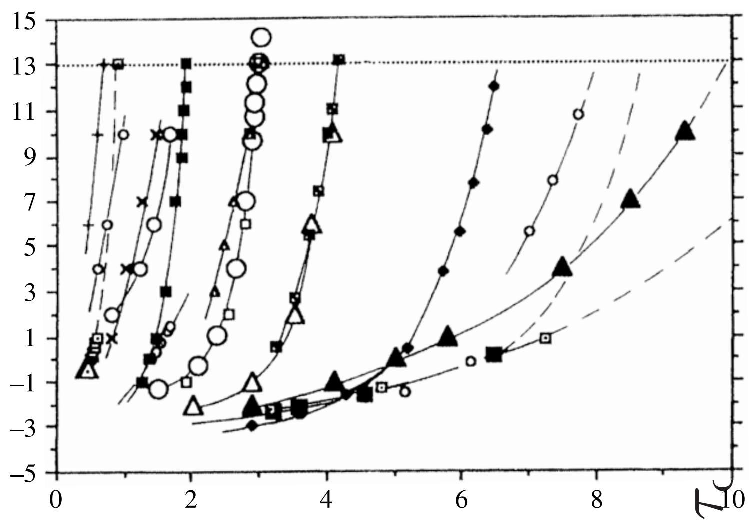
Dynamic facilitation → kinetically constrained models

free gas



$$\partial_t |P\rangle = \mathbb{W}|P\rangle$$

Triv

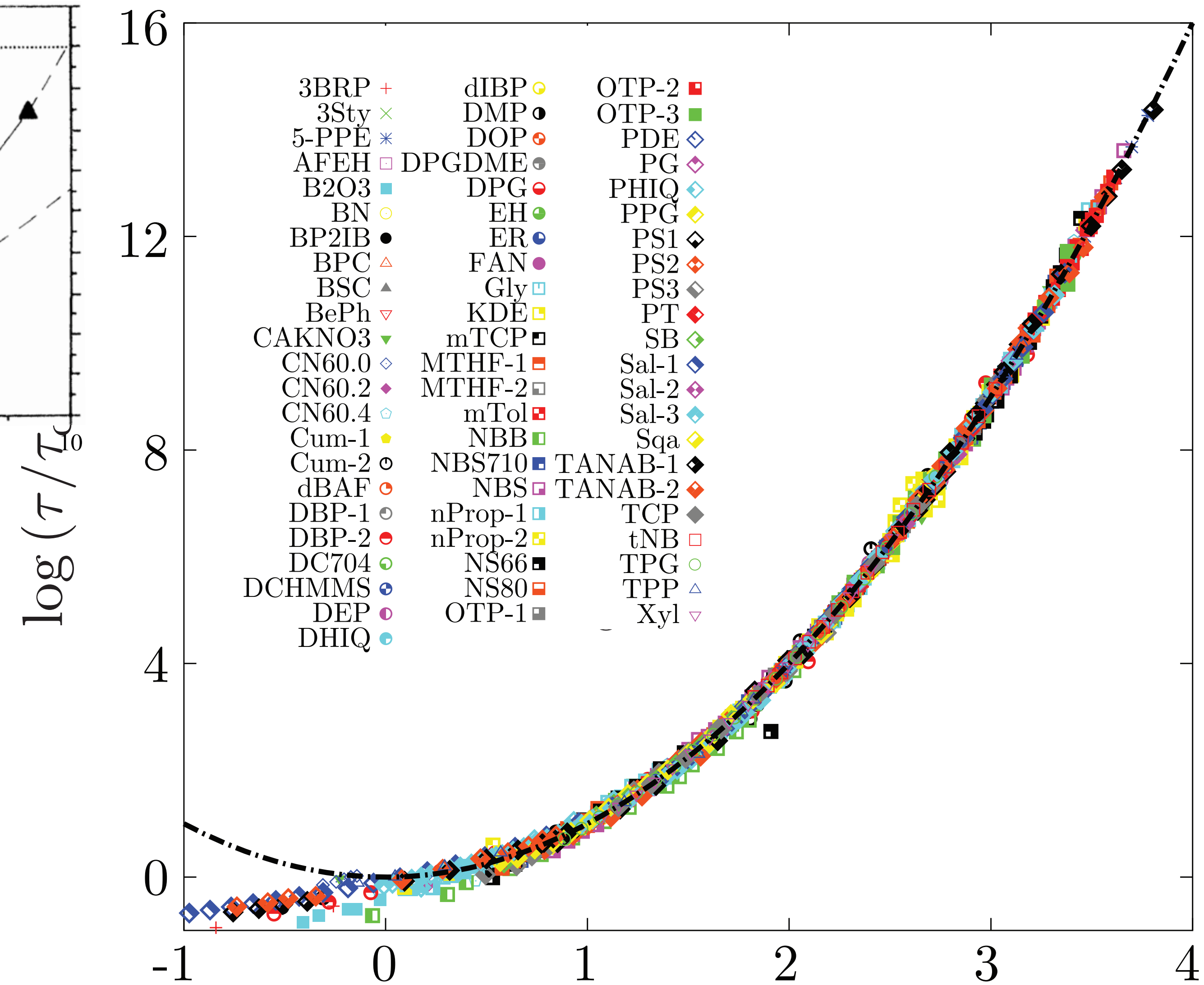


{Angell 1995}

NB: **no** VFT

$$\exp\left(\frac{C}{T - T_0}\right)$$

{cf. Bassler 1987, Rossler+ 1998, Hecksher+ 2007, McKenna+ 2013}



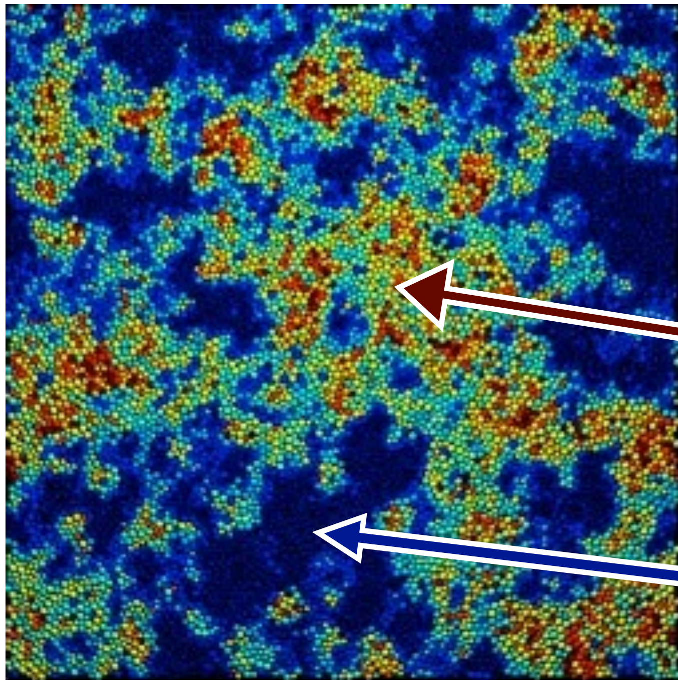
#1 $\quad \frac{J}{T_o}\left(\frac{T_o}{T} - 1\right)$

{Elmatad-Chandler-JPG, JPCB 2009/2010}

East model $\quad \tau_{\text{relax}} \approx \tau_0 \exp\left(\frac{A}{T^2} + \frac{B}{T}\right)$ {Sollich-Evans 1999}

“Thermodynamics” of trajectories: s-ensemble

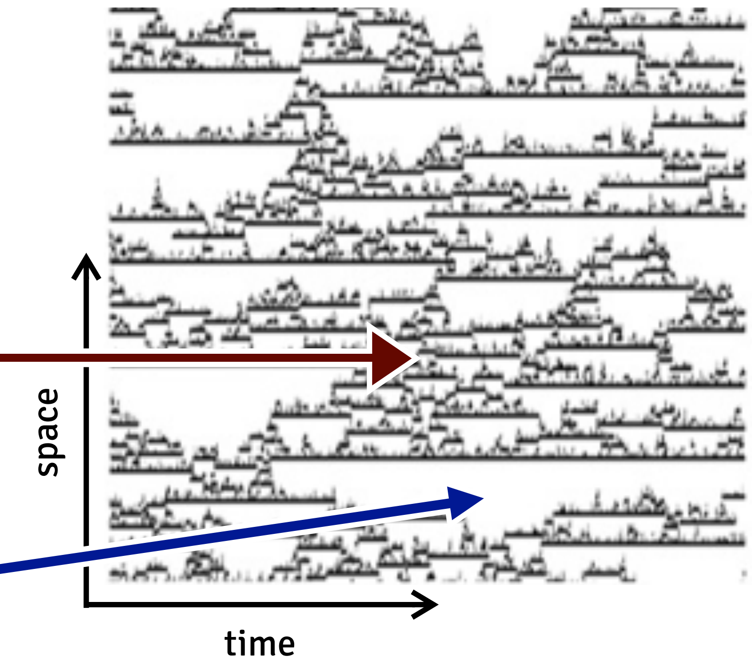
BMLJ



time-integrated
order parameter:
K = **activity**

active $K \gg 0$

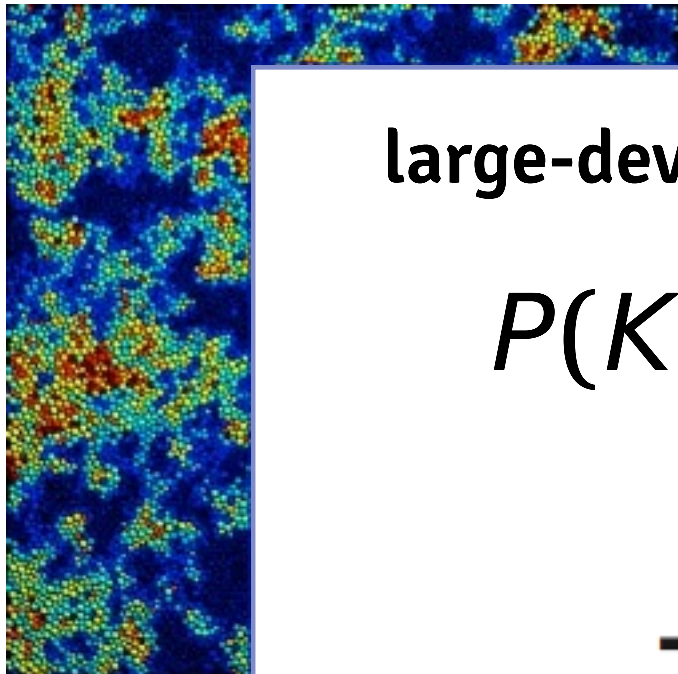
inactive $K \approx 0$



East

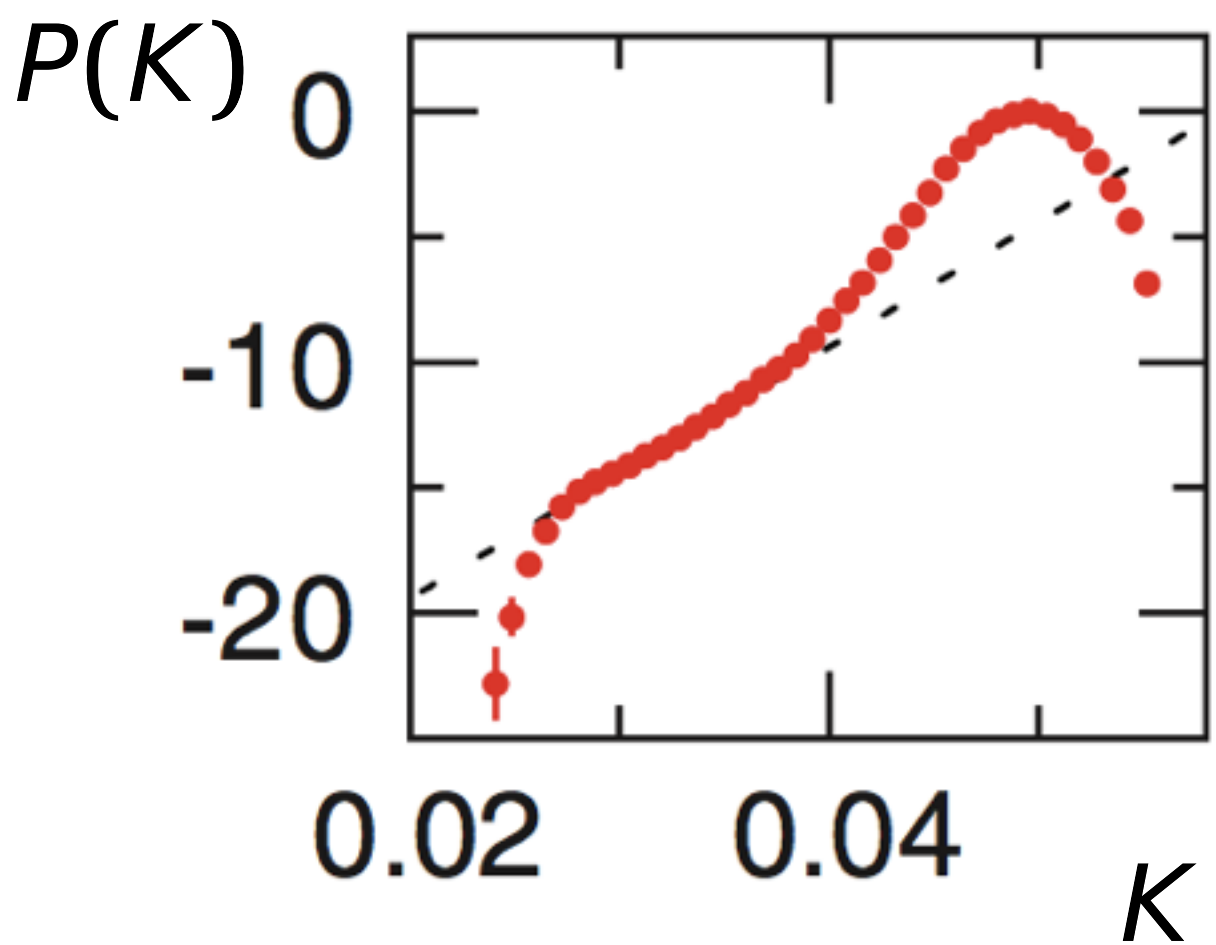
“Thermodynamics” of trajectories: s-ensemble

