Sampling, spectral gaps and stochastic localization

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Based on joint works with:

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Stochastic localization

[Eldan 2013]

Fix a measure μ on $\mathbb{R}^n$

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Exponential tilts: For any $y \in \mathbb{R}^n$ define the measure

$$\mu_{t,y}(\mathrm{d}x) = \frac{1}{Z(t,y)} e^{\langle y,x\rangle - t\|x\|^2/2} \mu(\mathrm{d}x)$$

Mean vector: $$m(t,y) = \int x \mu_{t,y}(\mathrm{d}x)$$

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Evolution of the tilting field: $$\mathrm{d}y_t = m(t,y_t)\mathrm{d}t + \mathrm{d}B_t, \quad y_0 = 0\,.$$

Let $\mu_t = \mu_{t,y_t}$ and $m_t = m(t,y_t)$

Stochastic localization

[Eldan 2013]

Properties:

1. $(\mu_t)_{t\geq 0}$ and $(m_t)_{t\geq 0}$ are martingales In particular $\mu = \mathbb{E}\mu_t$

2. $\forall t \geq 0$ $\mathbb{E}\mathrm{Cov}(\mu_t) \preceq \frac{1}{t} I$

3. Consequence of 1 and 2:

$$m_t \xrightarrow[t\to\infty]{\mathrm{d}} m_\infty \sim \mu$$

Powerful technique in High-dimensional Probability/Geometry

Stochastic analysis, KLS, functional inequalities, mixing times, …

Related to the Polchinski flow [Bauerschmidt, Bodineau, Dagallier 2023]

Information-theoretic characterization

[EA, Montanari 2021]

1. Sample $x_0 \sim \mu$
2. Let $\bar{y}_t = t x_0 + B_t$
3. Look at $\mu_t = \mathrm{Law}(x_0 \,|\, (y_s)_{s \le t})$

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Lemma: $(\bar{y}_s)_{s \le t} \stackrel{d}{=} (y_s)_{s \le t}$ and $(\mu_t)_{t \ge 0} \stackrel{\mathrm{d}}{=} \mathrm{SL\ process}$

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Consequence: $$W_2(\mathrm{Law}(y_T/T)\,,\,\mu)^2 \le \frac{\mathbb{E}\|B_T\|^2}{T^2} = \frac{d}{T}$$

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Equivalent to score-based diffusion sampling [Montanari 2023]

Rapidly growing theory in ML [Chen et al. 2022, Koehler et al. 22…]

A sampling algorithm

Sampling via stochastic localization (SL)

For $\ell = 0, 1, 2, \cdots$

1. Given a tilt vector y_ℓ compute the mean vector

$$\widehat{m}(y_\ell) \simeq m(y_\ell) = \int x \, \mu_{y_\ell}(\mathrm{d}x)$$

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Then output $y_L/(L\delta)$ for $L = T/\delta$ $\quad \delta \to 0,\ T \to \infty$

Mean-field spin glass measures

The Sherrington-Kirkpatrick model:

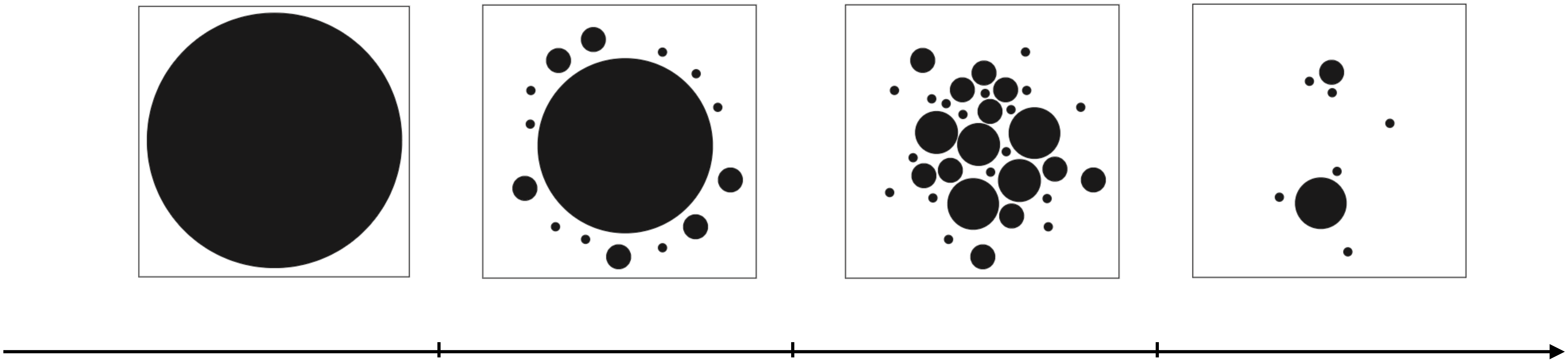
$$\mu(x) = \frac{1}{Z} \exp\left\{ \frac{\beta}{\sqrt{n}} \sum_{i<j} g_{ij} x_i x_j \right\}, \qquad x \in \{-1,+1\}^n$$

Mixed p-spin model:

$$\mu(x) = \frac{1}{Z} \exp\left\{ \sum_{p} \frac{\beta \gamma_p}{n^{(p-1)/2}} \langle G^{(p)}, x^{\otimes p} \rangle \right\}$$

The phase diagram, spherical

The pure **spherical** p-spin, p large:



$\beta_{d+} \simeq (e/2)\sqrt{\log p}^{-1}$

[Barra, Burioni, Mézard 96]

[Ben Arous, Jagannath 21]

$\beta_d \simeq \sqrt{e}$

[Crisanti, Horner, Sommers 93]

