

Glassy random walks: Large deviations and aging

Peter Sollich
with Fabián Aguirre López, Charles Marteau,
Diego Tapias, Vincent Wolff, Benedikt Grüger

Institute for Theoretical Physics, University of Göttingen
Disordered Systems Group, King's College London



GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

KING'S
College
LONDON
Founded 1829

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:

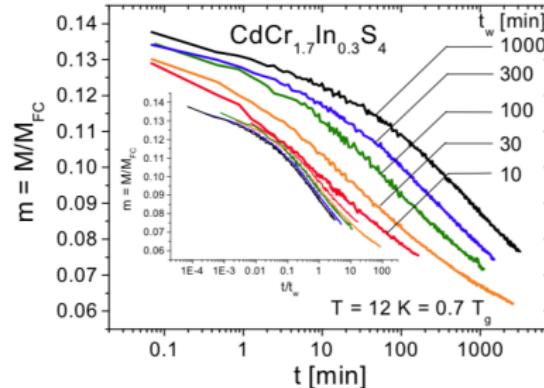
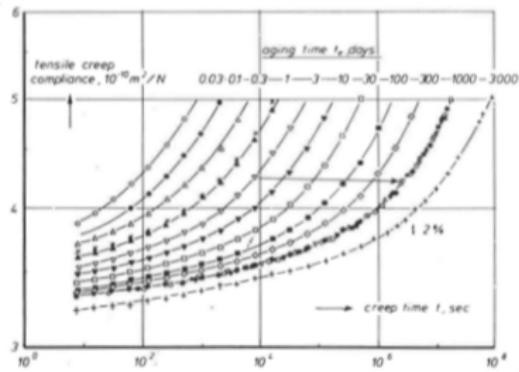
- Bacco, Guggiola, Kühn & Paga (2016):
*Rare events statistics of random walks on networks:
localisation and other dynamical phase transitions*

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...



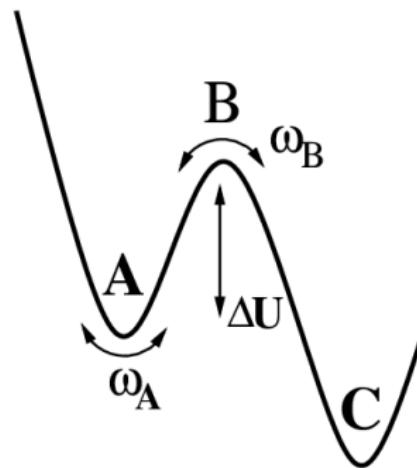
- Aging systems **could** reach equilibrium – but are too slow
- Significant dependence of properties on **age** since preparation
- Polymers, spin glasses, ...

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



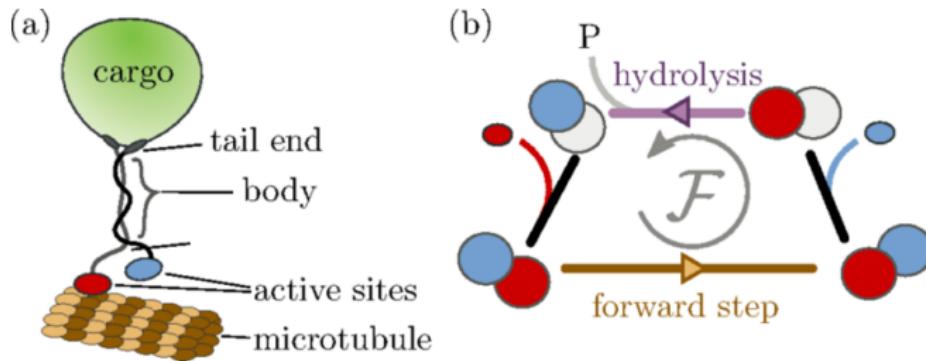
- Contrast with escape from single **metastable state**
- Beyond age \sim metastable lifetime, age-dependences disappear
- **Aging** requires many states, broad spectrum of lifetimes

Outline

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

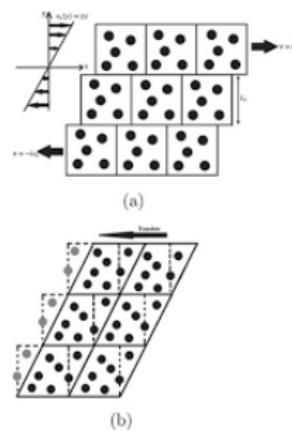
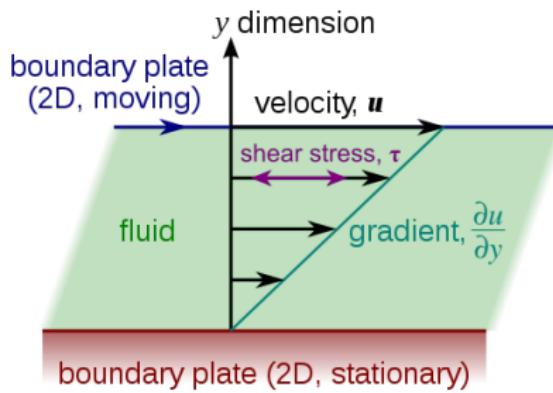
Driven systems

