Title: Quantum Algorithms for Classical Sampling Problems

Speakers: Dominik Wild

Series: Perimeter Institute Quantum Discussions

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Abstract: Sampling from classical probability distributions is an important task with applications in a wide range of fields, including computational science, statistical physics, and machine learning. In this seminar, I will present a general strategy of solving sampling problems on a quantum computer. The entire probability distribution is encoded in a quantum state such that a measurement of the state yields an unbiased sample. I will discuss the complexity of preparing such states in the context of several toy models, where a polynomial quantum speedup is achieved. The speedup can be understood in terms of the properties of classical and quantum phase transitions, which establishes a connection between computational complexity and phases of matter. To conclude, I will comment on the prospects of applying this approach to challenging, real-world tasks.

Quantum Algorithms for Classical Sampling Problems

Dominik S. Wild

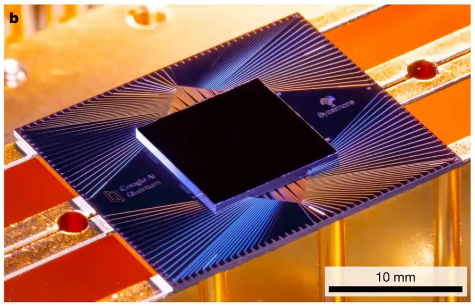
Quantum Information Seminar - Perimeter Institute

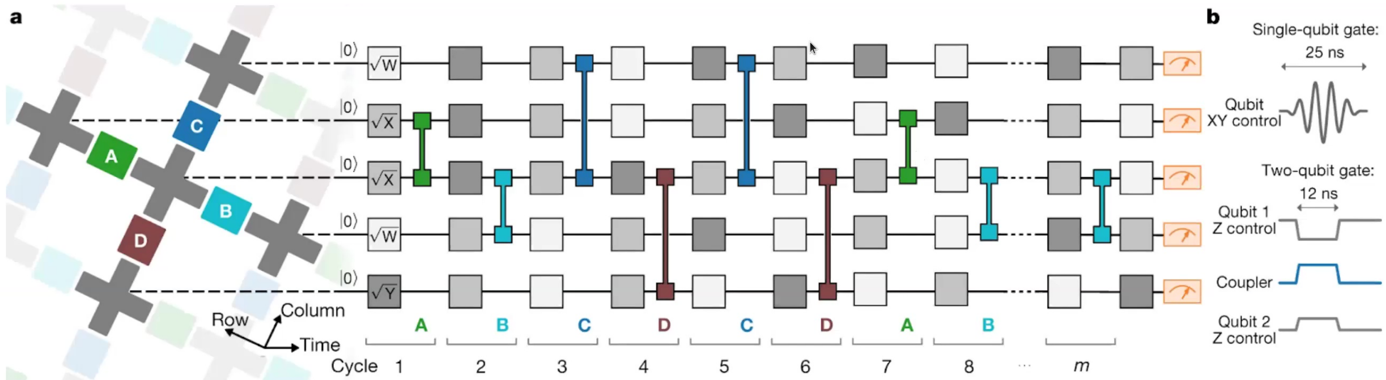
December 1, 2021

Phys. Rev. Lett. **127**, 100504 (2021)
Phys. Rev. A **104**, 032602 (2021)

Sampling problems

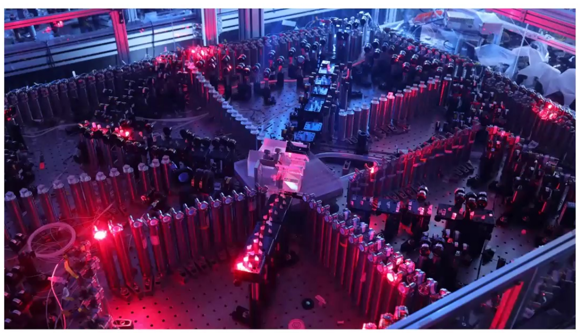
Sampling from random circuits

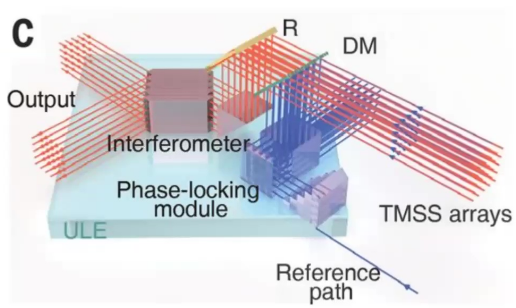




F. Arute *et al.*, Nature **574**, 505 (2019).

Boson sampling





H.-S. Zhong *et al.*, Science **370**, 1460 (2020).

