Large deviations of the dynamical activity in the East model: analysing structure in biased trajectories

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J. Phys. A, 47:015003, 2014

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Motivation

- Large deviations in time-integrated quantities
- Can be thought of as steady states generated by effective interaction
- Two-body? Many-body? Range?
- Dependence on strength of bias?
- Relevant e.g. for stable glassy states from activity bias, systems under steady shear
- Work so far mainly on one-body problems (Evans, Baule, Simha, Chetrite, Touchette) or extreme bias (Popkov, Schütz, Simon)
- Study effective interactions for East model
- . . . with bias towards large activity
- . . . across range of biases
- Hierarchy of responses, mirrors aging dynamics

Outline

1. Timescales, activity vs escape rate bias, observables
2. Response to bias: overview
3. Linear response theory
4. Variational approaches
5. Summary & outlook

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East model & timescale hierarchy

- Chain of N spins, $n_i = 1$ up, $n_i = 0$ down
- Facilitated spins: up-spin to left
- Facilitated spins flip up with rate c, down with rate $1 - c$
- Up-spin concentration $c = 1/(1 + \mathrm{e}^{\beta})$
- Hierarchy of timescales: to relax up-spin at distance ℓ, energy barrier $\alpha_\ell = \lceil \log_2 \ell \rceil$, timescale $\tau_\ell \sim \mathrm{e}^{\beta\alpha_\ell} \sim c^{-\alpha_\ell}$
- Path entropy matters once $\ell \sim 1/c$, timescale $\tau_{1/c} = \tau_0 \sim \mathrm{e}^{\beta^2/(2\ln 2)}$
- For larger ℓ, $\tau_\ell \sim c\ell\tau_0$ from $\approx$ independent events on length scale $1/c$

East model with activity bias

- Activity K = nr. of spin flips over time $t_{\rm obs}$
- Biased ensemble of trajectories $[\mathcal{C}(t)]$
  $\mathrm{Prob}[\mathcal{C}(t), s] \propto \mathrm{Prob}[\mathcal{C}(t), 0]\mathrm{e}^{-sK}/\langle \mathrm{e}^{-sK}\rangle_0$
- $s < 0$ favours large activity
- $s > 0$ gives inactive state
- Dynamical free energy $\mathrm{e}^{-N t_{\rm obs}\psi_K(s)} = \langle \mathrm{e}^{-sK}\rangle_0$
- $\psi_K(s)$ has kink at $s = 0$
- Dynamical phase transition there, bimodal distribution of K

Analogy with equilibrium statistical mechanics

Equilibrium:

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

Space-time:

- Bias trajectories by factor e^{-sK}
- Dynamical free energy

Activity vs escape rate bias

- Dynamical free energy is largest eigenvalue of deformed master operator $\mathbb{W}_K(s)$ (Spohn Lebowitz)
- $\mathbb{W}_K(s) = \mathbb{W}$ but with all off-diagonal elements mult. by e^{-s}
- So $\mathrm{e}^s \mathbb{W}_K(s) = \mathbb{W}$ with all diagonal elements mult. by e^s
- Diagonal elements are (negative) escape rates $-r(\mathcal{C})$

$$r(\mathcal{C}) = \sum_i r_i, \qquad r_i = (1-c)n_{i-1}n_i + cn_{i-1}(1-n_i)$$

- So $\mathrm{e}^s \mathbb{W}_K(s) = \mathbb{W} \; - r(\mathcal{C})(\mathrm{e}^s - 1)$ on diagonals
- Deformed master operator for ensemble biased w.r.t. integrated escape rate $R[\mathcal{C}(t)] = \int_0^{t_{\mathrm{obs}}} dt\, r(\mathcal{C}(t))$
- Trajectory weights $\mathrm{Prob}[\mathcal{C}(t), \nu] \propto \mathrm{Prob}[\mathcal{C}(t), 0]\mathrm{e}^{\nu R}$
- Here $\nu = 1 - \mathrm{e}^s$, free energies related by $\psi_R(\nu) = \mathrm{e}^s \psi_K(s)$

