Studying phase transitions in lattices using a superconducting quantum processor
Quantum Information: Quo Vadis?

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November 14, 2019


D:WAVE
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D:wave
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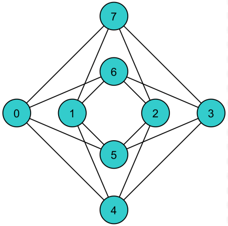
SYS:9

Initial plan:Solve classical optimization problems

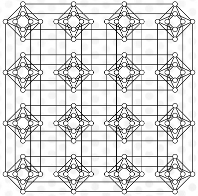
- Work with binary variables: ± 1 (**Ising model**)
- Energy function $\mathcal{E} : \{-1, +1\}^n \to \mathbb{R}$ represents "cost" of states
- Find minimum energy state: **ground state**
- Near-optima often useful, depending on application

$$H = \underbrace{\left[\sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z \right]}_{\text{classical Ising Hamiltonian}}$$

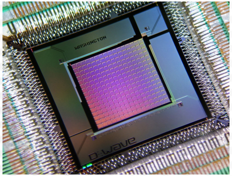
D-Wave quantum annealing system



unitcell



topology



processor (2000+ qubits)

- Qubits are not fully connected
- Chimera topology
- 8 qubits in a unitcell
- each unitcell is bipartite

Ising model can represent harder problems

frontiers in PHYSICS

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Ising formulations of many NP problems

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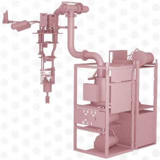
We provide Ising formulations for many NP-complete and NP-hard problems, including all of Karp's 21 NP-complete problems. This collects and extends mappings to the Ising model from partitioning, covering, and satisfiability. In each case, the required number of spins is at most cubic in the size of the problem. This work may be useful in designing adiabatic quantum optimization algorithms.

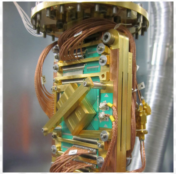
Keywords: spin glasses, complexity theory, adiabatic quantum computation, NP, algorithms

D-Wave quantum annealing system

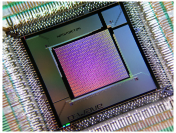
shielded room (1nT)



cryostat (10mK)



sample holder

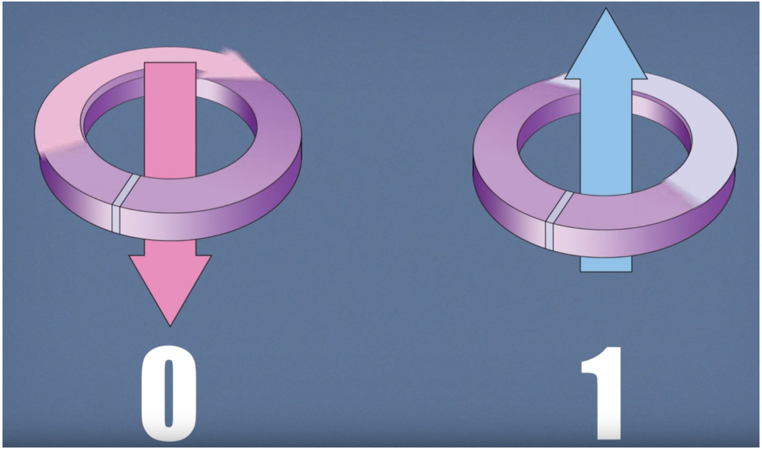


processor (2000+ qubits)

- Implementation of quantum annealing in transverse Ising model (not gate model quantum computing)
- Evolves a physical system of superconducting currents (± 1 spins). Default evolution time is 5 µs
- Finishes in a low-energy state of a classical Ising Hamiltonian.