Sampling problems

Quantum states naturally encode a sampling problem

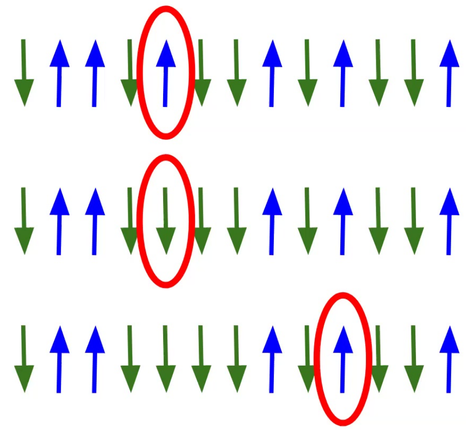
$$|\psi\rangle = \sum_s \sqrt{p(s)} e^{i\varphi(s)} |s\rangle$$

Focus on classical Gibbs distributions

$$|\psi(\beta)\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_s e^{-\beta H_c(s)/2} |s\rangle$$

Hard (spin glasses) and important (optimization, machine learning) problems can be formulated in terms of quantum state preparation.

Markov chain Monte Carlo



(i) Randomly select spin.

(ii) Flip spin with probability $p = \min(1, e^{-\beta \Delta E})$.

(iii) Repeat.

Markov chain defined in terms of generator *M*

$$p_{t+1}(s') = \sum_s p_t(s) M(s, s')$$

Detailed balance ensures convergence to Gibbs distribution

$$e^{-\beta H_c(s)} M(s, s') = e^{-\beta H_c(s')} M(s', s)$$

Parent Hamiltonian

$$H_q(\beta) = \mathbb{I} - e^{-\beta H_c/2} M(\beta) e^{\beta H_c/2}$$

- $H_q(\beta)$ is real and symmetric (detailed balance).
- $|\psi(\beta)\rangle$ is a ground state of $H_q(\beta)$ (detailed balance, *M* is stochastic matrix).
- Gap of $H_q(\beta)$ equals difference between largest and second largest eigenvalue of *M* (~ 1/mixing time).

F. Verstraete *et al.*, Phys. Rev. Lett. **96**, 220601 (2006).

Quantum sampling algorithm

Define sampling problem

$$p(s) = \frac{1}{\mathcal{Z}} e^{-\beta H_c(s)}$$

Pick Markov chain *M*.

Compute parent Hamiltonian

$$H_q(\beta) = \mathbb{I} - e^{-\beta H_c/2} M(\beta) e^{\beta H_c/2}$$

with ground state

$$|\psi(\beta)\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_s e^{-\beta H_c(s)/2} |s\rangle$$

Identify efficient adiabatic pathway from initial Hamiltonian H_0 with simple ground state to $H_q(\beta)$.

Adiabatically prepare $|\psi(\beta)\rangle$

Measure in computational basis to obtain sample from *p(s)*.

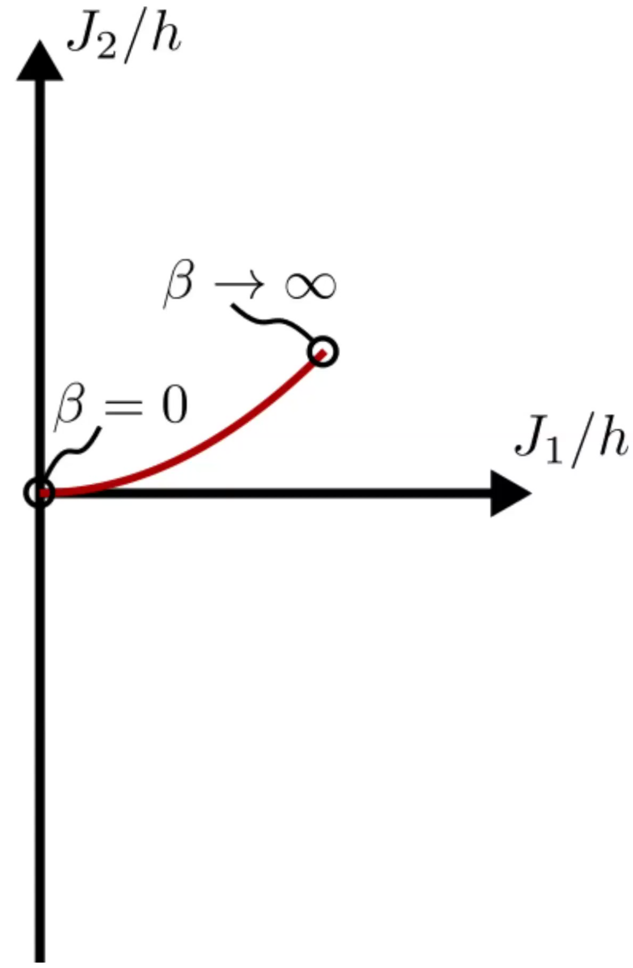
R. D. Somma, C. D. Batista, G. Ortiz, Phys. Rev. Lett. **99,** 030603 (2007).

