Driven dynamics of trap models

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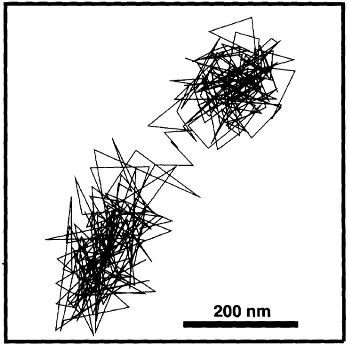
Overview

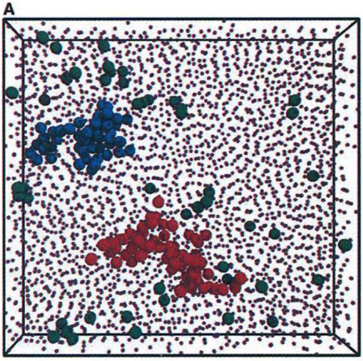
- Heterogeneities in KCM dynamics look in space-time plots like phase coexistence
- Probe by biasing activity of trajectories, equivalent to looking at large deviations of activity
- Dynamics in biased phases: auxiliary process with effective potential
- Non-trivial in KCMs (many-body), so study simpler models
- Trap models: interplay of aging dynamics and bias

Outline

1. Dynamical phase transitions and large deviations
2. Biased trajectory ensembles
3. Biased dynamics & effective potential
4. Bouchaud trap model

Dynamical heterogeneity

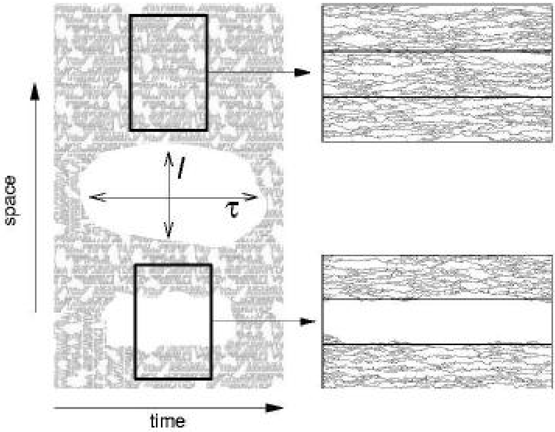




Dynamics in real (e.g. colloidal) glasses are intermittent, and heterogeneous

Space-time plots

FA model, $d = 1$

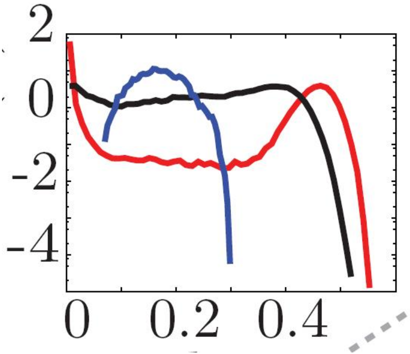


Domains of different space-time phases?

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

Distribution of total activity

Space-time boxes, length N, time t



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

Exploring phase coexistence

Equilibrium:

- Bias configurations by factor e^{hM}
- Gibbs free energy

Space-time:

- Bias trajectories by factor $\mathrm{e}^{-g\mathcal{A}}$
- Dynamical free energy

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Stochastic dynamics
Markov, unbiased

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

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

- Escape rate from $\mathcal{C}$: $r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \to \mathcal{C}')$
- 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 $\langle \mathcal{C} | \mathbb{W} | \mathcal{C}' \rangle = W(\mathcal{C}' \to \mathcal{C}) - \delta_{\mathcal{C}, \mathcal{C}'} r(\mathcal{C})$

Time-integrated quantities

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

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

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 $\mathcal{C}_0, \mathcal{C}_1, \ldots, \mathcal{C}_K$, 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 $\mathcal{C} \to \mathcal{C}'$ to total current, accumulated shear strain, entropy current, ...

Biasing trajectory probabilities

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

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

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

$$Z(g,t) = \sum_{\mathcal{C}_0 \ldots \mathcal{C}_M} \exp\{\Delta t \sum_{i=1}^{M} [W(\mathcal{C}_{i-1} \to \mathcal{C}_i) - g b(\mathcal{C}_{i-1})]\} p_0(\mathcal{C}_0)$$

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

- 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

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

- 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

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

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Bias as time-dependent master operator
(Transcribing from Chetrite & Touchette)

- Can we write biased path probability

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

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

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

- Idea: set

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

Bias as time-dependent master operator (cont)

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

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

- Hence the u_i can be determined backwards in time:

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

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

Effective transition rates

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

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

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

or explicitly

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

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

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

Effective exit rates

- Effective exit rates follow from normalization as

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

- Explicitly

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

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

Time dependence

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

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

  where $|V_\tau\rangle = \mathrm{e}^{\mathbb{W}(g)\tau}|0\rangle$
- Product of forward (from past) and backward (from future) factors