$\beta_c \simeq \sqrt{\log p}$

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Replica symmetry

Replica symmetry breaking

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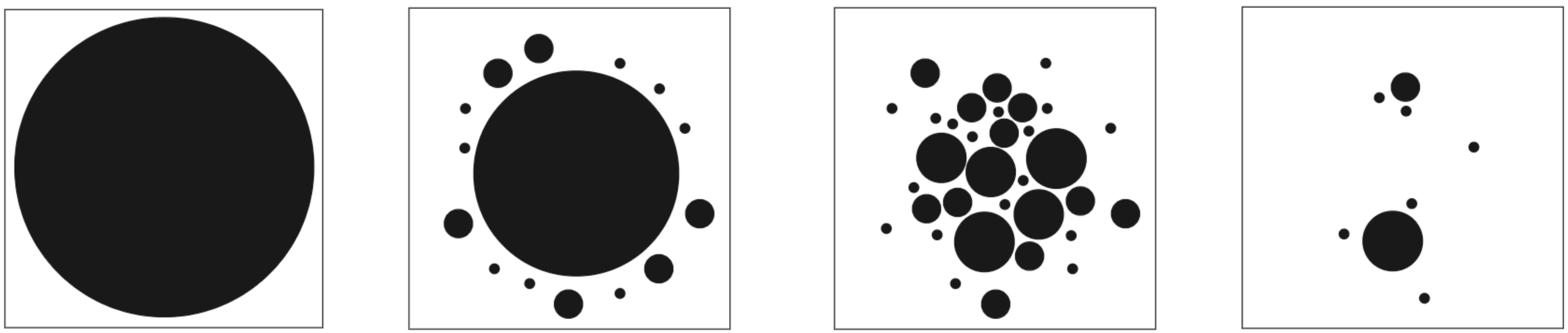

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[EA, Montanari, Sellke 2023, EA 24]

Thm: Shattering for all $\beta \geq \bar{\beta}_d \simeq 2.21$

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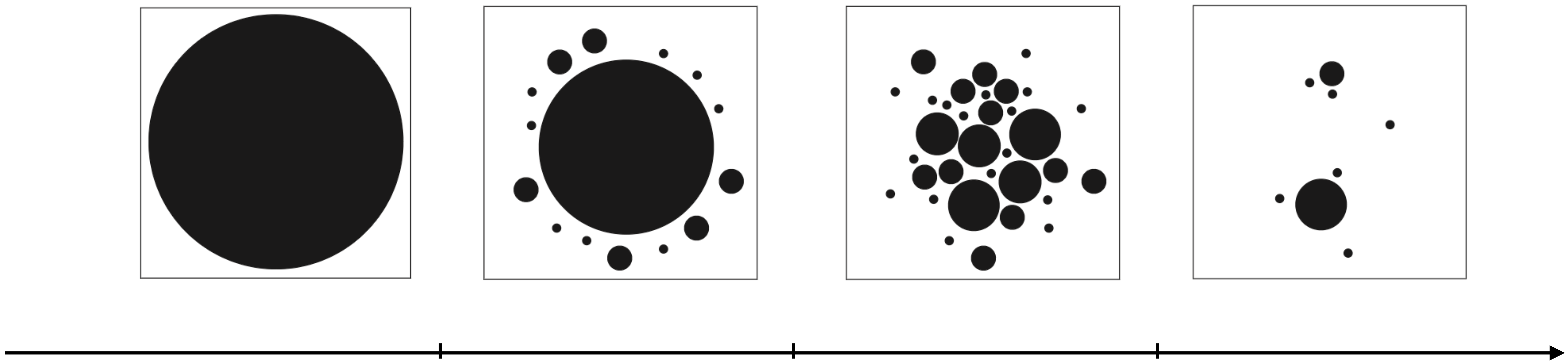

$\beta_{d+} \simeq ?$

$\beta_d \simeq \sqrt{(2 \log p)/p}$

[Montanari, Ricci-Tersenghi 03]

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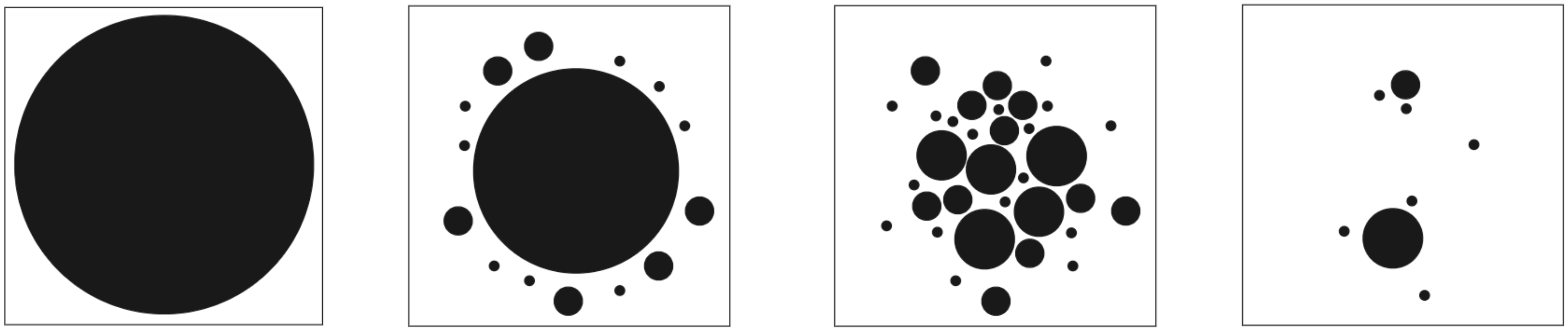

