Quantum Spin Systems and Phase Transitions

Ankur Moitra (MIT)
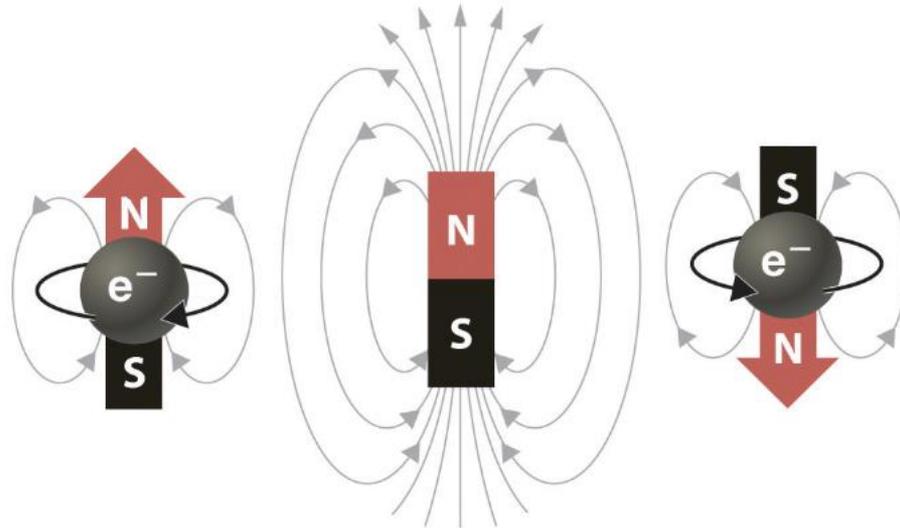
Swiss Winter School, Lecture #2

A GUIDING QUESTION

How do local interactions give rise to macroscopic behavior?

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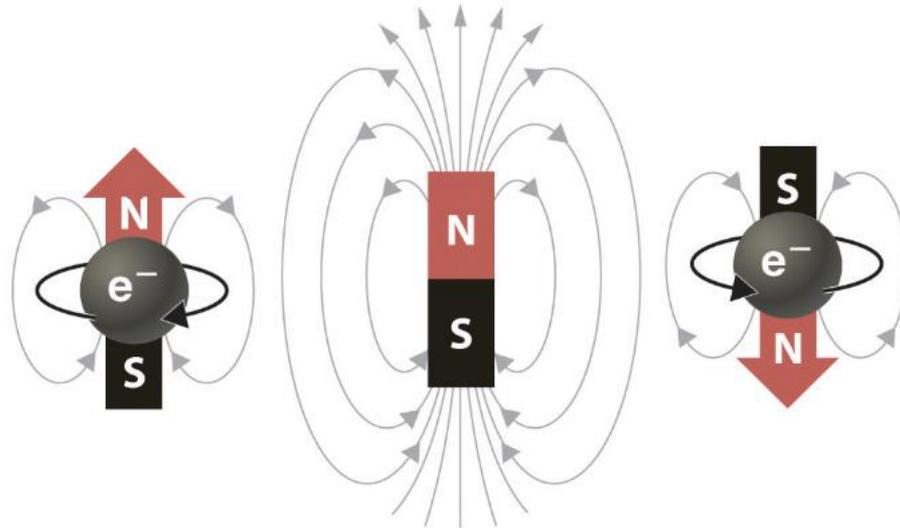
Running example: Consider **magnetism** – caused by most electron spins being oriented in same direction

