Phase Transitions in Quantum Spin Systems

Ankur Moitra (MIT)

UC Berkeley, February 26th

based on joint work with Ainesh Bakshi,
Allen Liu and Ewin Tang

A GUIDING QUESTION

How do local interactions give rise to macroscopic behavior?

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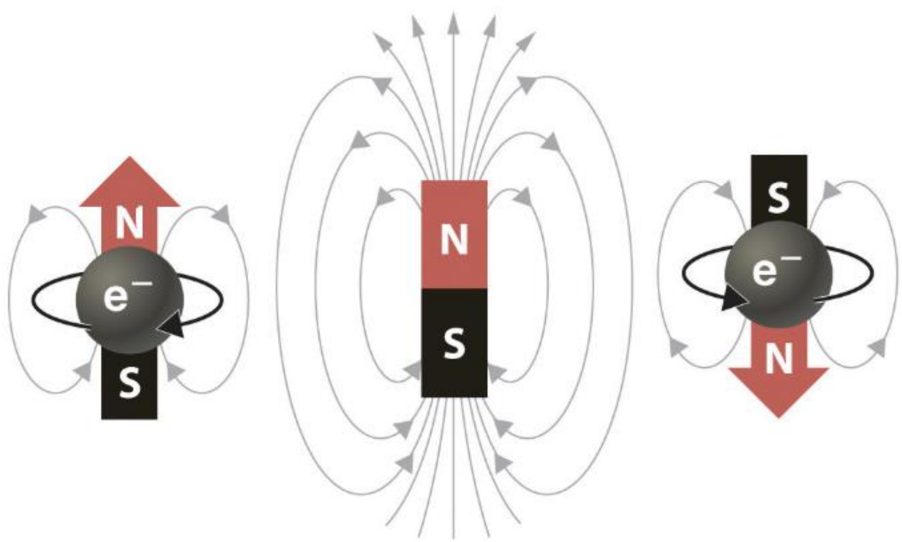
Running example: Consider **magnetism** – caused by most electron spins being oriented in same direction



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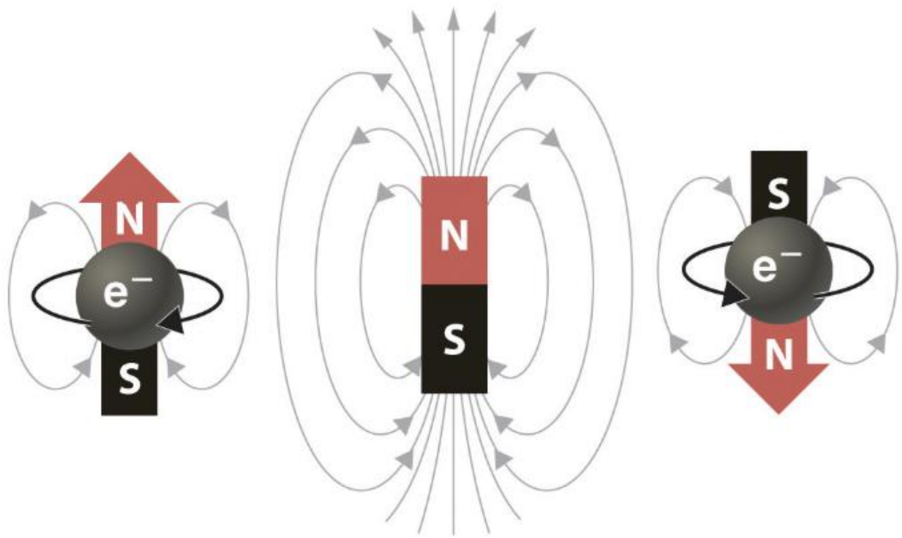

How do they know which way to point, if they don't all interact?

