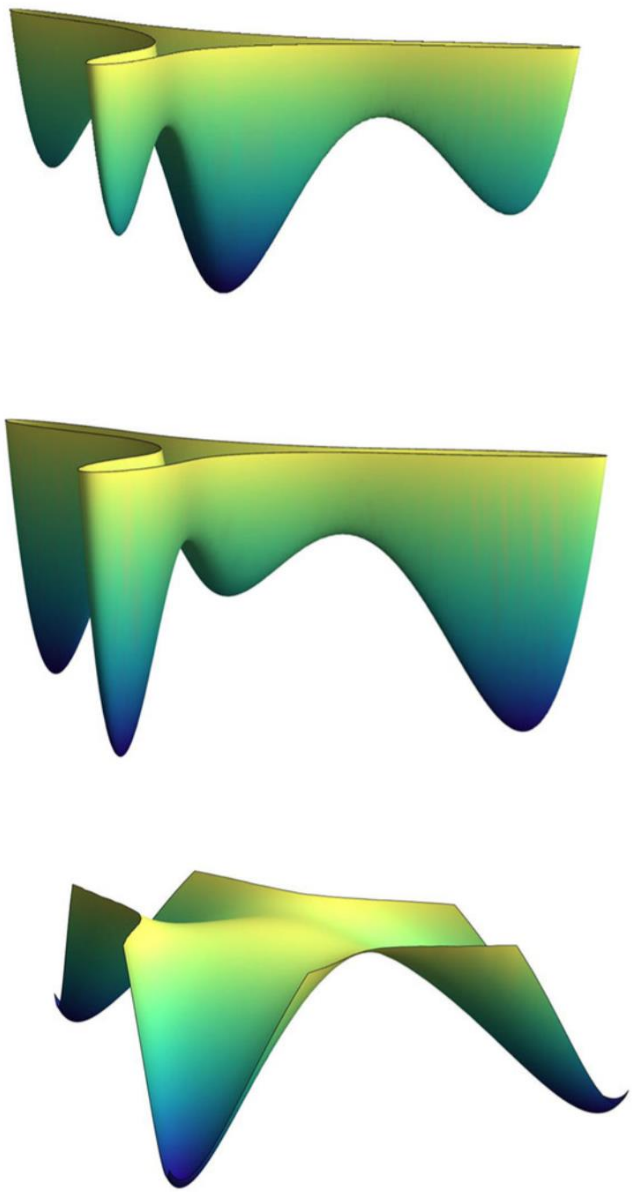

# Metastability For the DCWP Model with Glauber dynamics

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**Probability and geometry on configuration spaces**
**SPP2265: Random Geometric Systems**

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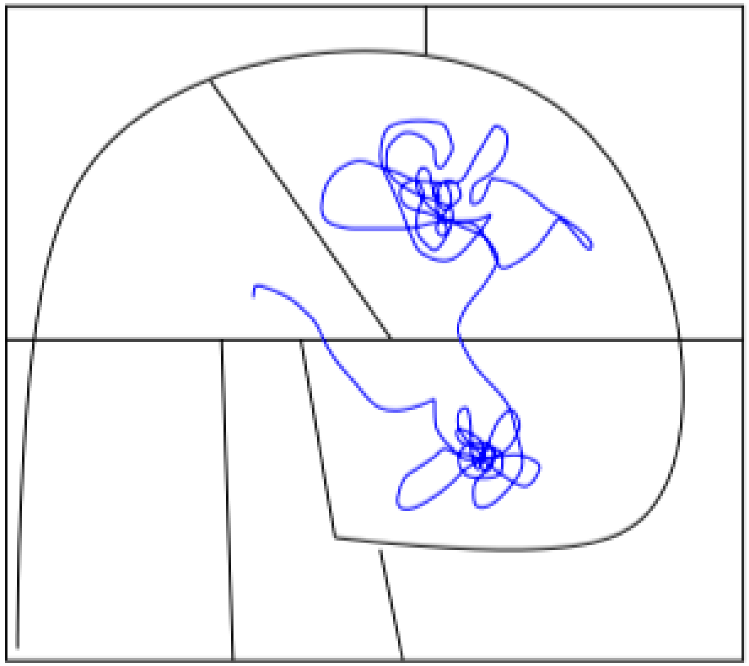
Joint work with Johan Dubbeldam, Elena Pulvirenti and Martin Slowik