Time-translation invariance

Restored for long $t - \tau$

- If $\mathbb{W}(g)$ has a non-degenerate maximal eigenvalue, $\mathbb{W}(g) = \psi(g)|V\rangle\langle U| + \ldots$ then

$$e^{\mathbb{W}(g)(t-\tau)} = e^{\psi(g)(t-\tau)} \left[|V\rangle\langle U| + \mathcal{O}(e^{-\Gamma(t-\tau)}) \right]$$

  in terms of gap Γ to next eigenvalue

- Neglecting exponentially small corrections for $\Gamma(t-\tau) \gg 1$,

$$\langle U_{t-\tau}| \approx \langle e|V\rangle e^{\psi(g)(t-\tau)} \langle U|$$

  hence $u_{t-\tau}(C) \propto u(C)$, time-independent effective potential

Time translation invariance: state probabilities
Need long $t - \tau$ and τ

- Partition function becomes

$$Z(g,t) = \langle e|\mathrm{e}^{\mathbb{W}(g)t}|0\rangle \approx \mathrm{e}^{\psi(g)t}\langle e|V\rangle\langle U|0\rangle$$

and similarly $|V_\tau\rangle \approx |V\rangle \mathrm{e}^{\psi(g)\tau}\langle U|0\rangle$

- State probabilities follow as:

$$p_\tau(\mathcal{C}) \approx \frac{\langle e|V\rangle \mathrm{e}^{\psi(g)(t-\tau)}\langle U|\mathcal{C}\rangle\langle\mathcal{C}|\mathrm{e}^{\psi(g)\tau}|V\rangle\langle U|0\rangle}{\mathrm{e}^{\psi(g)t}\langle e|V\rangle\langle U|0\rangle} = \langle U|\mathcal{C}\rangle\langle\mathcal{C}|V\rangle$$

- So if $\Gamma\tau \gg 1$ and $\Gamma(t-\tau) \gg 1$, state probabilities are (e.g. Giardina Kurchan Peliti 2006, Jack PS 2010, Popkov Schütz Simon 2010)

$$p^{\mathrm{TTI}}(\mathcal{C}) = u(\mathcal{C})v(\mathcal{C})$$

- Independent of time away from temporal boundaries

Time translation invariance: exit rates

- As $\langle U_\tau| \propto \langle U|$ for large $t - \tau$, shift of exit rates

$$\frac{\langle U_\tau|\mathbb{W}(g)|\mathcal{C}\rangle}{\langle U_\tau|\mathcal{C}\rangle} \approx \frac{\langle U|\mathbb{W}(g)|\mathcal{C}\rangle}{\langle U|\mathcal{C}\rangle} = \psi(g)$$

- So in TTI regime, all exit rates

$$r^{\mathrm{aux}}(\mathcal{C}) = r(\mathcal{C}) + \psi(g)$$

  are shifted by same amount (RML Evans)

- Implies bound $\psi(g) \geq -\min_{\mathcal{C}} r(\mathcal{C})$

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Trap models

- Picture of glassy dynamics: if(!) dominated by energy then 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

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

  where N = number of configurations
- Golf course landscape: always activate to "top" $(E = 0)$
- Mean field connectivity

Glass transition and aging

- Model specified by energies $\{E_i\}$
- For $N \to \infty$, distribution of energies $\rho(E)$
- Typically taken as $\rho(E) = \exp(-E)$
- 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 $E \sim T \ln(t)$

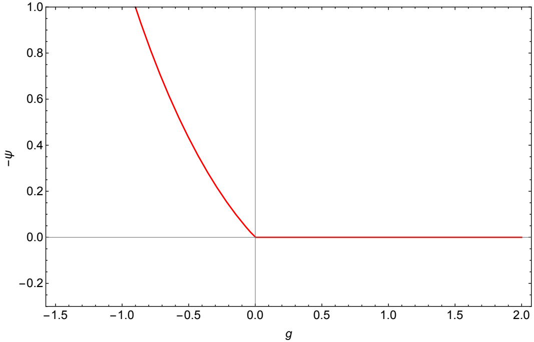
Focus

How do aging and activity bias interact?