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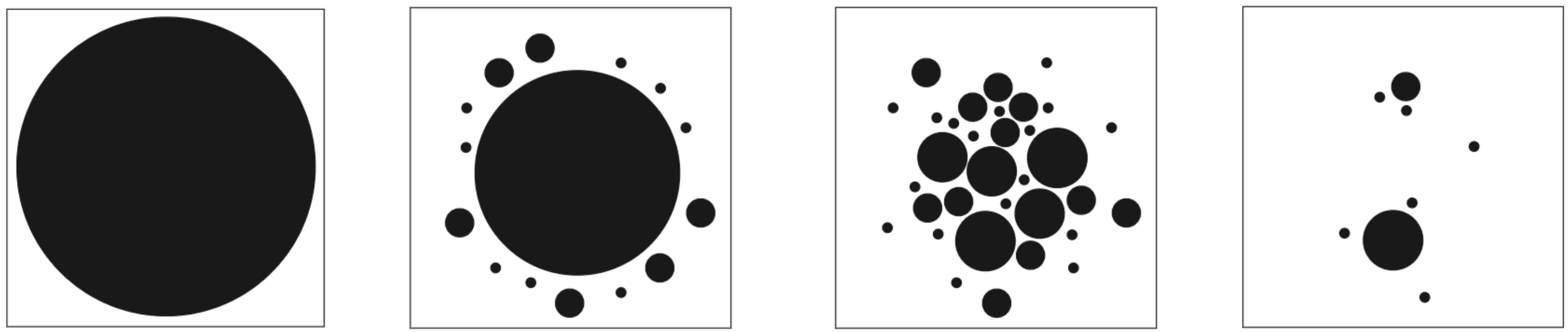

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Thm: Shattering *or* RSB implies hardness of sampling by “stable” algorithms.

[EA, Montanari, Sellke 2023]

Rapid mixing of Glauber dynamics

SK: for all $\beta < 1/4$ **p-spin**: for all $\beta < \frac{1}{\sqrt{p^3 \log p}}$

Poincaré inequality: Implying mixing in $t_{\mathrm{mix}} \leq Cn^2$

[Eldan-Koehler-Zeitouni 2020] [Adhikari, Brennecke, Xu, Yau 2022]

(Modified) **log-Sobolev inequality:** Implying mixing in $t_{\mathrm{mix}} \leq Cn \log n$

[Chen, Eldan 2022] [Anari, Jain, Koehler, Pham, Vuong 2023]

Very recently MLSI for SK: $\beta < 0.295 \cdots$ [Anari, Koehler, Vuong 2024]

Theorems

SK model:

Theorem: Wasserstein sampling guarantee for all $\beta < 1$

[EA, Montanari, Sellke 22, Celentano 23]

Theorems

Ising p-spin:

Theorem: Wasserstein sampling guarantee for $\beta < \beta_*(p) \asymp \dfrac{1}{p\sqrt{\log p}}$

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$\beta < \dfrac{1}{\sqrt{p^3 \log p}}$ (MLSI)

β_{d+}

$\beta_d \asymp \sqrt{(\log p)/p}$ (Shattering)

$\beta_c \asymp \sqrt{2 \log 2}$ (RSB)

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$\beta < \frac{1}{\sqrt{p^3 \log p}}$ (MLSI) — β_{d+} — $\beta_d \asymp \sqrt{(\log p)/p}$ (Shattering) — $\beta_c \asymp \sqrt{2 \log 2}$ (RSB)

Spherical p-spin:

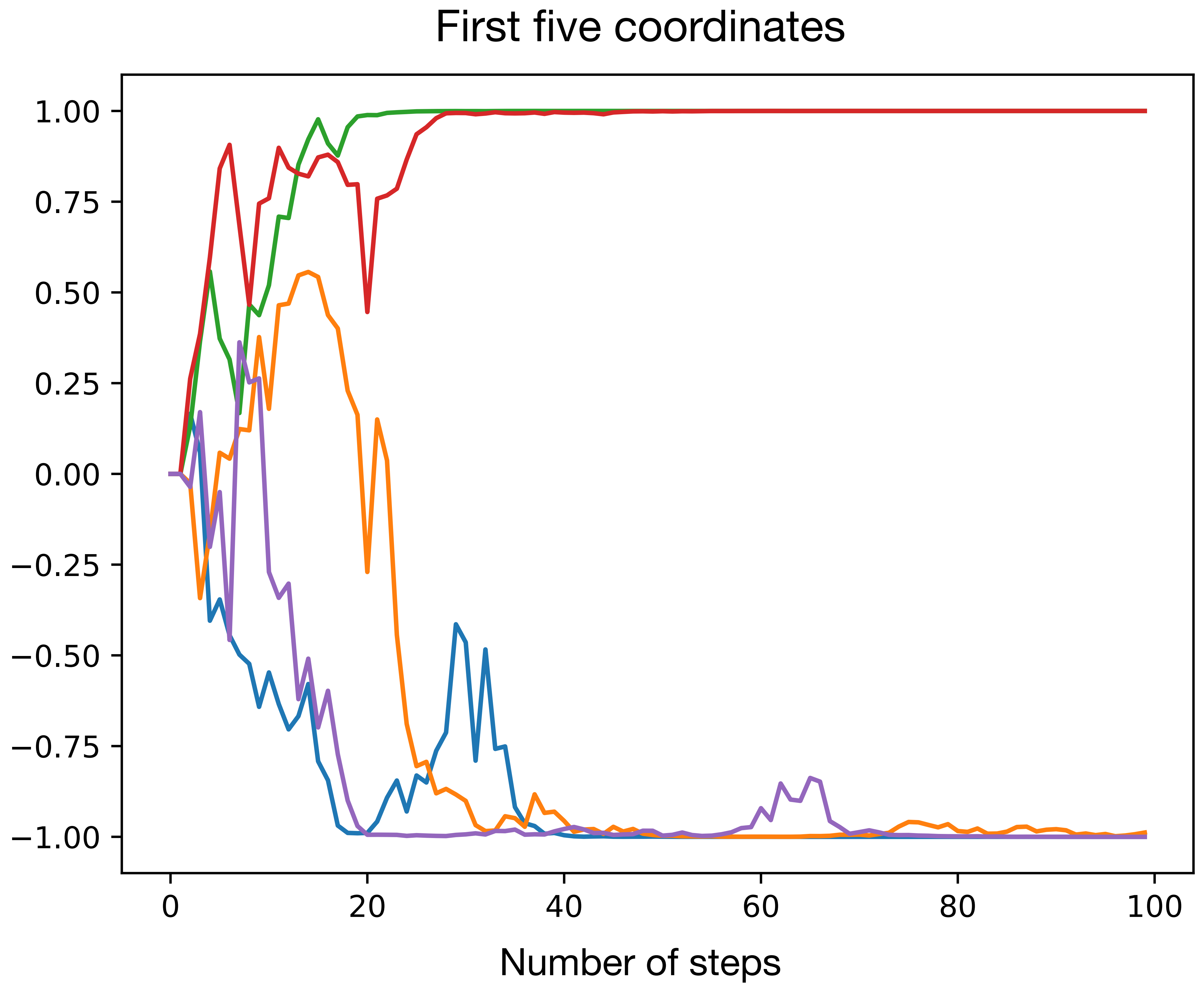
Theorem: Total variation sampling guarantee for $\beta < \beta_*(p) \asymp e/2$