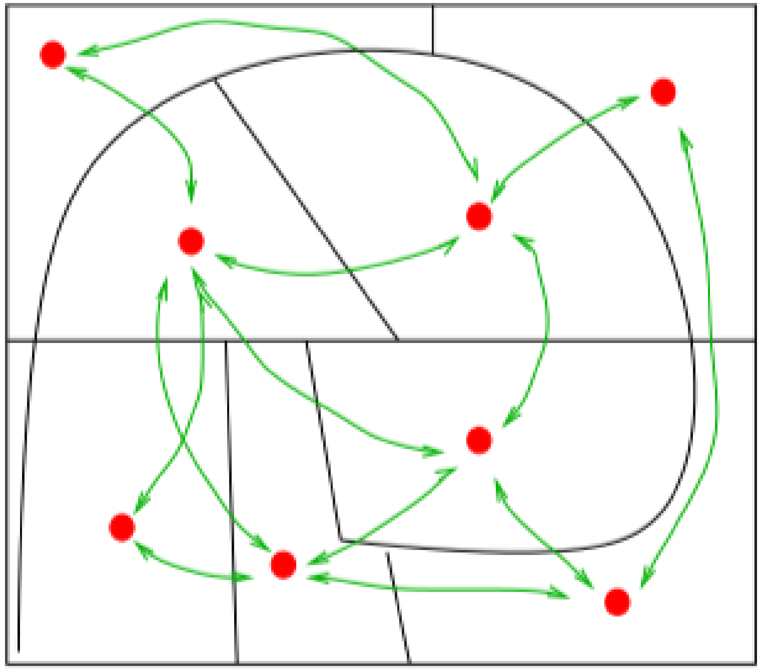
SPP2265 Random Geometric Systems

# What is metastability?

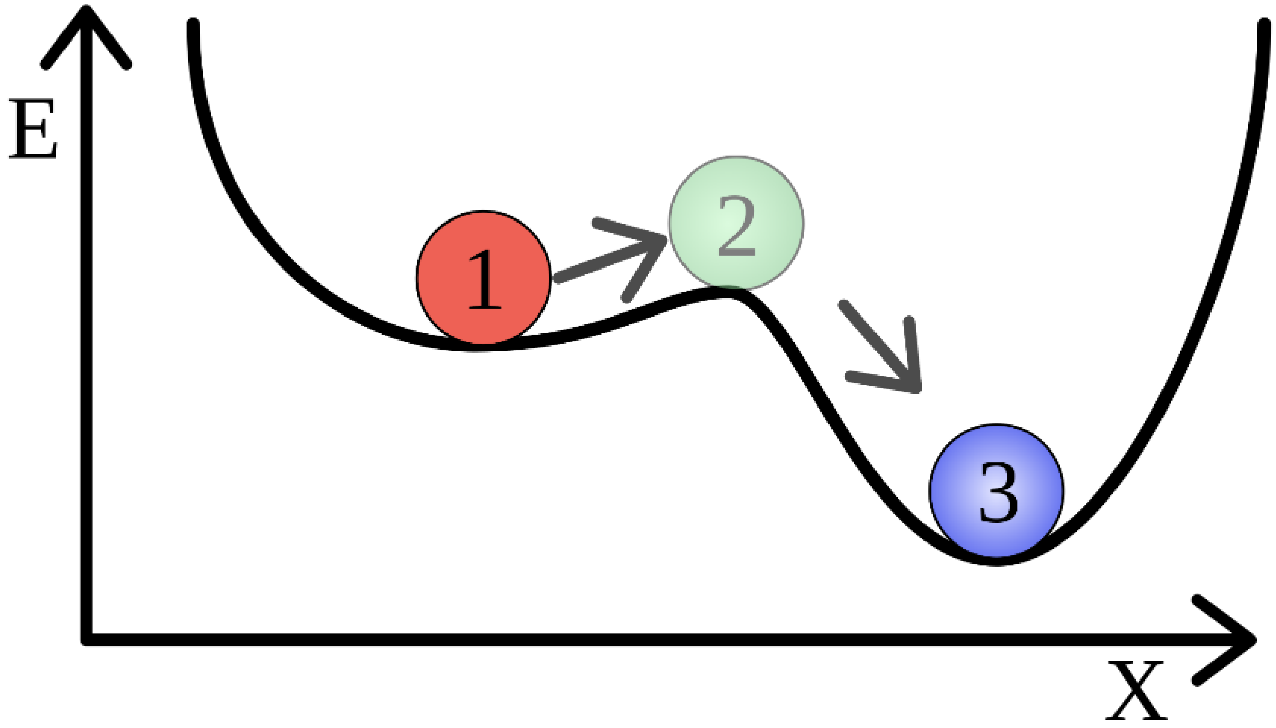
Metastability is a dynamical phenomenon where a system under the influence of stochastic dynamics moves between different regions **on different timescales.** Reword simpler

In physical systems, this takes the form of transitions between different local energy valleys.

