

# Glassy random walks: Large deviations and aging

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# Overview

- Two broad classes of non-equilibrium dynamics:  
**driven** and **aging**
- One general driving mechanism: trajectory biasing
- Directly linked to dynamical phase transitions and  
**large deviations**
- How **do driving and aging interact?**
- Probe in models of slow dynamics on networks:  
**glassy random walks**

# The Kühn connection

**Method** for finding dynamical free energies:

- Susca, Vivo & Kühn (2019):  
*Top eigenpair statistics for weighted sparse graphs*

**Physics** of localization transition in large deviations:

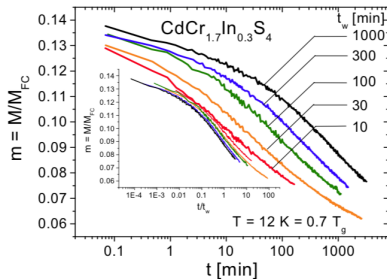
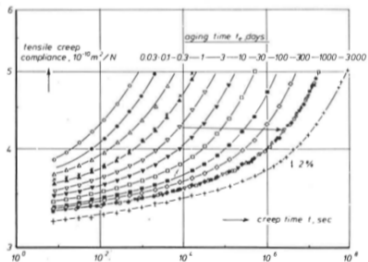
- Bacco, Guggiola, Kühn & Paga (2016):  
*Rare events statistics of random walks on networks:  
localisation and other dynamical phase transitions*

# Outline

- 1 Aging dynamics
- 2 Driven dynamics
- 3 Biased trajectory ensembles
- 4 Bouchaud trap model
- 5 Barrat-Mézard model
- 6 Finite network connectivity

# Aging

Occurs not just in living systems. . .



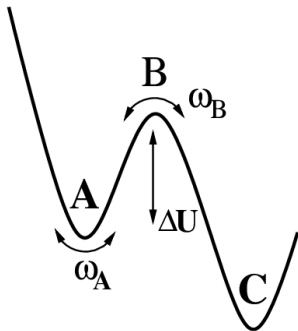
- Aging systems **could** reach equilibrium – but are too slow
- Significant dependence of properties on **age** since preparation
- Polymers, spin glasses, . . .

# Simple example of aging: coarsening



- Phase separation after quench from high  $T$
- Properties governed by growing **domain size**  $L(t)$
- E.g. two-time correlation functions decay with ratio of  $L$ 's

# Aging requires complex dynamics



- Contrast with escape from single **metastable state**
- Beyond age  $\sim$  metastable lifetime, age-dependences disappear
- **Aging** requires many states, broad spectrum of lifetimes

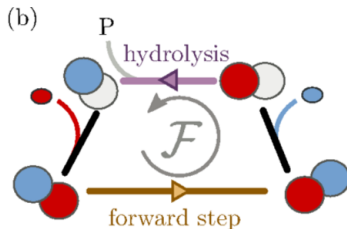
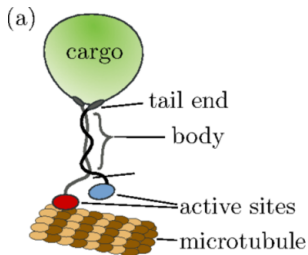
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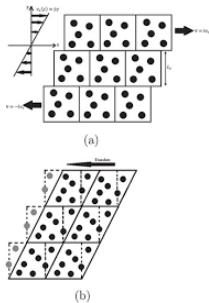
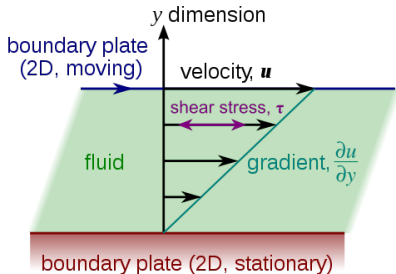
# Driven systems

- Break detailed balance
- E.g. sheared fluids, all living systems: energy input, dissipation
- **Probability currents** in steady state



# Modelling driven systems

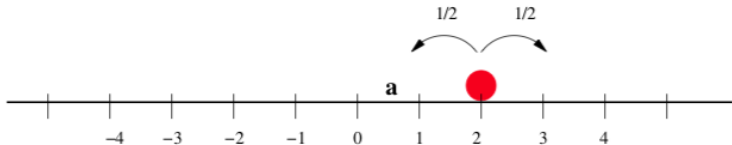
- Lack of detailed balance:  
More freedom to choose parameters – underconstrained?
- Is there a systematic way of assigning free parameters?
- E.g. for motion in bulk of **sheared fluid**



# Biased trajectory ensembles

Ruelle, Spohn, Evans, ...