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



Modelling driven systems

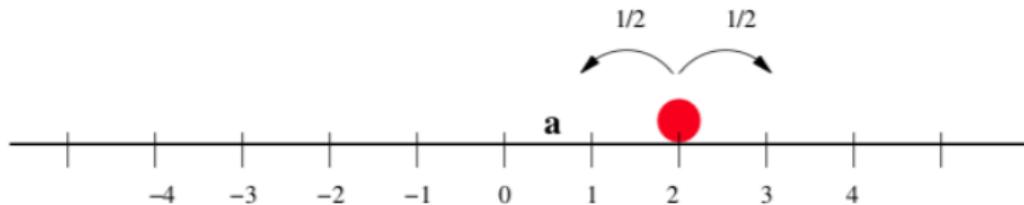
- Lack of detailed balance:
More freedom to choose parameters – underconstrained?
- Is there a systematic way of assigning free parameters?
- E.g. for motion in bulk of **sheared fluid**



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

Outline

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

Biasing trajectory probabilities

- Trajectory π ; 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**

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

Outline

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

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 $E \sim T \ln(t)$

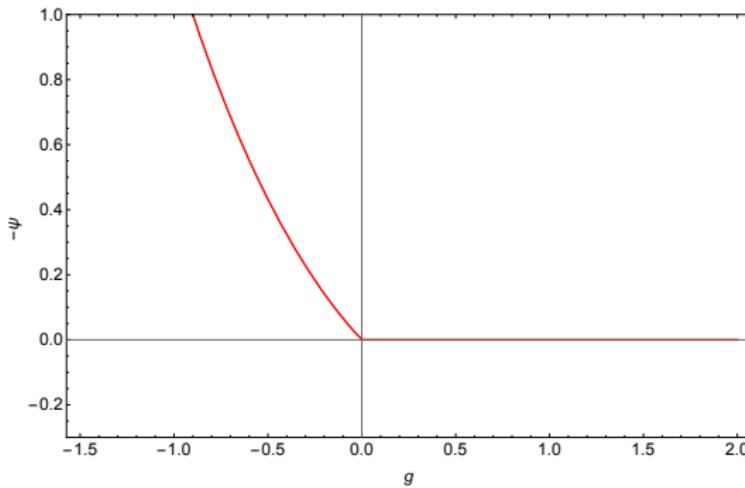
Focus

How do aging and driving (activity bias) interact?