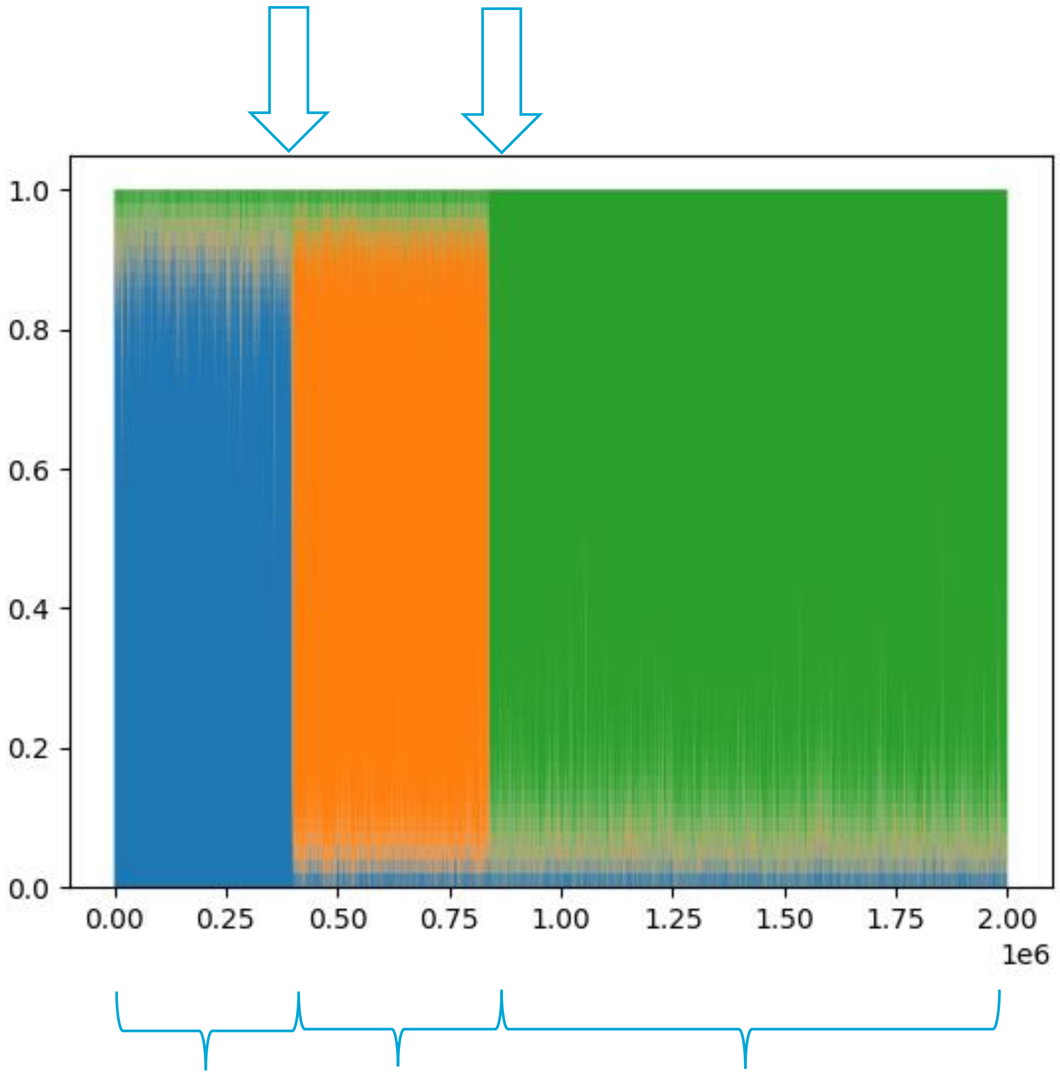




# Metastability continued

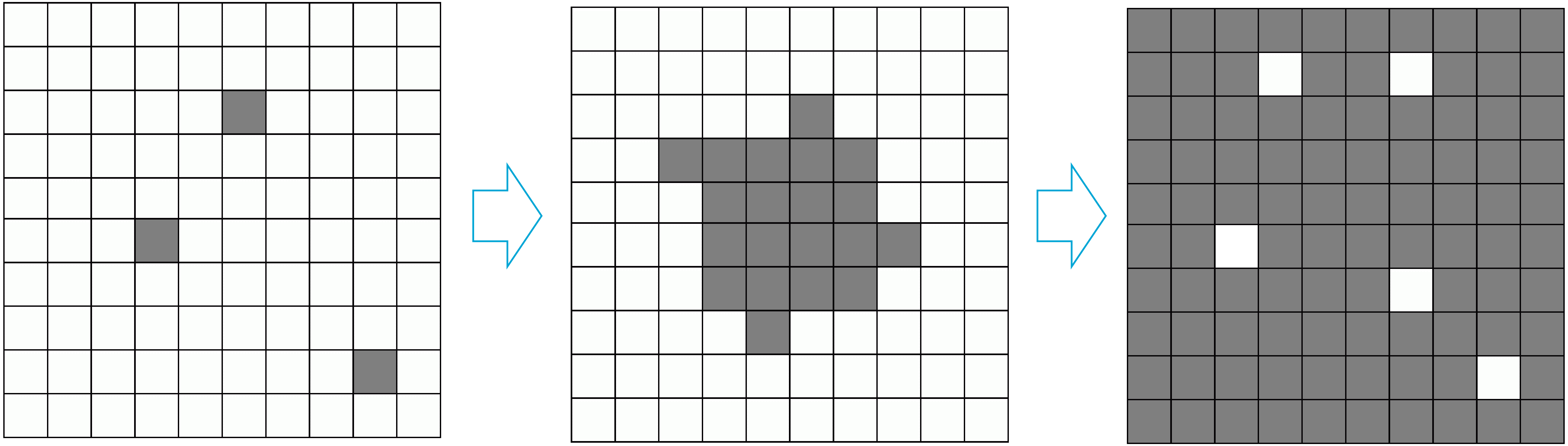


# Metastability continued



# Metastability continued

Ising model on a grid



# Metastability continued

Let $(X(t))_{t>0}$ be a Markov process over $\mathcal{S}$, and let $\mathcal{M} = \{\mathcal{M}_1, \ldots, \mathcal{M}_K\}, \mathcal{M}_i \subset \mathcal{S}$ be our candidate metastable set collection