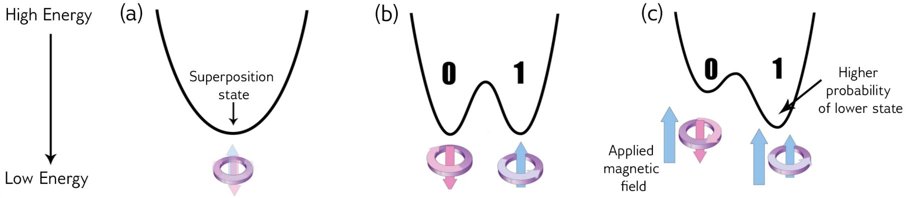
A qubit

A qubit's state is implemented as a circulating current.



Quantum annealing

Energy diagram changes over time as the quantum annealing process runs and a bias is applied

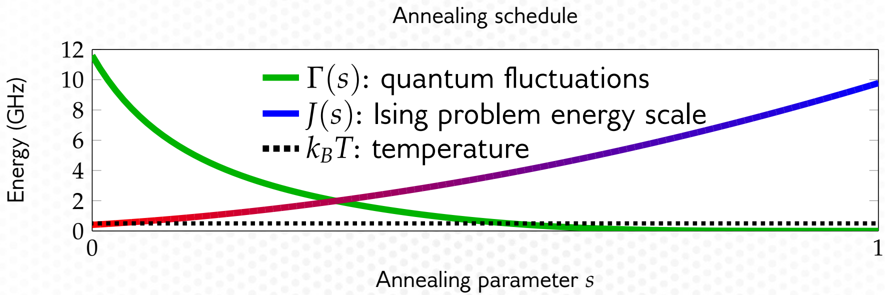


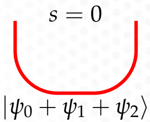
Hamiltonian: Transverse field Ising model

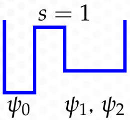
Annealing parameter $0 \leq s \leq 1$

$$H(s) = -\ \Gamma(s) \underbrace{\left[\sum_i \sigma_i^x\right]}_{\text{quantum fluctuations}} + J(s) \underbrace{\left[\sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z\right]}_{\text{classical Ising Hamiltonian}}$$

Quantum annealing (Kadowaki, Nishimori 1998)

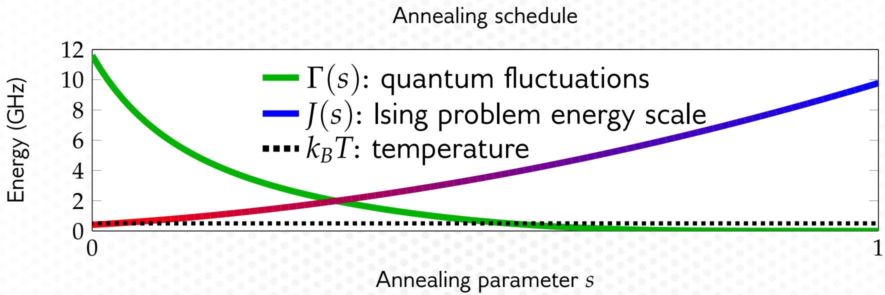






Bypass energy barriers: **tunnel through** (quantum) or **hop over** (classical)

Quantum annealing (Kadowaki, Nishimori 1998)



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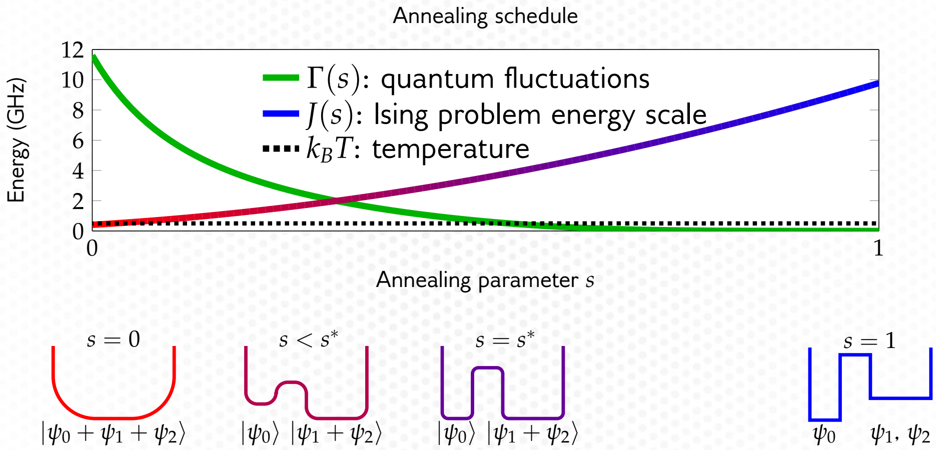