Example I: Ising chain

$$H_c = -\sum_i \sigma_i^z \sigma_{i+1}^z$$

Single spin flip updates with Glauber dynamics

$$H_q(\beta) = -h(\beta)\sum_i \sigma_i^x - J_1(\beta)\sum_i \sigma_i^z\sigma_{i+1}^z + J_2(\beta)\sum_i \sigma_{i-1}^z\sigma_i^x\sigma_{i+1}^z$$



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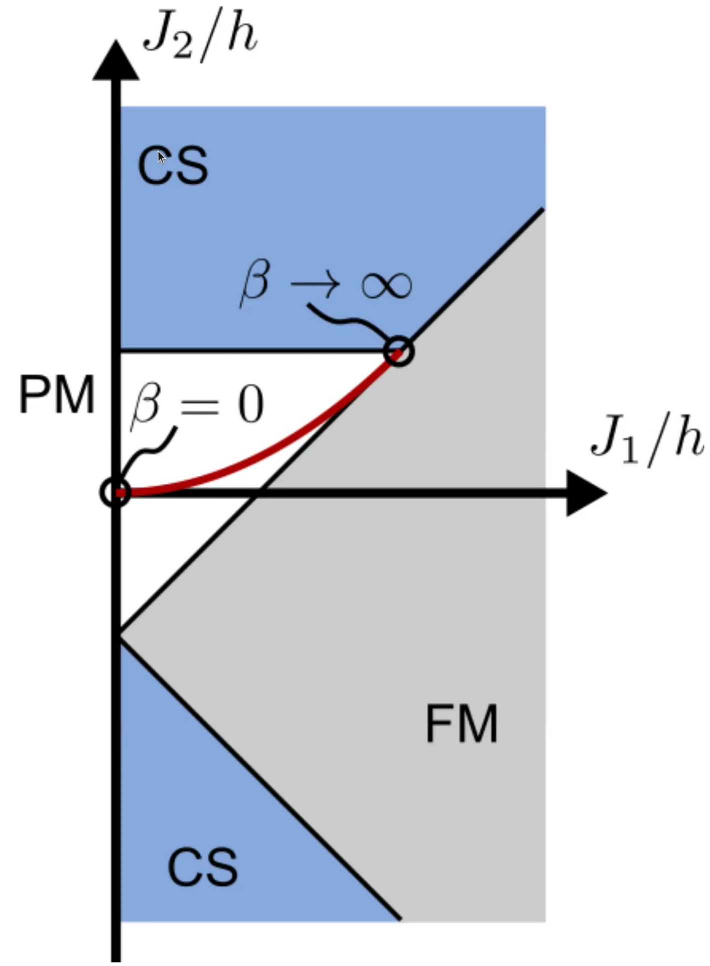