- Method: find Laplace transforms of $u_\tau(E)$, $v_\tau(E)$
- Then look at large $t-\tau$ or τ $(z \to 0)$

Dynamical free energy

$T = 2.5$



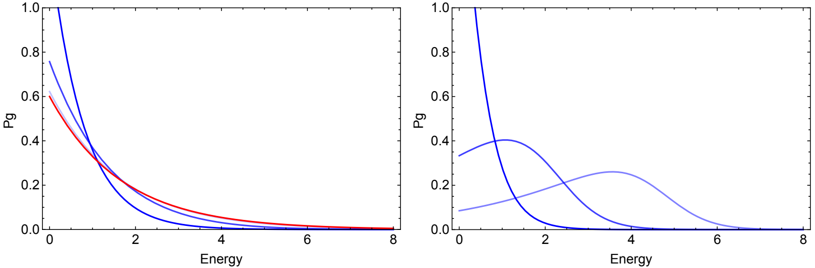
Dynamical phase transition

1^{st} order for $T > 1$, 2^{nd} order for $T < 1$

Note: $-\psi'(g) =$ average activity

Above average activity

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

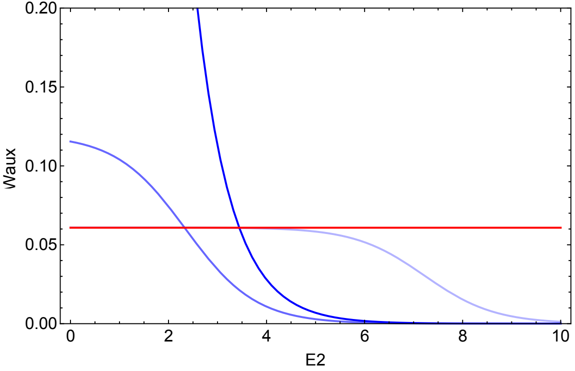


Left: $T = 2.5$; right: $T = 0.7$

For $T < 1$, typical energy increases as $g \to 0$;
remnant of transition to aging dynamics
Effective potential $E^{\text{eff}} = (2/\beta)\ln(1 + \psi e^{\beta E})$

Effective transition rates

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



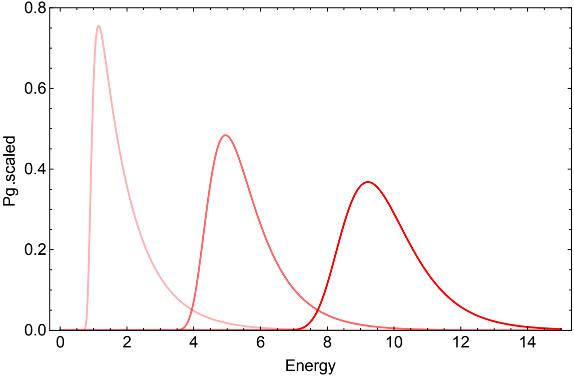
$W^{\text{aux}}(E_1 \to E_2)$ (for $E_1 = 2$, $T = 0.7$)

Jumps to shallow traps are favoured

Overall rate increases with $|g|$

Below average activity

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



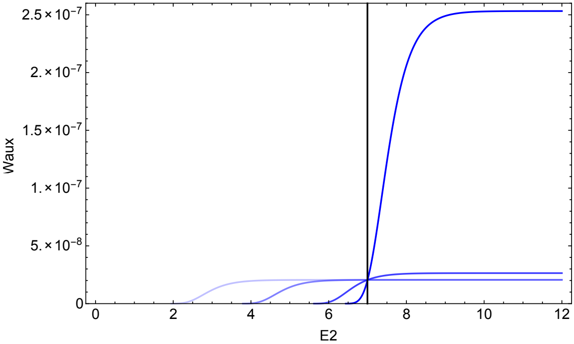
$p_\tau(E) \propto \rho(E) \exp(-t e^{-\beta E})$ (away from boundaries)

Independent of g and τ

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

Effective transition rates

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

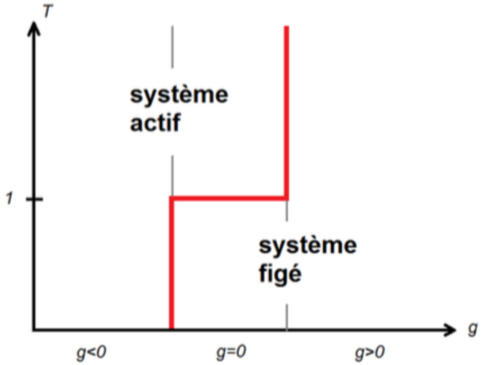


$$W^{\rm aux}(E_1 \to E_2) \text{ (at } E_1 = 7, T = 0.4)$$

At early times jumps only into deep traps

Effective threshold level rises towards end of trajectory

Phase diagram



Direct signature of glass transition only at $g = 0$

Summary & Outlook

Summary

- Activity bias in Bouchaud trap model has non-trivial effects
- Wipes out most signatures of glass transition
- Low-activity phase: time-dependent effective potential forces time-independent $p_\tau(E)$

Outlook

- Outlook: other trap models, e.g. Barrat-Mézard, transition rates $1/[1+\mathrm{e}^{\beta(E'-E)}]$
- At $T=0$ this shows (entropic) aging for any g
- Indications of dynamic transition at $g \neq 0$ for $T < 1/2$
- Trap models on graphs with finite connectivity – study using cavity method