[Huang, Montanari, Pham 24]

(MLSI) — $\beta_{d+} \simeq 1/\sqrt{\log p}$ — $\beta_d \simeq \sqrt{e}$ (Shattering) — $\beta_c \simeq \sqrt{\log p}$ (RSB)

Sampling from SK using SL

$n = 500, \ \beta = 0.5$



Functional inequalities and fast mixing

Proving PI/LSI using SL

Idea: Localizing the measure induces regularization

PI/LSI for localized measure + approximate variance/entropy conservation

implies PI/LSI for the original measure.

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Proving approximate conservation of variance/entropy relies on bounding the operator norm of the covariance matrix.

Poincare inequalities

We want to show: $$\mathrm{var}_\mu(f) \leq C\mathcal{E}_\mu(f,f)$$

where $$\mathcal{E}_\mu(f,f) = \sum_{\sigma\sim\sigma'} \frac{\mu(\sigma)\mu(\sigma')}{\mu(\sigma)+\mu(\sigma')}(f(\sigma)-f(\sigma'))^2$$

(Dirichlet form of Glauber dynamics)

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(Dirichlet form of Glauber dynamics)

Idea: Track the evolution of each term under SL

Lemma 1: $$\mathbb{E}\big[\mathcal{E}_{\mu_t}(f,f)\big] \le \mathcal{E}_\mu(f,f)$$

Lemma 2: $$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}\big[\mathrm{var}_{\mu_t}(f)\big] \ge -\mathbb{E}\big[\mathrm{var}_{\mu_t}(f)\|\mathrm{cov}(\mu_t)\|_{\mathrm{op}}\big]$$

Poincare inequalities

If $\|\mathrm{cov}(\mu_t)\|_{\mathrm{op}} \leq \alpha(t)$ a.s.

then $$\mathbb{E}\left[\mathrm{var}_{\mu_t}(f)\right] \geq e^{-\int_0^t \alpha(s)\mathrm{d}s}\ \mathrm{var}_{\mu}(f)$$

(Approx. variance conservation)

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Next, if $$\mathrm{var}_{\mu_t}(f) \leq C(t)\mathcal{E}_{\mu_t}(f,f)$$ a.s.

(PI for the localized measure)

then $$\mathrm{var}_\mu(f) \leq C(t)e^{\int_0^t \alpha(s)\mathrm{d}s}\mathcal{E}_\mu(f,f)$$

(PI for the original measure)

Much progress in the recent years

Spin systems (lattice, mean-field, disordered,…)

[Bauerschmidt-Bodineau 18]
[Eldan, Koehler, Zeitouni 20]
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Most constraining requirement: uniform bound on the covariance matrices

$$\|\mathrm{cov}(T_v\mu)\|_{\mathrm{op}} \leq \alpha \quad \forall\, v \in \mathbb{R}^n$$

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One example: **the Random Field Ising Model**

Random Field Ising Model

RFIM on a graph $G = (V, E)$:

$$\mu_G(\sigma) \propto \exp\left(\beta \sum_{(u,v)\in E} \sigma_u \sigma_v + \sum_{u \in V} h_u \sigma_u\right)$$

$$\beta \geq 0$$
$$h_u \sim N(0, \sigma^2)$$

Notation: $\mu_G = \mathrm{RFIM}_G(\beta, h)$

The (Random Field) Ising Model

The phase diagram:

- $d = 2$ Exponential decay of correlation **for all** β whenever $\sigma \neq 0$

  [Imry, Ma 75; Aizenman, Wehr 89; Chatterjee 18; Aizenman, Harel, Peled 19, 20]

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- $d \geq 3$ Phase transition in (β, σ^2)

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  ⟶ For $\beta < \beta_c(d)$ and any σ :

  Exp. decay of corr. and order-1 spectral gap

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  Long range order and very slow mixing

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$\longrightarrow$ For $\beta > \beta_c(d)$ and σ not too small :

There are large islands of small fields (low temp.)

…yet correlations decay exponentially *on average*.

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The Griffiths phase ⟶ For $\beta > \beta_c(d)$ and σ not too small :

There are large islands of small fields (low temp.)

