Approximation method to metastability: an application to Ising/Potts models without external fields

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Ferromagnetic Ising/Potts models without external field

Ising/Potts Hamiltonian

- Lattice $\Lambda = \{1, \ldots, L\} \times \{1, \ldots, L\}$ given periodic boundary conditions.
- Spins $S = \{1, 2, \ldots, q\}$ and configuration space $\mathcal{X} = S^\Lambda$.
- For each $\sigma \in \mathcal{X}$, the *Ising/Potts Hamiltonian* is

$$H(\sigma) = \sum_{\{x,y\} \subset \Lambda:\, x \sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\}.$$

For each $a \in S$, denote by $\mathbf{a} \in \mathcal{X}$ the configuration satisfying

$$\mathbf{a}(x) = a \quad \text{for all } x \in \Lambda.$$

Then, collect

$$\mathcal{S} = \{\mathbf{1}, \mathbf{2}, \ldots, \mathbf{q}\}.$$

Each $\mathbf{a} \in \mathcal{S}$ is called a *ground state*, since $\mathcal{S} = \arg\min_{\sigma \in \mathcal{X}} H(\sigma)$.

Gibbs distribution and Metropolis–Hastings dynamics

Gibbs distribution

For inverse temperature $\beta > 0$, the *Gibbs distribution* on $\mathcal{X}$ is

$$\mu_\beta(\sigma) = \frac{1}{Z_\beta} e^{-\beta H(\sigma)}.$$

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Continuous-time Markov chain $\sigma_\beta(t)$, $t \geq 0$ defined by an infinitesimal generator

$$(\mathcal{L}_\beta f)(\sigma) = \sum_{x \in \Lambda} \sum_{a \in S} e^{-\beta \max\{H(\sigma^{x,a}) - H(\sigma), 0\}} [f(\sigma^{x,a}) - f(\sigma)].$$

$\sigma^{x,a} \in \mathcal{X}$: configuration obtained from σ by updating the spin at $x \in \Lambda$ to $a \in S$.

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$\sigma^{x,a} \in \mathcal{X}$: configuration obtained from σ by updating the spin at $x \in \Lambda$ to $a \in S$.

The MH dynamics is irreducible and *reversible* w.r.t. to the Gibbs measure μ_β:

$$\mu_\beta(\sigma) r_\beta(\sigma, \sigma^{x,a}) = \mu_\beta(\sigma^{x,a}) r_\beta(\sigma^{x,a}, \sigma).$$

Comparison to Ising model with positive external field

Classical model: $S = \{1, 2\}$ and the Hamiltonian is

$$H(\sigma) = \sum_{\{x,y\} \subset \Lambda:\, x \sim y} \mathbb{1}\{\sigma(x) \neq \sigma(y)\} - h \sum_{x \in \Lambda} \mathbb{1}\{\sigma(x) = 1\},$$

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- Ben Arous–Cerf '96 : 3D analogue.
- Bovier–Manzo '02 : potential-theoretic approach.

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Features of Ising model with positive external field

1. **1** is stable and **2** is metastable.
2. There is exactly one metastable state, **2**, in the system.
3. The saddle structure is sharp.

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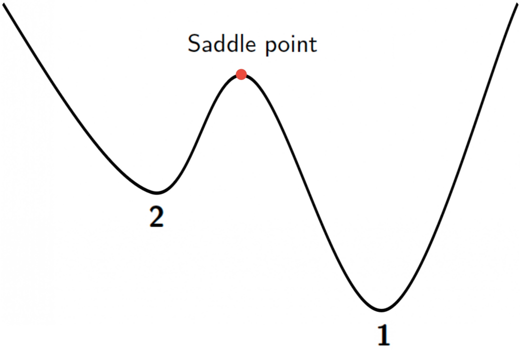

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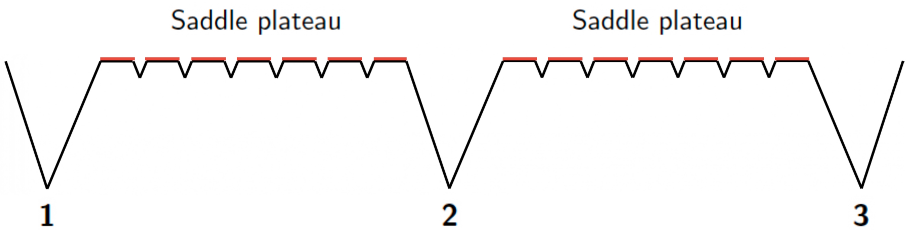

Features of Ising/Potts models with zero external field

1. The ground states in $\mathcal{S} = \{\mathbf{1}, \ldots, \mathbf{q}\}$ are equally metastable.
2. There are more than one metastable state.
3. The saddle structure is flat and forms a huge plateau.