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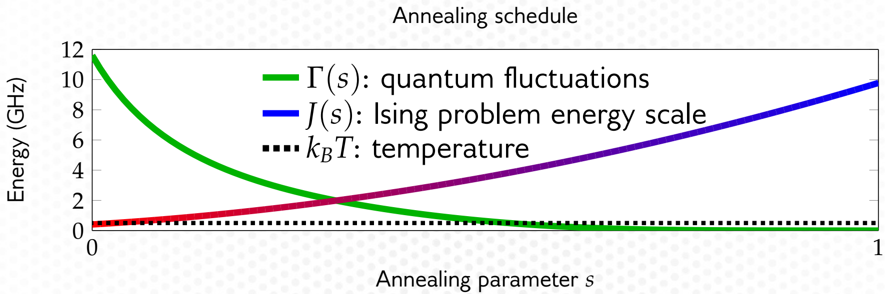
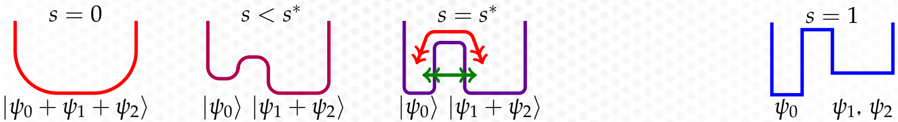




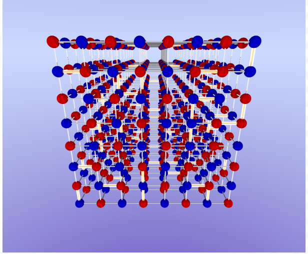
Bypass energy barriers: **tunnel through** (quantum) or **hop over** (classical)

Simulating quantum magnetic systems

Natural application

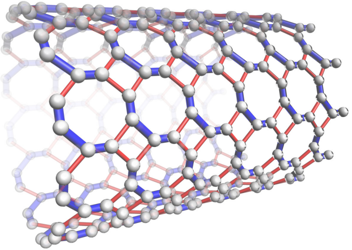
- Quantum annealing is performed in TFIM: Transverse field Ising model
- D-Wave processors = programmable TFIM