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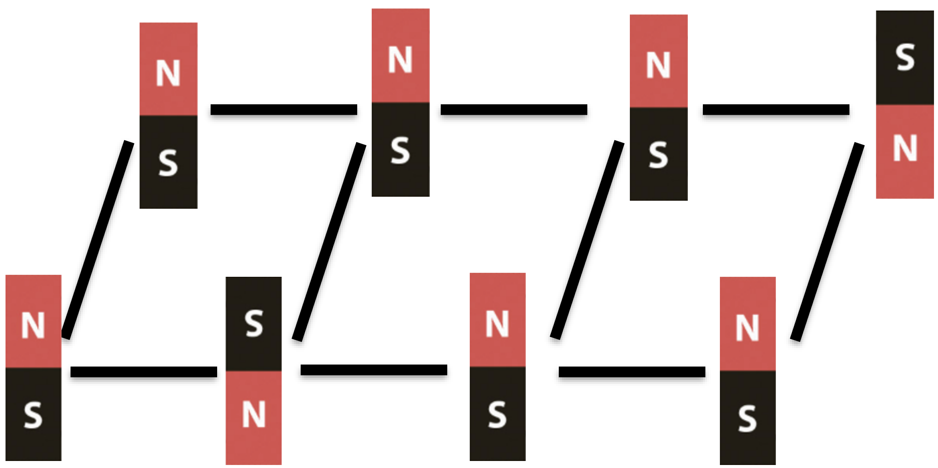

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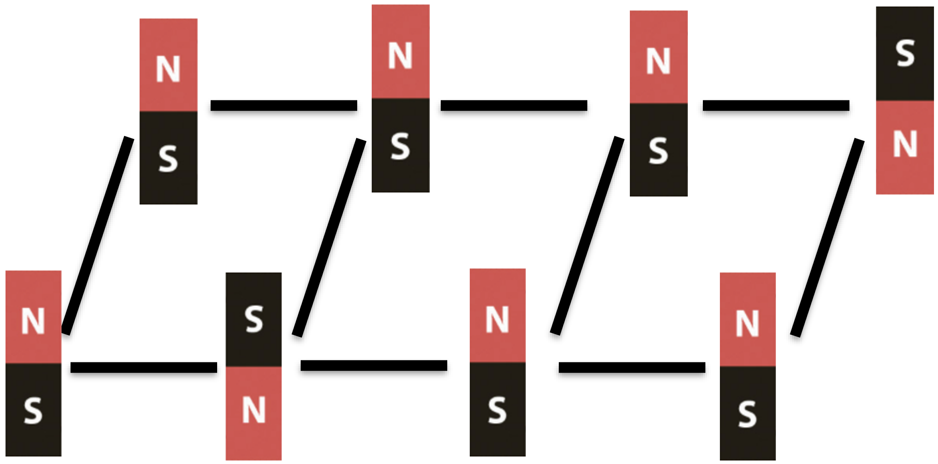

Statistical physics: Define a probabilistic model that captures behavior at thermal equilibrium and study its structural properties

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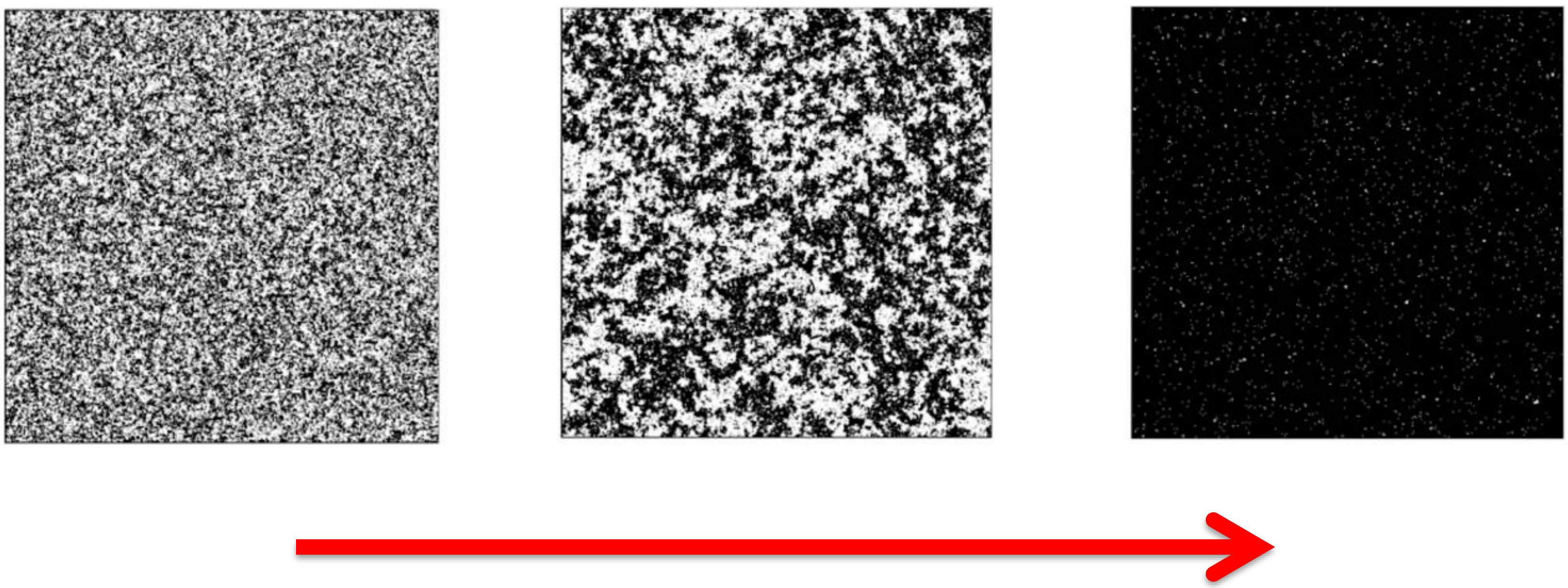
⚠ **Caution:** The Markov property fails in quantum spin systems