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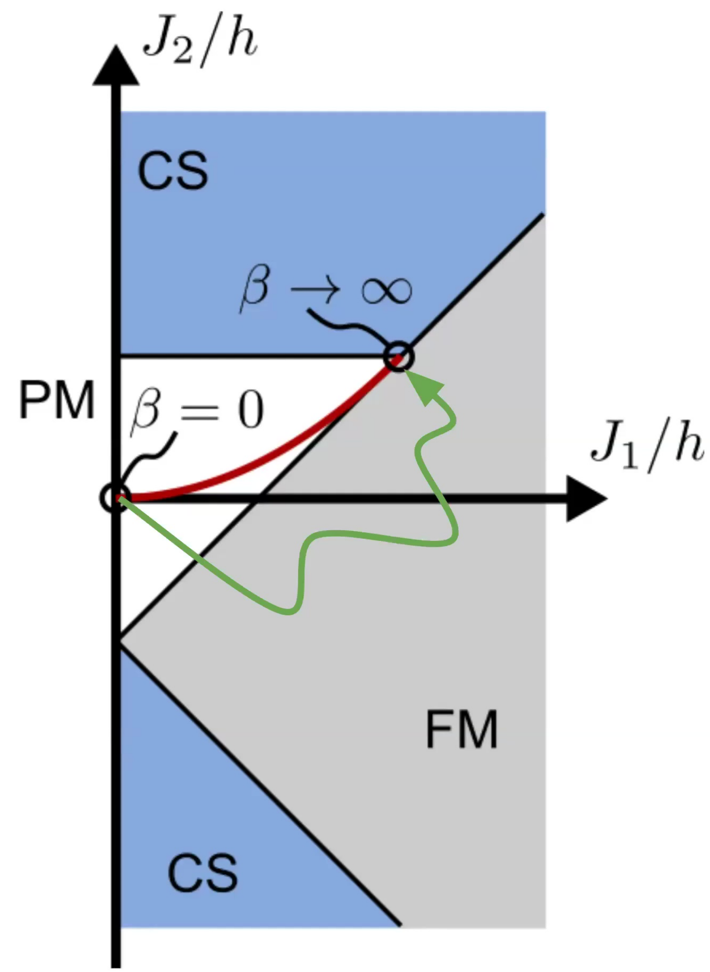
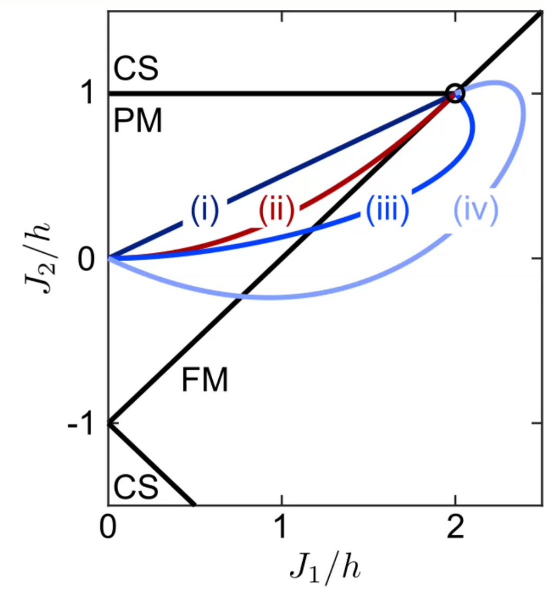
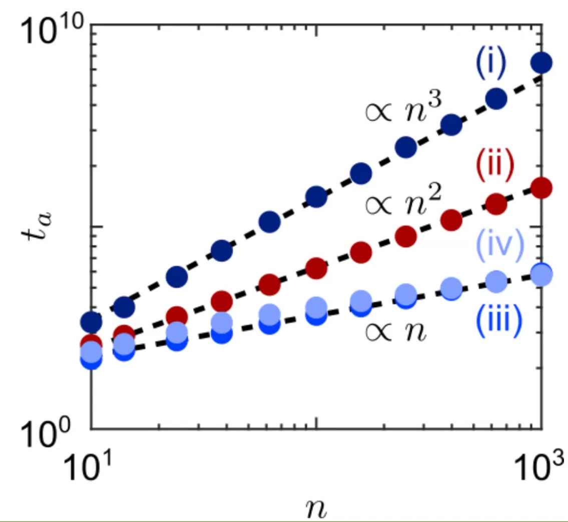
Key result: Trajectories in extended parameter space can lead to quantum speedup.



Speedup

- Can sample efficiently at any finite temperature, using Markov chain or adiabatic state preparation.
- Mixing time of Markov chain at zero temperature $t_m \sim n^2$ limited by diffusion.
- Adiabatic state preparation along $H_q(\beta)$ achieves same time complexity.
- Ballistic propagation of domain walls at Ising transition gives quadratic speedup for paths (iii) and (iv).





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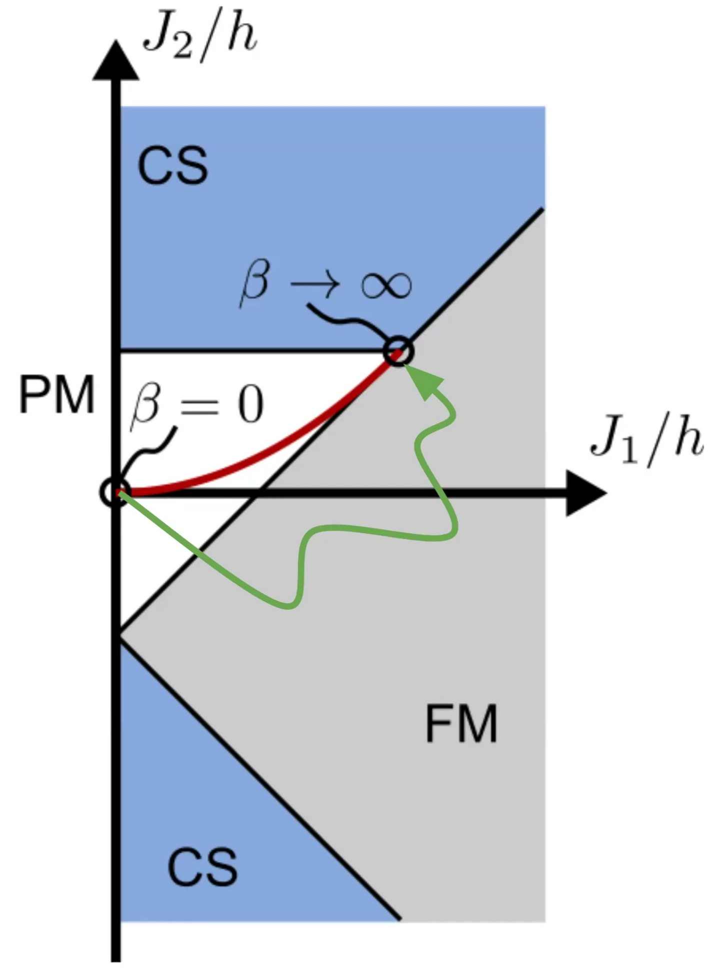
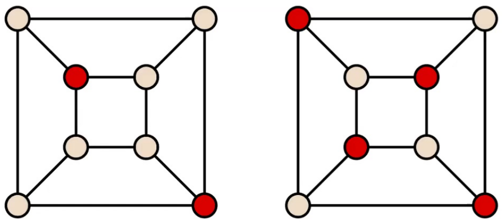