Auxiliary master operator & effective interaction

- Biased trajectories reach a steady state away from transients near $t = 0$ and $t = t_{\rm obs}$
- Steady state dynamics is governed by auxiliary master operator (e.g. Simon, Jack PS)
- Obtained from deformed (biased) operator by multiplying transition rates à la Metropolis, by $e^{[\Delta V(\mathcal{C})-\Delta V(\mathcal{C}')]/2}$ (Evans)
- Steady state $P_{\rm s}(\mathcal{C}) \propto e^{-\beta\sum_i n_i - \Delta V(\mathcal{C})}$
- $\Delta V(\mathcal{C})$ is effective interaction
- Can in principle be got from $u_{\mathcal{C}} = e^{-\Delta V(\mathcal{C})/2}$ = leading left eigenvector of deformed master operator

Observables

To understand the effects of bias ν will use:

- mean escape rate $r(\nu) = \langle R \rangle_\nu / (N t_{\rm obs}) = -\psi_R'(\nu)$
- susceptibility $\chi_R(\nu) = r'(\nu) = -\psi_R''(\nu)$,
  also gives variance of R
- spatial correlations $C(x) = \langle \delta n_i \delta n_{i+x} \rangle_\nu$,
  at equilibrium $C(x) = c(1-c)\delta_{x,0}$
- domain size distribution $p(d)$,
  for domains defined as $10\ldots001\ldots$

Range of ΔV?

- $p(d)$ useful probe of interaction range
- Exponential in equilibrium: $p(d) = c(1-c)^{d-1}$
- Can show: if ΔV has finite range, $p(d)$ remains exponential for $d >$ interaction range
- Will find that at any $\nu > 0$, $p(d)$ decays faster than exponential
- So ΔV must have infinite range
- May be related to question of whether effective potentials are "Gibbsian"

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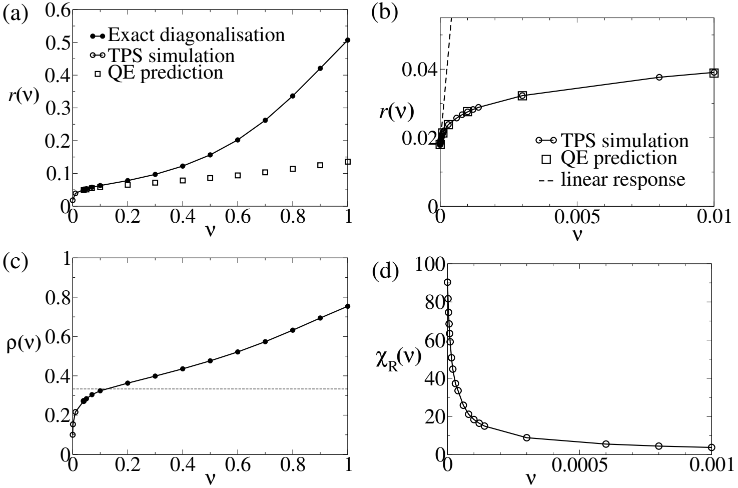
Numerical methods

- To sample biased ensemble numerically, can use transition path sampling ($N = 32 \dots 64$)
- Alternatively diagonalize deformed master operator exactly to find $\psi_R(\nu)$ and ΔV ($N = 14$)
- Checks for finite size effects
  - convergence to large $t_{\rm obs}$ results in TPS
  - comparison of $N = 12$ vs $N = 14$ for exact method
  - check that typical domain sizes $< N$

Mean escape rate, density, susceptibility

c=0.1



Susceptibility and linear response regime

- Susceptibility $\chi_R(\nu)$ grows for $\nu \to 0$
- Have (proportionality factor is $1/(Nt_{\text{obs}})$)

$$\chi_R(\nu) \propto \langle R^2 \rangle_\nu - \langle R \rangle_\nu^2 = \sum_{ij} \int_0^{t_{\text{obs}}} \mathrm{d}t \, \mathrm{d}t' \langle \delta r_i(t) \, \delta r_j(t') \rangle_\nu$$

- For $\nu \to 0$, correlation $\langle \delta r_i(t) \delta r_j(t') \rangle_0$ decays on timescale of order τ_0
- This gives dominant c-dependence of $\chi_R(\nu)$
- Linear response up to $\nu \simeq r(0)/\chi_R(0) \sim \tau_0^{-1}$
- Smallest of a hierarchy of scales for ν