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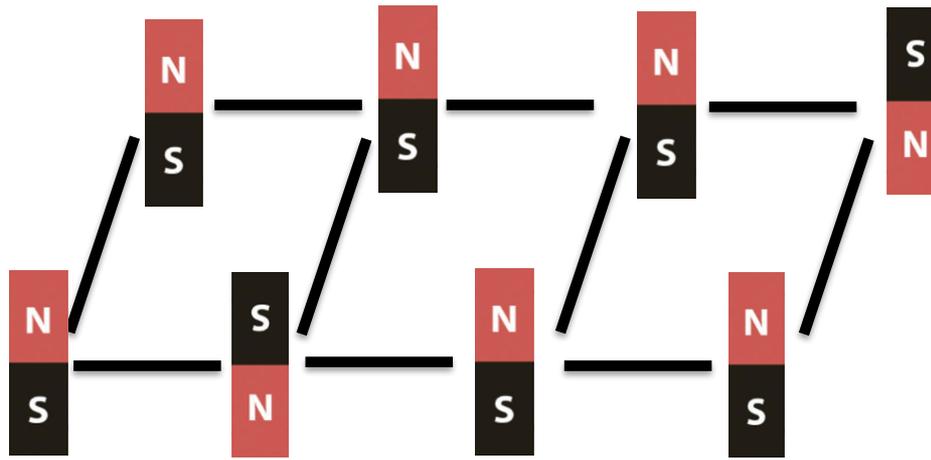How do local interactions give rise to macroscopic behavior?

Running example: Consider **magnetism** – caused by most electron spins being oriented in same direction

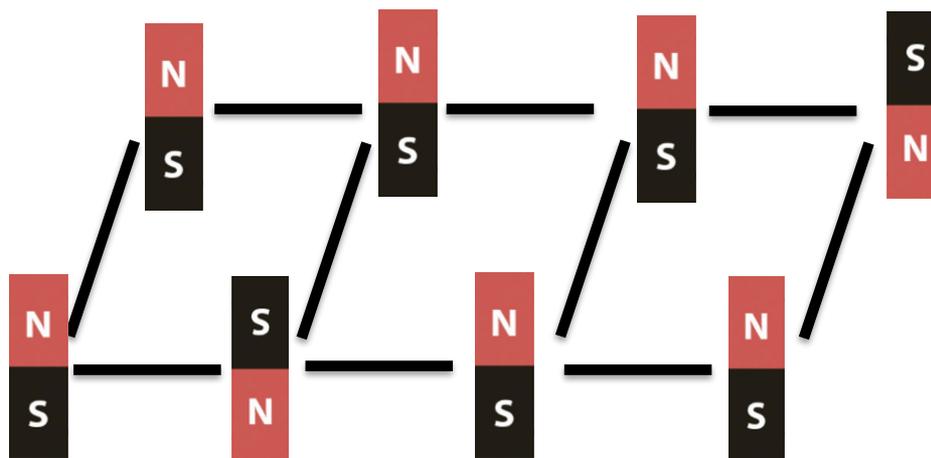How do they know which way to point, if they don't all interact?

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In **ferromagnets**, neighboring spin spins prefer to point in the same direction

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Statistical physics: Define a probabilistic model that captures behavior at thermal equilibrium and study its structural properties

CLASSICAL SPIN SYSTEMS

Definition: an **Ising model** is a distribution on $\{\pm 1\}^n$ with

inverse temperature   **Hamiltonian**

$$\mathbb{P}[X = x] = \frac{1}{Z}\exp\Big(-\beta H(x)\Big)$$

partition function

where $H(x) = -\sum_{i,j} J_{i,j} x_i x_j - \sum_i h_i x_i$

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Can generalize to higher degree polynomials etc

CONDITIONAL INDEPENDENCE

Often helpful to look at their graph structure:

$$G = (\{X_1, \cdots, X_n\}, E) \text{ with } E = \{(X_i, X_j) \text{ s.t. } J_{i,j} \neq 0\}$$