Sampling from independent sets

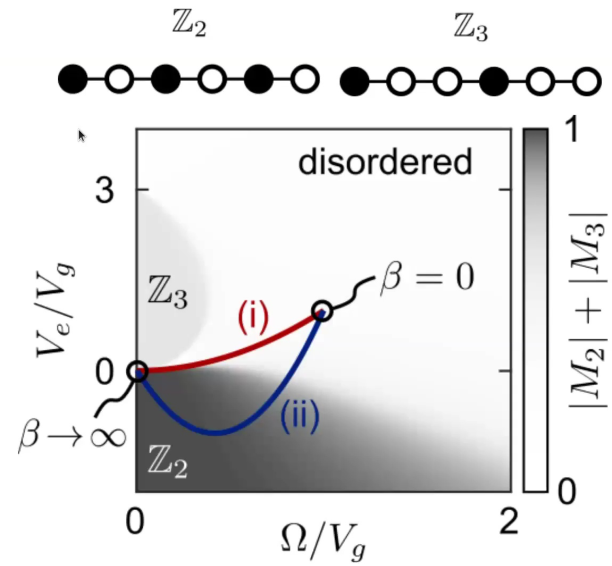


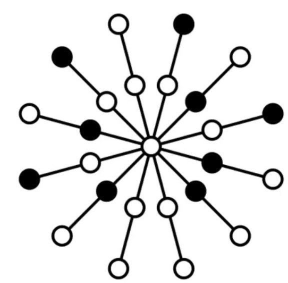
$$H_c = -\sum_{i \in V} n_i$$

The parent Hamiltonian derived from a single spin-flip Markov chain describes a generalized PXP model:

$$H_q(\beta) = \sum_{i \in V} P_i \left(e^{-\beta n_i} - e^{-\beta/2} \sigma_i^x \right)$$

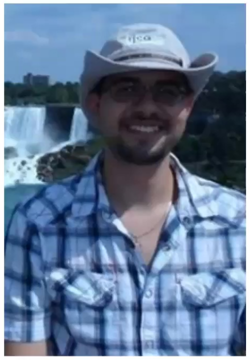
Can be implemented on certain graphs using Rydberg interactions.





Recap so far

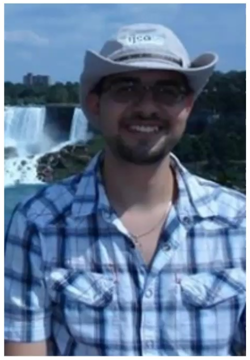
- Found quantum speedup for classical sampling problems by adiabatically preparing a state encoding the entire Gibbs distribution.
- Uncovered connection between computational complexity and quantum phases.



Cristian Zanoci
(MIT)

Recap so far

- Found quantum speedup for classical sampling problems by adiabatically preparing a state encoding the entire Gibbs distribution.
- Uncovered connection between computational complexity and quantum phases.
- Does this approach work beyond toy models?
  - ≥2 dimensions
  - disorder



Cristian Zanoci
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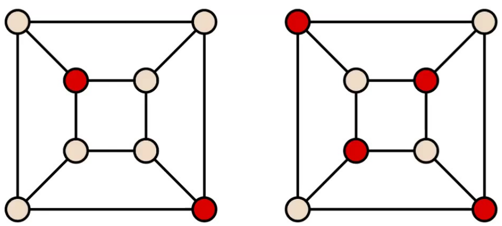
Sampling from independent sets



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Ising model in two dimensions

