Accelerating, to some extent, the p-spin dynamics

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1. Sampling Boltzmann

How to sample the Boltzmann distribution $\rho_B \propto e^{-\beta V}$?

- Brownian Dynamics (underdamped or overdamped)
- Molecular Dynamics with deterministic thermostats
- Markov Chain Monte Carlo

When is it hard? Supercooled liquids, protein folding, optimization problems...

2. Fast Convergence through smart dynamics

How to fight dynamical sluggishness?

One solution: Equilibrium & nonequilibrium alternatives to molecular dynamics that nevertheless sample the Boltzmann weight:

- Transition Path Sampling
- Event Chain Monte Carlo
- SWAP Monte Carlo
- Parallel tempering

Another possibility: local breaking of detailed balance. Why?

Irreversible samplers relax faster than their equilibrium counterparts [1]

$$\tau_{\rm irr} \le \tau_{\rm rev}$$

An example? Lifting: two copies of the system with probability flows allowed between them $\to$ theoretically appealing [2, 3, 4]

3. Ichiki-Ohzeki (IO) dynamics

Two copies of the same system with antisymmetric couplings:

$$\dot{\mathbf{x}}^{(1)} = -\boldsymbol{\nabla}_{\mathbf{x}^{(1)}} V(\mathbf{x}^{(1)}) + \gamma \boldsymbol{\nabla}_{\mathbf{x}^{(2)}} V(\mathbf{x}^{(2)}) + \sqrt{2T}\boldsymbol{\eta}^{(1)} \quad (1)$$
$$\dot{\mathbf{x}}^{(2)} = -\boldsymbol{\nabla}_{\mathbf{x}^{(2)}} V(\mathbf{x}^{(2)}) - \gamma \boldsymbol{\nabla}_{\mathbf{x}^{(1)}} V(\mathbf{x}^{(1)}) + \sqrt{2T}\boldsymbol{\eta}^{(2)} \quad (2)$$

Extra current $\mathbf{j}_\gamma$, divergenceless when $\rho_{ss} \propto \rho_{\rm B}^{(1)}\rho_{\rm B}^{(2)} = e^{-\beta V^{(1)}} e^{-\beta V^{(2)}}$

Nonequilibrium dynamics Entropy production $\dot{\Sigma} = 2\gamma^2 \langle \boldsymbol{\nabla}^2 V\rangle_{\rm B} > 0$

Previous works Abstract proof and numerical evidence for qualitative acceleration [5, 6]

Our goal Quantify the extent of the acceleration in activated processes and rugged landscapes

4. Rescaling Kramers time

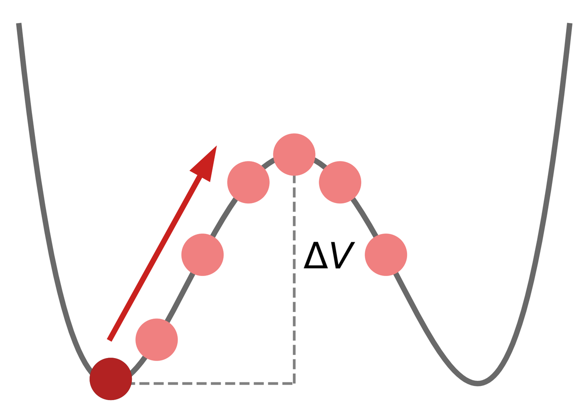
Standard Kramers' time $\tau \sim e^{\beta \Delta V}$

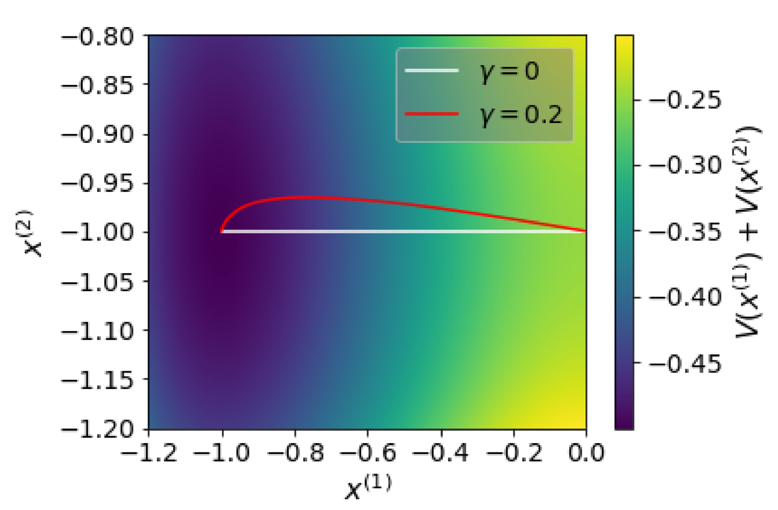
Heuristic reasoning System 2 confined in a very stiff harmonic well

$$\dot{x}^{(1)} = -(1+\gamma^2)V'(x^{(1)}) + \sqrt{2(1+\gamma^2)T}\eta^{(1)}$$

Equilibrium dynamics with rescaled mobility $\Rightarrow \tau \sim \frac{1}{1+\gamma^2} e^{\beta\Delta V}$