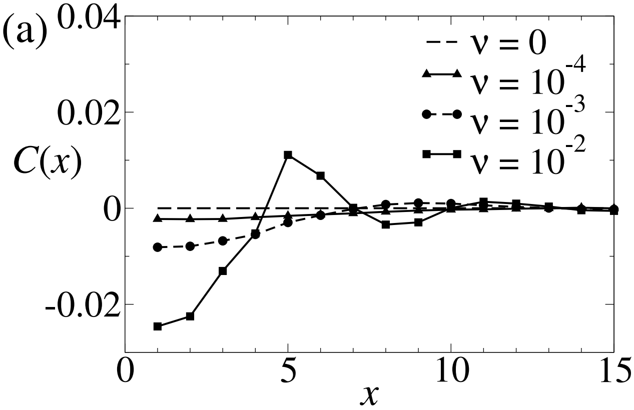
Quasiequilibrium

- Some degrees of freedom can remain quasiequilibrated
- Formally, some probability ratios $P_\mathrm{s}(\mathcal{C})/P_\mathrm{s}(\mathcal{C}')$ stay as for $\nu = 0$, and $\Delta V(\mathcal{C}) - \Delta V(\mathcal{C}')$ remains small
- E.g. if spin i is facilitated, typical lifetime of facilitating spin $i-1$ is $\sim \tau_0 \gg 1/c \Rightarrow$ spin i can flip many times
- Effect of ν on these local flips small if $\nu \ll 1$
- So probability ratio of configurations

  $$\mathcal{C} = \ldots 0 \ldots 010 \ldots$$
  $$\mathcal{C}' = \ldots 0 \ldots 011 \ldots$$

  is as in equilibrium
- For correlations get $\langle n_{i-1} n_i \rangle_\nu \approx \langle n_{i-1} \rangle_\nu c$
- ...and for mean escape rate $r(\nu) = 2c(1-c)\rho(\nu)$ where $\rho =$ up-spin density
- Each up-spin contributes $\approx 2c$ to escape rate

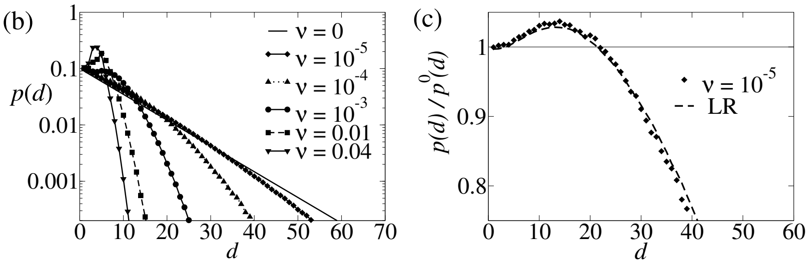
# Spatial correlations
c=0.1



Up spins repel each other, corresponding nearest-neighbour peak
But relatively weak effects

Domain size distribution

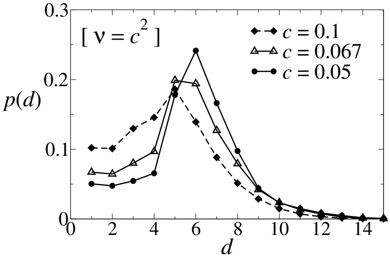
c=0.1



- Large domains suppressed as ν grows
- Eventually get peak at emergent lengthscale d^*
- Quasiequilibrium: $p(1) \approx c$, ok

Scaling for $c \to 0$

$\nu = c^2$



- Consider small c limit with $\nu = c^b$ (here $b = 2$)
- Peak becomes sharper: $p(d)$ for $d < d^*$ shrinks
- Consider linear response next to understand this

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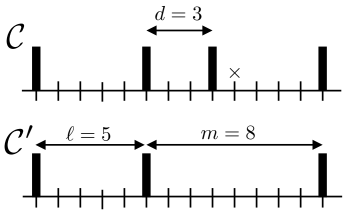
Effective interaction

- By linear response theory can relate effects of small ν to equilibrium correlations
- For effective interaction find $\Delta V_{\mathcal{C}} = -2\nu R_{\mathcal{C}} + O(\nu^2)$
- Here the propensity is

$$R_{\mathcal{C}} \equiv \sum_j \int_0^\infty dt\, \langle \delta r_j(t) \rangle_{\mathcal{C}}$$