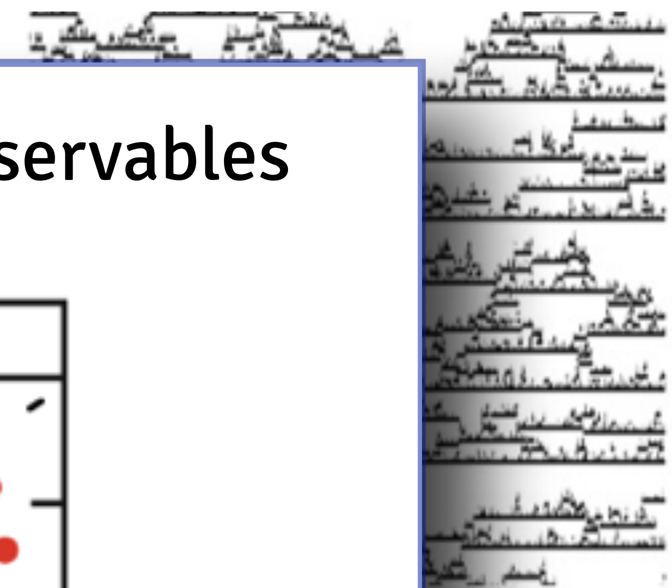
time-integrated



BMLJ

large-deviations of **time-integrated** observables

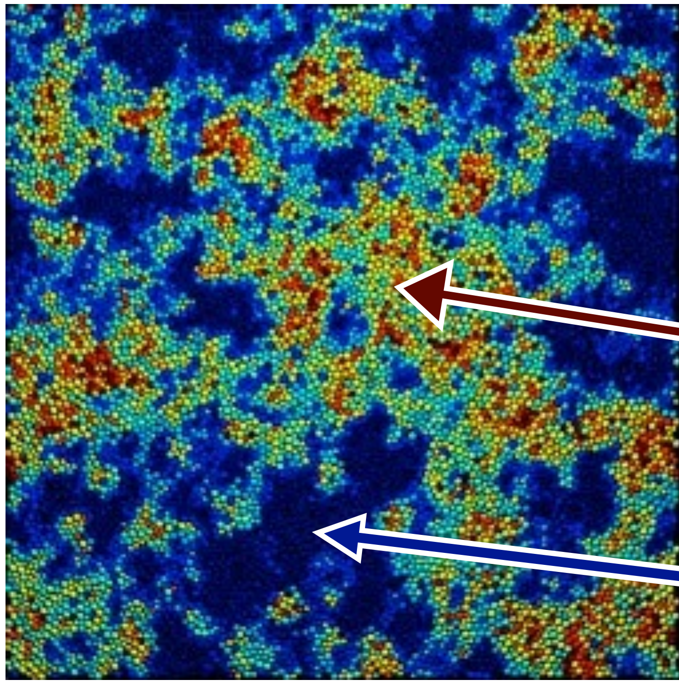




East

"Thermodynamics" of trajectories: s-ensemble

BMLJ

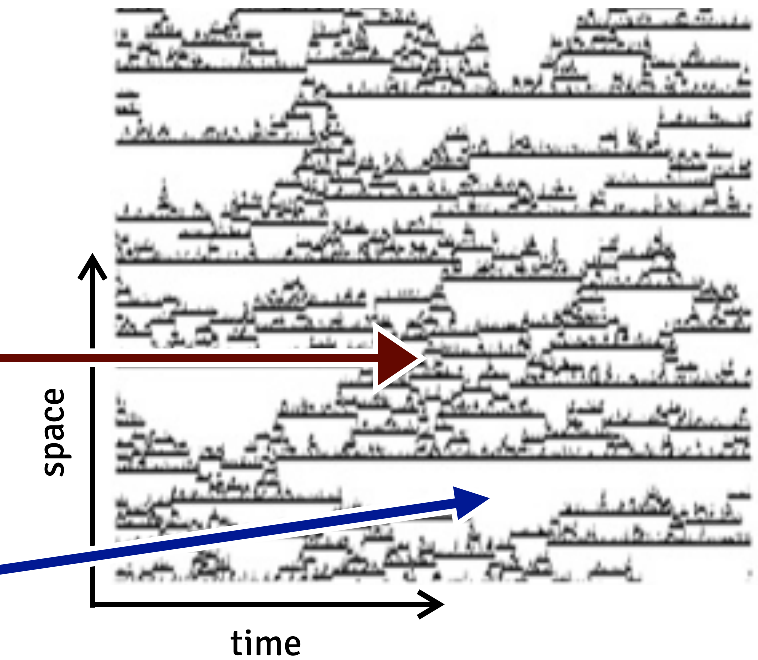


time-integrated order parameter:

K = **activity**

active $K \gg 0$

inactive $K \approx 0$



East

$$\mathrm{Prob}(K) \approx e^{-t\ \varphi(K)}$$

$$Z_t(s) \equiv \langle e^{-sK} \rangle \approx e^{t\ \theta(s)}$$

large deviations

{e.g. Ruelle, Lebowitz-Spohn, Gartner-Ellis, Donsker-Varadhan, Lecomte+, many others cf. **Full Counting Statisitcs**}

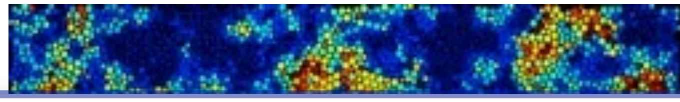
$s \leftrightarrow K$ φ = "entropy" θ = "free-energy" t = "volume"

$$\mathbb{W} \;\; \longrightarrow \;\; \mathbb{W}_s = \sum_i n_{i-1} \left[e^{-s} \left(\epsilon \sigma_i^+ + \sigma_i^- \right) - \epsilon (1 - n_i) - n_i \right]$$

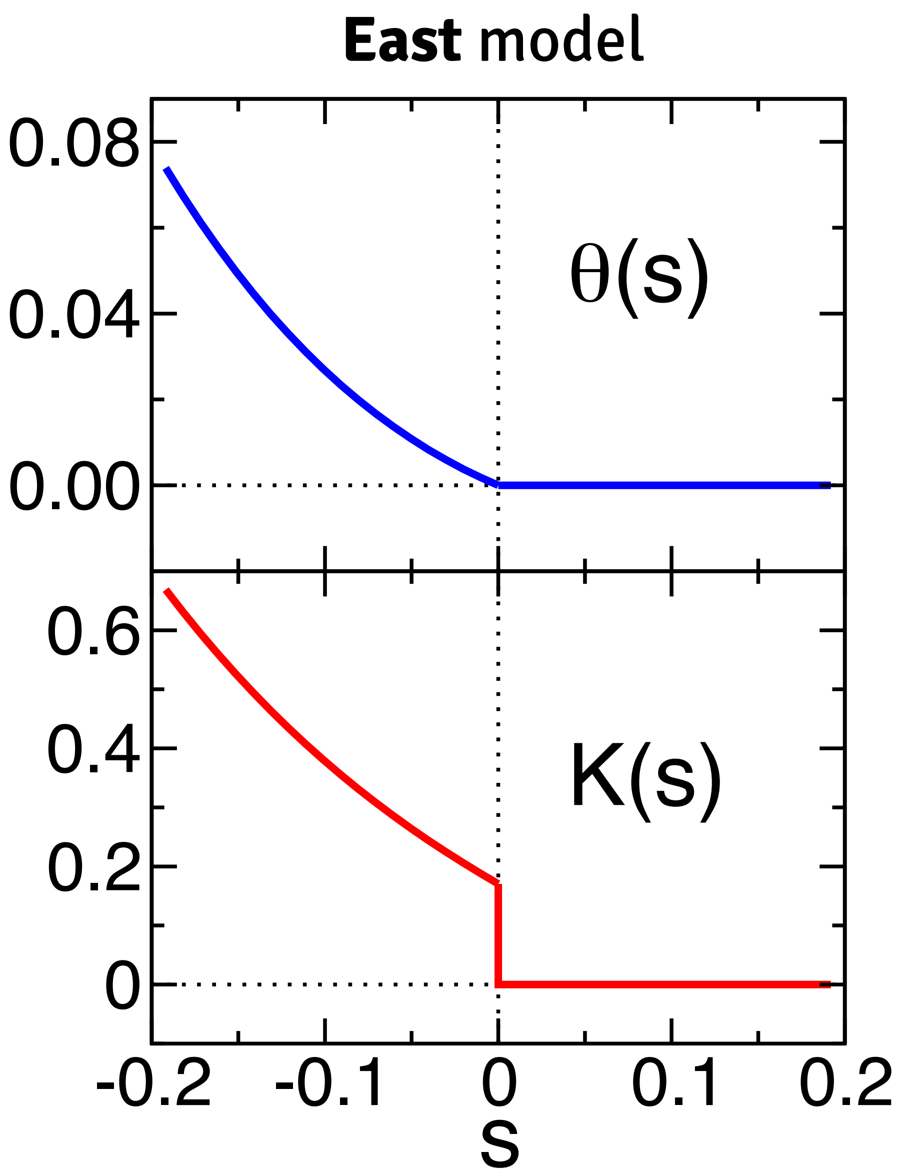
$\theta(s)$ **largest eigenvalue**

$\mathbb{W}_s$ is "transfer matrix" of "partition sum" $Z_t(s)$

“Thermodynamics” of trajectories: s-ensemble



time-integrated
order parameter:

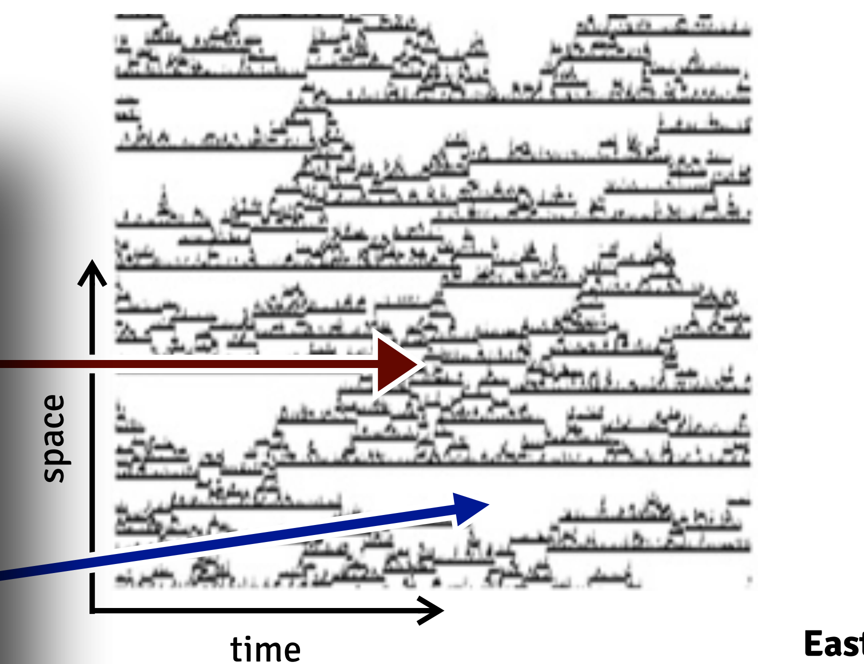


first-order dynamical transition

at $s_c = 0$

when $t_{obs} \to \infty$

{JPG-Jack-Lecomte-Pitard-van Duijvendijk-van Wijland, PRL 2007, JPA 2009}



iations

{e.g. Ruelle, Lebowitz-Spohn, Gartner-Ellis, Donsker-Varadhan, Lecomte+, many others cf. **Full Counting Statisitcs**}

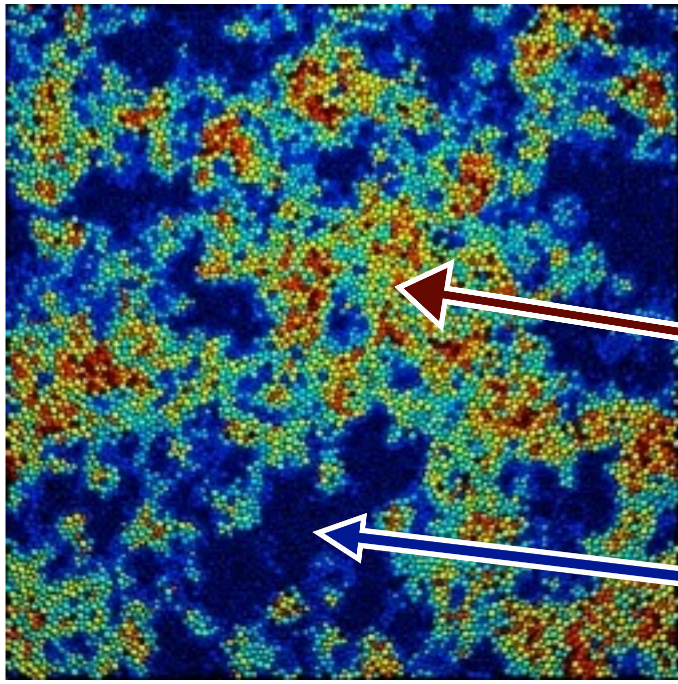
t = “volume”

$$\mathbb{W} \;\rightarrow\; \mathbb{W}_s = \sum_i n_{i-1}\left[\, e^{-s}\left(\epsilon\sigma_i^+ + \sigma_i^-\right) - \epsilon(1-n_i) - n_i \right]$$