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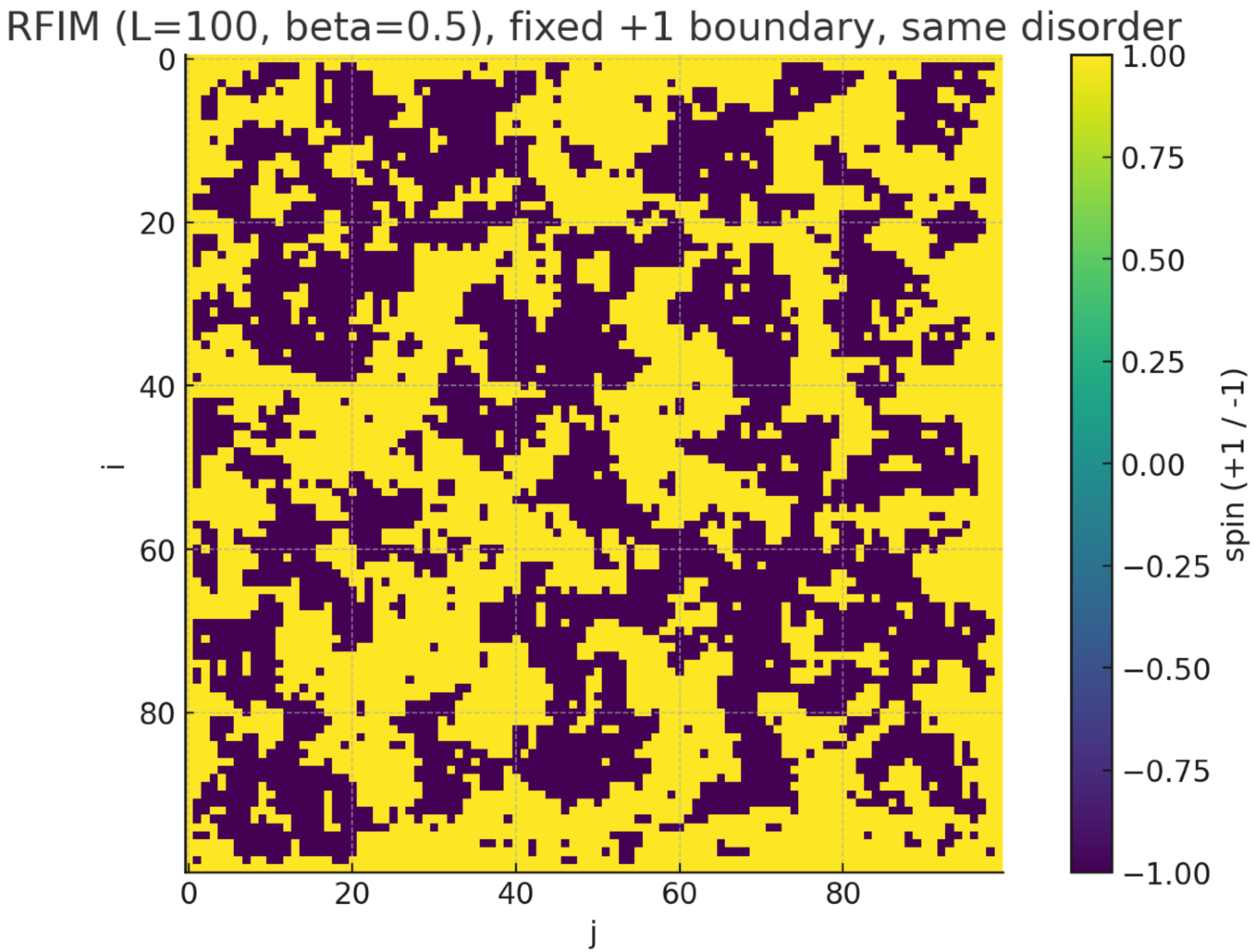
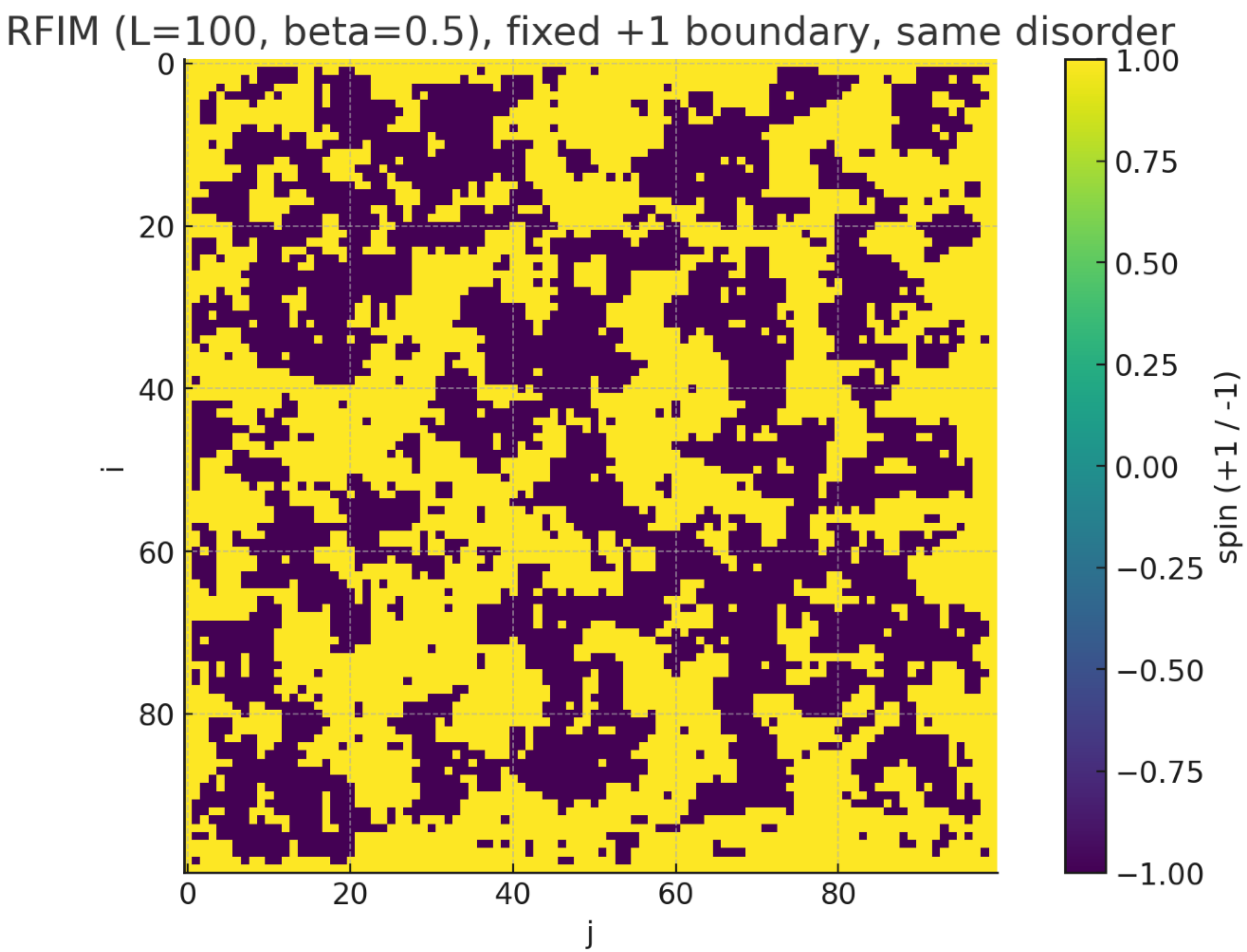
The Griffiths phase