PHASE TRANSITIONS

Dramatic changes in macroscopic properties as temperature varies

e.g. **average magnetization**



decreasing temperature

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QUANTUM SPIN SYSTEMS

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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. $H_e = A \otimes I \otimes \cdots \otimes I$

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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

In the limit as $\beta \to 0$ (i.e. **infinite temperature**) we have

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What happens at reasonable physical temperatures?

OUR RESULTS

We show that heat kills all entanglement

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

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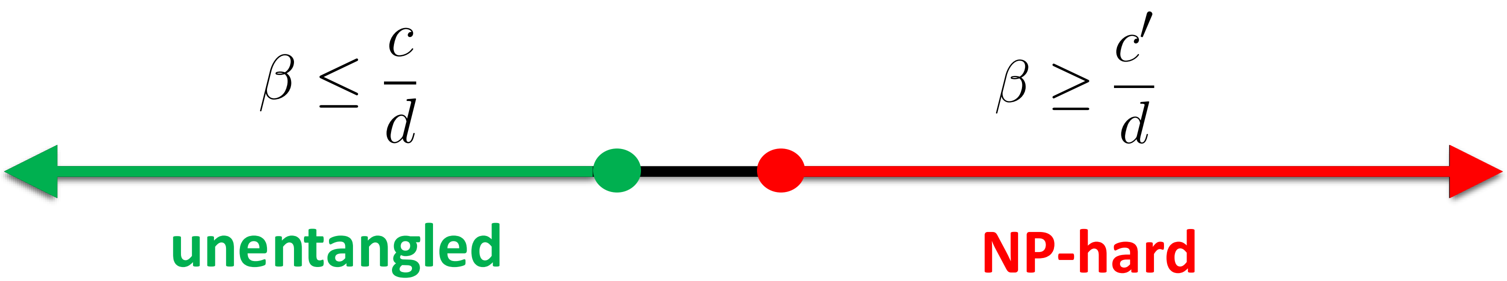
Theorem [Sly] [Sly,,Sun]: Even classical Gibbs sampling is NP-hard for k = 2 and $\beta \geq \frac{c'}{d}$ for some constant c'

And so the region you could hope for quantum advantage is now quite narrow for constant locality



INDEPENDENT WORK

Theorem [Rouze, Franca, Alhambra]: 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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This is too weak for our purposes, but there is a sharpening that points the way forward

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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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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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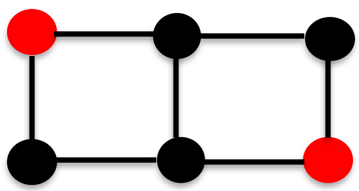
Natural Markov chain with local updates

choose node at random,
forget its state



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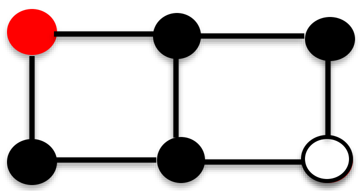