Cubic lattice



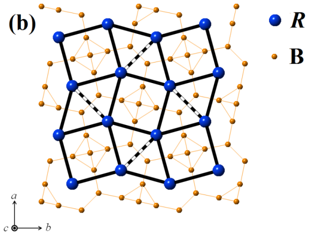
Science 2018,
See Richard Harris's Talk

Square-octagonal lattice



Nature 2018, and
arXiv:1911.03446

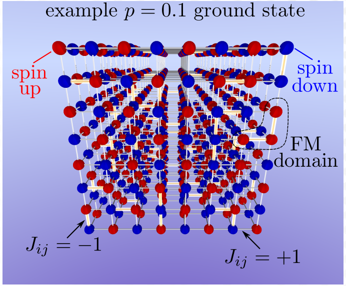
Shastry-Sutherland lattice

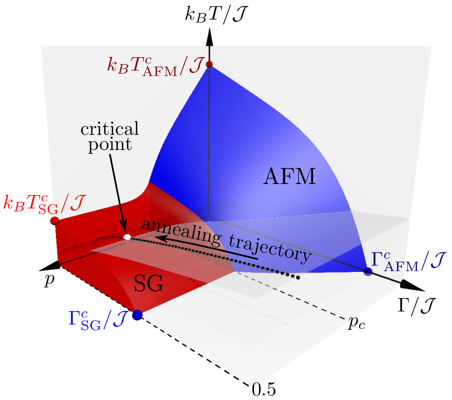


Paul Kairys, Oak Ridge
National Laboratories

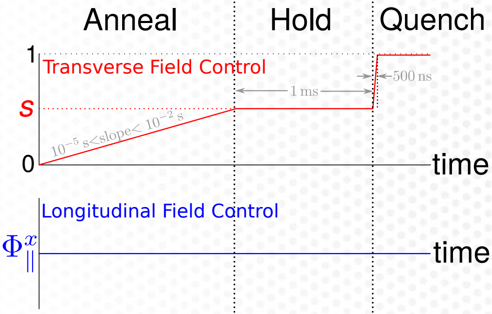
3D cubic lattice

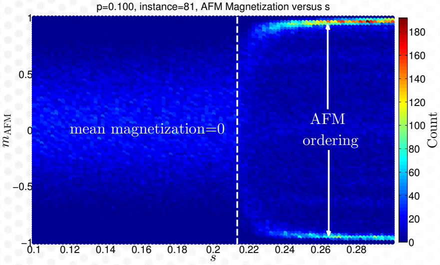
- Simulate quantum phase transition of doped AFM lattice
- The Hamiltonian: $H = \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z$
- Doping: $P(J_{ij} = 1) = 1 - p$ and $P(J_{ij} = -1) = p$
- Quantum phase transition at Γ_c / J





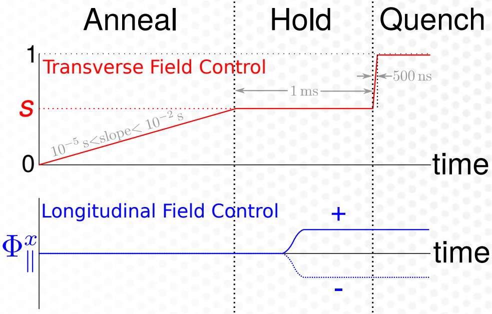
3D cubic lattice: Magnetization

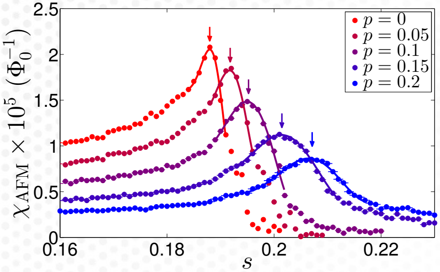




3D cubic lattice: PM to AFM transition

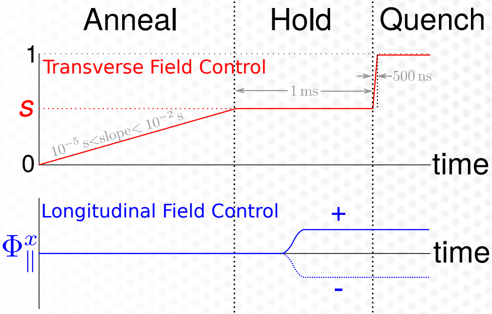
Susceptibility: $\chi_{AFM} = \frac{dm_{AFM}}{d\Phi^x_{\parallel}}$

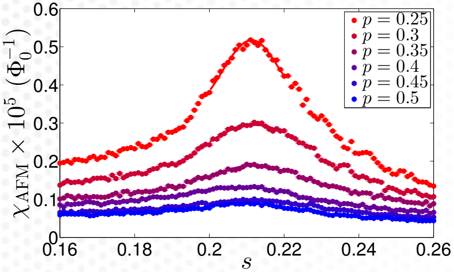




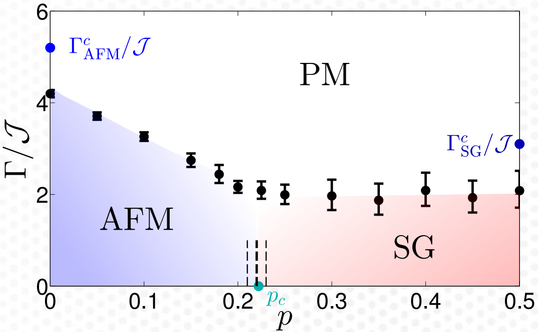
3D cubic lattice: PM to Spin Glass transition