Dynamics are expected to slow down, with vanishing spectral gap.
Mixing time is at least super-polylogarithmic.



The Griffiths phase

Persistence of correlations at small scale imply $\|\mathrm{cov}(\mu)\|_{\mathrm{op}}$ has non-trivial upper tail.



(Full) Poincaré inequality

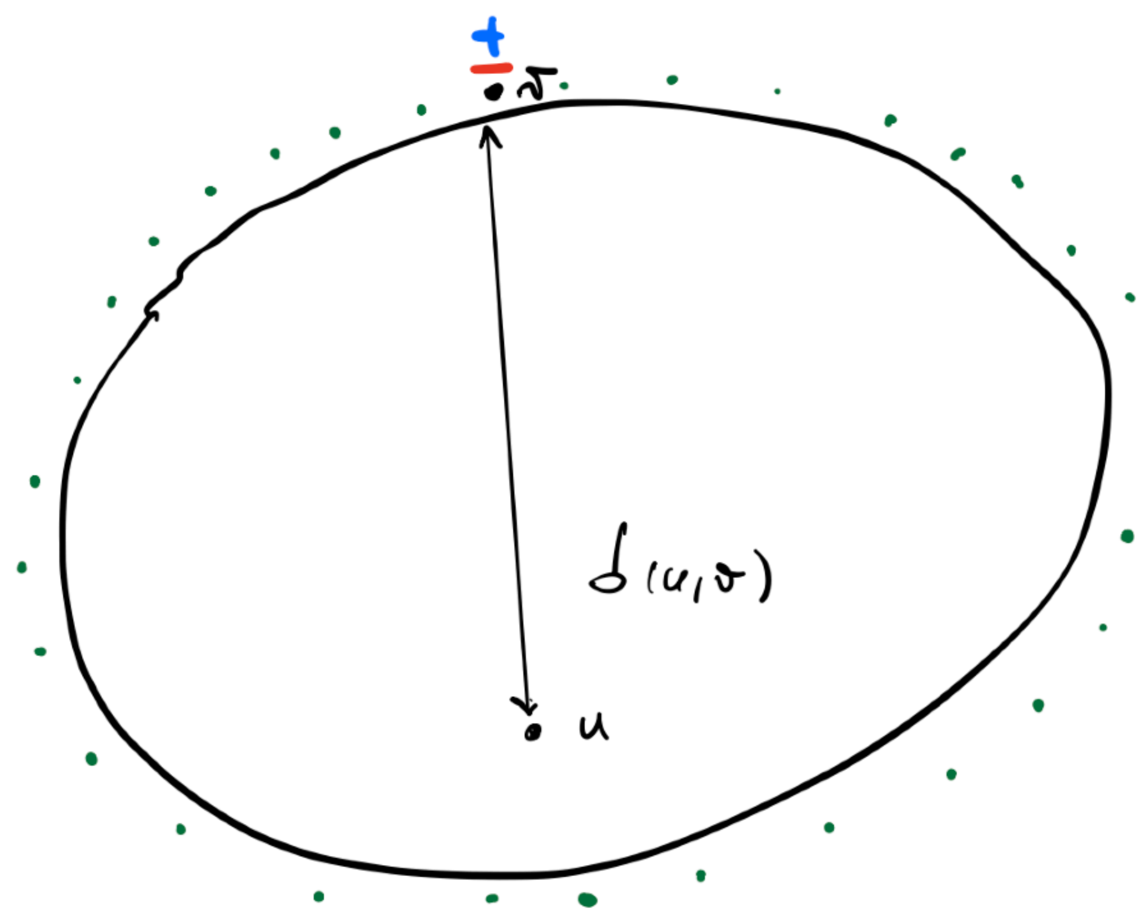
Theorem: If exponential decay of boundary influence on average, even in the presence of nearby pinnings, then

[EA, Eldan, Gheissari, Piana 24]

(i.e. **strong** spatial mixing)

$$\forall\, L \geq \kappa \log |V| \qquad \sup_f \frac{\mathrm{var}_\mu(f)}{\mathcal{E}_\mu(f,f)} \leq \exp\left\{L^{\frac{d-1}{d}+o(1)}\right\}, \qquad \text{with prob.} \quad 1-e^{-L}$$

Mixing time is $|V|^{o(1)}$ with high-probability.