$\theta(s)$ **largest eigenvalue**

$\mathbb{W}_s$ is “transfer matrix” of “partition sum” $Z_t(s)$

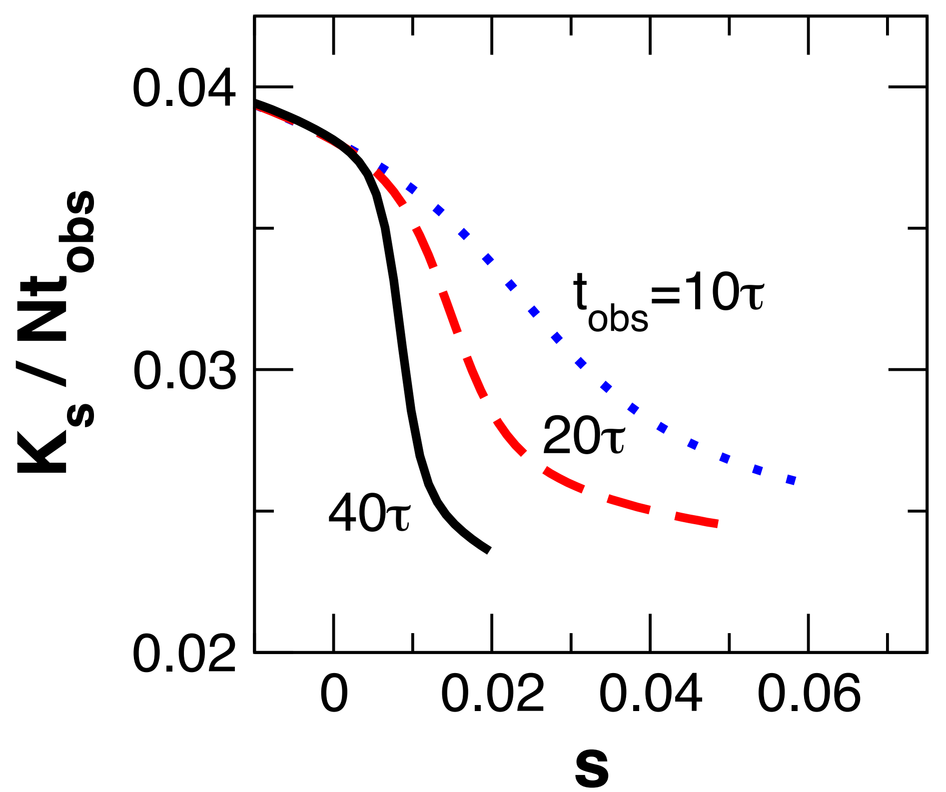
"Thermodynamics" of trajectories: s-ensemble



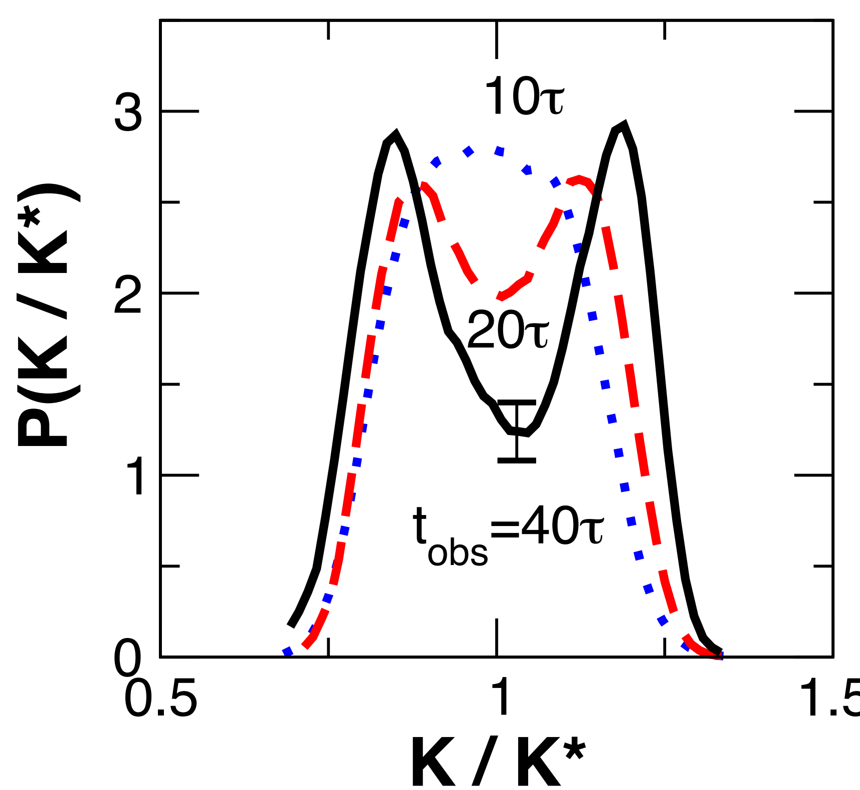
BMLJ

BMLJ (MD/TPS, N=150)

{Hedges-Jack-JPG-Chandler, **Science 2009**}



activity vs. counting field



first-order dynamical transition

at $s_c \gtrsim 0$

when $t_{obs} \gg \tau$

{see also,
Lecomte-Pitard-van Wijland 2011,
Speck-Chandler 2012
Speck-Malins-Royall 2012}

$\mathrm{Prob}(K) \approx e$

$Z_t(s) \equiv \langle e^{-sK} \rangle \approx$

$s \leftrightarrow K$ φ = "entropy"

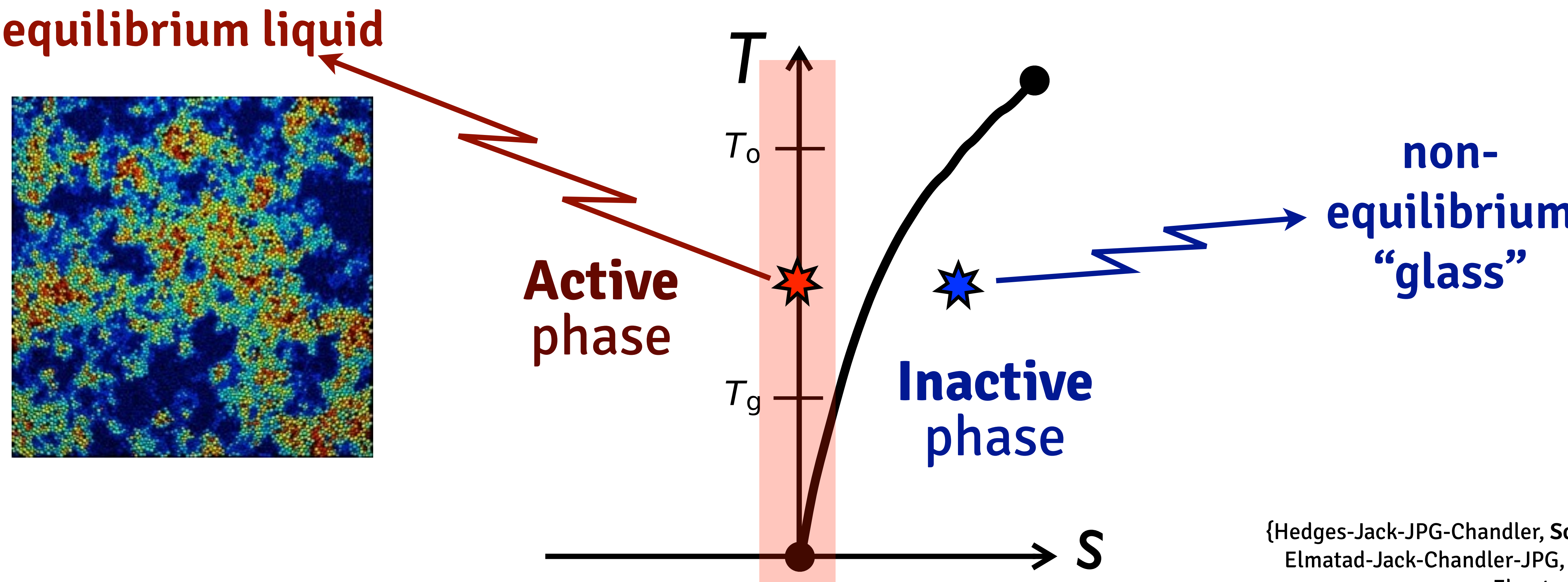
$\mathbb{W} \rightarrow \mathbb{W}_s = \sum_i n_{i-1} [e^{-s}$ (

$\mathbb{W}_s$ is "tra

“Thermodynamics” of trajectories: s-ensemble

dynamical phase-diagram

$(t_{\mathrm{obs}} \to \infty,\ N \to \infty)$



{Hedges-Jack-JPG-Chandler, **Science 2009**,
Elmatad-Jack-Chandler-JPG, **PNAS 2010**,
Elmatad-Jack 2013}

real dynamics $s = 0$ → **can we access** $s_c \gtrsim 0$ **?**

Accessible from **normal** dynamics via **cumulants** and **Lee-Yang** zeros

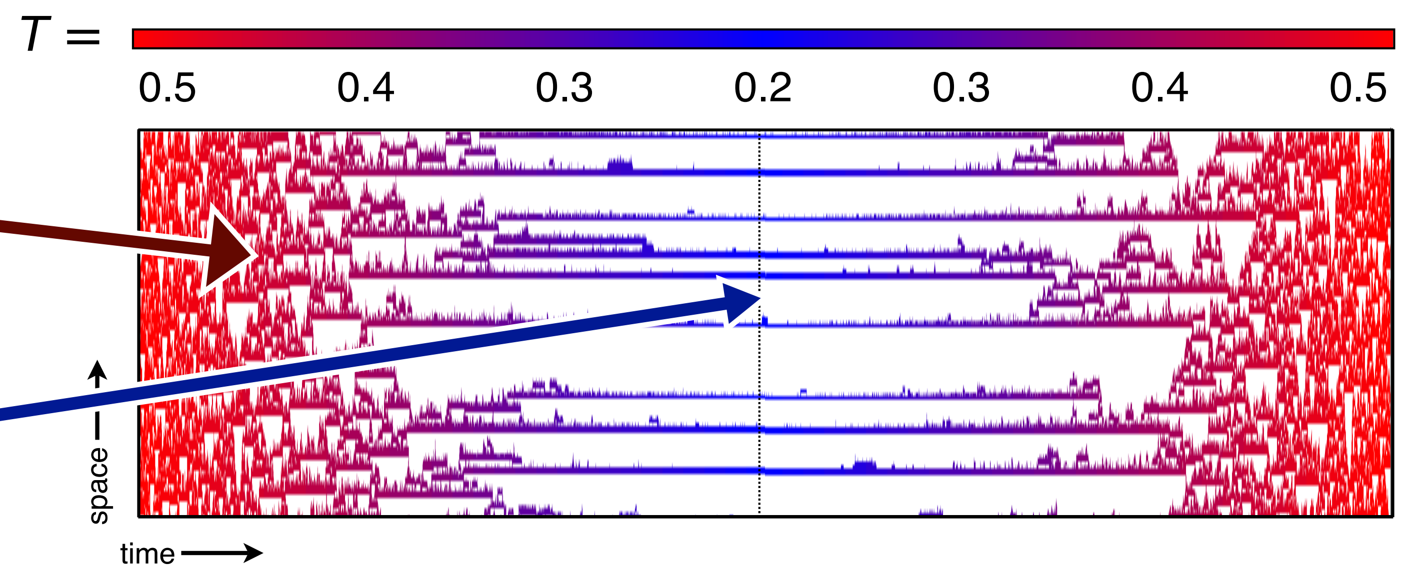
{Flindt-JPG, **PRL 2013**; Hickey-Flindt-JPG 2014}

Preparing glasses with s-ensemble

{Keys-JPG-Chandler, PNAS 2013 and arXiv:1401.7206}

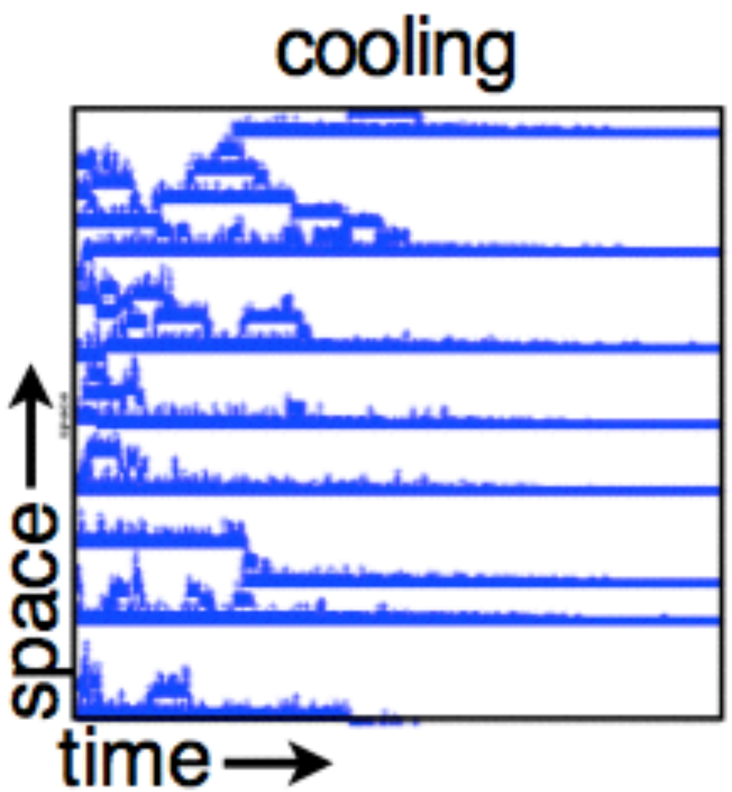
space-time bubbles (active & equil.)

space-time stripes (inactive & noneq.)