- Start from **equilibrium** dynamics
- Main idea: think of this as a distribution over **trajectories**
- Modify distribution to get e.g. some average current  $\mathcal{A}_t$
- Which trajectory distribution has **maximum entropy?**  
(relative to equilibrium dynamics)



# Biased trajectory ensembles – cont.

- Maximum entropy problem analogous to **equilibrium** statistical mechanics:  
Constraints on averages give **exponential weight factors**
- E.g. Boltzmann distribution constrains  $\langle E \rangle$ , gives weight  $e^{-\beta E}$   
Normalization defines free energy  $f$
- Similarly max ent **trajectory** ensemble:  
Equilibrium trajectory distribution biased by factor  $e^{-g \mathcal{A}_t}$   
Normalization defines a **dynamical free energy**  $\psi(g)$   
Legendre transform  $\Rightarrow$  large deviations  $P(\mathcal{A}_t) \sim e^{-t \phi(\mathcal{A}_t/t)}$

## Summary

A systematic way of describing driven systems is given by  
**trajectory thermodynamics**

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# Biasing trajectory probabilities

- Trajectory  $\pi$ ; bias probability to give large/small values of  $\mathcal{A}_t$ :

$$P[\pi, g] = Z(g, t)^{-1} P[\pi, 0] e^{-g\mathcal{A}_t}$$

- **Bias parameter  $g$** : analog of magnetic field  $h$
- **Dynamical free energy**: defined by analogy with equilibrium free energy

$$\psi(g) \equiv t^{-1} \ln Z(g, t)$$

- Derivatives give cumulants, e.g.

$$-\psi'(g) = t^{-1} \langle \mathcal{A}_t \rangle$$

# Setting: Stochastic dynamics

## Markov chain

- Consider stochastic model with configurations  $\mathcal{C}$
- **Transition rates**  $W(\mathcal{C} \rightarrow \mathcal{C}')$
- Escape rate from  $\mathcal{C}$ :  $r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \rightarrow \mathcal{C}')$
- Bias in a quantity measuring **transitions** that system makes:  
if configuration sequence is  $\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_K$

$$\mathcal{A}_t = \sum_{k=0}^{K-1} \alpha(\mathcal{C}_k, \mathcal{C}_{k+1})$$

- $\mathcal{A}_t =$  total nr. of transitions if  $\alpha(\mathcal{C}, \mathcal{C}') = 1$  for all  $\mathcal{C} \neq \mathcal{C}'$   
(activity)
- Or  $\alpha(\mathcal{C}, \mathcal{C}')$  could measure contribution of  $\mathcal{C} \rightarrow \mathcal{C}'$  to total current, accumulated shear strain, entropy current, ...

# Biased & auxiliary master operators

- Dynamical partition function is **largest eigenvalue** of **biased master operator**  $\mathbb{W}(g)$  with elements

$$\langle \mathcal{C} | \mathbb{W}(g) | \mathcal{C}' \rangle = \begin{cases} W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})}, & \mathcal{C} \neq \mathcal{C}' \\ -r(\mathcal{C}), & \mathcal{C} = \mathcal{C}' \end{cases}$$

- This does not conserve probability
- But can restore this by defining **effective rates** (Jack & PS, Chetrite & Touchette)

$$W^{\text{aux}}(\mathcal{C}' \rightarrow \mathcal{C}) = W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})} \frac{u_\tau(\mathcal{C})}{u_\tau(\mathcal{C}')}$$

- Metropolis-like factor  $\exp\{-\beta[E_\tau^{\text{eff}}(\mathcal{C}) - E_\tau^{\text{eff}}(\mathcal{C}')]/2\}$ , with **effective potential**

$$E_\tau^{\text{eff}}(\mathcal{C}) = (-2/\beta) \ln u_\tau(\mathcal{C})$$



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# Trap models

- Picture of glassy dynamics: at low  $T$  have **activated jumps**...
- ... between **local energy minima** in configuration space
- Take each minimum as a configuration  $\mathcal{C}_i$  or “trap”
- Trap depth  $E_i > 0$
- Simplest assumption on kinetics gives **Bouchaud trap model**

$$W(\mathcal{C}_i \rightarrow \mathcal{C}_j) = \frac{1}{N} \exp(-\beta E_i)$$

where  $N$  = number of configurations

- Golf course landscape: always activate to “top” ( $E = 0$ )
- **Mean field connectivity**

# Glass transition and aging

- Model specified by distribution of energies  $\rho(E)$
- Typically taken as  $\rho(E) = \exp(-E)$ , exponential tail
- Gibbs-Boltzmann equilibrium distribution  
 $\propto \exp(\beta E) \exp(-E)$  normalizable only for  $\beta < 1$
- **Glass transition** at  $T = 1/\beta = 1$
- For  $T < 1$  system must **age**, typical  $E \sim T \ln(t)$

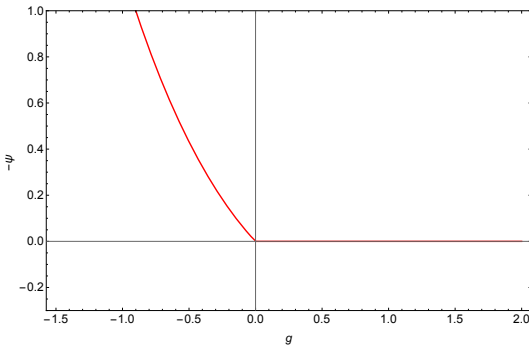
## Focus

# How do aging and driving (activity bias) interact?

Method: Laplace transforms,  
then look at large  $t - \tau$  or  $\tau$  ( $z \rightarrow 0$ )