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Lemma: SSM holds if $\sigma > \sigma_0(d,\beta)$

Weak Poincaré inequality

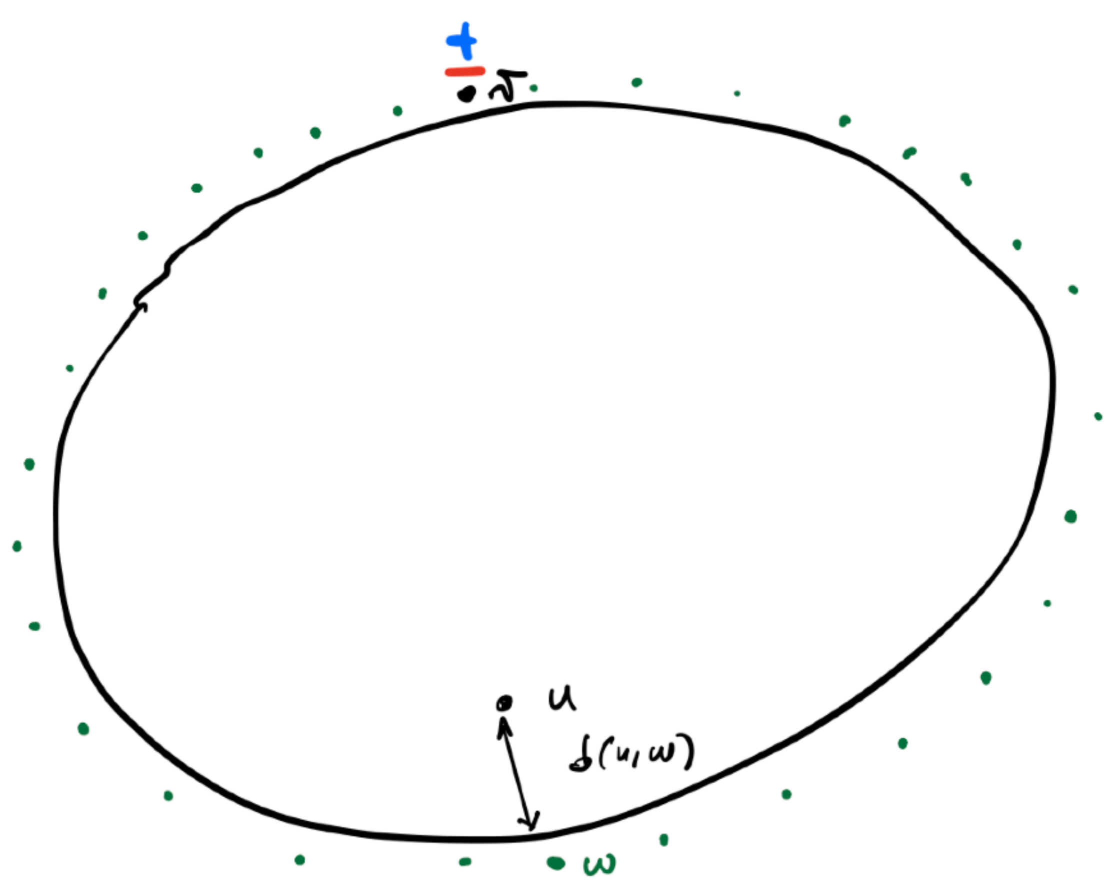
Theorem: If exponential decay of boundary influence on average then

(i.e. **weak** spatial mixing)

[EA, Eldan, Gheissari, Piana 24]

$$\mathrm{var}_\mu(f) \leq |V|^\kappa \, \mathcal{E}_\mu(f,f)^{1/p} \, \mathrm{osc}(f)^{1/q}$$

$\kappa = \kappa(d, \beta, \sigma^2) > 0$ $\quad$ $1/p + 1/q = 1$ $\quad$ (p a large constant)



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Implies *algebraic* relaxation of the dynamics on **polynomial time scales**:

$$\mathrm{var}_\mu(P_t f) \leq \frac{n^\kappa}{t^\alpha} \|f\|_\infty .$$

and existence of a polynomial time sampling (in TV distance) algorithm.

At a high-level

- Proving PI/LSI for the localized measure:

$$\mu = \mathrm{RFIM}_G(\beta, h) \qquad \Longrightarrow \qquad \mu_t = \mathrm{RFIM}_G(\beta, h + y_t)$$