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

Dynamical free energy

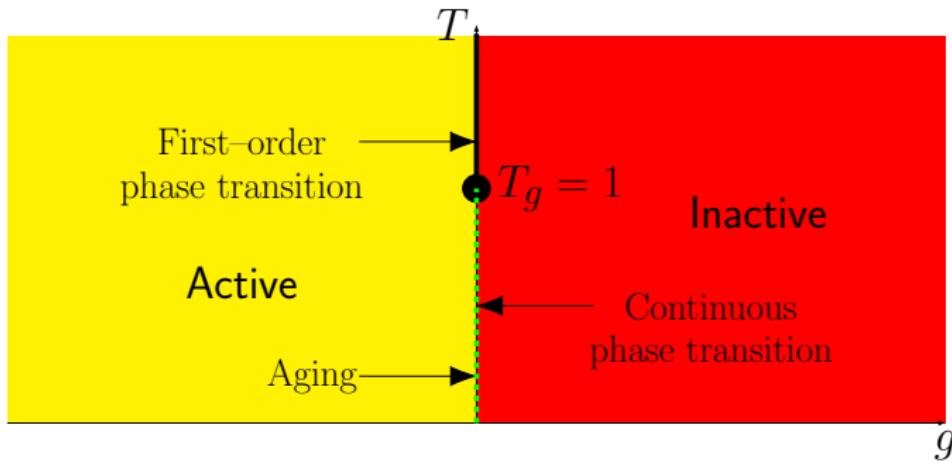
$T = 2.5$



Dynamical phase transition, active to inactive

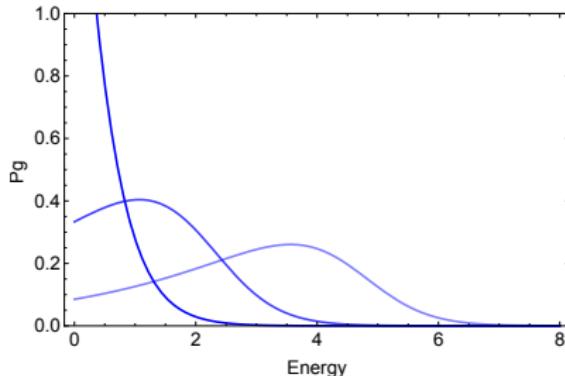
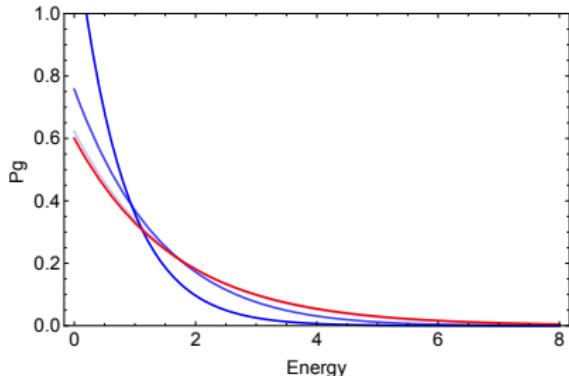
Reminder: $-\psi'(g) = \text{average activity}$

Phase diagram



Above average activity: active phase

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



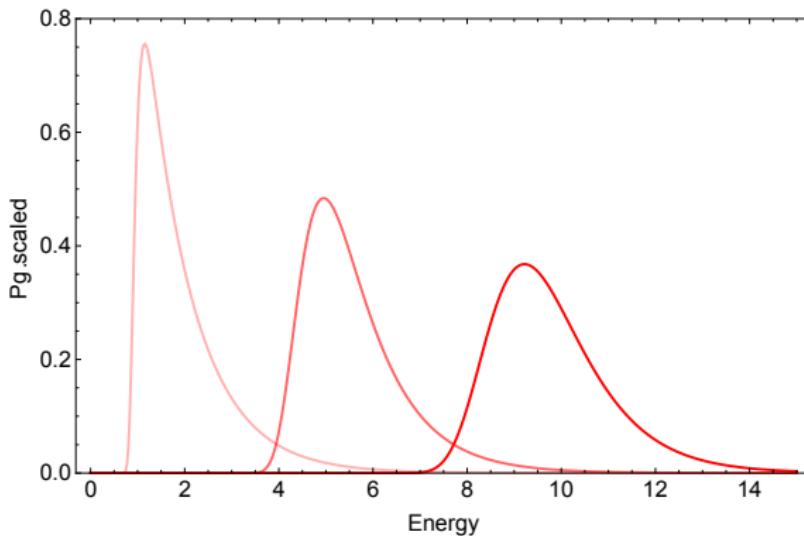
Left: $T = 2.5$; right: $T = 0.7$

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



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

Independent of g and τ

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

Outline

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

BM model basics

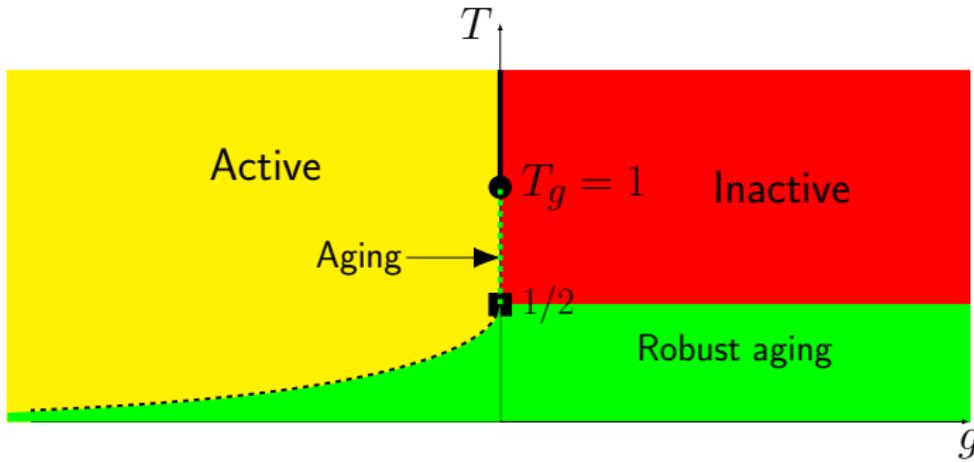
- Like Bouchaud model but Glauber rates:

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

- 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

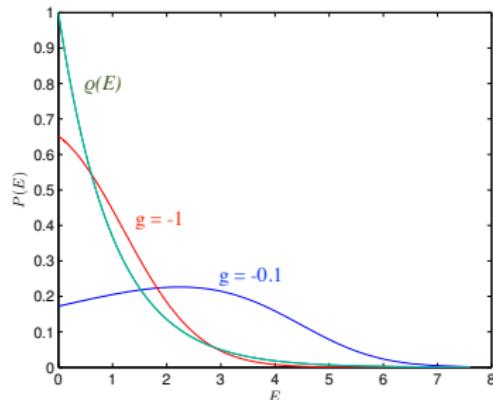
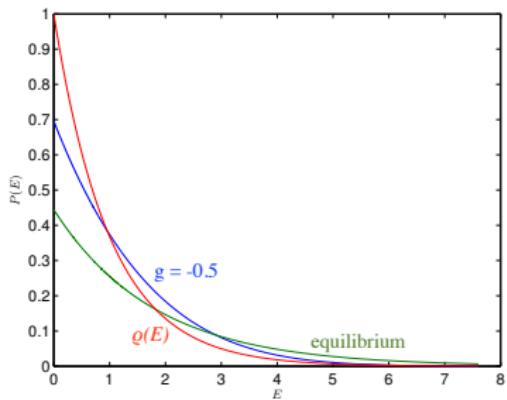
Analytical prediction, confirmed numerically by finite-size scaling



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

Trap depth distributions in active phase

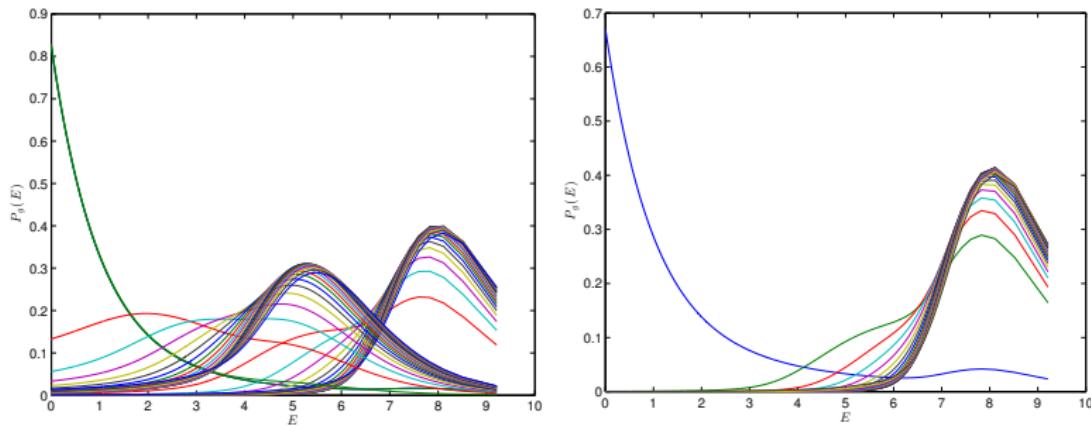
$T = 1.5, g = -0.5$ (left), $T = 0.8, g = -0.1, -1$ (right)



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

Inactive phase, $T > 1/2$

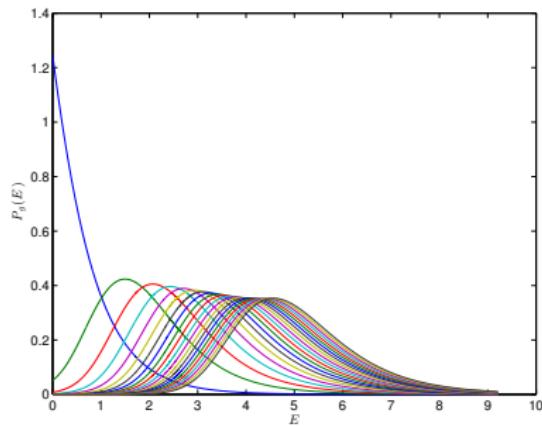
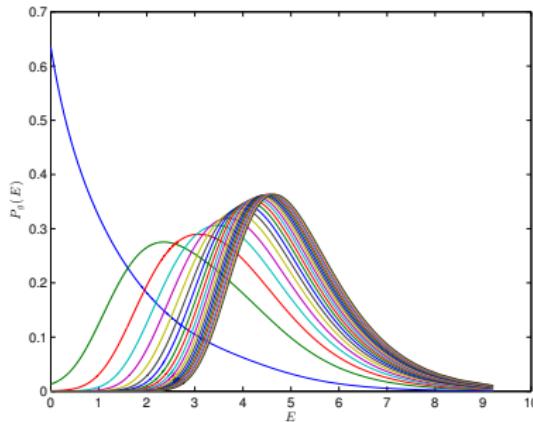
$T = 0.8$, $g = 0.25$, $t = 100$ and 1000 (left), $g = 0.5$, $t = 1000$ (right)