# Dynamical free energy

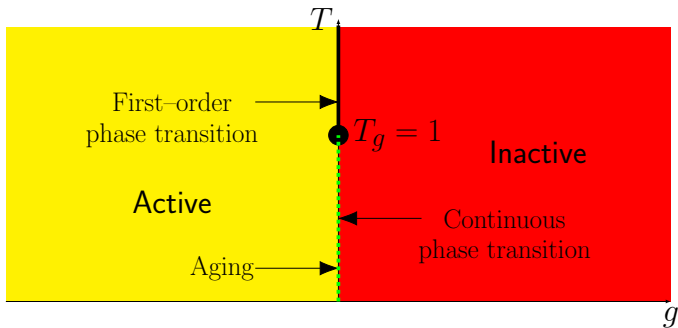
$T = 2.5$



**Dynamical phase transition**, active to inactive

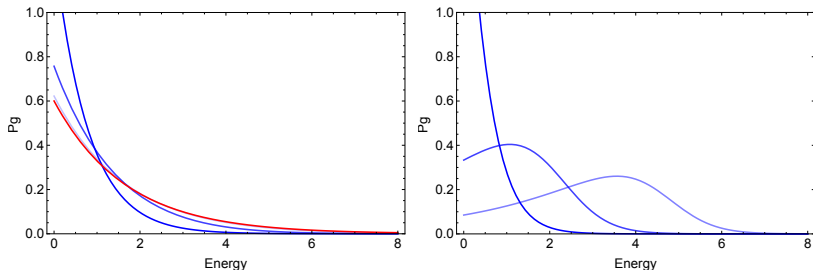
Reminder:  $-\psi'(g) = \text{average activity}$

# Phase diagram



## Above average activity: active phase

$g = -2$  (dark),  $-0.2$ ,  $-0.02$  (light), steady state trap depth distributions



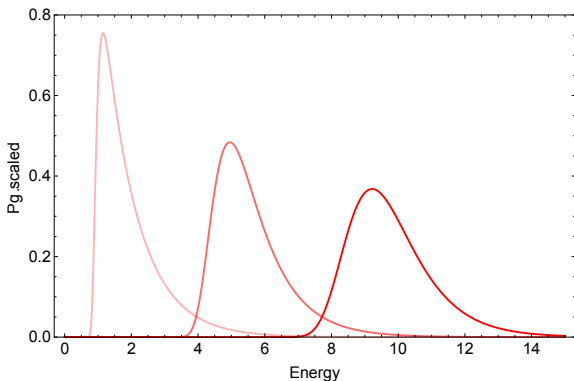
Left:  $T = 2.5$ ; right:  $T = 0.7$

For  $T < 1$ , typical trap depth increases as  $g \rightarrow 0$ ;  
remnant of transition to aging dynamics

**Effective potential**  $E^{\text{eff}} = (2/\beta) \ln(1 + \psi e^{\beta E})$

# Below average activity: inactive phase

$g > 0$ , large  $t$ ,  $p_0(E) = \rho(E)$ ,  $T = 0.1, 0.5, 1.0$  left to right



$$p_\tau(E) \propto \rho(E) \exp(-te^{-\beta E}) \quad (\text{away from boundaries})$$

Independent of  $g$  and  $\tau$

$$E^{\text{eff}} = 2T(t - \tau)e^{-\beta E} \text{ is time-dependent}$$



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# BM model basics

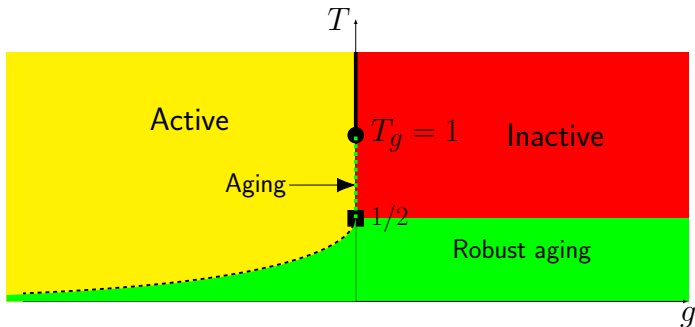
- Like Bouchaud model but Glauber rates:

$$W(\mathcal{C}_i \rightarrow \mathcal{C}_j) = \frac{1}{N} \frac{1}{1 + \exp[\beta(E_i - E_j)]}$$

- Same equilibrium state, same glass transition temperature
- Aging different: **entropic aging** at low  $T$ ,  
running out of lower energy states
- Dynamics not frozen even at  $T = 0$

# Phase diagram

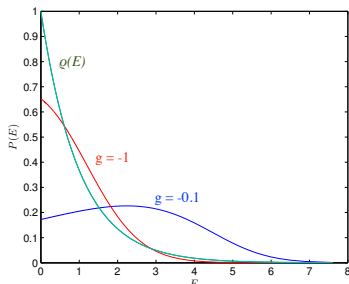
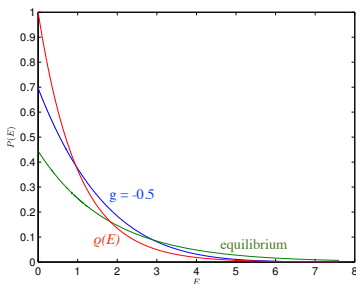
Analytical prediction, confirmed numerically by finite-size scaling



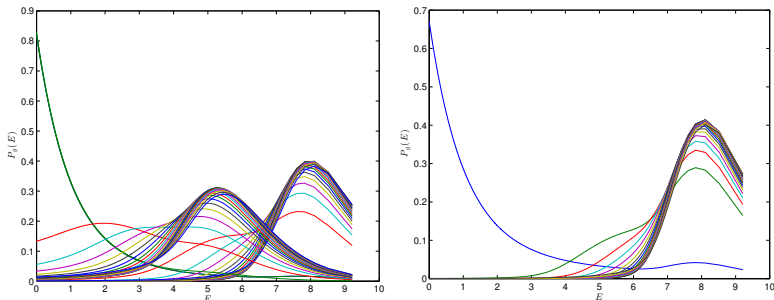
- **Qualitative change** at  $T = 1/2$
- $T > 1/2$ : shows Bouchaud-like behaviour, can be confirmed by explicit coarse-graining (Cammara & Marinari)
- $T < 1/2$ : qualitatively different, mainly **downward jumps**