Metastability from pathwise approach

LDP-type results (Nardi–Zocca '19)

Let $\Gamma := 2L + 2$. Suppose that the process starts from $\mathbf{a} \in \mathcal{S}$.

1. $\lim_{\beta\to\infty} \frac{1}{\beta} \log \tau_{\mathcal{S}\setminus\{\mathbf{a}\}} = \Gamma$ in probability.
2. $\lim_{\beta\to\infty} \frac{1}{\beta} \log \mathbb{E}_{\mathbf{a}}[\tau_{\mathcal{S}\setminus\{\mathbf{a}\}}] = \Gamma$.
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Tools: analysis on the energy landscape (energy barrier, depth of valleys, etc.) & pathwise approach applied to the path trajectories.

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Objective 1. Prefactor estimate of $\mathbb{E}_{\mathbf{a}}[\tau_{\mathcal{S}\setminus\{\mathbf{a}\}}]$.

Objective 2. Scaling limit of the successive metastable transitions in $\mathcal{S}$.

Main results

Eyring–Kramers law (K.–Seo '21)

Recall that $\Gamma = 2L + 2$. There exists an explicit prefactor $\kappa = \kappa(L) > 0$ such that

$$\mathbb{E}_{\mathbf{a}}[\tau_{\mathcal{S} \setminus \{\mathbf{a}\}}] \simeq \frac{\kappa}{q-1} \cdot e^{\Gamma\beta}.$$

Moreover, the constant κ satisfies $\lim_{L \to \infty} \kappa(L) = \frac{1}{8}$.

Markov chain model reduction (K.–Seo '21)

The law of the accelerated process $\sigma_\beta(e^{\Gamma\beta}t)$ converges, as $\beta \to \infty$, to the law of a Markov chain $Y(t)$ defined by jump rate $r_Y(\cdot, \cdot) \equiv \frac{1}{\kappa}$.

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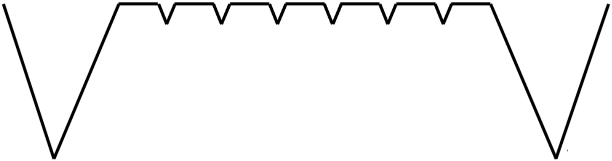
Tools: *precise analysis* on the energy landscape & potential-theoretic and martingale approach to metastability.

Precise analysis on the energy landscape



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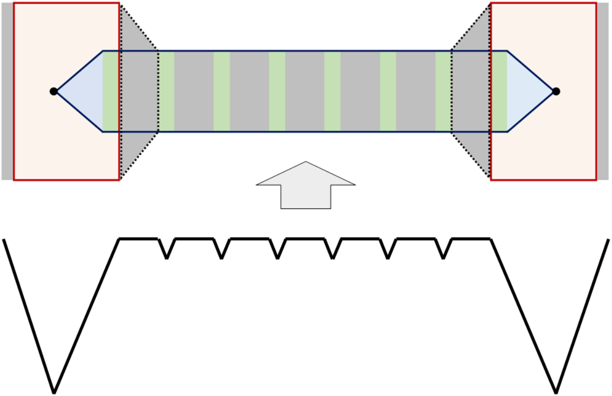

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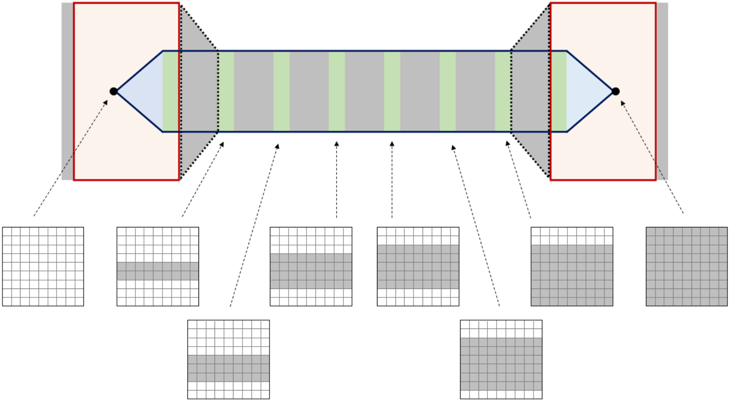