Let us define the return time to a set $\mathcal{A} \subset \mathcal{S}$ by

$$\tau_{\mathcal{A}} := \inf \{t > 0 : X(t) \in \mathcal{A}, X(t-) \notin \mathcal{A}\}$$

Then $(X(t))_{t>0}$ is said to be $\rho$-metastable with respect to the collection $\mathcal{M}$ if and only if

Each $\mathcal{M}_j$ is hard to leave for the others

$$K \frac{\max_{j\in\{1,\ldots,K\}} \mathrm{P}_{\mu|\mathcal{M}_j}\left[\tau_{\cup\mathcal{M}\setminus\mathcal{M}_j} < \tau_{\mathcal{M}_j}\right]}{\min_{\mathcal{B}\subset\mathcal{S}\setminus\cup\mathcal{M}} \mathrm{P}_{\mu|\mathcal{B}}\left[\tau_{\cup\mathcal{M}} < \tau_{\mathcal{B}}\right]} \leq \rho \ll 1$$

There must not be other hard to leave sets

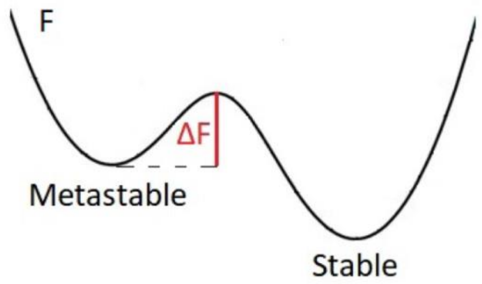
# How to study metastability?

The geometry of the free energy landscape gives us information about metastability

- Global minimum
- Local minima
- Saddle points

⇨

stable state
metastable state
gates/critical droplets




A central quantity is the mean hitting time from a metastable to a metastable set.

Hitting times between metastable sets behave like exponential RVs (no memory)

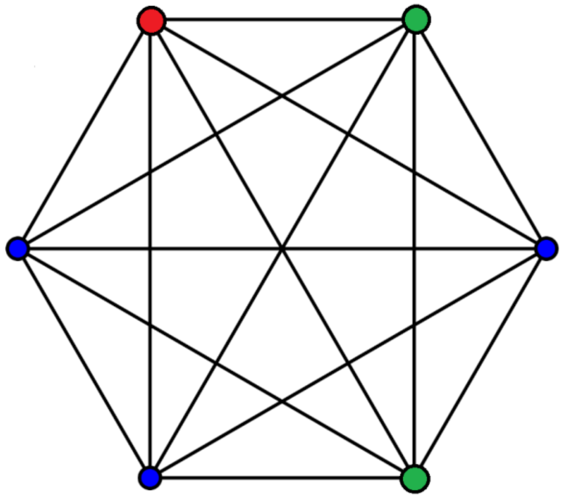
Metastable systems recover **Arrhenius law:** for $N \to \infty,\ \mathrm{E}(\tau) \sim \exp(N\Delta F)$

Typically, trajectories in state space pass through from gates/critical droplets.

Trough **potential theory** we will obtain explicit expressions for the hitting time.

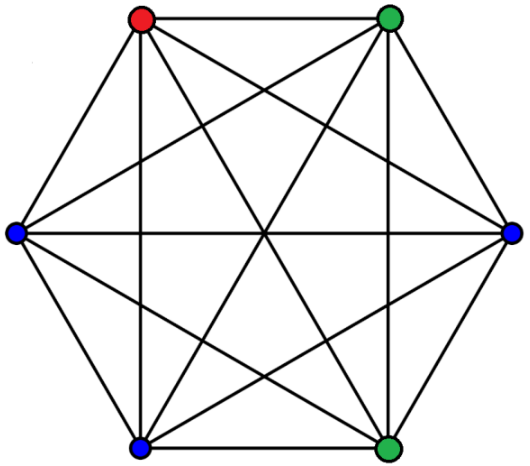
# The CWP model

- Mean field spin particle model, with configuration space
  $\mathcal{S}_N = \{1, \dots, q\}^N, \quad \sigma = (\sigma_1, \cdots, \sigma_N) \in \mathcal{S}_N$
- CWP Hamiltonian given by $\tilde{H}_N(\sigma) := \frac{-1}{N} \sum_{i<j}^{N} \mathbb{1}_{\sigma_i = \sigma_j} \propto N$
- Equilibrium Gibbs measure given by $\tilde{\mu}_N(\sigma) = \frac{e^{-\beta \tilde{H}_N(\sigma)}}{\tilde{Z}_N},$
- **Can** be expressed in terms of empirical magnetization.
- **Symmetry** on both **colors** and **positions.**