# Trap depth distributions in active phase

$T = 1.5, g = -0.5$  (left),  $T = 0.8, g = -0.1, -1$  (right)



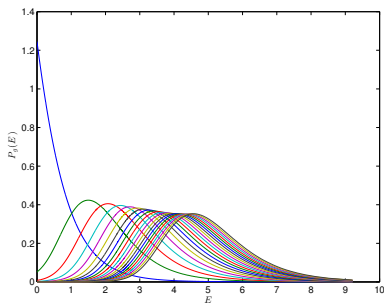
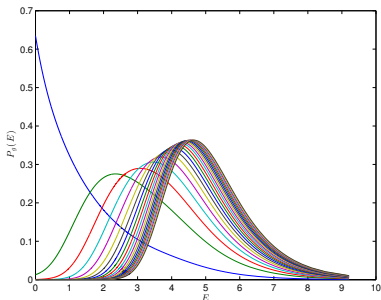
- For  $T < 1$ , distributions again shift to large  $E$  on approaching inactive phase

Inactive phase,  $T > 1/2$  $T = 0.8, g = 0.25, t = 100$  and  $1000$  (left),  $g = 0.5, t = 1000$  (right)

- $p_\tau(E)$  for increasing  $\tau$  approaches shape **only dependent on  $t$**
- System rapidly descends to deep traps
- Total nr. of jumps finite, average activity decays as  $\tau^{-1-\alpha}$

# Inactive phase, $T < 1/2$

$T = 0.2$ ,  $g = 0.5$ ,  $t = 1000$  (left) and  $g = -0.5$  (right)



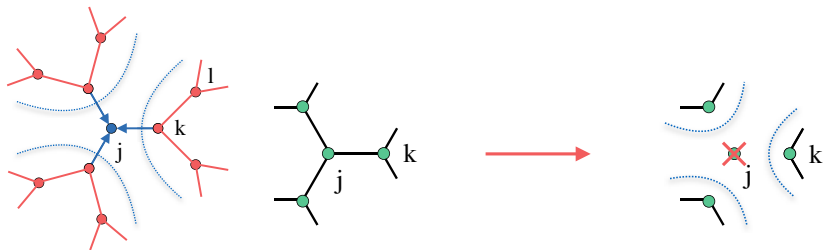
- **Aging persists** in presence of bias: “robust aging”
- Activity decays as  $\tau^{-1}$ , like for  $g = 0$
- Total number of jumps diverges with  $t$

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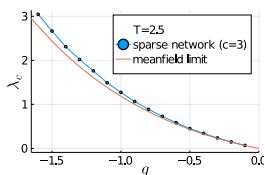
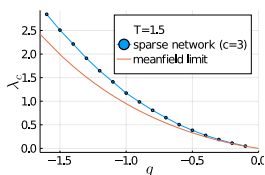
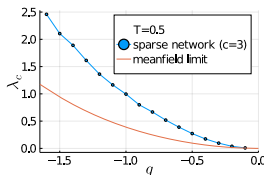
# Bouchaud model on random regular network

- Fixed **finite** connectivity  $c$
- Use cavity theory to find largest eigenvalue of  $\mathbb{W}(g)$  and associated eigenvector (Kabashima, Susca et al)
- Apply to large single instances of networks (population dynamics subtle)

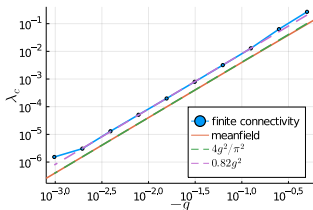
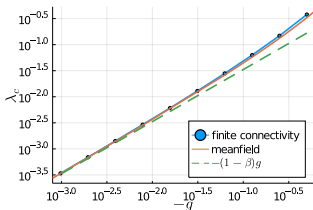
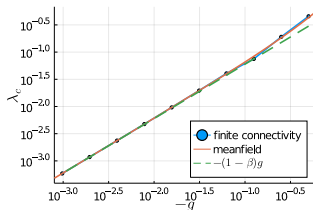




# Dynamical free energy



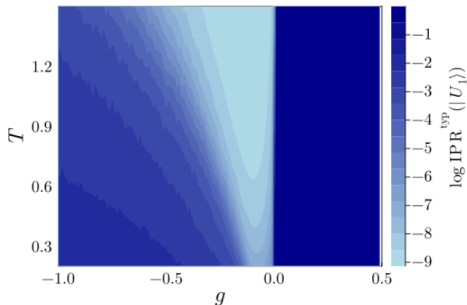
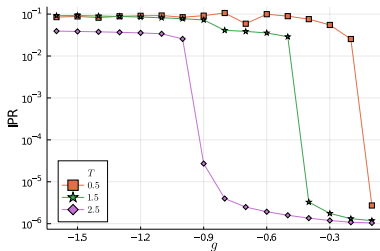
- $\psi(g)$  **qualitatively similar** to mean field limit  $c \rightarrow \infty$
- **High temperature limit** can be taken in cavity equations:  
independent of  $c$