Susceptibility: $\chi_{AFM} = \frac{dm_{AFM}}{d\Phi^x_{\parallel}}$





3D cubic lattice: Phase diagram

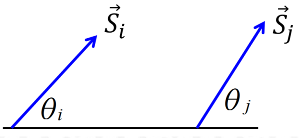


Sketching out the phase diagram

- m versus p gives p_c (from Binder cumulant crossing)
- Susceptibility peaks give Γ_c

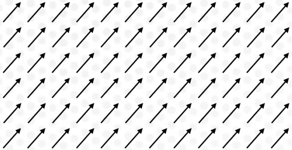
Square Octagonal Lattice: XY model

Classical 2D spin:



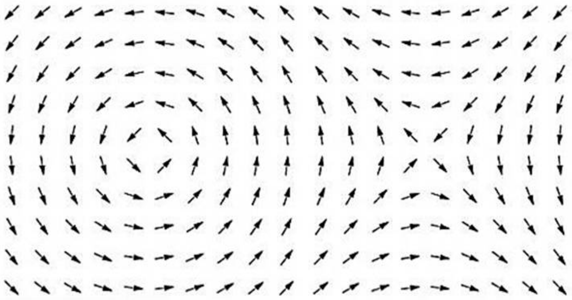
XY-Hamiltonian $H = -J_{\text{XY}} \sum_{i,j} \vec{S}_i \cdot \vec{S}_j = -J_{\text{XY}} \sum_{i,j} \cos\left(\theta_i - \theta_j\right)$

Ground state:
all spins aligned



Continuous rotational symmetry: $O(2)$ or $U(1)$

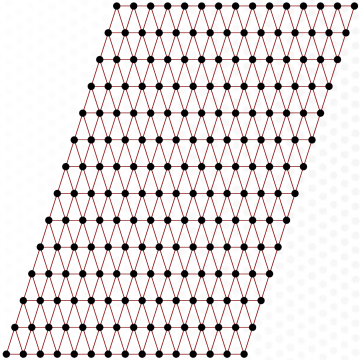
Square Octagonal Lattice: Topological excitations



Defects appear in vortex/antivortex pairs (Stokes' Theorem)

But when are these pairs tightly bound?
Below the KT phase transition

Square Octagonal Lattice: Transverse Field Ising Model in Triangular Lattice



Hamiltonian

$$H = \sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x$$

Theoretical predictions

- Blankschtein, Ma, Berker, Grest & Soukoulis, PRB 29, 5250 (1984)
- Moessner, Sondhi & Chandra, PRL 84, 4457 (2000)
- Moessner & Sondhi, PRB 63, 224401 (2001)
- Isakov & Moessner, PRB 68, 104409 (2003)
- Wenzel, Coletta, Korshunov & Mila, PRL 109, 187202(2012)

Square Octagonal Lattice: Order by disorder (transverse field Γ)

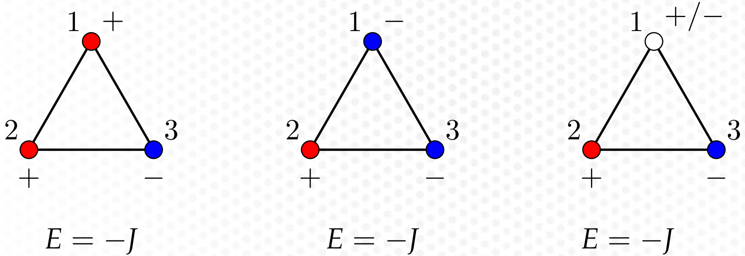
Hamiltonian

$$H = \sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma \sum_i \sigma_i^x$$