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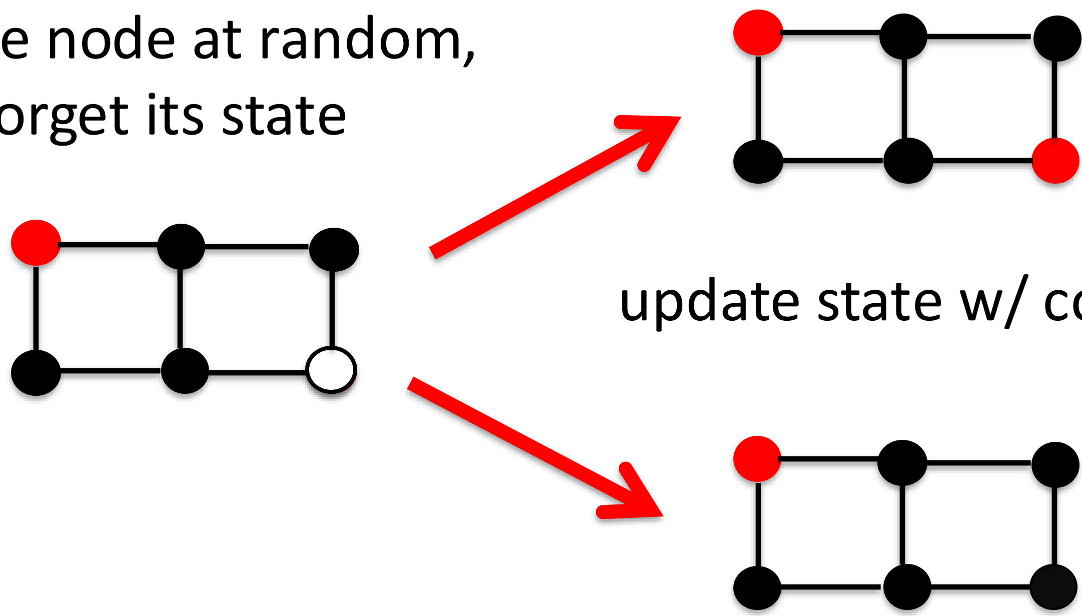

update state w/ correct probability

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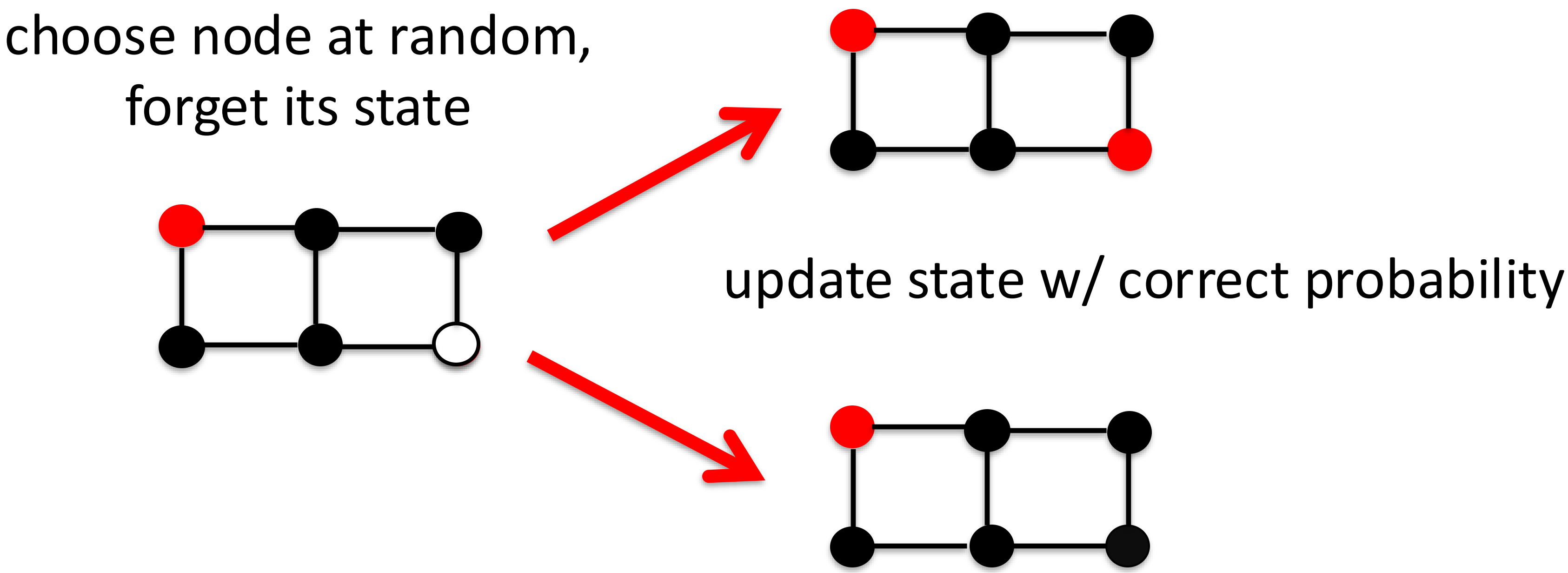
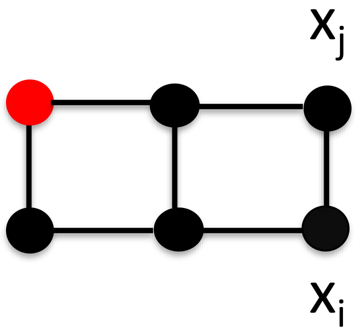