Dynamical free energy near  $g = 0$ (a)  $T = 0.5$ (b)  $T = 1.5$ (c)  $T = 2.5$ 

Activity  $-\psi'(g)$  for  $g \rightarrow 0$  independent of  $c$  (for  $T > 1$ )

# Localization transitions & phase diagram

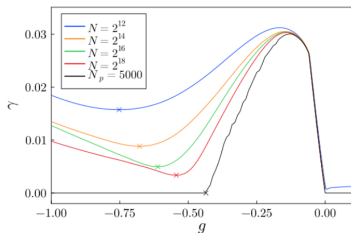
Left: single instance with  $N = 2^{20}$  nodes



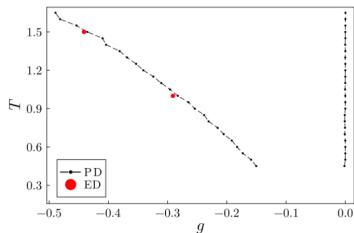
- Dynamical transition at  $g = 0$  is always a **localization** transition
- **Additional** localization transition at  $T$ -dependent  $g < 0$

# Spectral gap

Single instance vs population dynamics



(a) spectral gap

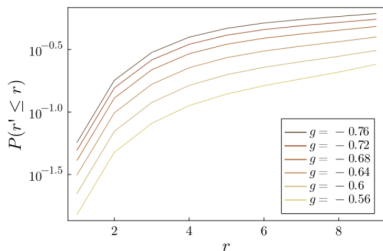


(b) phase transitions

# Structure of localized eigenvectors for $g < 0$



(a) typical localisation cluster



(b) cumulative probability

- Localization on **shallow** traps
- Requires **clusters** of shallow traps (compare De Bacco et al)

# Conclusion & Outlook

## Summary

- Driving by activity bias in **Bouchaud trap model** has non-trivial effects
- Aging is **fragile**: bias towards inactivity  $\Rightarrow$  freezing
- Low-activity phase: time-dependent effective potential forces time-independent  $p_\tau(E)$
- **Barrat-Mézard**: qualitatively different for  $T < 1/2$
- Aging is **robust** to biasing towards inactivity

## Outlook

- **Universality classes** of aging (robust, fragile, ...)?
- **Aging** in “directly” driven systems?
- Nature & **dynamical consequences** of localization transitions

# Link to large deviations

- E.g. in Ising model magnetization distribution

$$P(M) \sim e^{-N\phi(m)}$$

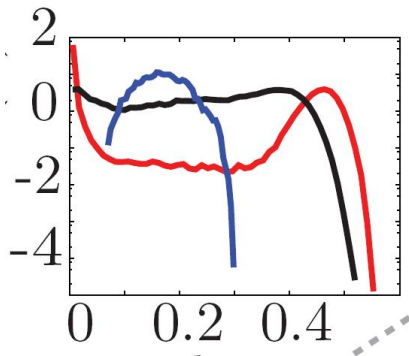
- **Large deviation function**  $\phi(m)$ , with  $m = M/N$
- Free energy as function of magnetic field  $h$

$$f(h) = -N^{-1} \ln \langle e^{hM} \rangle \approx \min_m \phi(m) - hm$$

- So **Legendre transform** links  $\phi(m)$  and  $f(h)$ :  
change of ensemble, fixed  $m$  vs fixed  $h$
- Works the same for **trajectories**: can get  $P(\mathcal{A}_t) \sim e^{-t\phi(\mathcal{A}_t/t)}$   
from dynamical free energy  $\psi$

# Example: Distribution of total activity

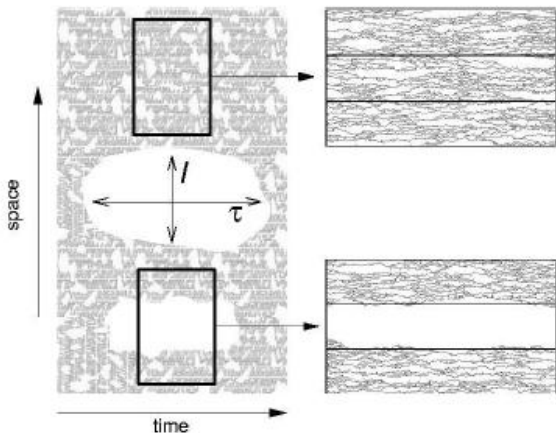
Spin model with constrained kinetics



- $\mathcal{A}_t$  = total number of transitions (spin flips)
- **Two peaks** in  $\ln P(\mathcal{A}_t)$ : phase coexistence
- Analogous to magnetization in Ising model at  $h = 0$



# Space-time plots: Dynamical heterogeneity

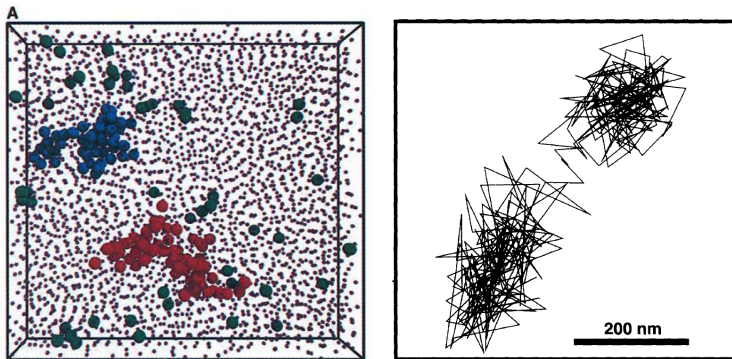


**Domains** of different space-time phases

(Jack, Garrahan, Chandler, Lecomte, van Wijland, Lecomte, Pitard, ...)