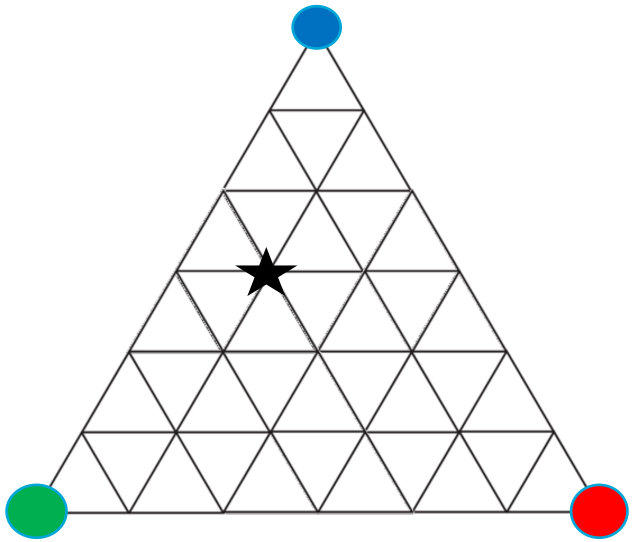


$\sigma \in \mathcal{S}_6, \quad q = 3$

# The CWP model: empirical magnetization



$\sigma \in \mathcal{S}_6, \quad q = 3$



$\mathcal{P}^1_{3,4}$

$$\rho_N : S_N \to \mathcal{P}^1_{q,N} := \left\{ x \in N^{-1}\mathbb{N}^q : \sum_{k=1}^{q} x_k = 1 \right\},$$

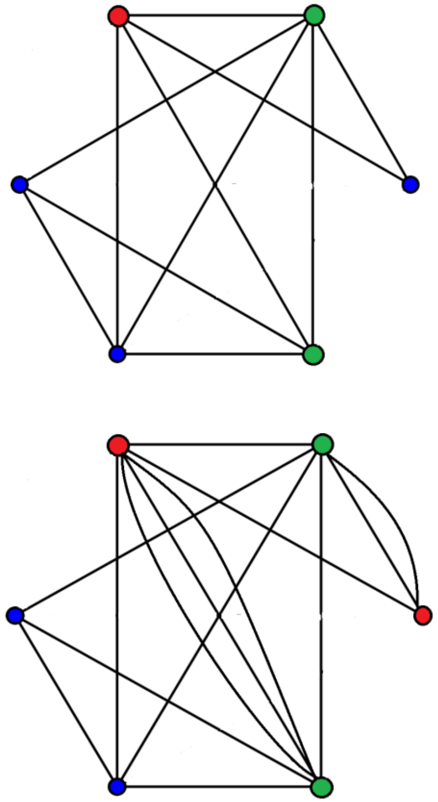
$$\sigma \mapsto \left( \rho_N^{(1)}(\sigma), \dots, \rho_N^{(q)}(\sigma) \right),$$

$$\tilde{H}_N(\sigma) = \frac{-N}{2} \|\rho_N(\sigma)\|_2^2 + \frac{1}{2} := \frac{N}{2} E_N(\rho_N(\sigma))$$

$$\rho_N^{(r)}(\sigma) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{\sigma_i = r}$$

# The DCWP model

- $J = (J_{ij})_{1\leq i<j\leq\infty}$ triangular array with i.i.d mean 1 entries variance $v$ (+regularity conditions)
- CWP Hamiltonian given by $H_N(\sigma) := \frac{-1}{N}\sum_{i<j}^{N} J_{ij}\mathbb{1}_{\sigma_i=\sigma_j}$
- Gibbs measure $\mu_N$ analogously defined
- Close to CWP Hamiltonian: $\mathbb{E}[H_N(\sigma)] = \tilde{H}_N(\sigma), \quad \mathbb{V}[H_N(\sigma)] \leq \frac{v}{2}$
- **Can't** be expressed in terms of the empirical magnetization.
- Depending on the edge weights, can thought as a Potts model over a random graph (Erdős–Rényi, multiedge)
- Breaks the position symmetry (edge weights)
- Maintains color symmetry (absence of magnetic field)



# Glauber dynamics

Both models can be endowed with spin flip dynamics: let $\sigma, \eta \in \mathcal{S}_N$ adjacent configurations, then define $(\Sigma_N(n))_{n\geq 0}$ on $\mathcal{S}_N$ with transition probabilities

$$p_N(\sigma,\eta) = \begin{cases} \frac{1}{qN} e^{-\beta[H_N(\eta)-H_N(\sigma)]_+} & \text{if} \quad d(\sigma,\eta)=1 \\ 0 & \text{otherwise} \end{cases},$$

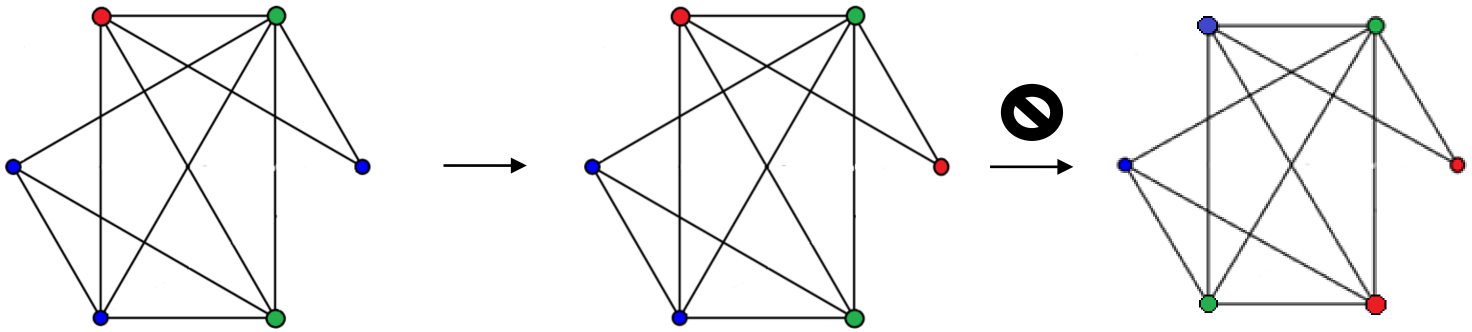
Analogously define $(\tilde{\Sigma}_N(n))_{n\geq 0}$.
$\mu_N, \tilde{\mu}_N$ are their reversible measures