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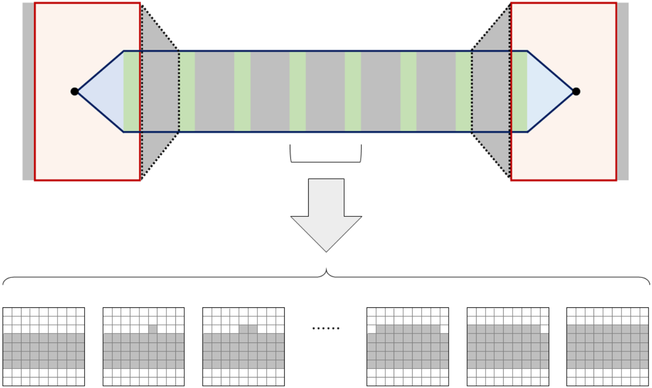

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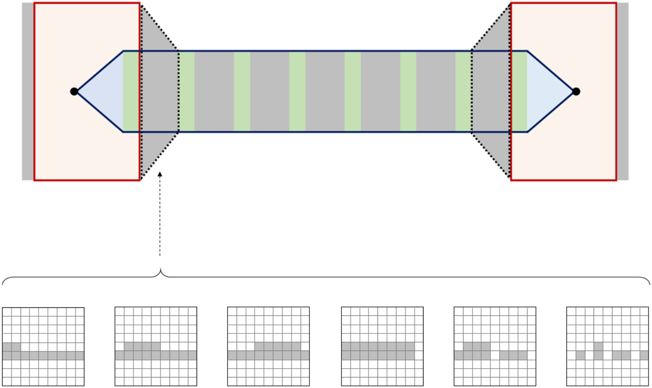
Precise analysis on the energy landscape



1. Transition on the bulk part is one-dimensional.
2. Transition on the edge part is more complex.

Extension 1: non-reversible cyclic dynamics

Cyclic dynamics for $q \geq 3$ (Landim–Seo '16)

Continuous-time Markov chain $\sigma_\beta^{\mathrm{cyc}}(t)$, $t \geq 0$ defined by an infinitesimal generator

$$(\mathcal{L}_\beta^{\mathrm{cyc}} f)(\sigma) = \sum_{x \in \Lambda} e^{-\beta \max_{a \in S} \{H(\sigma^{x,a}) - H(\sigma)\}} [f(\tau_x \sigma) - f(\sigma)].$$

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The cyclic dynamics is irreducible, but *non-reversible* w.r.t. to μ_β, since spins can only rotate in one direction $(1 \to 2 \to \cdots \to q \to 1)$ and not in the opposite direction $(1 \to q \to \cdots \to 2 \to 1)$:

$$r_\beta^{\mathrm{cyc}}(\sigma, \tau_x \sigma) > 0, \quad \text{whereas} \quad r_\beta^{\mathrm{cyc}}(\tau_x \sigma, \sigma) = 0.$$

Main results for cyclic dynamics

Eyring–Kramers law and MC model reduction (K.–Seo '22)

Define $\Gamma' = 2L + 4$. Then, there exists $\kappa' = \kappa'(L) > 0$ such that

$$\mathbb{E}_{\mathbf{a}}[\tau_{\mathcal{S}\setminus\{\mathbf{a}\}}] \simeq \frac{\kappa'}{q-1} \cdot e^{\Gamma'\beta},$$

where $\lim_{L\to\infty} \kappa'(L) = \frac{1}{8}$. Moreover, the law of $\sigma_\beta^{\mathrm{cyc}}(e^{\Gamma'\beta} t)$ converges to the law of a Markov chain $Y'(t)$ defined by jump rate $r_{Y'}(\cdot,\cdot) \equiv \frac{1}{\kappa'}$.

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Remarks.

1. Constants κ and κ' are different (cf. $\lim_{L\to\infty} \kappa(L) = \lim_{L\to\infty} \kappa'(L) = \frac{1}{8}$).
2. Although the microscopic system $\sigma_\beta^{\mathrm{cyc}}(t)$ updates the spins in one direction only, the macroscopic limit $Y'(t)$ becomes symmetric. This suggests a *coarse-graining effect* in the limit which removes the cyclic feature.
3. LDP-type results are also attainable [Cirillo–Nardi–Sohier '15].

Extension 2: three-dimensional model

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where $\lim_{L\to\infty} \kappa^{3D}(L) = \frac{1}{48}$. Moreover, the law of $\sigma_\beta(e^{\Gamma^{3D}\beta} t)$ converges to the law of a Markov chain $Y^{3D}(t)$ defined by jump rate $r_{Y^{3D}}(\cdot,\cdot) \equiv \frac{1}{\kappa^{3D}}$.

Difficulties in three-dimensional model

Energy landscape analysis is far more complicated in the 3D model.