# Dynamical heterogeneity in colloidal glasses

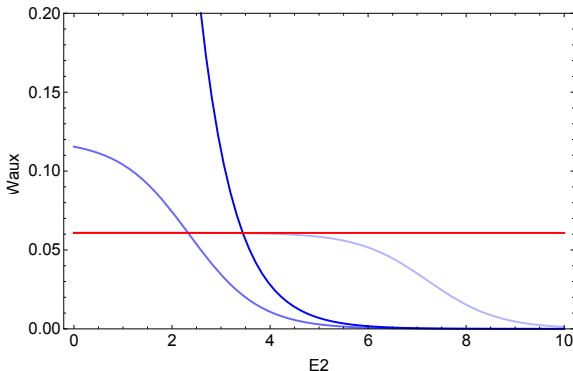
(Eric Weeks group)



Dynamical heterogeneity makes individual particle motion intermittent

# Bouchaud model: Effective transition rates

$$g = -2, -0.2, -0.02$$

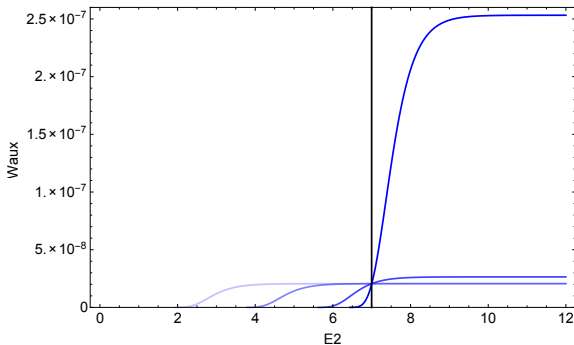


$$W^{\text{aux}}(E_1 \rightarrow E_2) \quad (\text{for } E_1 = 2, T = 0.7)$$

Jumps to shallow traps are favoured

Overall rate increases with  $|g|$

## Bouchaud model: Effective transition rates

 $t - \tau = 10^3(\text{light}), 10^4, 10^5, 10^6(\text{dark})$ 

 $W^{\text{aux}}(E_1 \rightarrow E_2) \text{ (at } E_1 = 7, T = 0.4\text{)}$ 

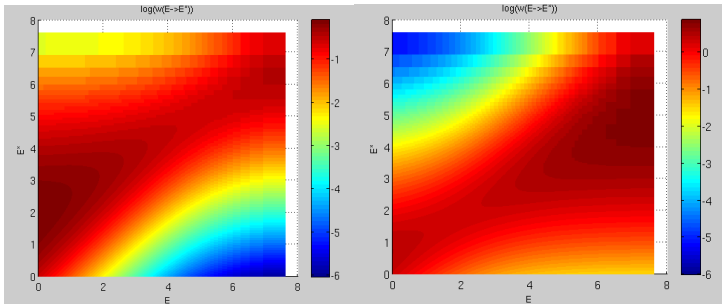
At **early times** jumps only into deep traps  
 Effective threshold level rises towards end of trajectory

# Time-dependent activity

- Average activity now depends on time  $\tau$  along trajectory
- Goes as  $\tau^{-1-T}$  (away from temporal boundaries)
- Jumps concentrated in initial part of trajectory (for  $T < 1$ )
- Total activity is  $\propto (e^g - 1)^{-1}$ , only finite number of jumps
- Bias towards inactivity **freezes** system

# BM model: Effective transition rates in active phase

$T = 0.8, g = -0.1$  (left),  $T = 0.8, g = -1$  (right)



- Jumps biased towards more shallow traps
- Resulting rates are non-monotonic in arrival trap depth

# Stochastic dynamics

## Markov, unbiased

- Start from stochastic model with configurations  $\mathcal{C}$
- **Transition rates**  $W(\mathcal{C}' \rightarrow \mathcal{C})$
- Master equation:

$$\frac{\partial}{\partial t} p(\mathcal{C}, t) = -r(\mathcal{C})p(\mathcal{C}, t) + \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C}' \rightarrow \mathcal{C})p(\mathcal{C}', t)$$

- Escape rate from  $\mathcal{C}$ :  $r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \rightarrow \mathcal{C}')$
- Matrix/vector form: let  $|P(t)\rangle = \sum_{\mathcal{C}} p(\mathcal{C}, t)|\mathcal{C}\rangle$ , then

$$\frac{\partial}{\partial t} |P(t)\rangle = \mathbb{W}|P(t)\rangle$$

- Master operator  $\mathbb{W}$  has matrix elements  
 $\langle \mathcal{C} | \mathbb{W} | \mathcal{C}' \rangle = W(\mathcal{C}' \rightarrow \mathcal{C}) - \delta_{\mathcal{C}, \mathcal{C}'} r(\mathcal{C})$

# Time-integrated quantities

- In simplest case, might want to bias trajectories according to cumulative value of some observable

$$\mathcal{B}_t = \int_0^t dt' B(t')$$

where  $B(t') = b(\mathcal{C}(t'))$  depends only on configuration  $\mathcal{C}(t')$

- Or bias depending on **transitions** that system makes:  
if configuration sequence is  $\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_K$ , use

$$\mathcal{A}_t = \sum_{k=0}^{K-1} \alpha(\mathcal{C}_k, \mathcal{C}_{k+1})$$

- $\mathcal{A}_t =$  total number of moves if  $\alpha(\mathcal{C}, \mathcal{C}') = 1$  for all  $\mathcal{C} \neq \mathcal{C}'$  (activity)
- Or  $\alpha(\mathcal{C}, \mathcal{C}')$  could measure contribution of  $\mathcal{C} \rightarrow \mathcal{C}'$  to total current, accumulated shear strain, entropy current, ...