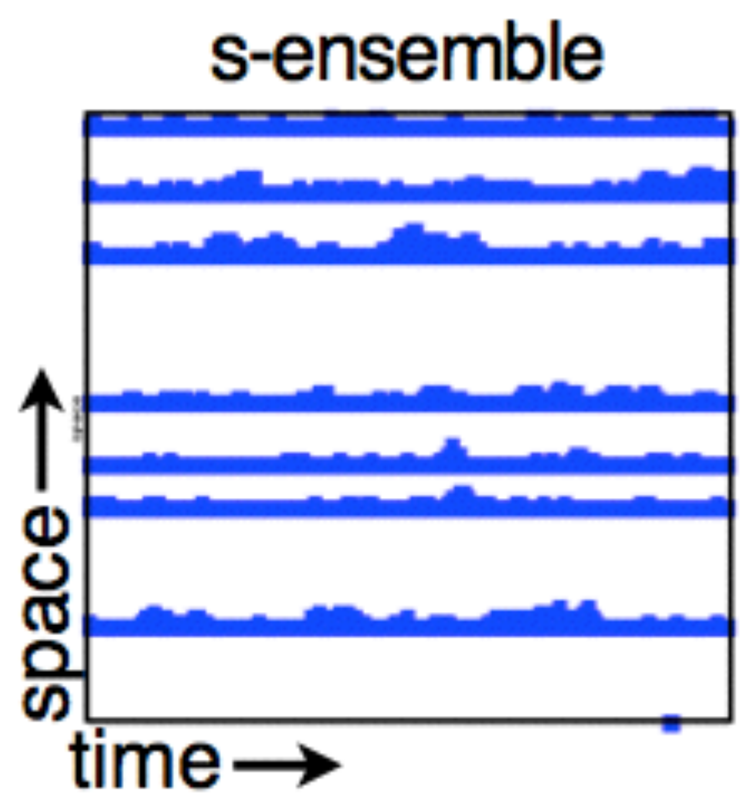


East model

{cf. Sollich-Evans 2003}



$$\} \; l = \left(\frac{\tau_g}{\tau_o}\right)^{T_g}$$



$$\} \; l = \left(\frac{t_{obs}}{\tau_o}\right)^{T}$$

non-equilibrium characteristic **length** in glassy state

Preparing glasses with s-ensemble

{Keys-JPG-Chandler, **PNAS 2013** and **arXiv:1401.7206**}

space-time bubbles (active & equil.)

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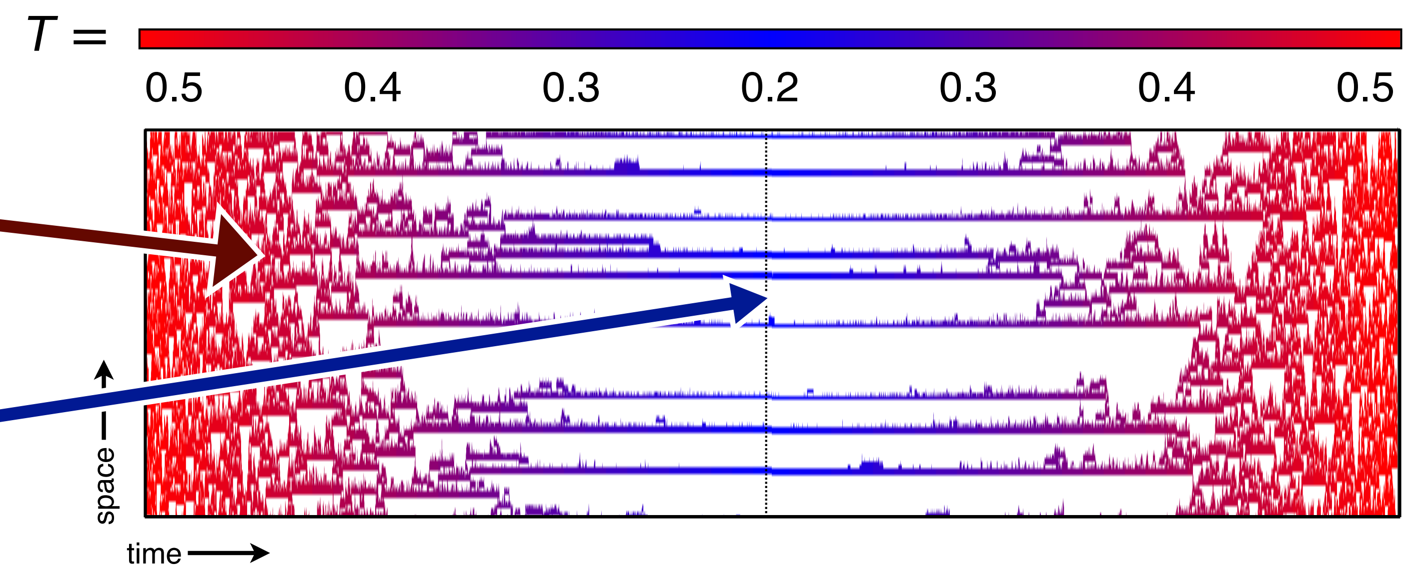

East model

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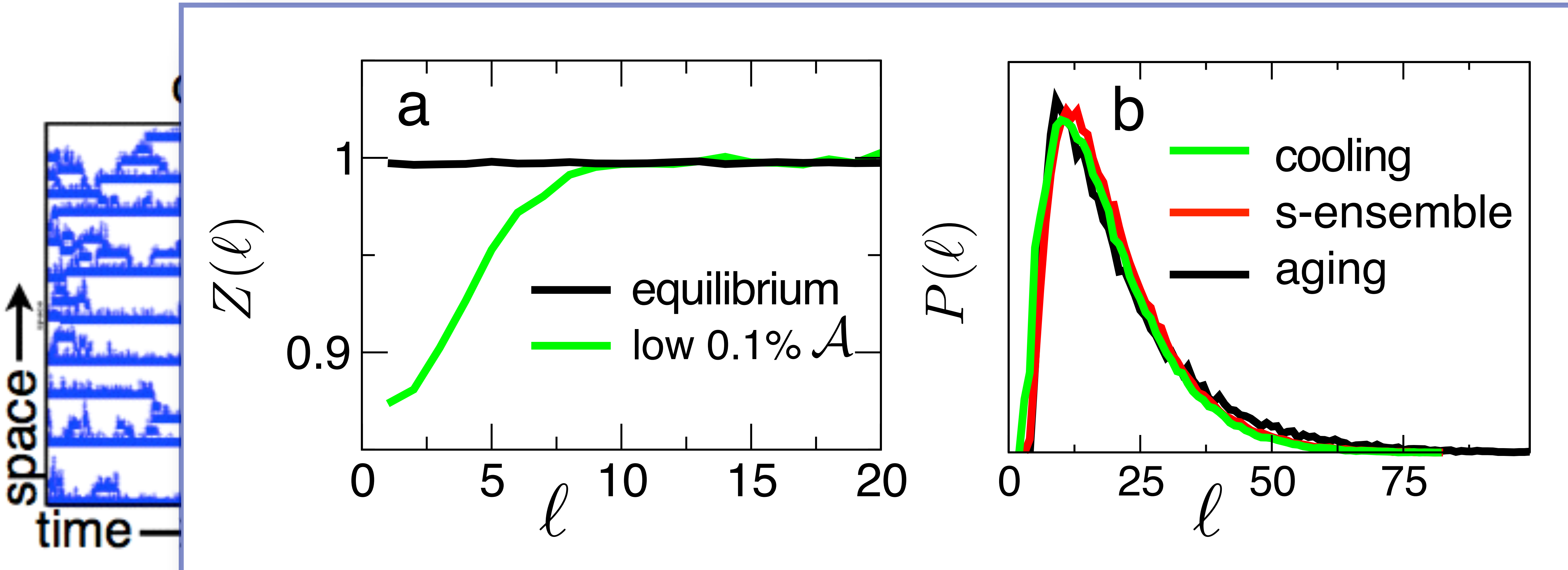
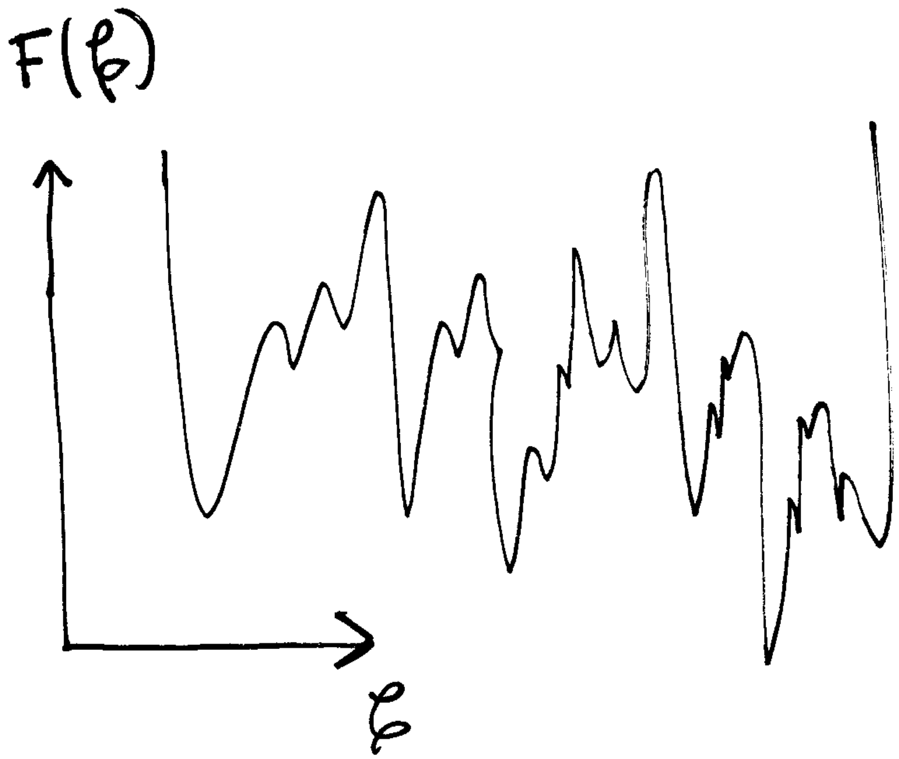


non-equilibrium characteristic **length** in glassy state

Perspectives on glass transition

Thermodynamic



Statics ⇒ Dynamics

eg. **RFOT**

{Parisi+Wolynes+many others}

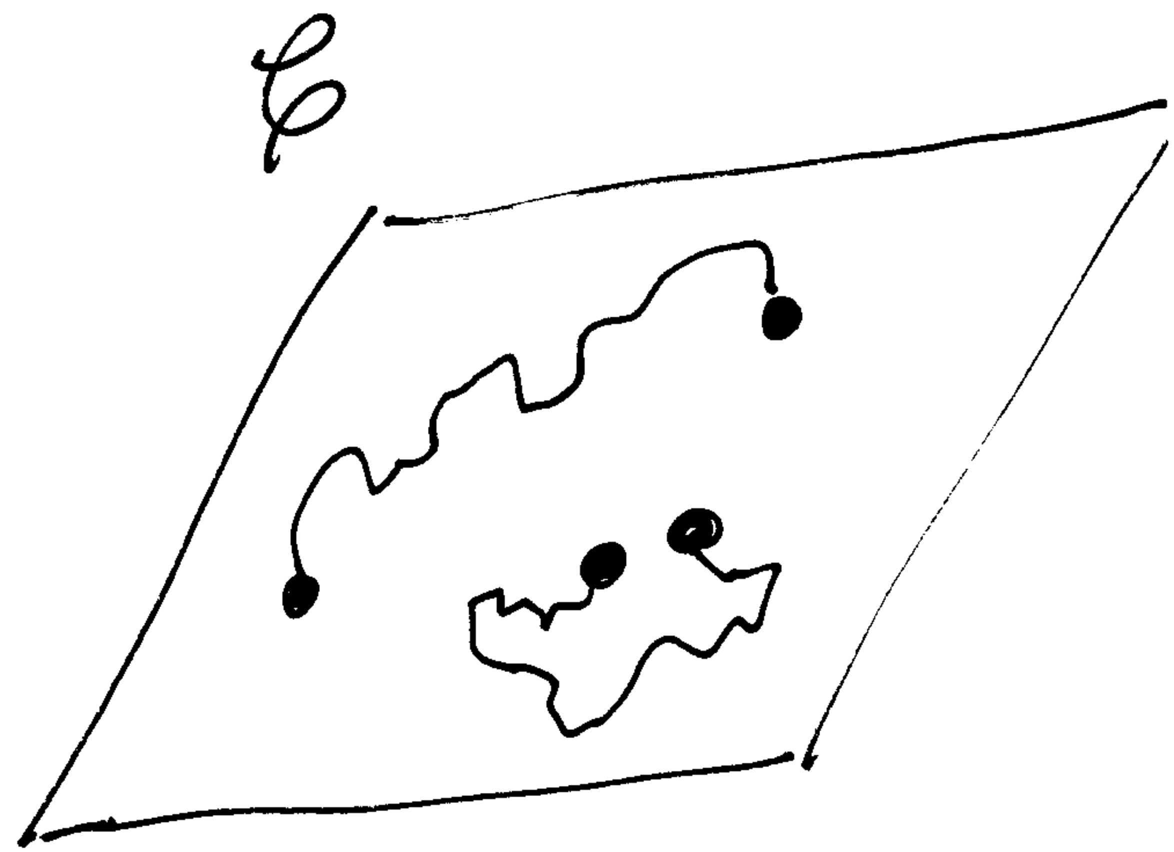
ideal models e.g. **p-spin spin glass**

low overlap (liquid) → **high** overlap (glass)