- Mean change in escape rate when starting in configuration $\mathcal{C}$
- Still need to understand how $R_{\mathcal{C}}$ depends on $\mathcal{C}$ (2^N numbers)
- But useful for intuition

Propensity differences



- If $\alpha_d < \alpha_{m-d}, \alpha_l$ then $\mathcal{C}$ relaxes to $\mathcal{C}'$ on timescale τ_d
- Main contribution to propensity difference from site $\times$
- Facilitating up-spin has lifetime τ_d, so $R_\mathcal{C} - R_{\mathcal{C}'} \approx 2c\tau_d$
- Hence $\Delta V_{\mathcal{C}'} - \Delta V_\mathcal{C} \approx 4\nu c\tau_d$
- Depends strongly on d (for $d = 1$ get $O(1)$ difference), e.g. $\sim \nu c^{-b}$ for $d = 1 + 2^b$
- Configurations are favoured for having more spins, but far apart (large d)

Domain size distribution

With same arguments can estimate linear response of $p(d)$:

$$\frac{p(d)}{p^0(d)} \simeq 1 + A_1\nu + O(\nu^2), \qquad d = 1$$

$$\frac{p(d)}{p^0(d)} \simeq 1 + A_d\nu/c^{\alpha_d - 1} + O(\nu^2), \qquad 2 \le d \lesssim 1/c$$

$$\frac{p(d)}{p^0(d)} \simeq 1 - A_d\nu\tau_0 c^2 d(cd-1) + O(\nu^2), \qquad d \gtrsim 1/c$$

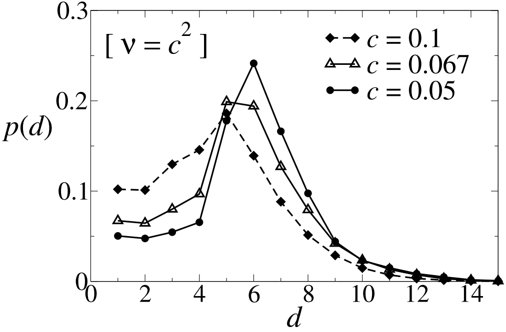
Suppression of very large domains: reduction in propensity from down-spins in interior of domain significant

Hierarchy of responses

- Generalization of quasiequilibrium argument for $\nu \ll 1$
- Consider $\nu \ll c^{b-1}$
- Domains of sizes $d \leq 2^b$ weakly affected by ν
  (relative linear response correction is $\ll 1$)
- So $p(d) = O(c)$ for $d \leq 2^b$
- Larger d: relative response large, expect $p(d) = O(1)$

Revisit earlier results

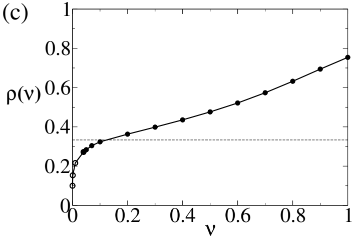
$\nu = c^2$



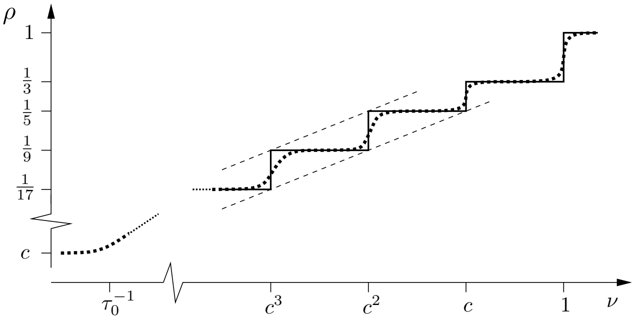
- $\nu = c^2 \ll c = c^{b-1}$ with $b = 2$
- So expect $p(d) = O(c)$ for $d \leq 2^b = 4$
- Larger domains have finite probability

Plateau regions

- Consider ν between two scales, $c^b \ll \nu \ll c^{b-1}$
- $p(d) = O(c)$ for $d \leq 2^b$ as before
- Larger domains can have $p(d) = O(1)$
- System can maximize its escape rate by making most (all?) domains of size $d = 2^b + 1$
- So should get density $\rho = 1/(2^b + 1)$
- E.g. $\rho = 1/3$ for $c \ll \nu \ll 1$
- Numerical results consistent with this



Summary of hierarchy



- Close similarity to hierarchical density evolution during aging
- Entropy vanishing in plateaux so non-monotonic in ν?