Single spin flips on a hexagonal lattice

$$H_q(\beta) = -h(\beta)\sum_i \sigma_i^x - J_1(\beta)\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z$$
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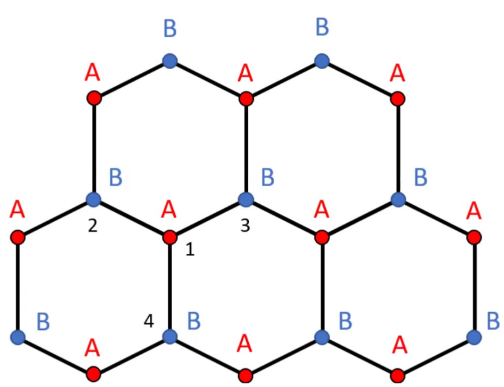
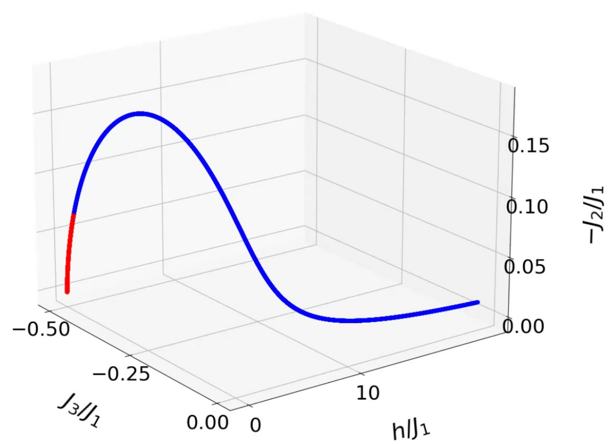
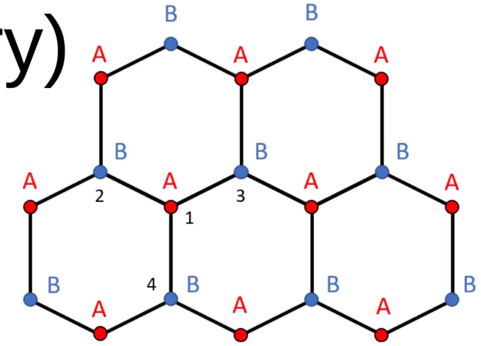




Ising model in two dimensions (preliminary)



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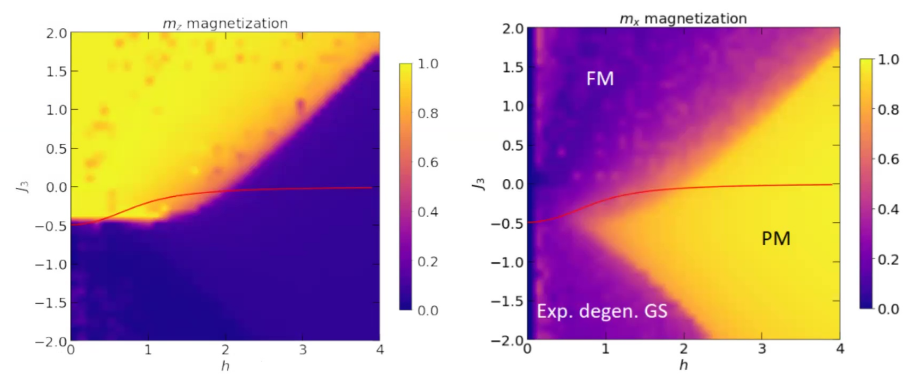

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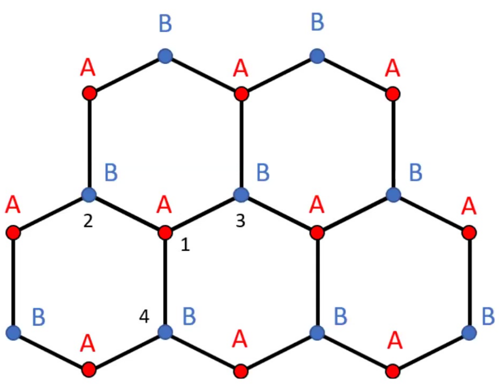

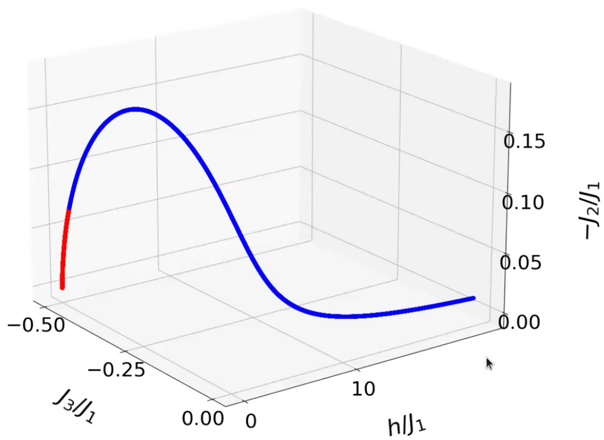

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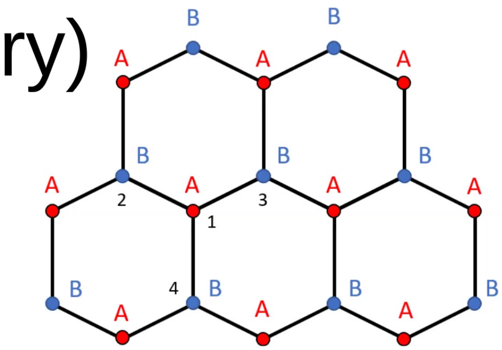