{Franz-Parisi}

numerical **evidence** {Berthier 2013, Parisi-Seoane 2013}

Dynamic



Statics **does not** ⇒ Dynamics

metric → Dynamic facilitation

ideal models **KCMs**

{Anderson+Andersen+Jackle+many others}

transition in space of **trajectories**

active (liquid) → **inactive** (glass)

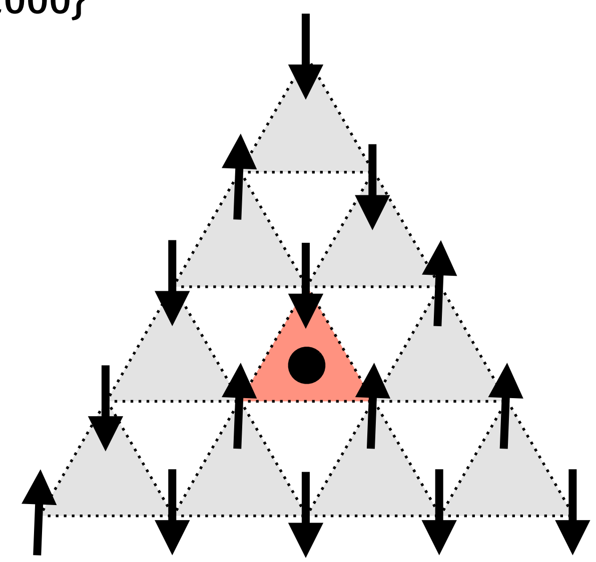
Overlap transitions and facilitation

{JPG, **PRE 2014**; Turner-Jack-JPG 2014}

Triangular plaquette model (TPM):

{Newman-Moore 1999, JPG-Newman 2000}

$$E = -\frac{J}{2}\sum_{\triangle} s_i s_j s_k$$

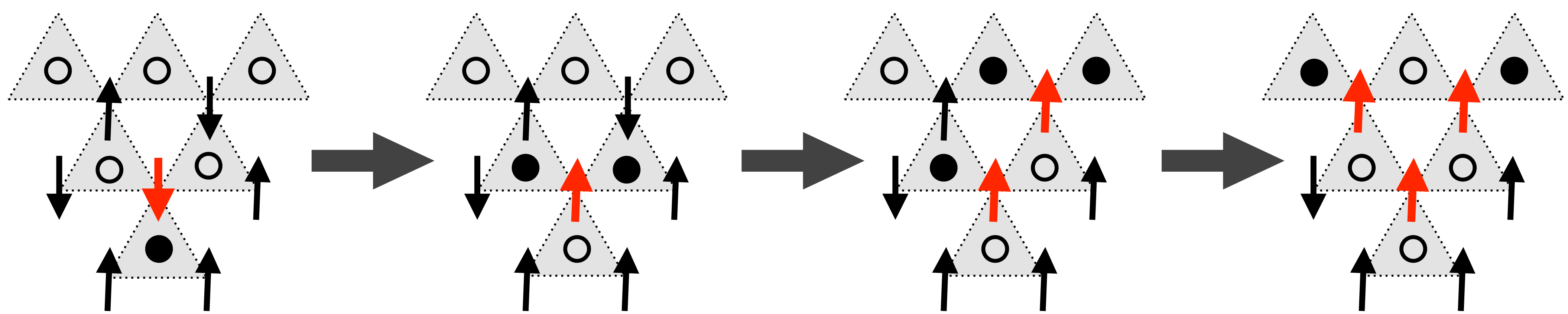


Thermodynamics:

1-1 mapping **spins-plaquettes**

free plaquettes → **free localised** defects
⇒ disordered ∀ T

Dynamics: (effectively) **kinetically constrained**



Relaxation is **hierarchical** $\longrightarrow$ $\tau = e^{1/T^2}$ cf. **East facilitated model** {Sollich-Evans 1999}

Statics **trivial**, dynamics **complex** & glassy, but singular **only at T=0** (cf. dynamic facilitation)

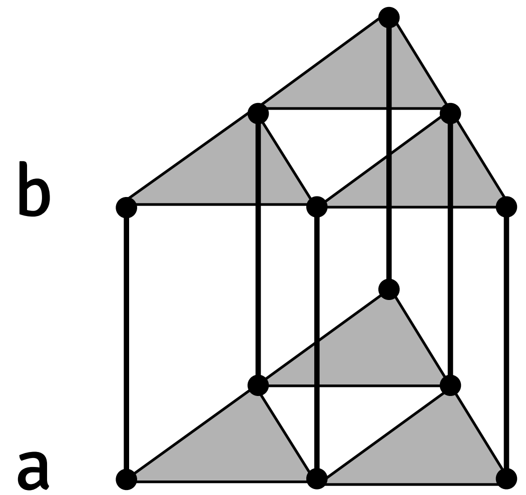
Overlap transitions and facilitation

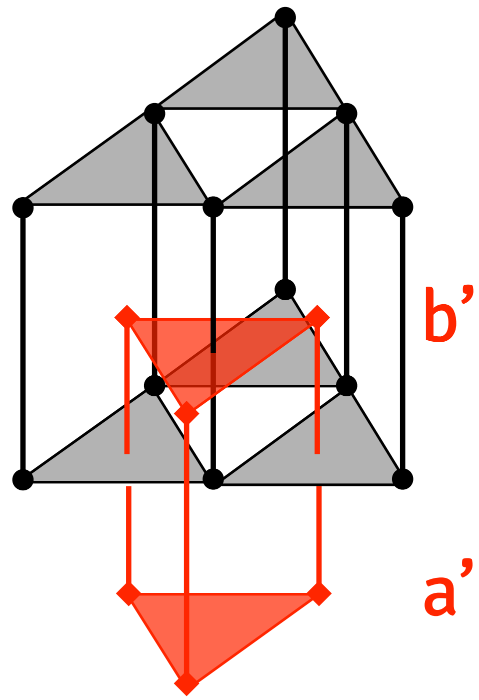
{JPG, PRE 2014; Turner-Jack-JPG 2014}

Two coupled TPMs (annealed): $E = -\frac{J}{2}\sum_{\triangle}\left(s_i^a s_j^a s_k^a + s_i^b s_j^b s_k^b\right) - \varepsilon \sum_i s_i^a s_i^b$

{cf. Franz-Parisi}

Exact duality:





$$e^{-2K_1'} = \tanh K_3$$

$$e^{-2K_3'} = \tanh K_1$$

$$Z(K_J, K_\varepsilon) = \left(\sinh 2K_J \sinh K_\varepsilon\right)^N Z(K_J^*, K_\varepsilon^*) \qquad (2K_J = \beta J, \quad K_\varepsilon = \beta\varepsilon)$$

$$e^{-K_\varepsilon^*} = \tanh K_J, \quad \tanh K_J^* = e^{-K_\varepsilon}$$

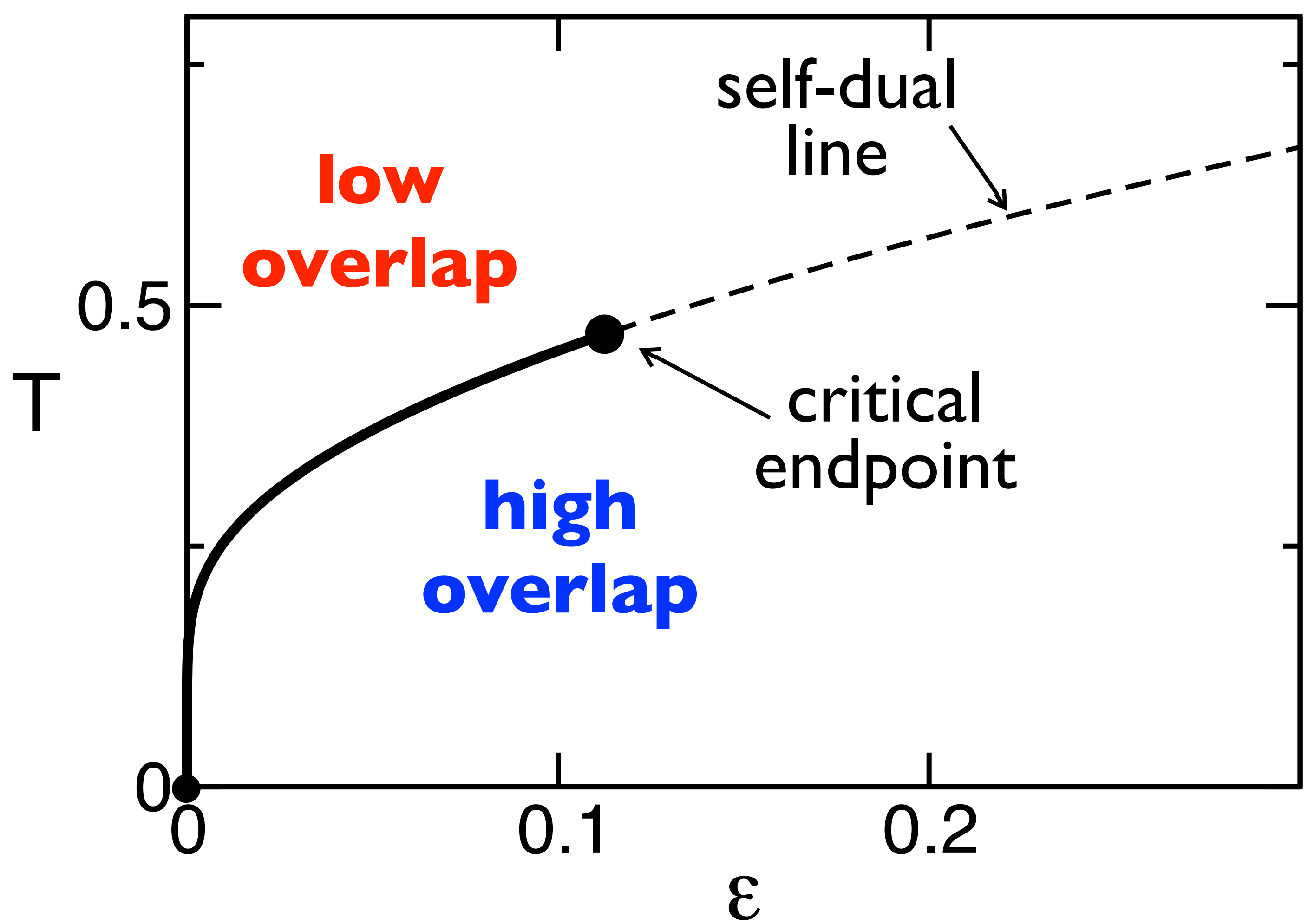
Overlap transitions and facilitation

{JPG, PRE 2014; Turner-Jack-JPG 2014}

Two **coupled** TPMs (annealed): $E = -\frac{J}{2}\sum_{\triangle}\left(s_i^a s_j^a s_k^a + s_i^b s_j^b s_k^b\right) - \varepsilon \sum_i s_i^a s_i^b$

Self-dual: $\left(\sinh \frac{J}{T}\right)\left(\sinh \frac{\varepsilon}{T}\right) = 1$