6-degenerate frustrated ground state

Classical $E_{\mathrm{GS}} = -J$

Quantum $E_{\mathrm{GS}} = -J - \Gamma$



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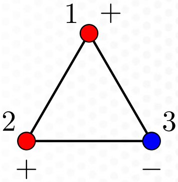
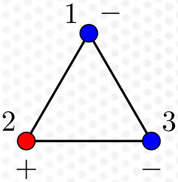


$E = -J$



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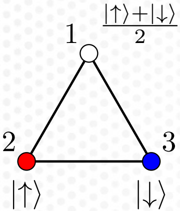

$E = -J - \Gamma$

Perturbative picture

Floppy spins (no net effective field) align with transverse field

Square Octagonal Lattice: Order by disorder (transverse field Γ)

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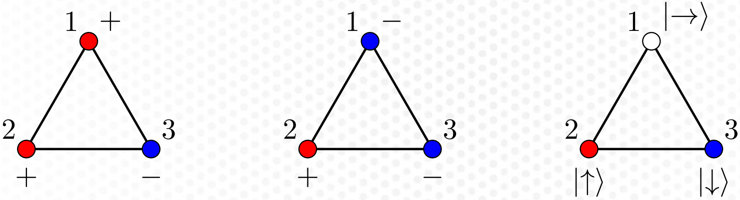

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Perturbative picture

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Square Octagonal Lattice: Order by disorder (transverse field Γ)

Hamiltonian

$$H = \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

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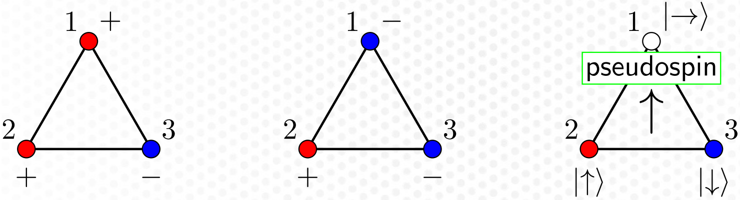

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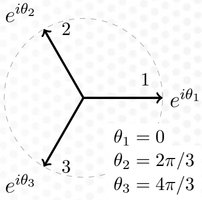
Perturbative picture

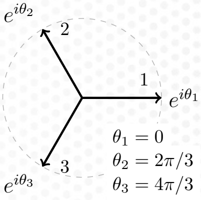
Floppy spins (no net effective field) align with transverse field

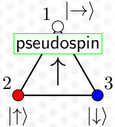
Square Octagonal Lattice: Order Parameter

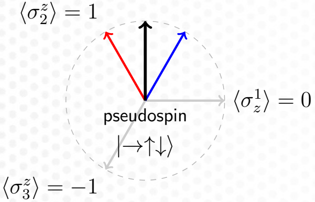


$$\psi = me^{i\theta} = (m_1 + m_2 e^{i2\pi/3} + m_3 e^{i4\pi/3})/\sqrt{3}$$

Square Octagonal Lattice: Order Parameter







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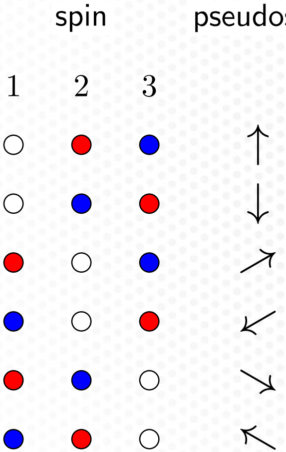
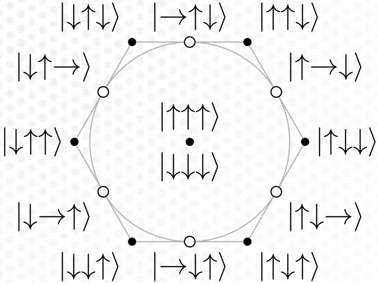
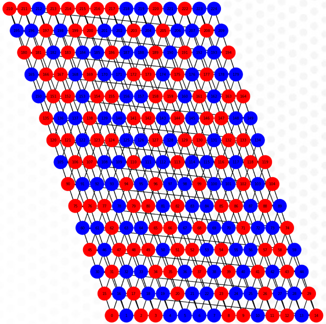
Square Octagonal Lattice: Pseudospin ⇒ 6 clock states (in perturbative picture)