- $p_\tau(E)$ for increasing τ 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)



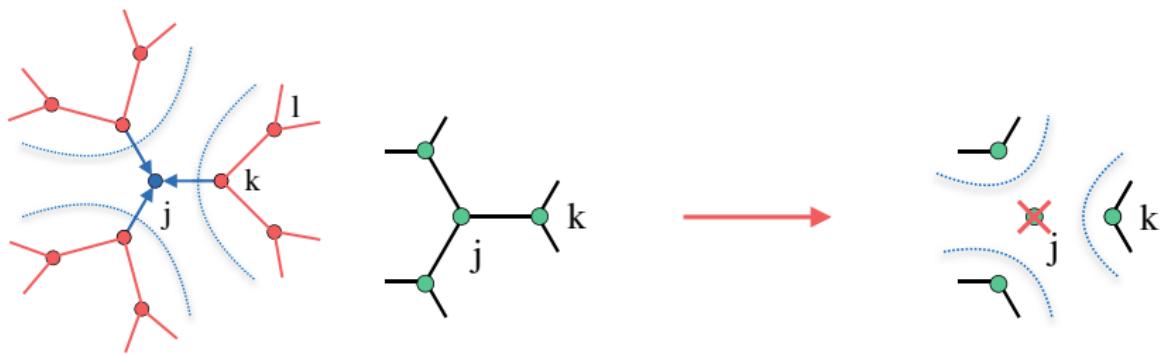
- Aging persists in presence of bias: “robust aging”
- Activity decays as τ^{-1} , like for $g = 0$
- Total number of jumps diverges with t

Outline

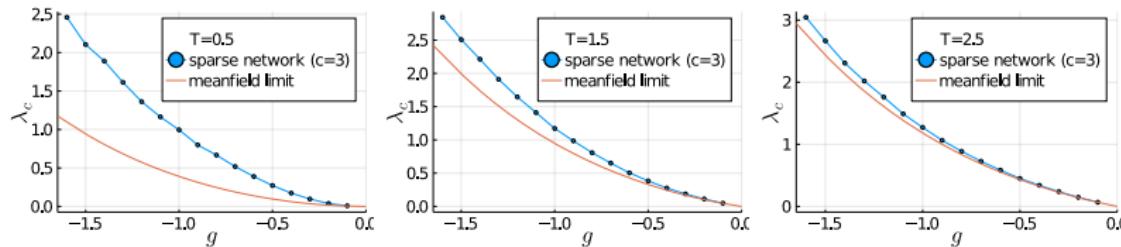
- 1 Aging dynamics
- 2 Driven dynamics
- 3 Biased trajectory ensembles
- 4 Bouchaud trap model
- 5 Barrat-Mézard model
- 6 Finite network connectivity

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)

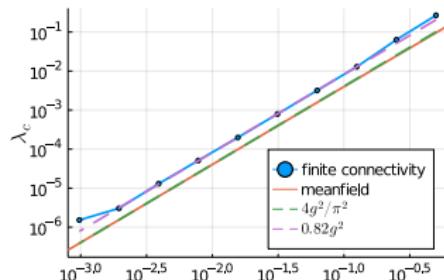
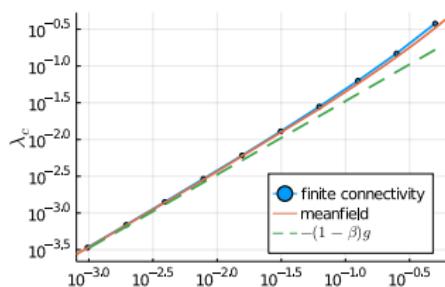
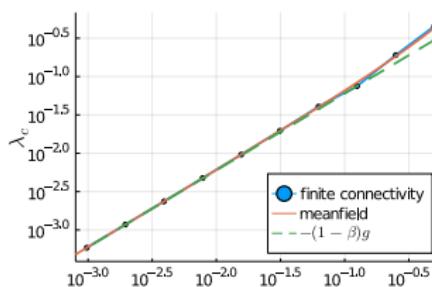