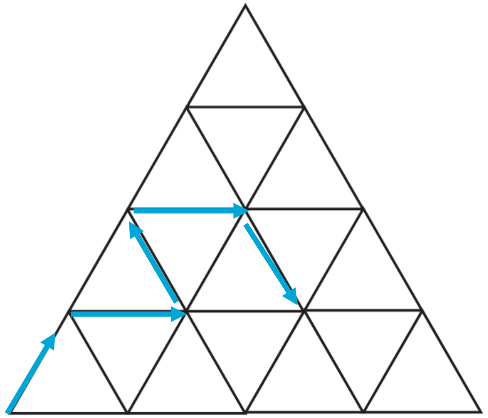
$(\rho_N(\Sigma_N(n)))_{n\geq 0}$ **is not** a Markov process.

$(\rho_N(\tilde{\Sigma}_N(n)))_{n\geq 0}$ **is** a Markov process (lumping property). Closest neighbor weighted random walk with reversible measure

$$\eta(x) = \tilde{\mu}_N(\rho_N^{-1}(x)) \approx \frac{\exp(-\beta N F_\beta(x))}{(2\pi N)^{\frac{q-1}{2}} \tilde{Z}_N}$$

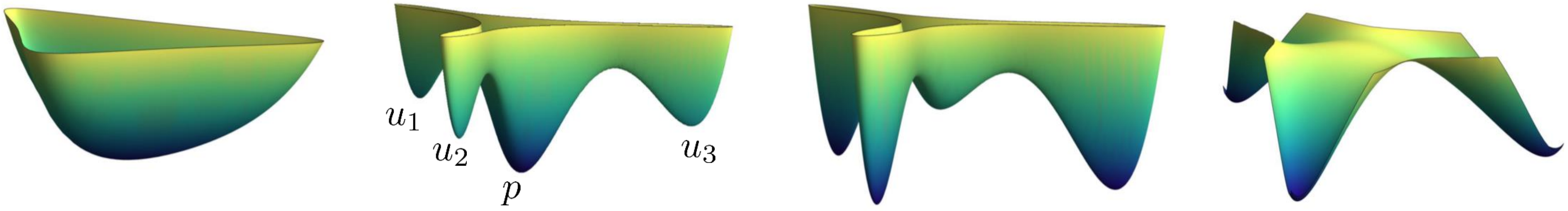
# Glauber dynamics





# Lumped annealed free energy landscape, q=3

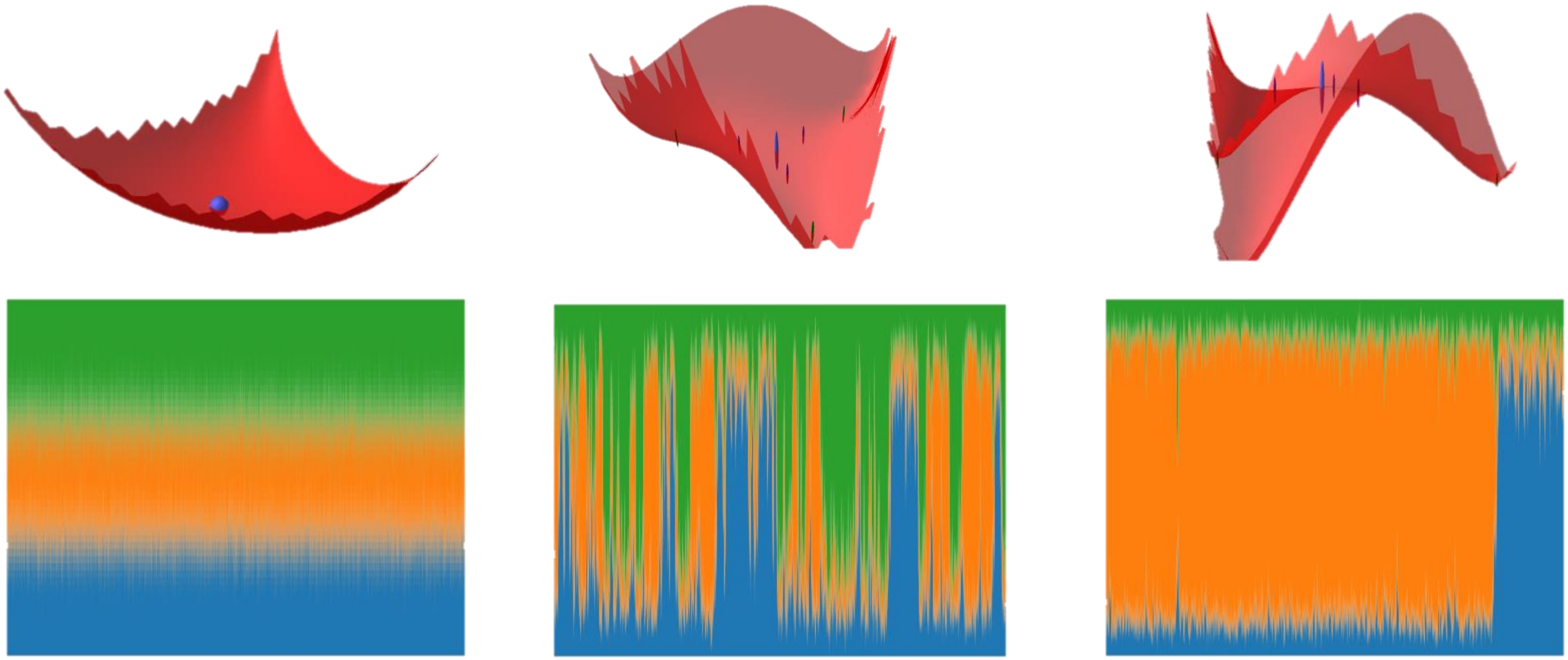
$$F_\beta(x) = -\frac{\|x\|_2^2}{2} + \frac{1}{\beta}\sum_{k=1}^{q} x_k \ln x_k$$