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$$X_i \perp X_j | X_U$$

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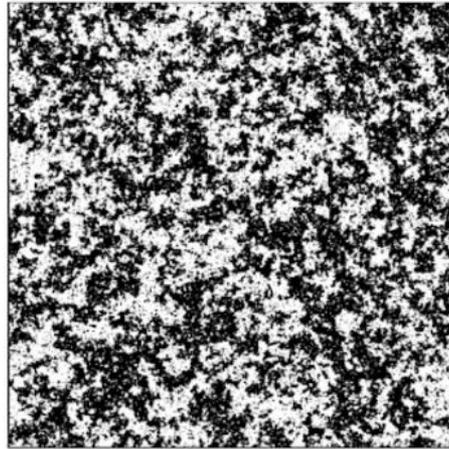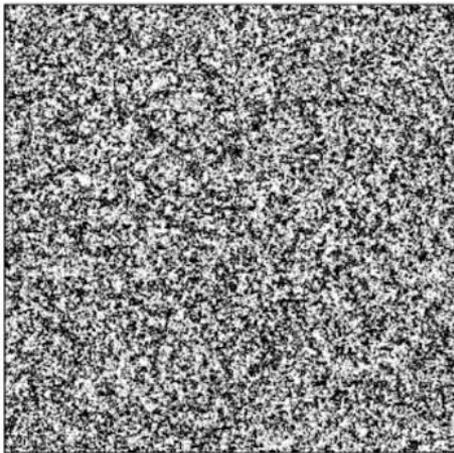
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⚠ **Caution:** The Markov property fails in quantum spin systems

PHASE TRANSITIONS

Dramatic changes in macroscopic properties as temperature varies

e.g. **average magnetization**
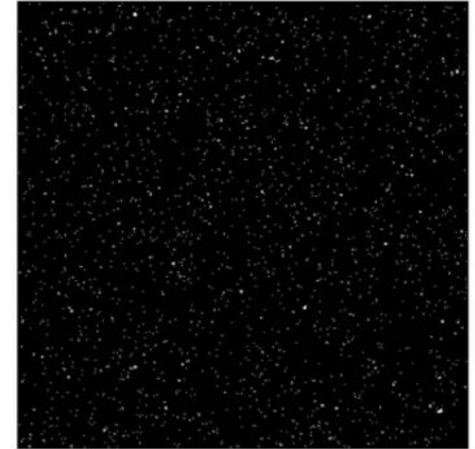
decreasing temperature

OUTLINE

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- Density Matrices, Operators and Quantum Spin Systems

- Sudden Death of Entanglement

Part II: Showing Separability

- Perturbations of the Identity

Intermission: Glauber Dynamics

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QUANTUM SPIN SYSTEMS

How do we describe quantum systems at thermal equilibrium?

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💡 Think of it as a generalization of classical distributions for which
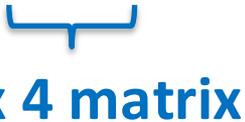
$$\rho = \begin{bmatrix} \rho_1 & & \\ & \rho_2 & \\ & & \ddots \end{bmatrix}$$

i.e. entries along the diagonal are probabilities of each of the 2^n possible configurations

QUANTUM STATES AND OPERATORS

We will also be interested in operators that act on at most k qubits

all other sites
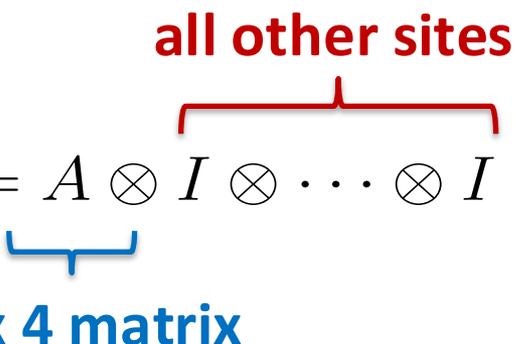
e.g. $H_e = A \otimes I \otimes \cdots \otimes I$

4 x 4 matrix

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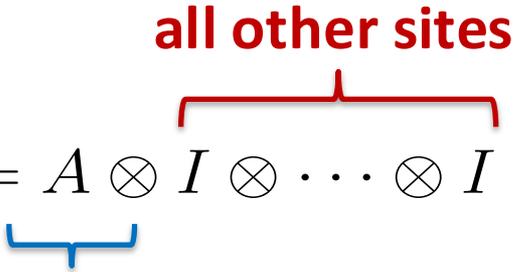$$\text{e.g. } H_e = A \otimes I \otimes \cdots \otimes I$$

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More generally a 2^k x 2^k matrix and a list of qubits, called its **support**, that it acts on

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💡 Think of it as a generalization of local interactions in a graphical model

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How does temperature affect properties of a quantum system?

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💡 Think of separable states as ones that have only classical correlations

BOUNDS ON ENTANGLEMENT

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What happens at reasonable physical temperatures?