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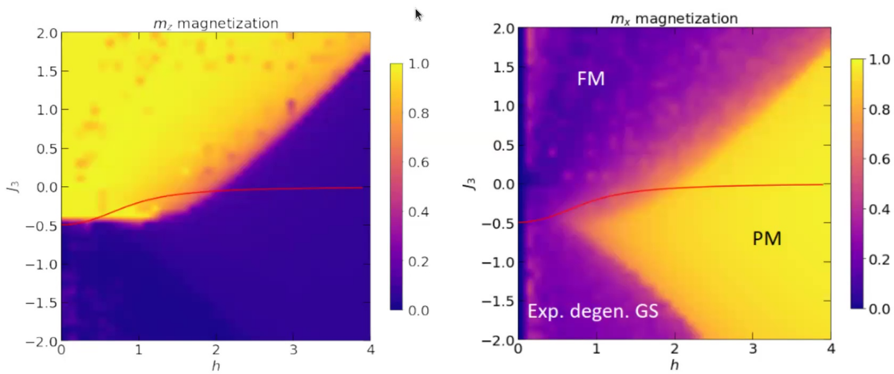

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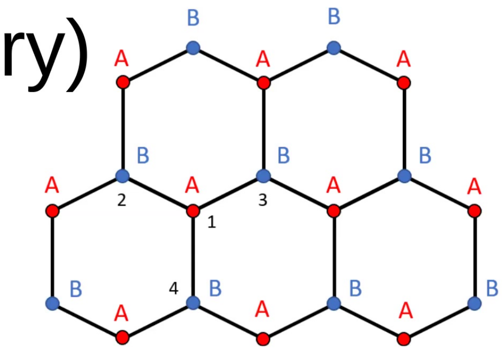

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- Extremely rich phase diagram
- Classical ferromagnetic phase corresponds to boundary between quantum phases.
- Adiabatic evolution along “thermal line” is extremely slow. Exponentially faster paths exist.

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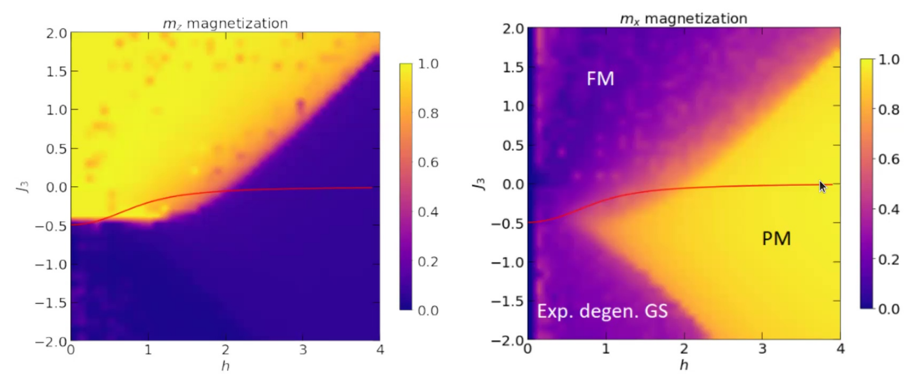
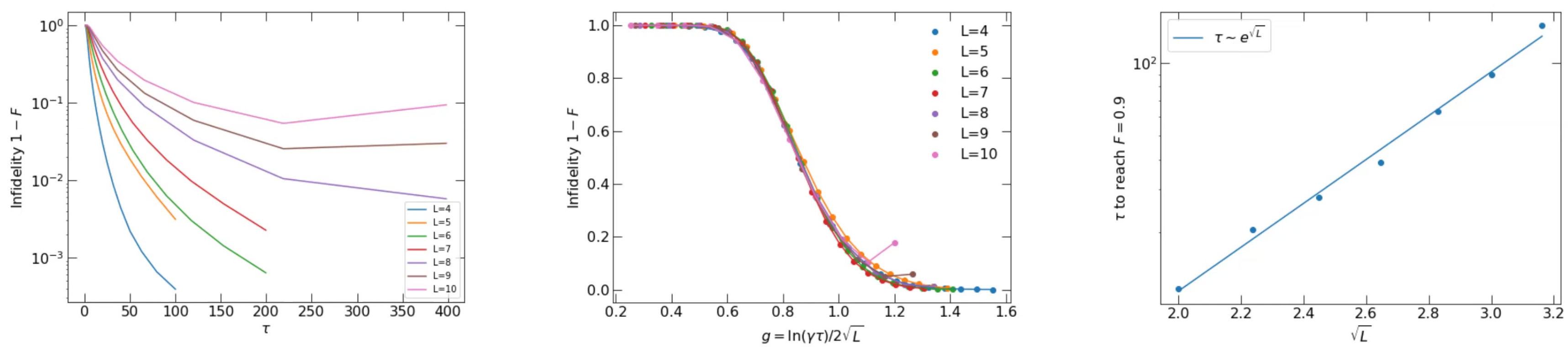