Cf. TMP in field {Sasa 2010}
& generalised Baxter-Wu {Nienhuis 2010}



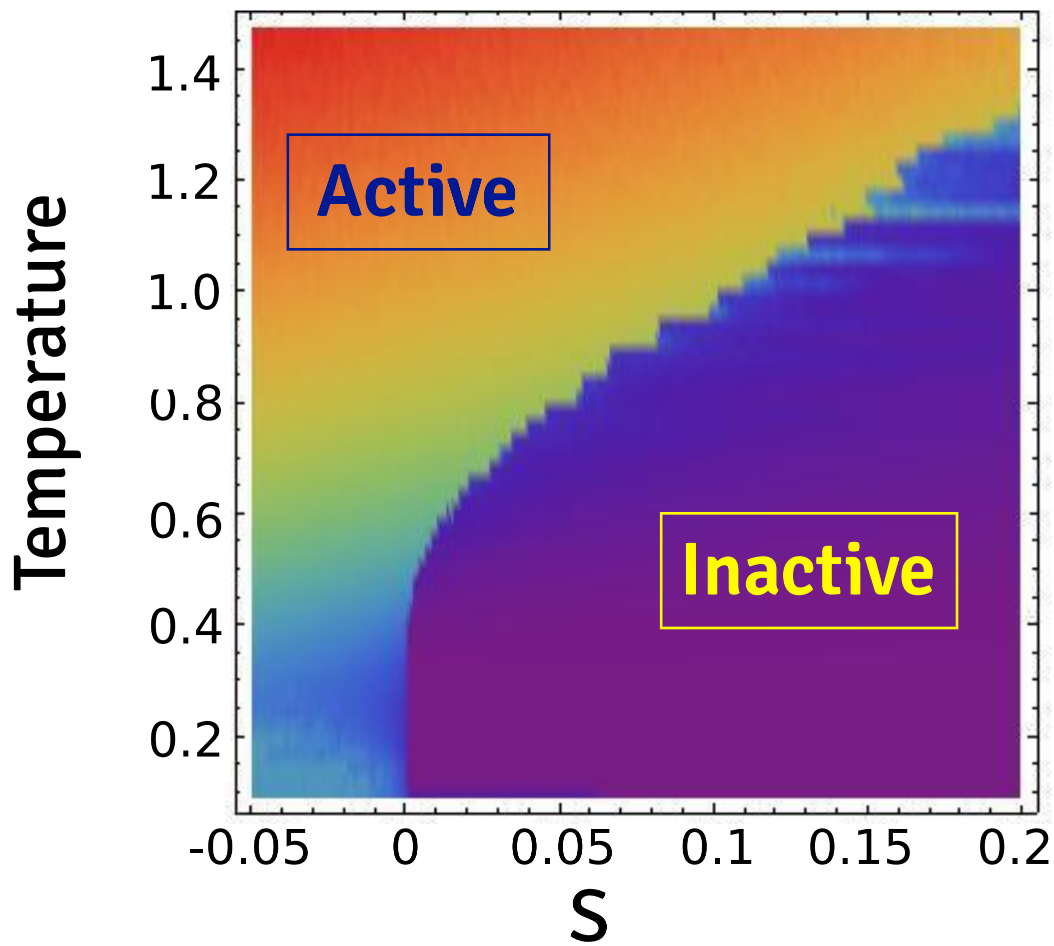
1st order static transition
at **finite** coupling
ending at CP (***Ising***)
{Turner-Jack-JPG 2014}

<u>transition **vanishes** at ε → 0</u>

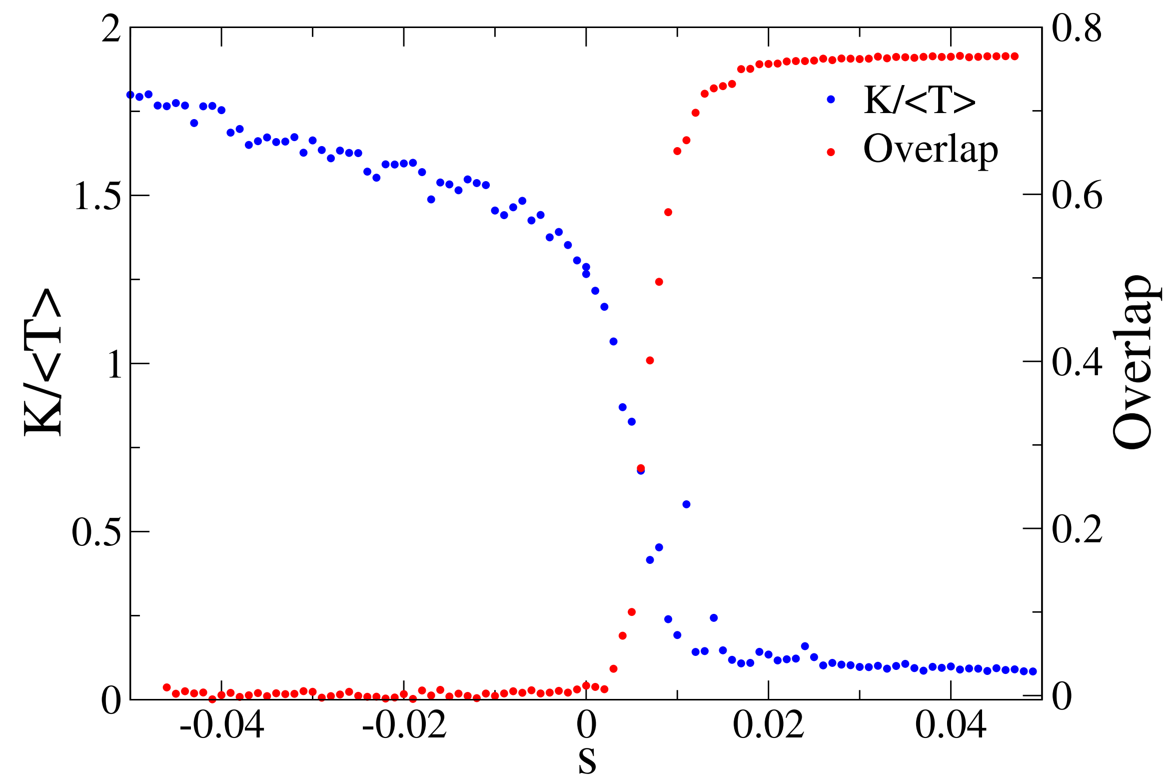
Overlap transitions and facilitation

{JPG, PRE 2014; Turner-Jack-JPG 2014}

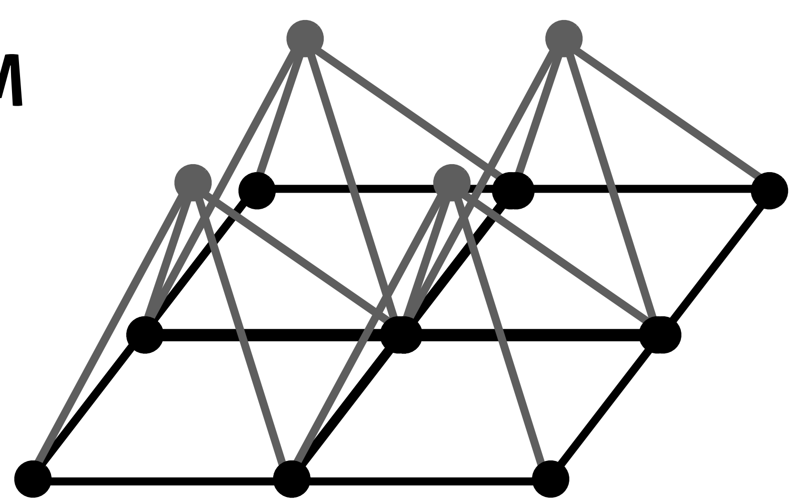
Classify trajectories of TPM according to **dynamical activity → s-ensemble**