$$y_t = t\sigma_0 + \sqrt{t}g$$

$$\sigma_0 \sim \mu \qquad g \sim N(0, I)$$

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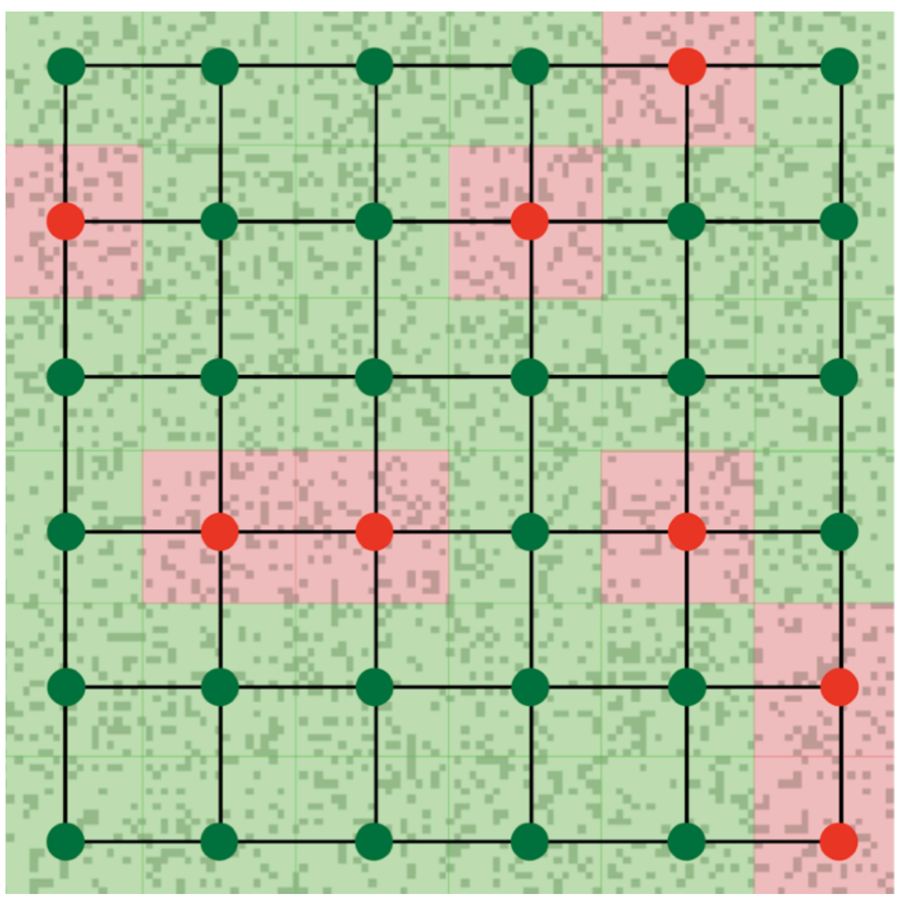

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Larger t means variance field variance!

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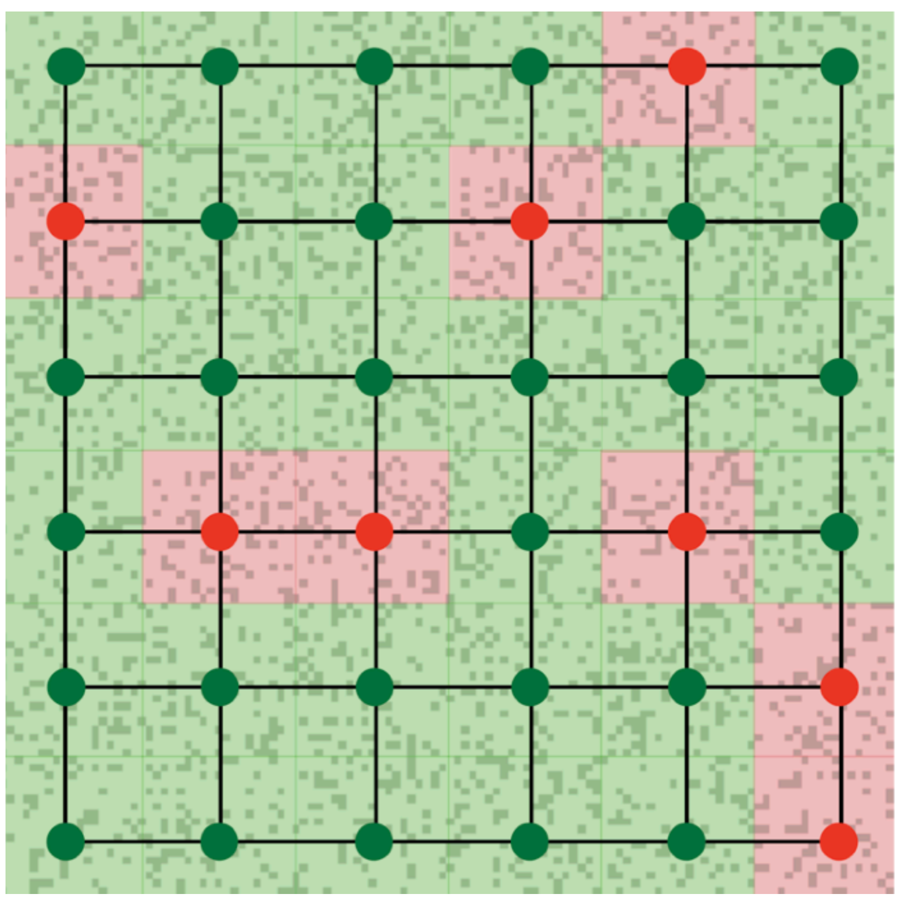

$$y_t = t\sigma_0 + \sqrt{t}g$$

$$\sigma_0 \sim \mu \qquad g \sim N(0, I)$$

Larger t means variance field variance!

Show PI for μ_t via coarse-graining the lattice + disagreement percolation

Green = strong fields -> SSM

Red = weak fields -> low temperature

At a high-level

- Proving PI/LSI for the localized measure:

- Proving approximate conservation of variance/entropy relies on bounding **the operator norm of the covariance matrix**.

We prove an exponential upper tail $\mathbb{P}\Big(\|\mathrm{cov}(\mu_t)\|_{\mathrm{op}} \geq R\Big) \leq |V|\, e^{-c_0 R}$

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Implies the weak PI $\mathrm{var}_\mu(f) \leq |V|^\kappa\, \mathcal{E}_\mu(f,f)^{1/p}\, \mathrm{osc}(f)^{1/q}$

A few open questions

Prove PI/LSI for

1. RFIM under weak spatial mixing
2. SK for all $\beta < 1$
3. SK with external field

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Thanks!