# Biasing trajectory probabilities

- Trajectory  $\pi$ ; bias probability to give large/small values of  $\mathcal{B}_t$ :

$$P[\pi, g] = Z(g, t)^{-1} P[\pi, 0] \exp[-g\mathcal{B}_t]$$

- **Bias parameter**  $g$ ; canonical version of hard constraint on  $\mathcal{B}_t$
- Trajectory partition function (discretize,  $t = M\Delta t$ )

$$Z(g, t) = \sum_{\mathcal{C}_0 \dots \mathcal{C}_M} \exp\left\{\Delta t \sum_{i=1}^M [W(\mathcal{C}_{i-1} \rightarrow \mathcal{C}_i) - gb(\mathcal{C}_{i-1})]\right\} p_0(\mathcal{C}_0)$$

$$\rightarrow \langle e | e^{\mathbb{W}(g)t} | 0 \rangle, \quad \mathbb{W}(g) = \mathbb{W} - g \sum_{\mathcal{C}} b(\mathcal{C}) |\mathcal{C}\rangle \langle \mathcal{C}|$$

- Projection state  $\langle e | = \sum_{\mathcal{C}} \langle \mathcal{C} |$
- Unbiased initial (e.g. steady) state  $|0\rangle = \sum_{\mathcal{C}} p_0(\mathcal{C}) |\mathcal{C}\rangle$

# Dynamical free energy

- Define by analogy with equilibrium free energy as

$$\psi(g) \equiv \lim_{t \rightarrow \infty} t^{-1} \ln Z(g, t)$$

- If configuration space is finite, can decompose  $\mathbb{W}(g) = \sum_i \omega_i |V_i\rangle \langle U_i|$
- Then  $\psi(g) = \max_i \omega_i$  (Lebowitz Spohn)
- Maximum eigenvalue “generically” non-degenerate
- Same for bias in  $\mathcal{A}_t$  (**activity**, current etc), with

$$\langle \mathcal{C} | \mathbb{W}(g) | \mathcal{C}' \rangle = \begin{cases} W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})}, & \mathcal{C} \neq \mathcal{C}' \\ -r(\mathcal{C}), & \mathcal{C} = \mathcal{C}' \end{cases}$$

# Bias as time-dependent master operator

(Transcribing from Chetrite & Touchette)

- Can we write biased path probability

$$P[\pi, g] = Z(g, t)^{-1} \prod_{i=1}^M \langle \mathcal{C}_i | e^{\mathbb{W}(g)\Delta t} | \mathcal{C}_{i-1} \rangle \times p_0(\mathcal{C}_0)$$

- ... as resulting from effective time-dependent master equation:

$$P[\pi, g] = \prod_{i=1}^M \langle \mathcal{C}_i | e^{\mathbb{W}_{i-1}^{\text{aux}}(g)\Delta t} | \mathcal{C}_{i-1} \rangle \times p_0^{\text{aux}}(\mathcal{C}_0)$$

- Idea: set

$$\langle \mathcal{C}_i | e^{\mathbb{W}_{i-1}^{\text{aux}}(g)\Delta t} | \mathcal{C}_{i-1} \rangle = \frac{u_i(\mathcal{C}_i)}{u_{i-1}(\mathcal{C}_{i-1})} \langle \mathcal{C}_i | e^{\mathbb{W}(g)\Delta t} | \mathcal{C}_{i-1} \rangle$$

## Bias as time-dependent master operator (cont)

- Require:  $u_M(\mathcal{C}_M) = 1$ ,  $p_0^{\text{aux}}(\mathcal{C}_0) = p_0(\mathcal{C}_0)u_0(\mathcal{C}_0)/Z(g, t)$  and **normalization**

$$\sum_{\mathcal{C}_i} \langle \mathcal{C}_i | e^{\mathbb{W}_{i-1}^{\text{aux}}(g)\Delta t} | \mathcal{C}_{i-1} \rangle \equiv \sum_{\mathcal{C}_i} \frac{u_i(\mathcal{C}_i)}{u_{i-1}(\mathcal{C}_{i-1})} \langle \mathcal{C}_i | e^{\mathbb{W}(g)\Delta t} | \mathcal{C}_{i-1} \rangle = 1$$

- Hence the  $u_i$  can be determined **backwards in time**:

$$u_{i-1}(\mathcal{C}_{i-1}) = \sum_{\mathcal{C}_i} u_i(\mathcal{C}_i) \langle \mathcal{C}_i | e^{\mathbb{W}(g)\Delta t} | \mathcal{C}_{i-1} \rangle$$