ALGORITHMS

Heat kills all entanglement

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Theorem [Bakshi, Liu, Moitra, Tang '24]: There is a constant c > 0 so that for any $\beta \leq \dfrac{c}{dk^2}$ the Gibbs state is separable

Here k is the locality and d is the graph degree

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Moreover there is an efficient randomized algorithm that outputs the description of a product state that works under similar parameters

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Show there are efficient quantum Gibbs samplers that succeed where classical algorithms do not

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Would be applications in **quantum chemistry** for understanding material properties

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Theorem [Sly '10] [Sly, Sun '14]: Even classical Gibbs sampling is NP-hard for k = 2 and $\beta \geq \dfrac{c'}{d}$ for some constant c'

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Theorem [Sly '10] [Sly, Sun '14]: Even classical Gibbs sampling is NP-hard for k = 2 and $\beta \geq \dfrac{c'}{d}$ for some constant c'

And so the region you could hope for quantum advantage is now quite narrow for constant locality
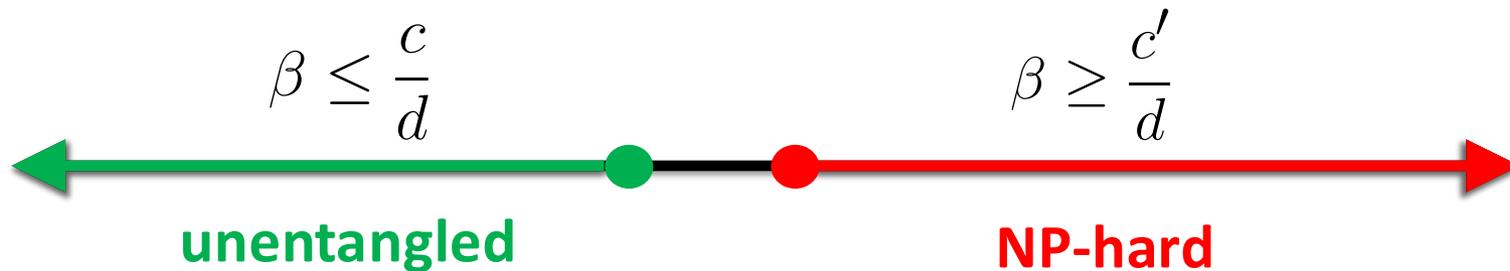
$$\beta \leq \frac{c}{d} \qquad\qquad \beta \geq \frac{c'}{d}$$

unentangled   **NP-hard**

INDEPENDENT WORK

Theorem [Rouze, Franca, Alhambra '24]: Polynomial mixing time bounds for quantum Gibbs sampling at high enough temperature

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Better dependence on locality (k vs k^2), but worse dependence on degree (d vs $d^{O(1)}$)

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$$\rho = \frac{I + cE}{2^n}$$

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This is too weak for our purposes, but there is a sharpening that points the way forward

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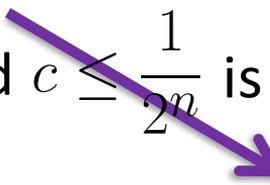
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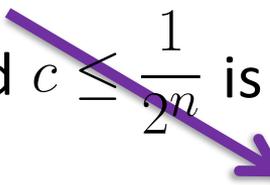
$$c \leq \frac{1}{2^k}$$

Can we approximate the Gibbs state by local perturbations of the identity?