| | | | |
|---|---|---|---|
| $0 < \beta < \beta_1$ | $\beta_1 < \beta < \beta_2$ | $\beta_2 < \beta < \beta_3$ | $\beta_3 < \beta$ |
| Not metastable | Metastable,<br>one global minimum<br>3 local minima | Metastable,<br>one local minimum<br>3 global minima | Metastable,<br>3 global minima |

- Due to symmetry metastable regimes are degenerate: multiple minima with the same energy.

# Simulations for the DCWP model



$-\ln \mu_N(\rho_N^{-1}(x))$

Sampling via simulations

$0 < \beta < \beta_1$ | $\beta_2 < \beta < \beta_3$ | $\beta_3 < \beta$

# Key questions

Start defining $\mathcal{M}_0 = \rho_N^{-1}(p), \quad , \mathcal{M}_k = \rho_N^{-1}(u_k), \quad , k \in \{1,2,3\}$

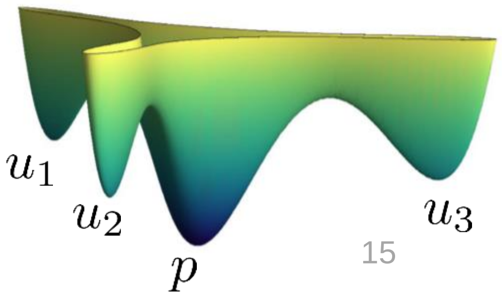
Assume $\beta_1 < \beta < \beta_2$ is such that the CWP model is $e^{-k_1 N}$-metastable with respect to the sets $\mathcal{M}_0, \cdots, \mathcal{M}_q$

Q: Is the DCWP model metastable for the **same** $\beta$ and metastable sets?
**A: Yes ,with probability going to 1 and metastability constant** $e^{-k_2 N}, k_2 < k_1$ .

Let $\mathcal{A} = \mathcal{M}_1 \cup \mathcal{M}_2 \cup \mathcal{M}_3, \, \mathcal{B} = \mathcal{M}_0$ and $\nu_{\mathcal{A},\mathcal{B}}$ the last exit biased distribution.

Q: What can we say about the mean hitting time $\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]$ ?
**A: Two types of results: moment and tail estimates.**

Q: What can we say about different $\mathcal{A}$ , $\mathcal{B}$ ?
**A:**



# Main Theorems

**Assumption** *Let $\beta_1 < \beta < \beta_2$. The CWP model is $e^{-k_1 N}$ metastable with respect to the collection $\mathcal{M} = \mathcal{M}_0, \cdots, \mathcal{M}_3$.*

**Theorem 1:** *There exists $0 < k_2 < k_1$ such that the event $\{(\Sigma_N(t))_{t\geq 0}$ is $e^{-k_2 N}$-metastable with respect to $\mathcal{M}\}$ has probability going to 1 as $N \to \infty$.*

Strategy of proof: from the potential-theoretic definition of metastability

$$|\mathcal{M}| \frac{\tilde{\text{cap}}(\mathcal{M}_l, \cup\mathcal{M} \setminus \mathcal{M}_l)/\tilde{\mu}[\mathcal{M}_l]}{\tilde{\text{cap}}(\mathcal{C}, \cup\mathcal{M})/\tilde{\mu}[\mathcal{C}]} \leq e^{-k_1 N}$$

The CWP and DCWP capacities and measures deviate by an order of $e^{C\sqrt{N}}$ with probability going to 1, preserving the exponential order on the r.h.s..