- In vector notation:  $\langle U_{i-1} | = \langle U_i | e^{\mathbb{W}(g)\Delta t}$
- Solution:  $\langle U_i | = \langle e | e^{\mathbb{W}(g)(M-i)\Delta t}$
- Thus  $p_0^{\text{aux}}(\mathcal{C}) = \langle e | e^{\mathbb{W}(g)t} | \mathcal{C} \rangle p_0(\mathcal{C}) / \langle e | e^{\mathbb{W}(g)t} | 0 \rangle$ , normalized

# Effective transition rates

Continuous time:  $\tau = i\Delta t$ ,  $\Delta t \rightarrow 0$

- Expanding relation between  $\mathbb{W}^{\text{aux}}$  and  $\mathbb{W}(g)$  to  $O(\Delta t)$  gives **effective rates**

$$\langle \mathcal{C} | \mathbb{W}_\tau^{\text{aux}} | \mathcal{C}' \rangle = \langle \mathcal{C} | \mathbb{W}(g) | \mathcal{C}' \rangle \frac{u_\tau(\mathcal{C})}{u_\tau(\mathcal{C}')}$$

or explicitly

$$W^{\text{aux}}(\mathcal{C}' \rightarrow \mathcal{C}) = W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})} \frac{u_\tau(\mathcal{C})}{u_\tau(\mathcal{C}')}$$

- Effect of  $u_\tau(\mathcal{C})$  can be interpreted as Metropolis-like factor  $e^{-\beta[E_\tau^{\text{eff}}(\mathcal{C}) - E_\tau^{\text{eff}}(\mathcal{C}')]/2}$ , with **effective potential**

$$E_\tau^{\text{eff}}(\mathcal{C}) = (-2/\beta) \ln u_\tau(\mathcal{C})$$

# Effective exit rates

- **Effective exit rates** follow from normalization as

$$-\langle \mathcal{C} | \mathbb{W}_\tau^{\text{aux}} | \mathcal{C} \rangle = -\langle \mathcal{C} | \mathbb{W}(g) | \mathcal{C} \rangle + \frac{\langle U_\tau | \mathbb{W}(g) | \mathcal{C} \rangle}{\langle U_\tau | \mathcal{C} \rangle}$$

- Explicitly

$$r^{\text{aux}}(\mathcal{C}) = r(\mathcal{C}) + \frac{\langle U_\tau | \mathbb{W}(g) | \mathcal{C} \rangle}{\langle U_\tau | \mathcal{C} \rangle}$$

- Shift in general dependent on  $\mathcal{C}$  (and  $\tau$ )

# Biased & auxiliary master operators

- Dynamical partition function derived from a **biased master operator**  $\mathbb{W}(g)$  with elements

$$\langle \mathcal{C} | \mathbb{W}(g) | \mathcal{C}' \rangle = \begin{cases} W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})}, & \mathcal{C} \neq \mathcal{C}' \\ -r(\mathcal{C}), & \mathcal{C} = \mathcal{C}' \end{cases}$$

- This does not conserve probability
- But can restore by multiplicative reweighting (Jack & PS, Chetrite & Touchette)

$$\langle \mathcal{C}_{\tau+\Delta t} | e^{\mathbb{W}_{\tau}^{\text{aux}}(g)\Delta t} | \mathcal{C}_{\tau} \rangle = \frac{u_{\tau+\Delta t}(\mathcal{C}_{\tau+\Delta t})}{u_{\tau}(\mathcal{C}_{\tau})} \langle \mathcal{C}_{\tau+\Delta t} | e^{\mathbb{W}(g)\Delta t} | \mathcal{C}_{\tau} \rangle$$

- Normalization forces  $\langle U_{\tau} | = \langle e | e^{\mathbb{W}(g)(t-\tau)}$

# Effective transition rates

Continuous time:  $\tau = i\Delta t$ ,  $\Delta t \rightarrow 0$

- Relation between  $\mathbb{W}^{\text{aux}}$  and  $\mathbb{W}(g)$  gives **effective rates**

$$W^{\text{aux}}(\mathcal{C}' \rightarrow \mathcal{C}) = W(\mathcal{C}' \rightarrow \mathcal{C}) e^{-g\alpha(\mathcal{C}', \mathcal{C})} \frac{u_\tau(\mathcal{C})}{u_\tau(\mathcal{C}')}$$

- Effect of  $u_\tau(\mathcal{C})$  can be interpreted as Metropolis-like factor  $e^{-\beta[E_\tau^{\text{eff}}(\mathcal{C}) - E_\tau^{\text{eff}}(\mathcal{C}')]/2}$ , with **effective potential**

$$E_\tau^{\text{eff}}(\mathcal{C}) = (-2/\beta) \ln u_\tau(\mathcal{C})$$



# Time dependence

- Effective master operator and potential in general time-dependent
- Also **state probabilities**

$$p_\tau(\mathcal{C}) = \frac{\langle e | e^{\mathbb{W}(g)(t-\tau)} | \mathcal{C} \rangle \langle \mathcal{C} | e^{\mathbb{W}(g)\tau} | 0 \rangle}{Z(g, t)} = \frac{u_\tau(\mathcal{C}) v_\tau(\mathcal{C})}{Z(g, t)}$$

where  $|V_\tau\rangle = e^{\mathbb{W}(g)\tau} |0\rangle$

- Product of forward (from past) and backward (from future) factors
- Time-dependences disappear if driven system reaches stationary state – but not if there is **aging**