This is not so straight forward

this is local, by assumption

$$\rho = \frac{I}{2^n} + \left(\frac{e^{-\beta H}}{Z} - \frac{I}{2^n} \right)$$
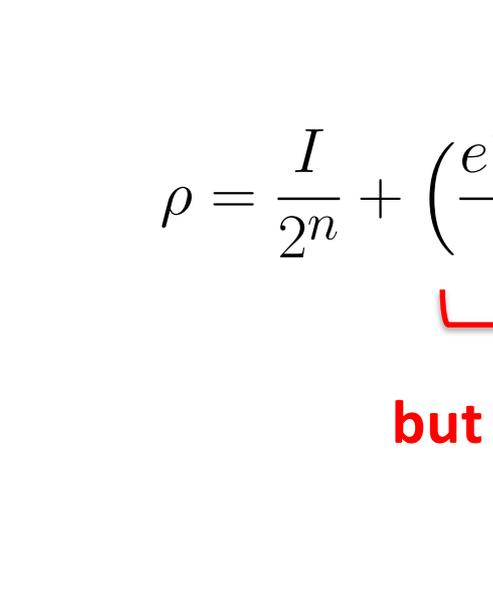
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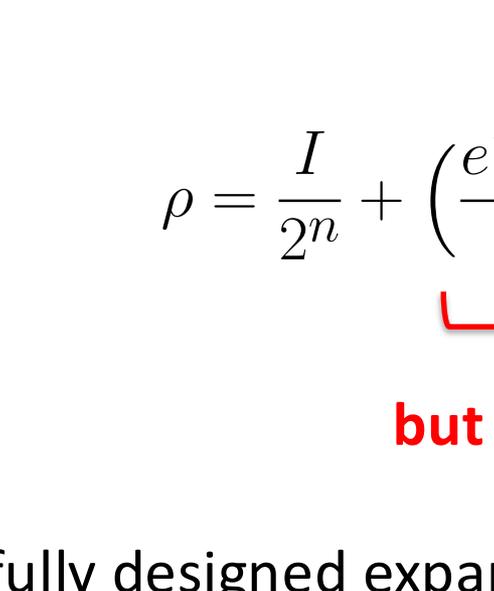
but what about this??

Need carefully designed expansions, let's take a detour to explain where they come from

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CLASSICAL SAMPLING

How do you sample from an Ising model?

GLAUBER DYNAMICS

Natural Markov chain with local updates

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Natural Markov chain with local updates

choose node at random,
    forget its state
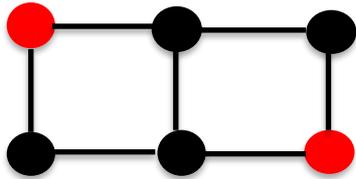
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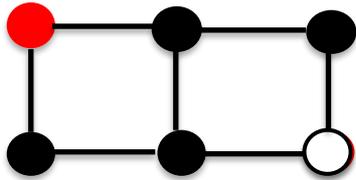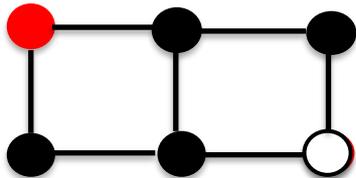
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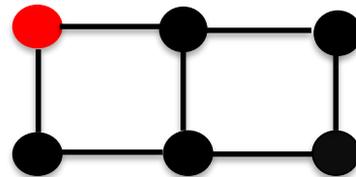forget its state
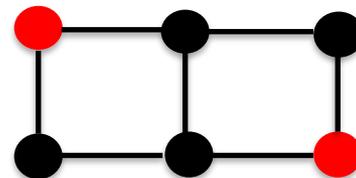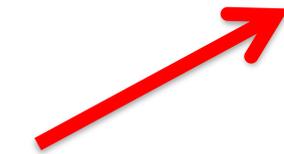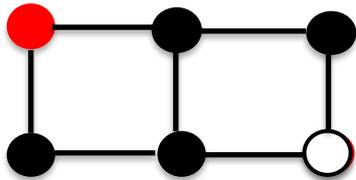
update state w/ correct probability
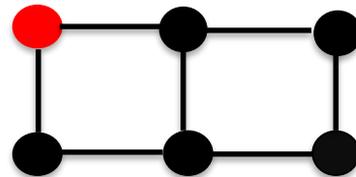
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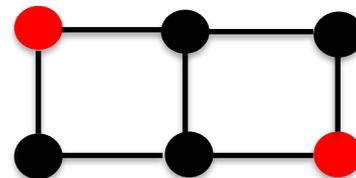
update state w/ correct probability