1st order transition in activity & overlap



TPM in D=3 → **SPyM**



$$E = -J \sum_{py} s_i s_j s_k s_l s_m$$

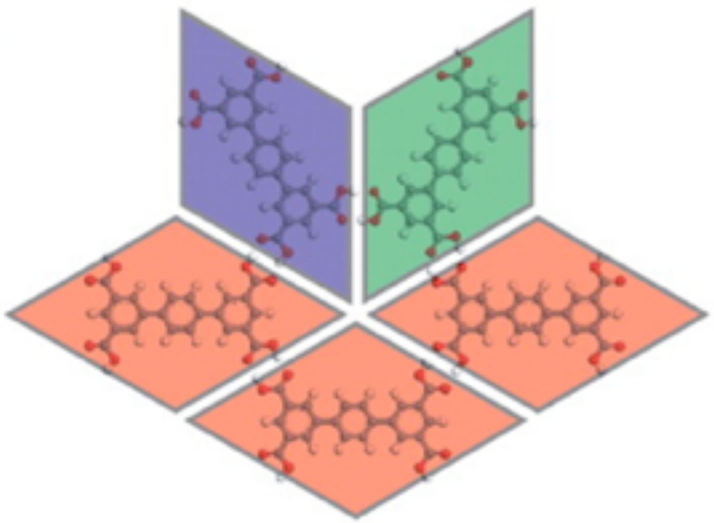
spins-pyramids 1-1

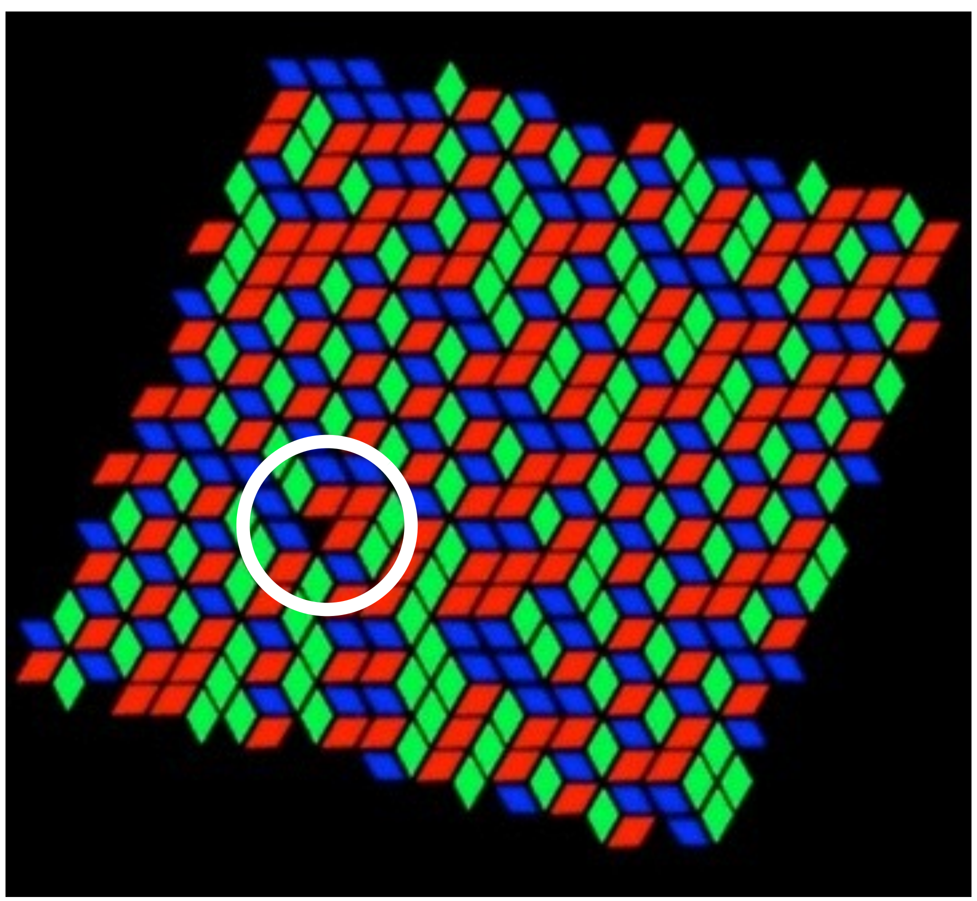
same dualities as TPM

Similar features in tilings / dimer coverings / “spin-ice”-like systems

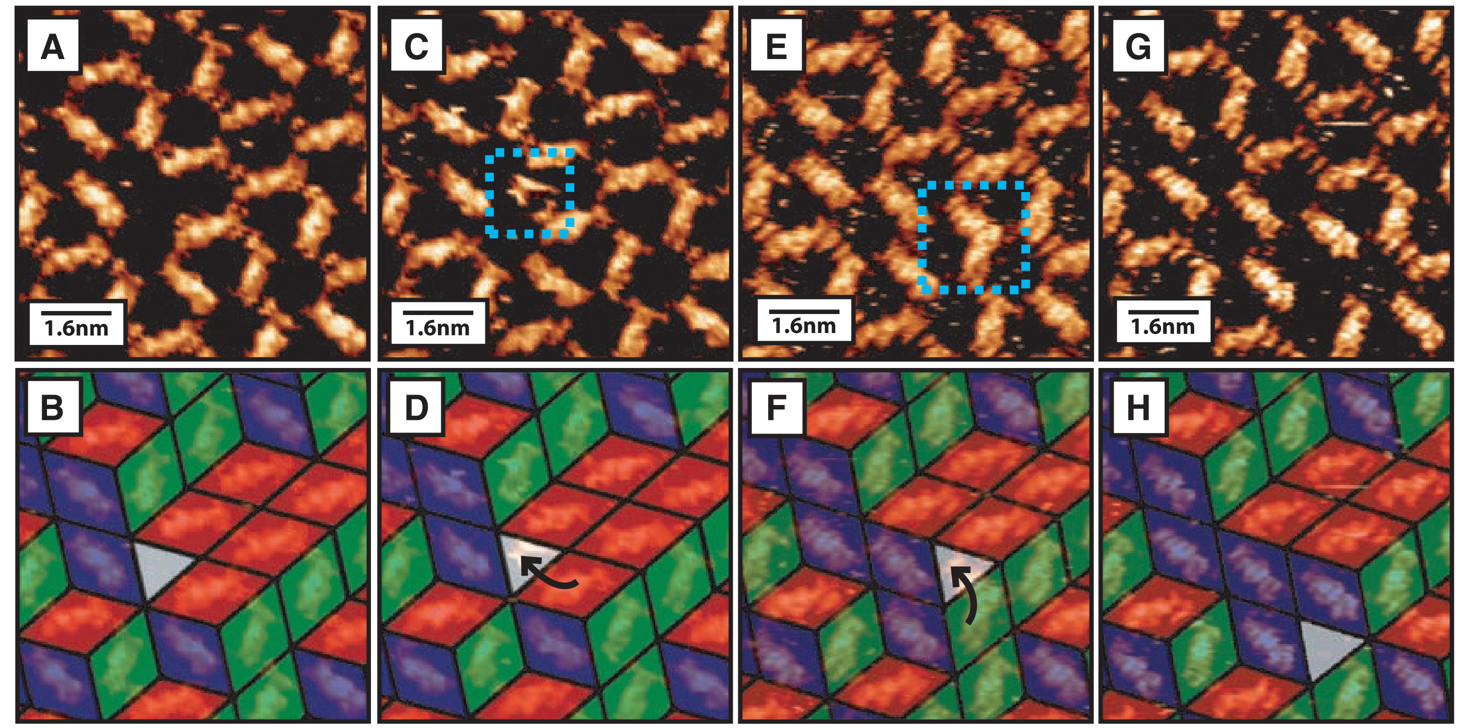
Eg. **molecular random tilings**

{Beton+Champness+Blunt+Whitelam+Stannard+...+JPG}

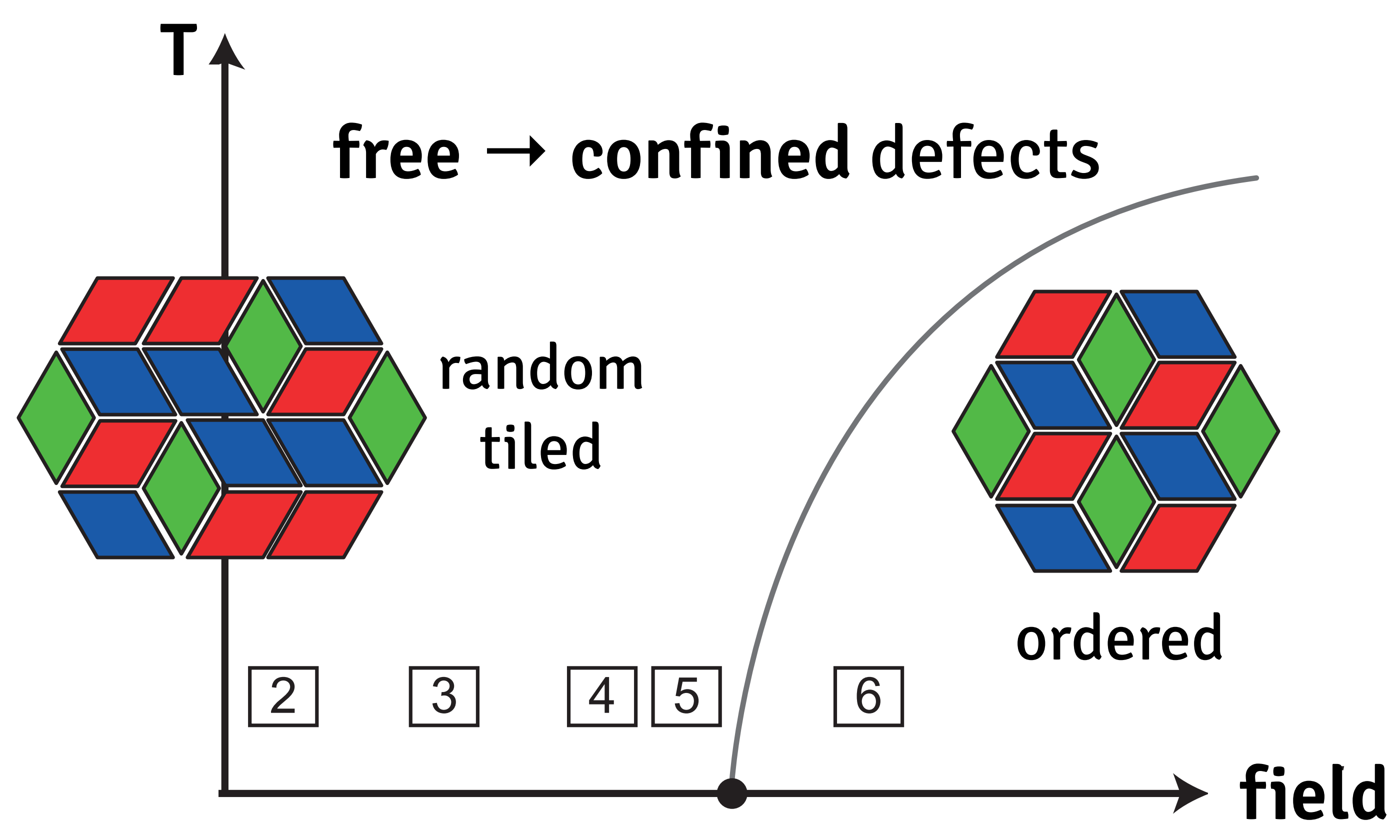




“**mosaics**” for real



dynamics **facilitated** by localised free **defects**



KCMs and many-body localisation in closed quantum systems

{Hickey-Genway-JPG, **arXiv:1405.5780**}

Many-body localisation (**MBL**) transition:

{**Basko-Aleiner-Altshuler 2006**, Huse+, many others}

- Cf. Anderson localisation but for **interacting** system
- Singular change **throughout spectrum**
- Eigenstates change from "thermal" (**ETH** {Deutsch, Sdrenicki}) to **MBL**
- Observables **do not relax** in MBL phase
- Often thought of as **"glass transition"** but modelled with **disorder**

Can KCMs (as models for classical glasses) say anything about quantum MBL?

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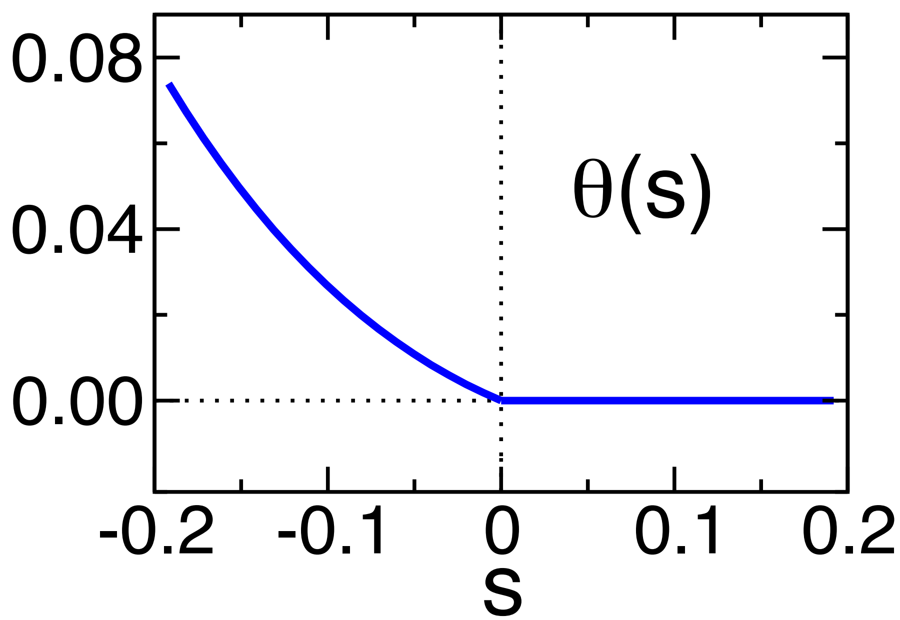
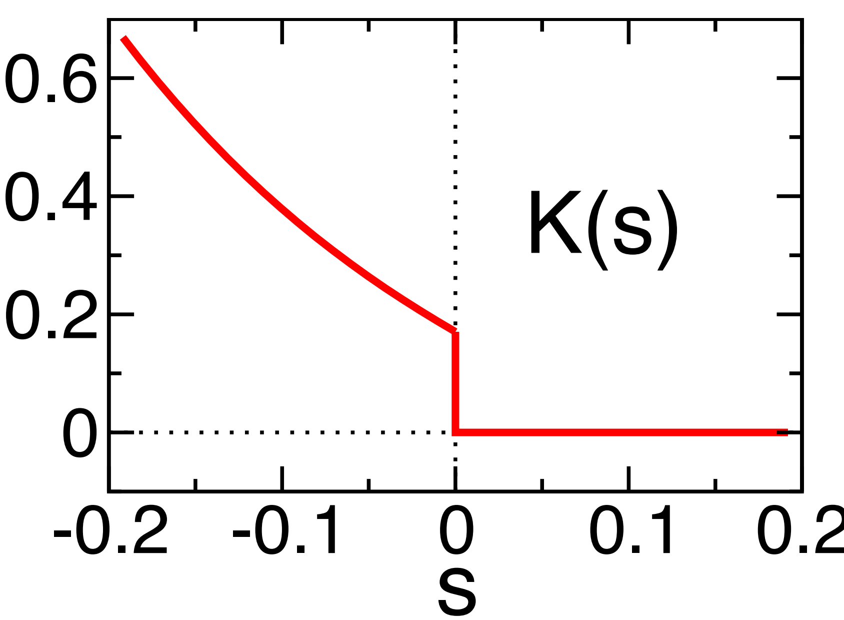
{Hickey-Genway-JPG, **arXiv:1405.5780**}

Recap: active-inactive "space-time" transitions in KCMs (eg. East/FA)

$$\mathbb{W} \;\rightarrow\; \mathbb{W}_s = \sum_i n_{i-1}\left[e^{-s}\left(\epsilon\sigma_i^+ + \sigma_i^-\right) - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1)$$

Largest e/value = cumulant G.F. for **activity** → **1st order phase transition**





{Merolle-Chandler-JPG, 2005, JPG+Jack+Lecomte+van Wijland+, PRL 2007, JPA 2009, + others}

Can transform into **Hermitian** operator through equilibrium distribution

$$\mathbb{H}_s \equiv -\mathbb{P}^{-1}\mathbb{W}_s\mathbb{P} = -\sum_i n_{i-1}\left[e^{-s}\sqrt{\epsilon}\,\sigma_i^x - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1)$$

Consider as **Hamiltonian** and corresponding **quantum unitary dynamics** $|\psi_t\rangle = e^{-it\mathbb{H}_s}|\psi_0\rangle$

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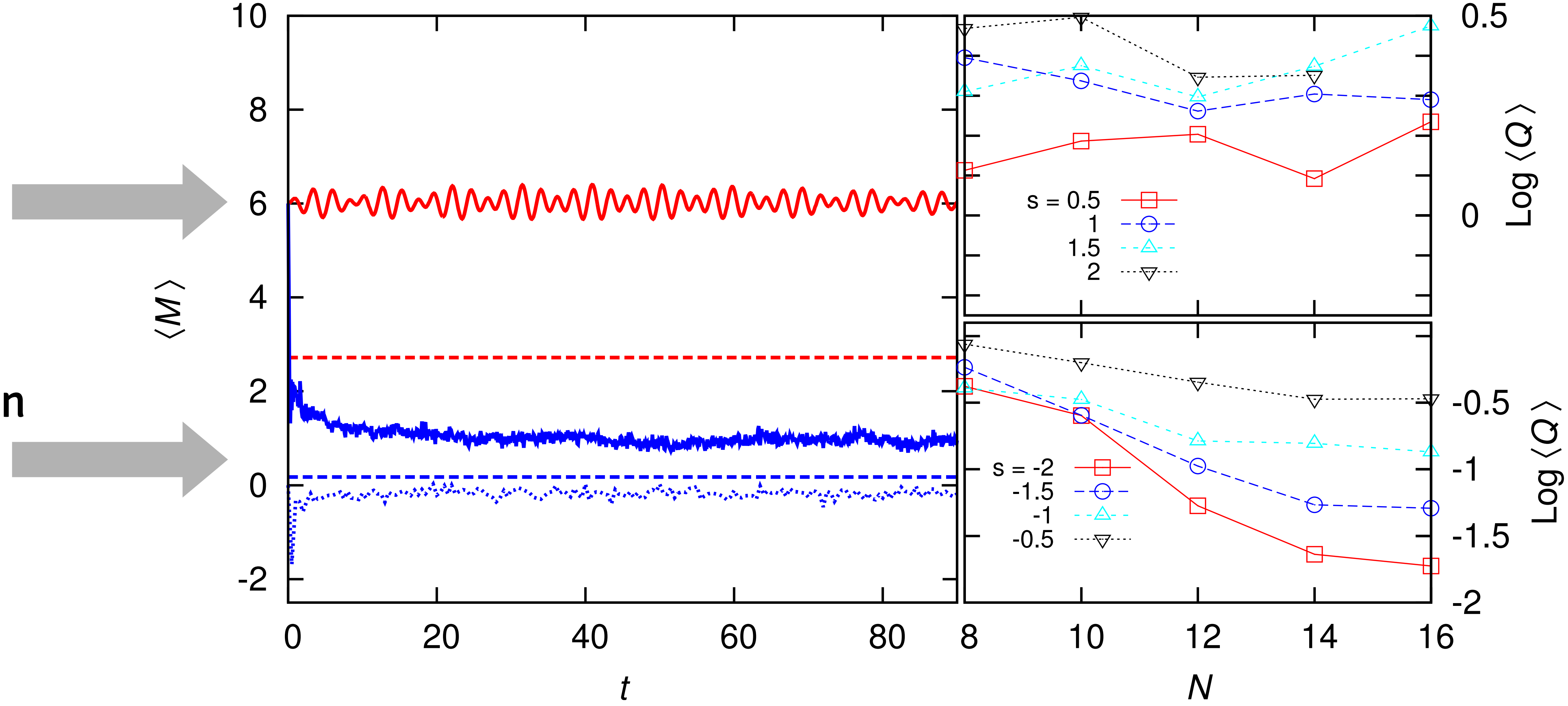
$$\mathbb{H}_s = -\sum_i n_{i-1}\left[e^{-s}\sqrt{\epsilon}\sigma_i^x - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1) \qquad |\psi_t\rangle = e^{-it\mathbb{H}_s}|\psi_0\rangle$$