Disordered models (preliminary)

- Few general statements are known about quantum annealing of disordered systems.
- Disordered, ferromagnetic Ising model in 2D:

$$H(t) = -\sum_{\langle ij \rangle} J_{ij}\sigma_i^z\sigma_j^z - \Gamma(t)\sum_i h_i\sigma_i^x$$



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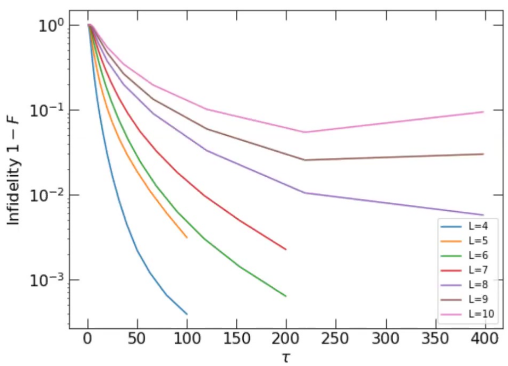
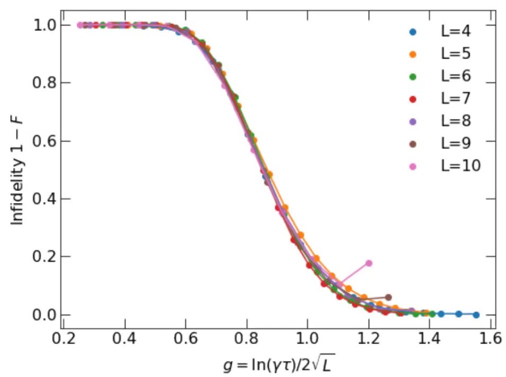
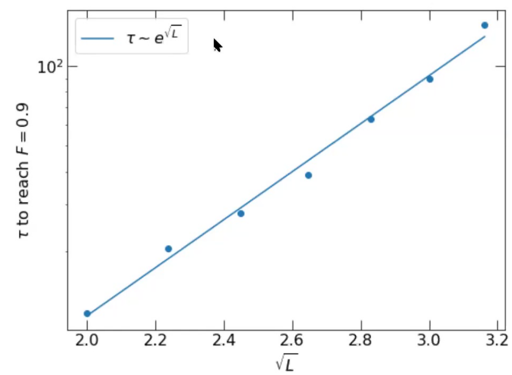
- Suspect that (classical) simulated annealing requires τ ~ exp(L)





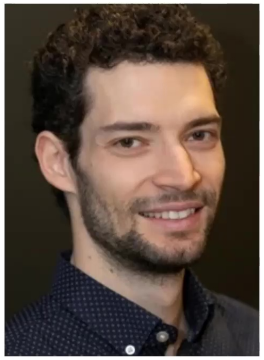


Summary and Outlook

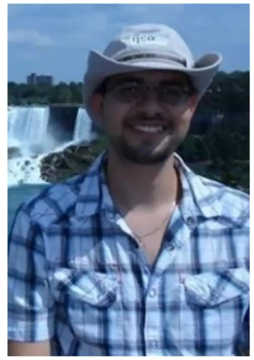
- Found quantum speedup for classical sampling problems by adiabatically preparing a state encoding the entire Gibbs distribution.
- Uncovered connection between computational complexity and quantum phases.
- Interesting physics for harder problems with potential speedup over simulated annealing.
- Use hybrid approaches to find good adiabatic paths.

Acknowledgments

Dries Sels
(NYU & Flatiron)



Hannes Pichler
(Innsbruck)



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Mikhail Lukin
(Harvard)

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J. Ignacio Cirac
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Marie Skłodowska-Curie
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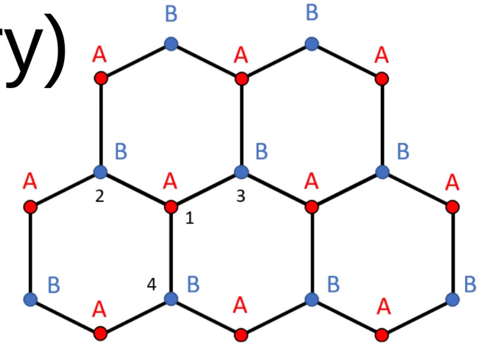

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