Its unique steady state distribution is the Gibbs distribution
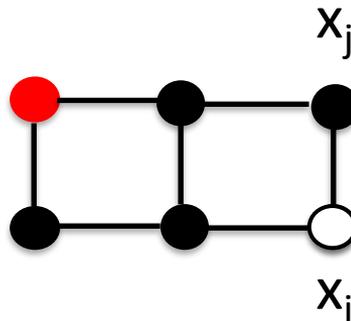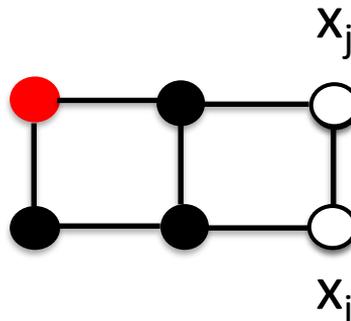
PINNING TO A PRODUCT DISTRIBUTION
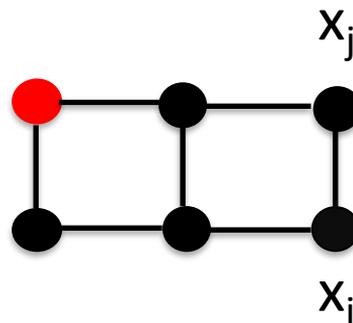
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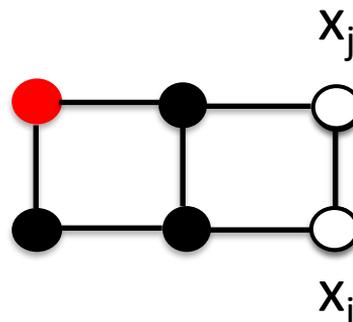
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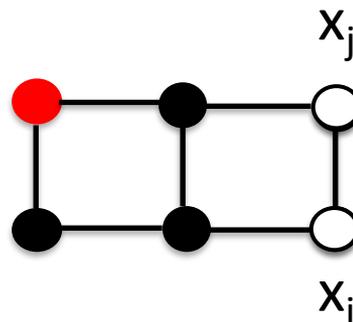
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x_j

both options almost equally likely

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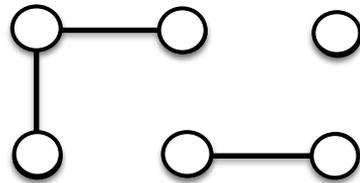# PINNING TO A PRODUCT DISTRIBUTION

A classical thought experiment

x_j

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Claim: At high temperature, there is a good chance that their updates can be made independently, in which case we can ignore their edge
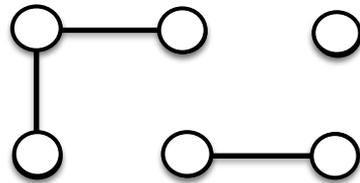
PINNING TO A PRODUCT DISTRIBUTION

Try to make x_i independent of the rest, but keep only edges that are needed as correction terms

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And you end up with small connected components – **this is where locality comes from**

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Key is to define an **extraction operator** and write its expansion with **exponentially decaying coefficients**

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$$M_1 = e^{\beta(H - H_1)/2} e^{-\beta H/2}$$

THE KEY LEMMA

Lemma: We can write

$$M_1 = \sum_{k=0}^{\infty} \frac{(\beta/2)^k}{k!} f_k(H, H_1) \quad \text{where} \quad f_k(H, H_1) = \sum_{a \in \mathcal{S}} c_a E_a$$

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The point is, when $\beta << 1/d$ the terms are exponentially decaying, and can get a handle on entanglement via **Fact'**

PUTTING THINGS TOGETHER

Corollary: Hence we know that $M_1 M_1^*$ is separable

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Induction is involved because $M_1 M_1^*$ is not literally the identity, need a careful potential function argument

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Part II: Showing Separability

- Perturbations of the Identity

Intermission: Glauber Dynamics

- Proof Strategy and the Extraction Operator

- The Expansion and its Interpretation via Commutators

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$f_k(H,H_1)$

Now let's try to interpret these expressions

A RECURRENCE

Easy to check that this expression

$$f_k(H, H_1) = \sum_{j=0}^{k} \binom{k}{j} (H - H_1)^{k-j} (-H)^j$$

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$$= [H, f_{k-1}(H, H_1)] - H_1 f_{k-1}(H, H_1)$$

where $[A, B] = AB - BA$ is the **commutator**

UNDERSTANDING COMMUTATORS

Key Fact: For any A and B, we have

$$[A, B] = \begin{cases} 0 & \text{if their supports are disjoint} \\ & \text{supported on the union of their supports otherwise} \end{cases}$$