Full expression of τ with theory of Bouchet and Reygner [7] $\Rightarrow$ we compute prefactor and instanton trajectories





5. Rugged landscapes - The model

The spherical p−spin A fully connected graph of spin σ_i with quenched disordered couplings and a spherical constraint $\sum_{i=1}^N \langle \sigma_i(t)^2 \rangle = N$

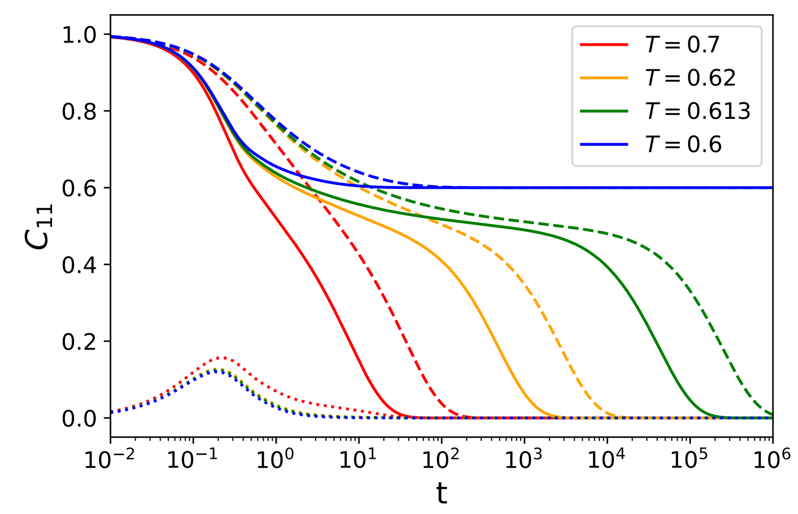
$$\mathscr{H}[\{\sigma_i\}_{i=1,\dots,N}] = -\sum_{i_1<\dots<i_p} J_{i_1\dots i_p}\sigma_{i_1}\dots\sigma_{i_p} \quad (3)$$
$$\overline{J_{i_1\dots i_p}} = 0 \qquad \overline{J^2_{i_1\dots i_p}} = \frac{2J^2}{p!N^{p-1}} \quad (4)$$
$$\partial_t \sigma_i = -\frac{\partial \mathscr{H}}{\partial \sigma_i} - \mu(t)\sigma_i + \sqrt{2T}\eta_i \quad (5)$$

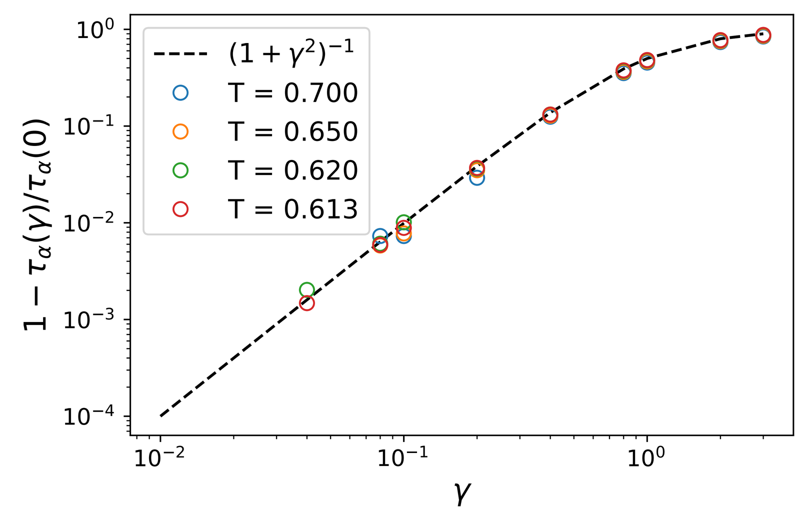
- $\mathbf{T > T_d}$ Ergodic paramagnet
- $\mathbf{T_c < T < T_d}$ Paramagnet with many metastable states $\to$ dynamical ergodicity breaking
- $\mathbf{T < T_c}$ Spin glass

p-spin under IO dynamics: what happens?

6. Rugged landscapes: Results

- T_d is the same, but correlations decay **faster** in the ergodic phase
- We **quantify** the acceleration by looking at the relaxation time τ_α: a factor of $1+\gamma^2$ in the explored regime
- We find an *accidental* fluctuation-dissipation theorem $\to$ **analytical derivation** of the speed-up and of T_d





7. Outlook

- **What we did**: Quantitative analysis of the acceleration of an irreversible sampler of the Boltzmann distribution:
  - One energy barrier
  - A system with rugged landscape
- **Possible developments**:
  - IO dynamics in supercooled liquids and its numerical efficiency
  - Many other irreversible samplers to explore: run and tumble, active Brownian, active Ornstein-Uhlenbeck
  - Combination of IO with underdamped, Nosé-Hoover...

8. References

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