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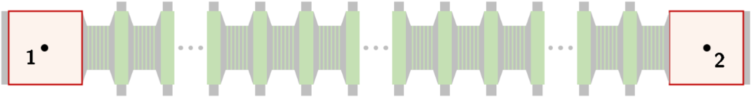

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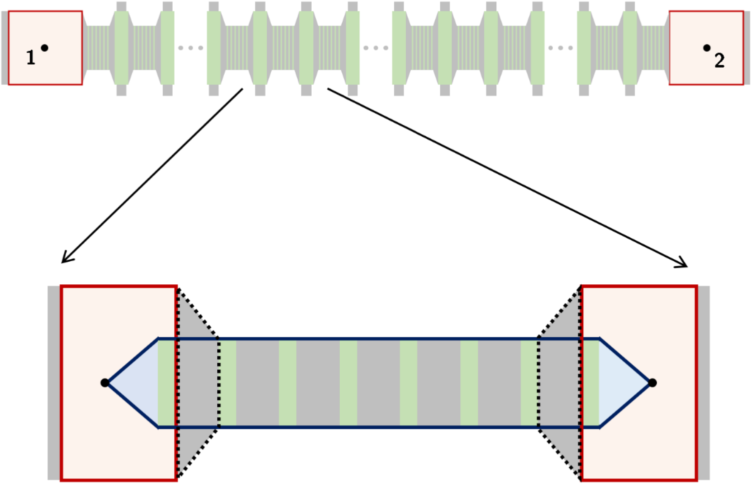

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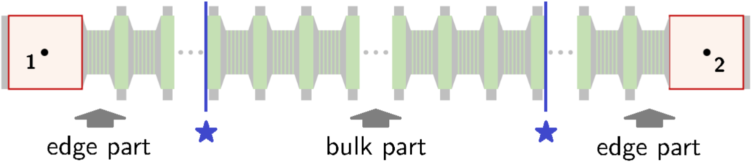

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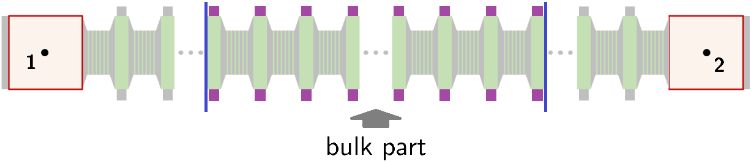

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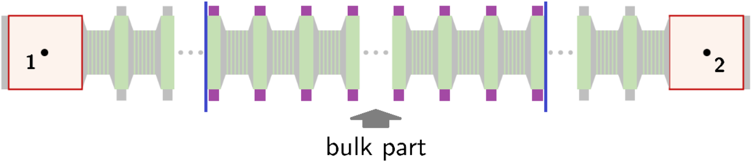

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Remark. In higher dimensions, $d \geq 4$, the energy barrier is conjectured as

$$\Gamma(d) = 2L^{d-1} + 2L^{d-2} + \cdots + 2L + 2.$$

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Sharp thresholds of energy vs. entropy (K.–Seo '22)

1. If $L^{1/2} \ll e^{\beta}$, then the ground states in $\mathcal{S}$ are metastable.
2. If $L^{1/4} \ll e^{\beta} \ll L^{1/2}$, then the valleys around $\mathcal{S}$ are metastable.
3. If $e^{\beta} \ll L^{1/4}$, then the valleys are not metastable.

Idea of proof: analyze the Gibbs distribution μ_β.

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Recall that $\Gamma = 2L + 2$. If $L^3 \ll e^\beta$, it holds that

$$\mathbb{E}_{\mathbf{a}}[\tau_{\mathcal{S} \setminus \{\mathbf{a}\}}] \simeq \frac{1}{8(q-1)} \cdot e^{\Gamma\beta}.$$

Moreover, the law of $\sigma_\beta(e^{\Gamma\beta}t)$ converges to the law of $Y''(t)$ where $r_{Y''}(\cdot, \cdot) \equiv 8$.

Remark. Also applicable to the same model on the 2D hexagonal lattice.

Other extensions and related recent works

Degenerate Potts model with external field towards one direction:

- (negative external field) Bet–Gallo–Nardi '22.
- (positive external field) Bet–Gallo–Nardi '21.

Blume–Capel model with zero chemical potential and zero external field: K. '21.

Potts model with general interaction constants: Bet–Gallo–K. '22.

Potts model with general external fields: Ahn '23+.

Ising model on the hexagonal lattice: Apollonio–Jacquier–Nardi–Troiani '22.

Ising model under Kawasaki dynamics:

- (square lattice) Baldassarri–Nardi '22.
- (hexagonal lattice) Baldassarri–Jacquier '23.

Thank you! Merci!