Dynamical free energy



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

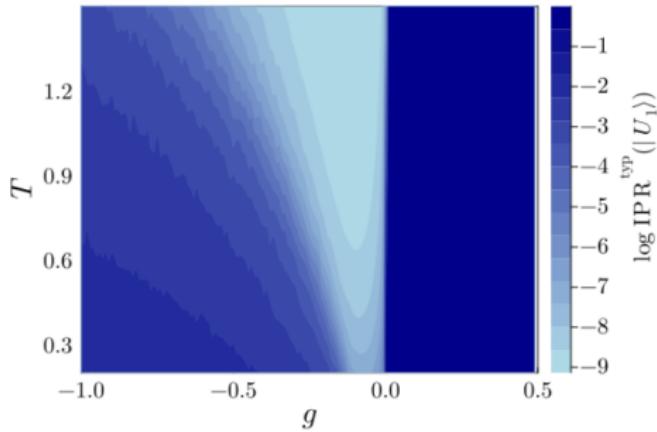
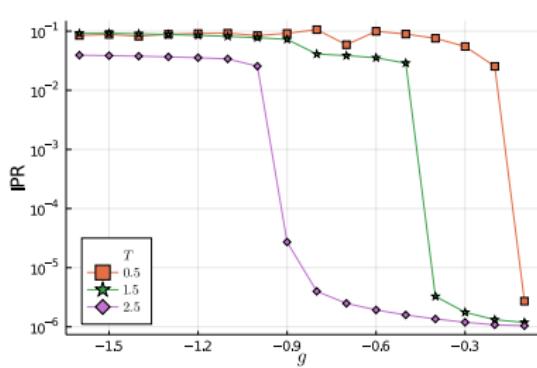
Dynamical free energy near $g = 0$

(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

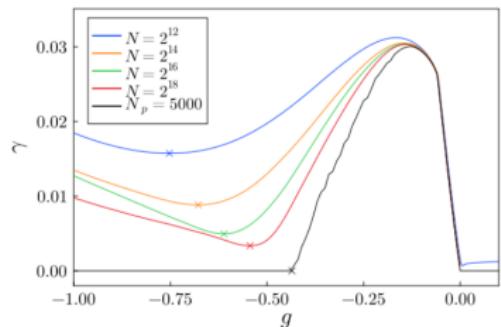
Left: single instance with $N = 2^{20}$ nodes



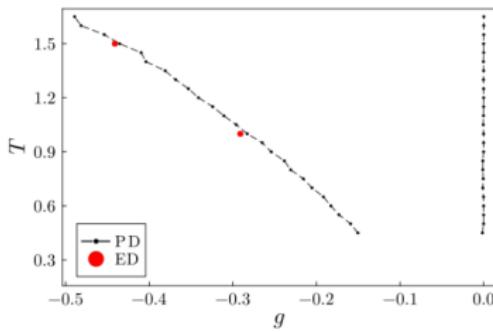
- Dynamical transition at $g = 0$ is always a **localization** transition
- **Additional** localization transition at T -dependent $g < 0$

Spectral gap

Single instance vs population dynamics



(a) spectral gap

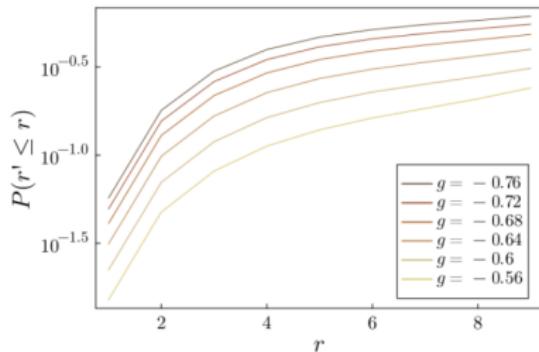


(b) phase transitions

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

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

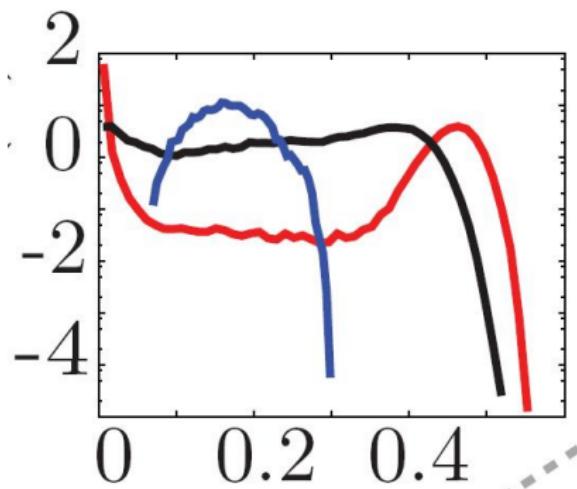
- Large deviation function $\phi(m)$, with $m = M/N$
- Free energy as function of magnetic field h