# Main Theorems

**Theorem 2:** *for any* $r > 0$, *and* $N$ *big enough we have*

$$e^{-\frac{\beta^2 v}{4}}(1 + o(1)) \leq \frac{\mathbb{E}\left[\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]^r\right]^{\frac{1}{r}}}{\tilde{\mathrm{E}}_{\tilde{\nu}_{\mathcal{A},\mathcal{B}}}[\tilde{\tau}_{\mathcal{B}}]} \leq e^{4r\frac{\beta^2 v}{4}}(1 + o(1)).$$

**Theorem 3:** *Let* $\beta$ *be such that* $\mathcal{A}, \mathcal{B}$ *as previously defined. Then are constants* $c_1, c_2, c_3, c_4, \alpha$ *such that* $\forall s > 0$

$$\lim_{N\to\infty} \mathbb{P}\left[c_1 e^{-t-\alpha}(1 + o(1)) \leq \frac{\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]}{\tilde{\mathrm{E}}_{\tilde{\nu}_{\mathcal{A},\mathcal{B}}}[\tilde{\tau}_{\mathcal{B}}]} \leq c_2 e^{t+\alpha}(1 + o(1))\right] \geq 1 - c_3 e^{-c_4 s^2}.$$

# Main Theorems

**Sketch of proof for Theorem 3:**

$$\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}] = \frac{\sum_{x\in\mathcal{S}} \mu(x) h_{\mathcal{A},\mathcal{B}}(x)}{\mathrm{cap}(\mathcal{A},\mathcal{B})}$$

$$\ln\left(\frac{\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]}{\tilde{\mathrm{E}}_{\tilde{\nu}_{\mathcal{A},\mathcal{B}}}[\tilde{\tau}_{\mathcal{B}}]}\right) = \ln\big(\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]\big) - \mathbb{E}[\ln\big(\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]\big)] + \mathbb{E}[\ln\big(\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}]\big)] - \ln\Big(\tilde{\mathrm{E}}_{\tilde{\nu}_{\mathcal{A},\mathcal{B}}}[\tilde{\tau}_{\mathcal{B}}]\Big)$$

⇩ Concentration inequality for Lipschitz functions

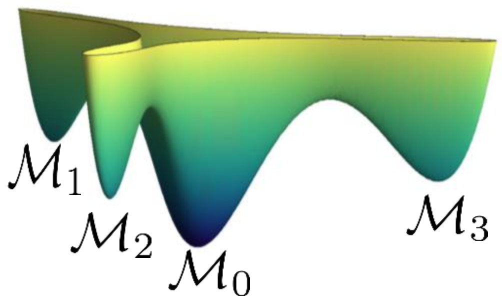
⇩ Annealed estimates

$e^{-k_1 N}$ metastability let's us approximate the log of the harmonic sum by the depth of the valley, which is Lipschitz on the random weights.

Variational principles let us estimate capacity.

# Challenges

Consider the regime defined by




$$\sum_{x\in\mathcal{S}} \mu(x) h_{\mathcal{M}_1,\mathcal{M}_0}(x)$$

$$= \mu[\mathcal{S}_1] \sum_{x\in\mathcal{S}_1} \mu|_{\mathcal{S}_1}(x) h_{\mathcal{M}_1,\mathcal{M}_0}(x) + \sum_{k\in\{2,3\}} \mu[\mathcal{S}_k] \sum_{x\in\mathcal{S}_k} \mu|_{\mathcal{S}_k}(x) h_{\mathcal{M}_1,\mathcal{M}_0}(x) + \mu[\mathcal{S}_0] \sum_{x\in\mathcal{S}_0} \mu|_{\mathcal{S}_0}(x) h_{\mathcal{M}_1,\mathcal{M}_0}(x)$$

$\approx \mu[\mathcal{S}_1]$

$$\mu[\mathcal{S}_1] = \mu[\mathcal{S}_2] = \mu[\mathcal{S}_3]$$

$\approx \mu[\mathcal{S}_1] e^{-CN}$

No estimates for $h_{\mathcal{M}_1,\mathcal{M}_0}$ in $\mathcal{S}_2, \mathcal{S}_3$

This can be solved by use of symmetries for the CWP model via lumped process and color symmetry use, but not (yet) for DCWP.

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# Potential theory

Translates the problem of understanding the metastable behaviour of Markov processes to the study of capacities of electric networks/boundary problems.

Key formulas: $\mathcal{A}, \mathcal{B} \subset \mathcal{S},\ x \in \mathcal{S}$

$$h_{\mathcal{A},\mathcal{B}}(x) = \mathrm{P}_x[\tau_{\mathcal{A}} < \tau_{\mathcal{B}}]$$

Harmonic function

$$\mathrm{cap}(\mathcal{A},\mathcal{B}) = \sum_{x\in\mathcal{A}} \mu(x)(-Lh_{\mathcal{A},\mathcal{B}})(x)$$

Capacity between two sets

$$\mathrm{E}_{\nu_{\mathcal{A},\mathcal{B}}}[\tau_{\mathcal{B}}] = \frac{\sum_{x\in\mathcal{S}} \mu(x) h_{\mathcal{A},\mathcal{B}}(x)}{\mathrm{cap}(\mathcal{A},\mathcal{B})}$$

Expression for (biased) hitting time

The capacity has upper and lower bounds coming from variational principles!
Metastability can be rephrased in terms of comparison of capacities.