Its unique steady state distribution is the Gibbs distribution

PINNING TO A PRODUCT DISTRIBUTION

A classical thought experiment



First update x_i then update x_j

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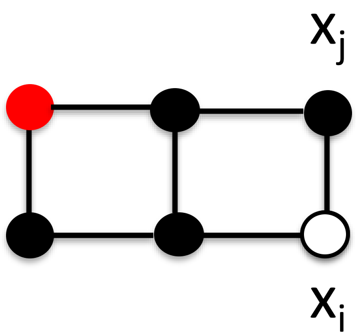

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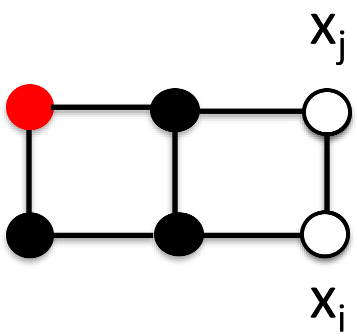

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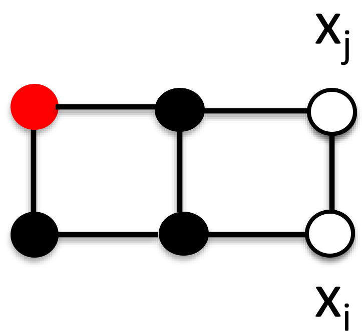

both options almost equally likely

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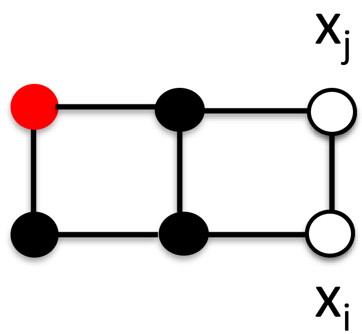

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Claim: At high temperature, there is a good chance that their updates can be made independently, in which case we can ignore their edge

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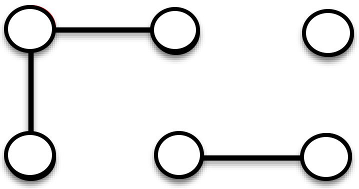
Try to make x_i independent of the rest, but keep only edges that are needed as correction terms



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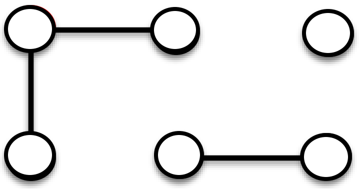

And you end up with small connected components – **this is where locality comes from**

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

THE EXTRACTION OPERATOR

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Definition: The **extraction operator** is

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

THE KEY LEMMA

Lemma: We can write

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

and…

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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

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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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EXPANDING THE EXTRACTION OPERATOR

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$$M_1 = \left(\sum_{i=0}^{\infty} \frac{(\beta/2)^i}{i!} (H - H_1)^i \right) \left(\sum_{j=0}^{\infty} \frac{(\beta/2)^j}{j!} (-H)^j \right)$$

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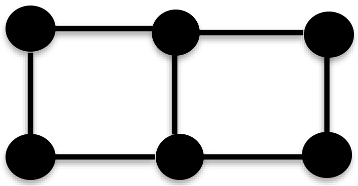
Hence, for each new term, its support grows by one incident edge