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

- 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 ψ

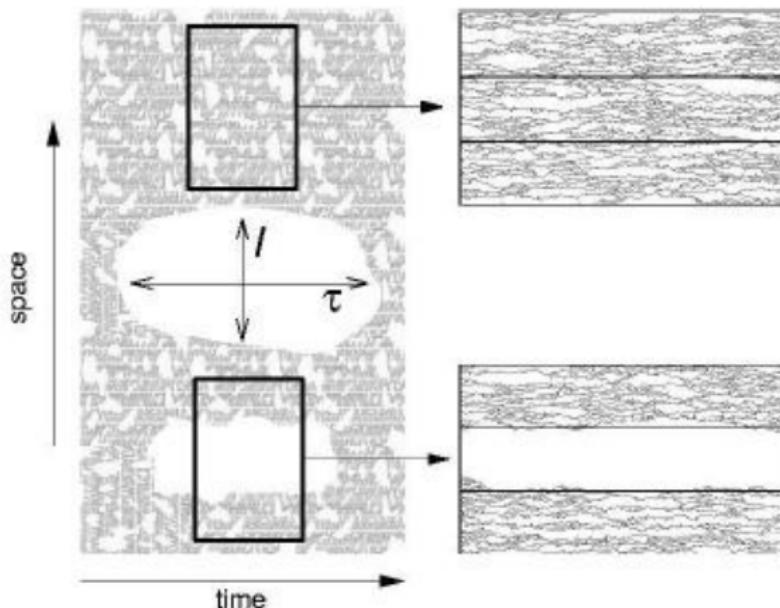
Example: Distribution of total activity

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

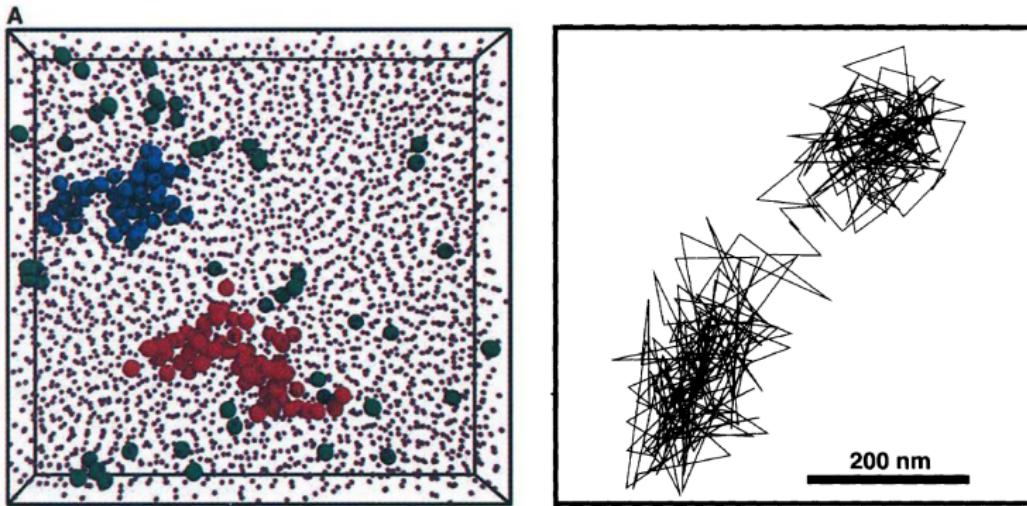


Domains of different space-time phases

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

Dynamical heterogeneity in colloidal glasses

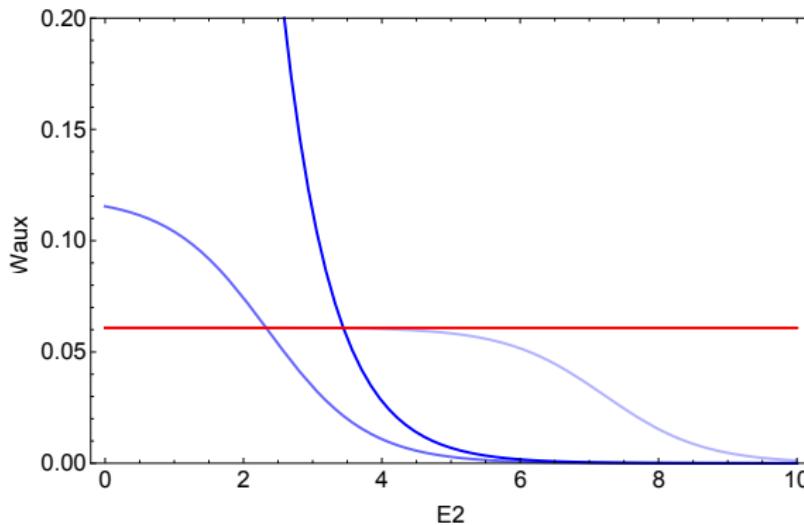
(Eric Weeks group)