Signatures of **MBL** transition: **(i) relaxation / non-relaxation of observables**

time evolution of magnetisation $\langle M\rangle_t = \sum_i \langle\psi_t|\sigma_i^z|\psi_t\rangle$

does not relax on **inactive** side s>0

relaxes on **active** side s<0

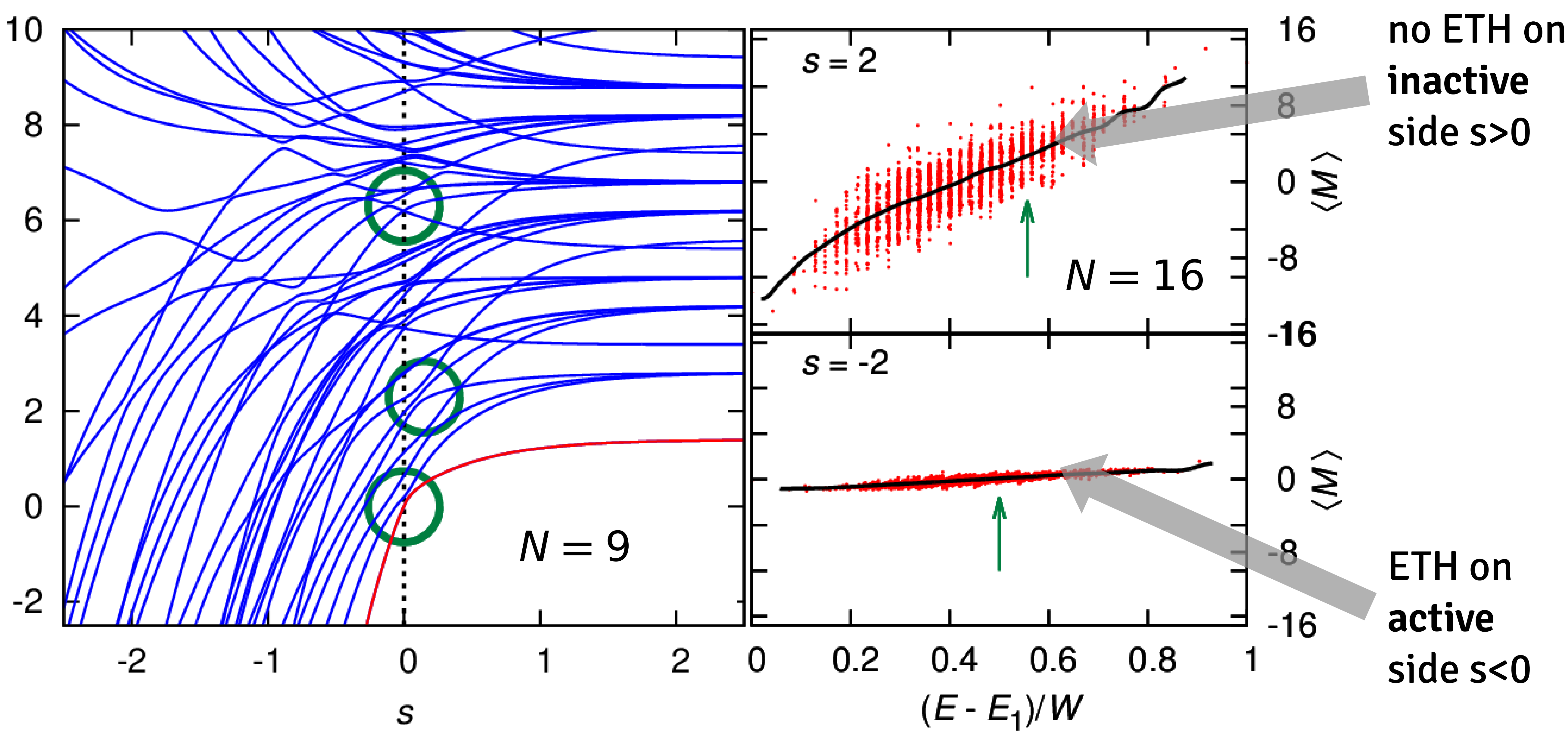


KCMs and many-body localisation in closed quantum systems

{Hickey-Genway-JPG, arXiv:1405.5780}

$$\mathbb{H}_s = -\sum_i n_{i-1}\left[e^{-s}\sqrt{\epsilon}\sigma_i^x - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1) \qquad |\psi_t\rangle = e^{-it\mathbb{H}_s}|\psi_0\rangle$$

Signatures of **MBL** transition: **(ii) transitions throughout spectrum**



KCMs and many-body localisation in closed quantum systems

{Hickey-Genway-JPG, **arXiv:1405.5780**}

$$\mathbb{H}_s = -\sum_i n_{i-1}\left[e^{-s}\sqrt{\epsilon}\sigma_i^x - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1) \qquad |\psi_t\rangle = e^{-it\mathbb{H}_s}|\psi_0\rangle$$

Signatures of MBL transition: **(iii) level spacing statistics**

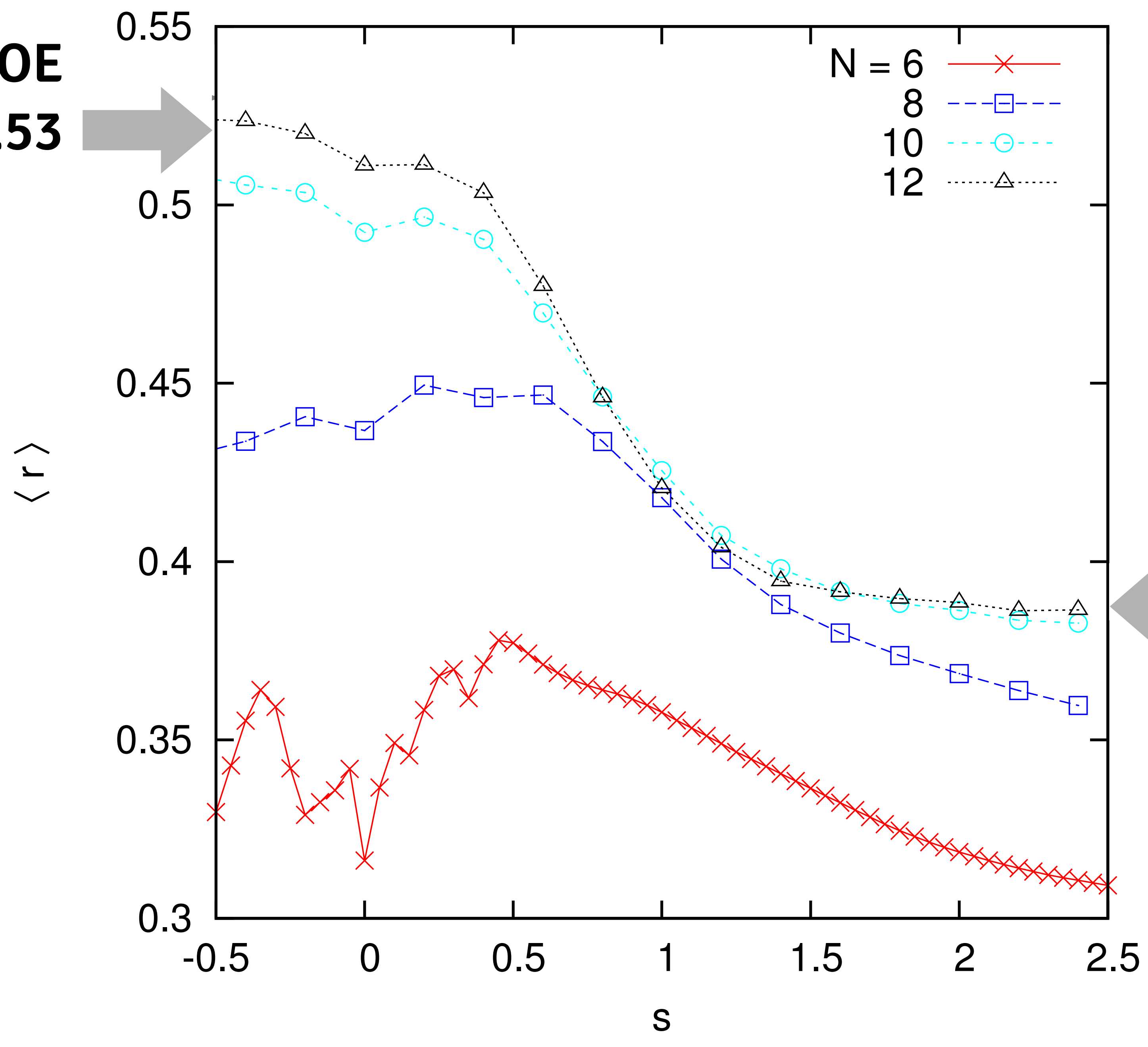
Many symmetries in clean system

Can remove with site disorder:

$\epsilon \rightarrow |\epsilon - g\pi_i| \quad (g \ll \epsilon)$

KCM dynamics unchanged

GOE 0.53



Poisson 0.39

KCMs and many-body localisation in closed quantum systems

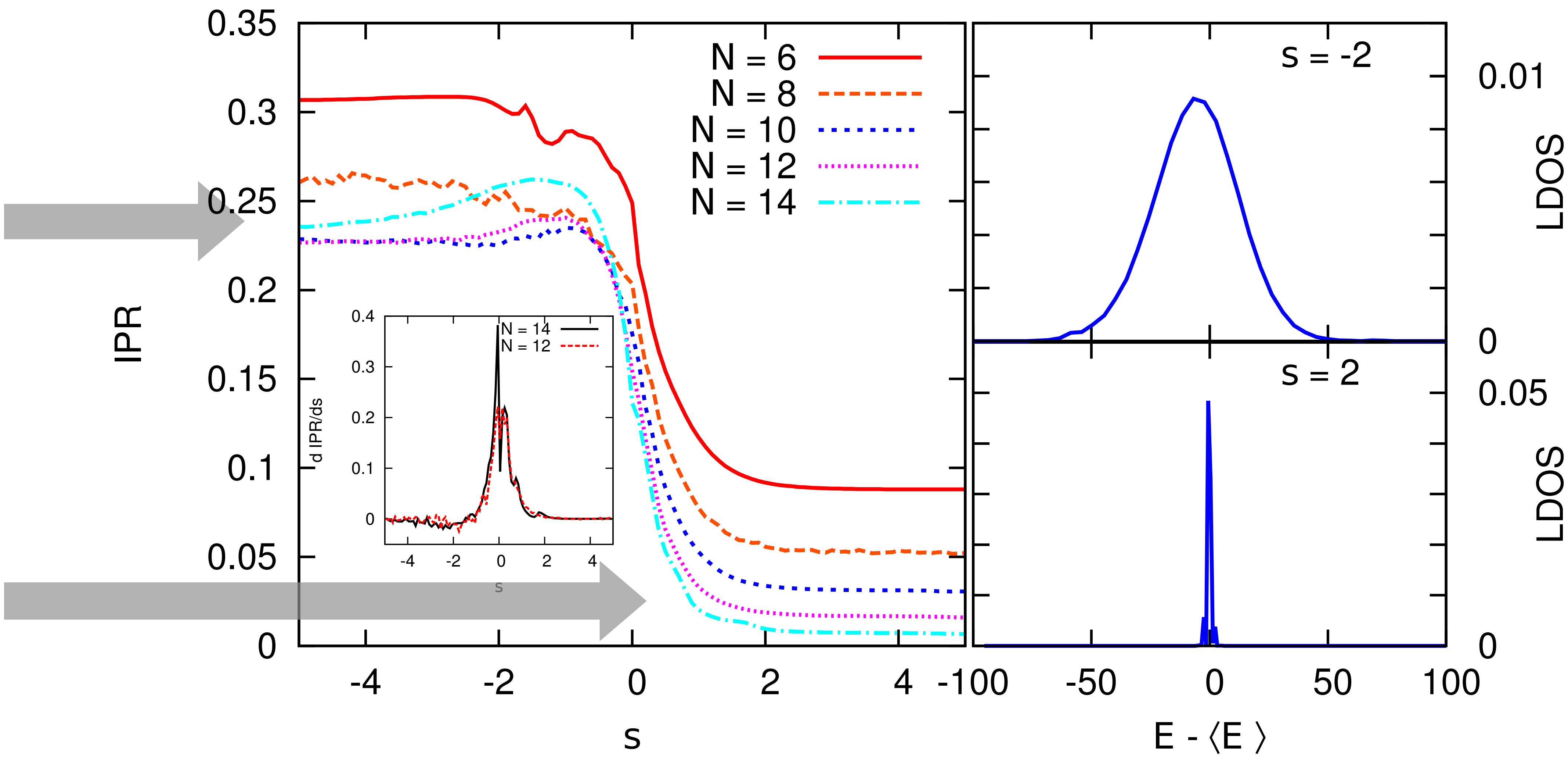
{Hickey-Genway-JPG, arXiv:1405.5780}

$$\mathbb{H}_s = -\sum_i n_{i-1}\left[e^{-s}\sqrt{\epsilon}\sigma_i^x - \epsilon(1-n_i) - n_i\right] + (i \leftrightarrow i-1) \qquad |\psi_t\rangle = e^{-it\mathbb{H}_s}|\psi_0\rangle$$

Signatures of **MBL** transition: **(iv) localisation onto classical basis**

widely spread active s<0

e/states concentrated inactive s>0



⇒ active-inactive transition → 1st order MBL transition in whole spectrum

MBL transition without disorder

SUMMARY

"Thermodynamics of **trajectories"** based on **LD** theory

Glass transition as a active/inactive transition in **trajectory space**

KCM glass models as models for **MBL without disorder**