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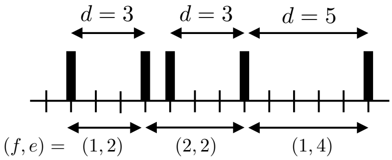
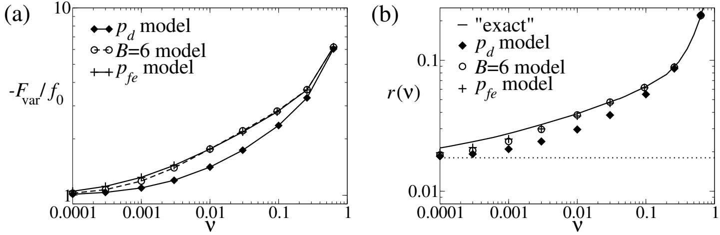
Variational approach

- Escape rate bias acts only on diagonal elements of $\mathbb{W}$ so does not destroy detailed balance
- Can determine dynamical free energy $\psi_R(\nu)$ variationally
- Choose tractable classes of effective interactions
  - Interactions of blocks of B spins: maximal range $B-1$, up to B-body
  - Bias on $p(d)$: interaction of 1's separated by string of 0's
  - Bias on $p(f,e)$: same with domains defined as string of 1's followed by string of 0's



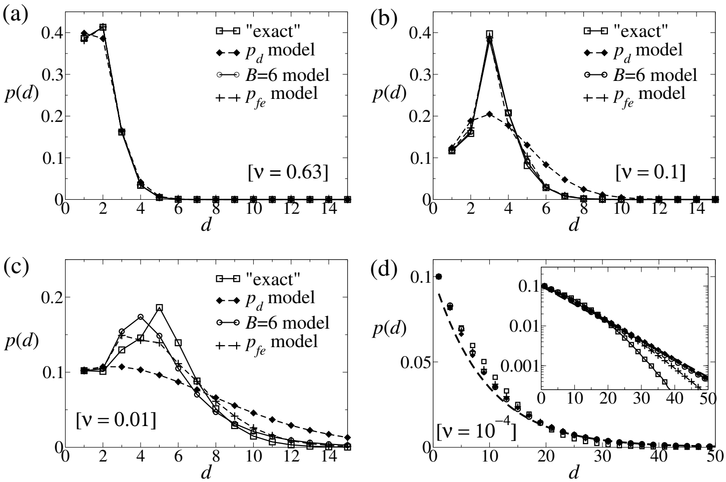
# Free energy and mean escape rate
c=0.1



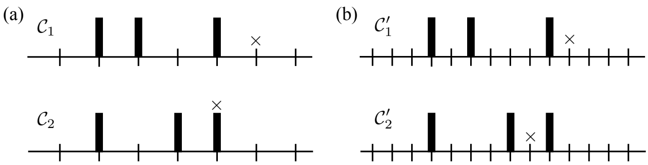
- Free energy plotted as ratio with linear baseline $-f_0 = \nu r(0)$
- All approximations decent for larger ν but become worse as ν decreases
- $p(f, e)$ model best

Domain size distributions

c=0.1



Where do variational approaches fail?



- $\mathcal{C}_1$ has longer-lived "superspin" than $\mathcal{C}_2$ so is favoured
- $p(d)$ model cannot represent this; $p(f,e)$ can, and captures quasiequilbrium by $p(f+1,e) \approx cp(f,e+1)$
- But $p(f,e)$ model fails similarly at next level up (all lengthscales doubled)
- Block model will fail once preferred domain size $> B-1$

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Summary & outlook

- In linear response, have found general link between effective interaction and propensity
- For East model specifically, hierarchical structure of response
- Similar to aging case
- Conjecture for simple ordered structure of system in plateau regions of ν, non-monotonic entropy
- Variational approaches can be useful but need physical insight
- Timescale separation leads to weak interactions on short lengthscales, may be helpful in other contexts