Dynamical heterogeneity makes individual particle motion
intermittent

Bouchaud model: Effective transition rates

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



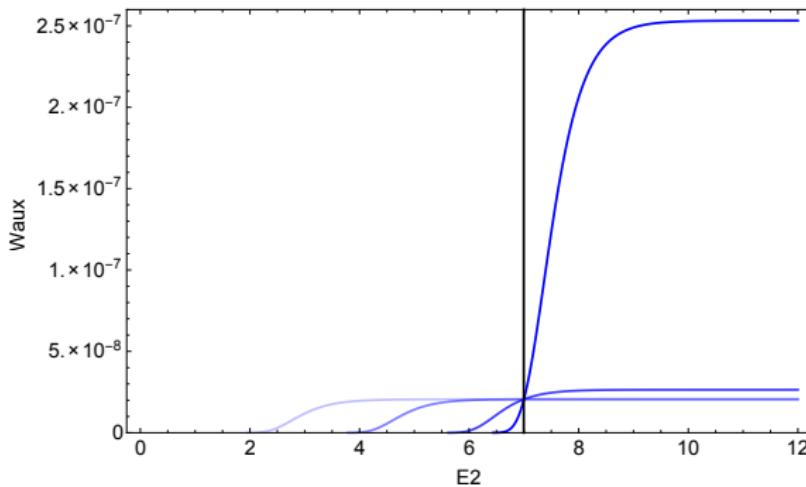
$W^{\text{aux}}(E_1 \rightarrow E_2)$ (for $E_1 = 2$, $T = 0.7$)

Jumps to shallow traps are favoured

Overall rate increases with $|g|$

Bouchaud model: Effective transition rates

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



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

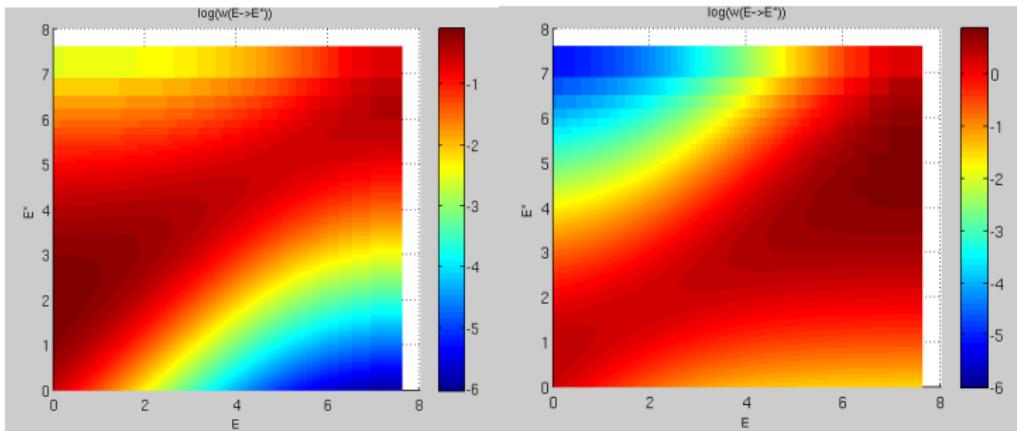
At **early times** jumps only into deep traps
 Effective threshold level rises towards end of trajectory

Time-dependent activity

- Average activity now depends on time τ along trajectory
- Goes as τ^{-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 π ; 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, $t = M\Delta t$)

$$\begin{aligned} Z(g, t) &= \sum_{\mathcal{C}_0 \dots \mathcal{C}_M} \exp \left\{ \Delta t \sum_{i=1}^M [W(\mathcal{C}_{i-1} \rightarrow \mathcal{C}_i) - g b(\mathcal{C}_{i-1})] \right\} p_0(\mathcal{C}_0) \\ &\rightarrow \langle e | e^{\mathbb{W}(g)t} | 0 \rangle, \quad \mathbb{W}(g) = \mathbb{W} - g \sum_{\mathcal{C}} b(\mathcal{C}) |\mathcal{C}\rangle \langle \mathcal{C}| \end{aligned}$$

- 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}^{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 τ)

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}^{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**