VISUALIZING THE RECURRENCE

If our base graph is



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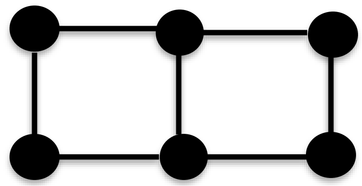
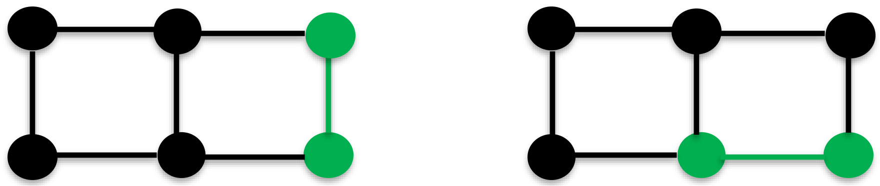


we can visualize the support of the terms in f_1



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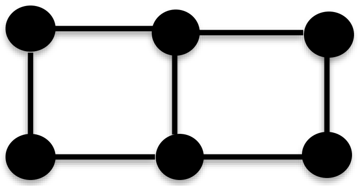
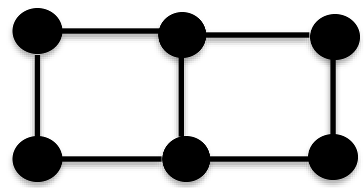
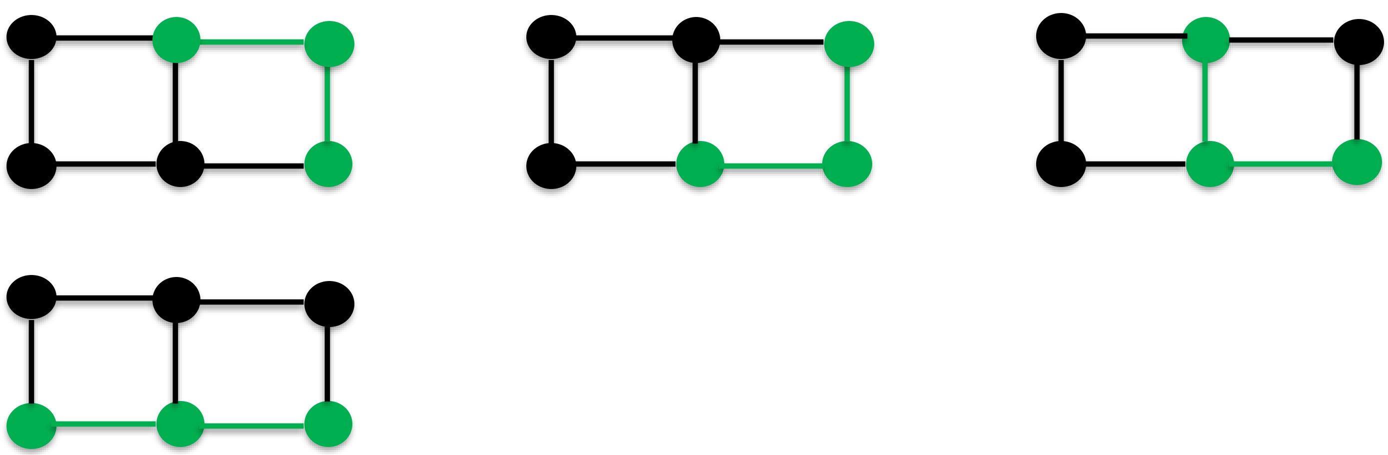


VISUALIZING THE RECURRENCE

If k = 2 and our base graph is



And the support of the terms in f_2



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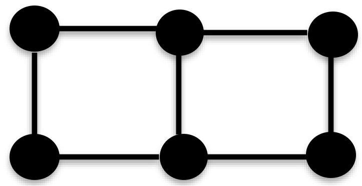

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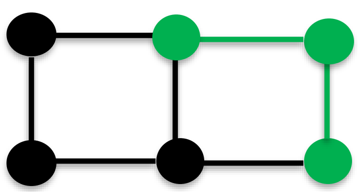

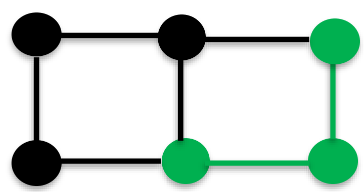

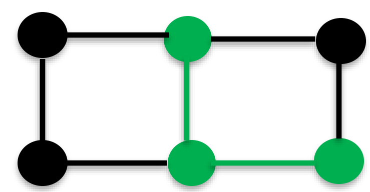

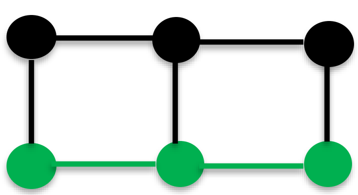

Can also track how the coefficients grow

OPEN QUESTIONS

Does entanglement exhibit a sharp phase transition?

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And does that transition happen earlier than NP-hardness

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Related to classical notions like **spatial mixing**

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?