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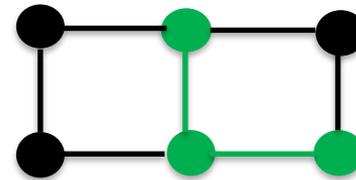
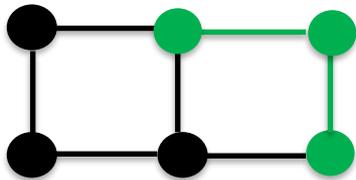Hence, for each new term, its support grows by one incident edge

VISUALIZING THE RECURRENCE
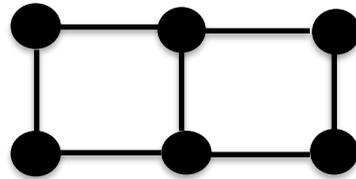
If our base graph is

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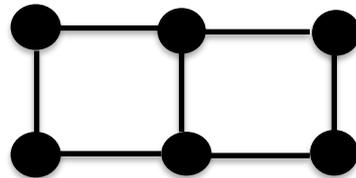
If our base graph is

we can visualize the support of the terms in f_1

VISUALIZING THE RECURRENCE
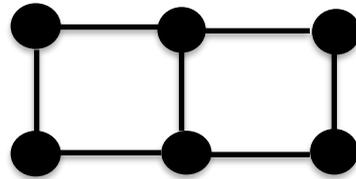
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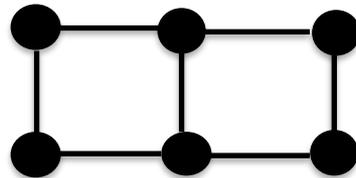
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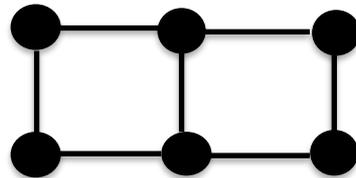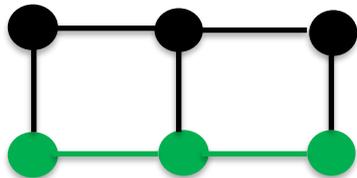

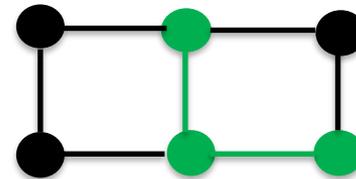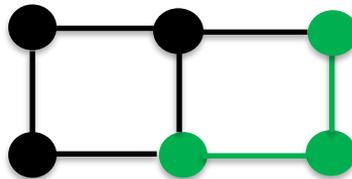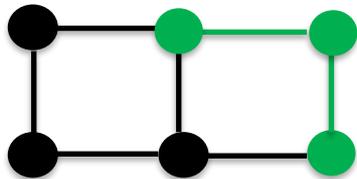And the support of the terms in f_2
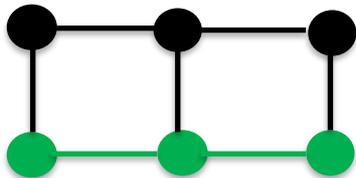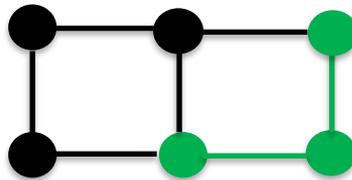
VISUALIZING THE RECURRENCE

If our base graph is

And the support of the terms in f_2

Can also track how the coefficients grow

OPEN QUESTIONS

Does entanglement exhibit a sharp phase transition?

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Lot of **missing metaphors** with the classical theory

Summary:

- New physical law: At high temperature, quantum spin systems have **zero entanglement**

- Proof via carefully designed expansions and the **extraction operator**

- **For what kind of quantum spin systems should we expect quantum advantage in preparing the Gibbs state?**

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Thanks! Any Questions?