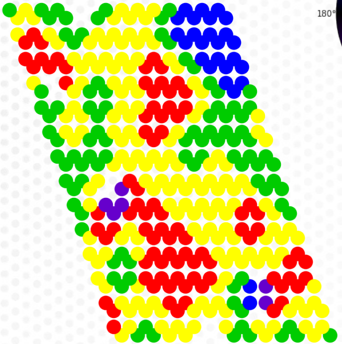


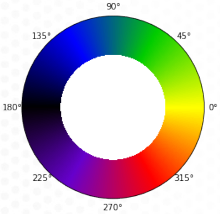


Square Octagonal Lattice: Dual Lattice

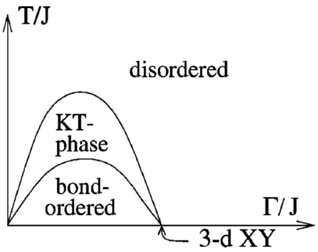


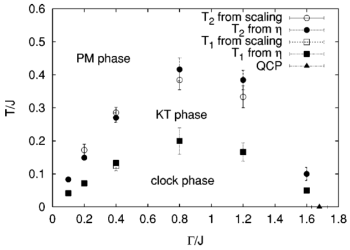
effective 2D XY model
on the dual lattice





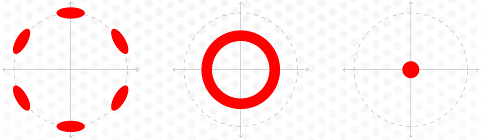
Square Octagonal Lattice: Triangular Lattice Phase Diagram





Moessner & Sondhi, 2001

Isakov & Moessner, 2003



Square Octagonal Lattice: Kosterlitz-Thouless phase transition

Above T_c

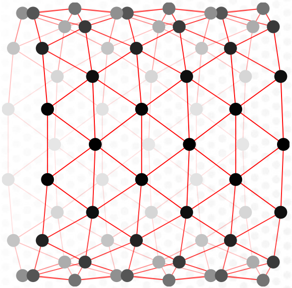
- V/AV pairs are unbound, not attracted
- Phase correlations decay **exponentially**

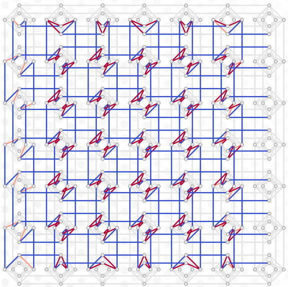
Below T_c

- V/AV pairs are bound
- Phase correlations decay **power-law**

Thermal + Quantum
Fluctuations

Square Octagonal Lattice: An Embedded Triangular Lattice

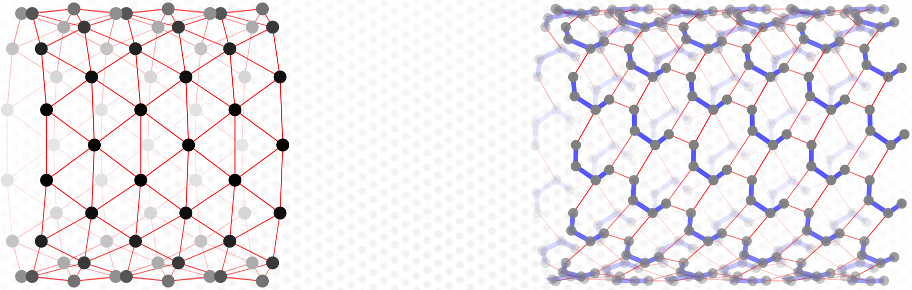




No native triangular lattice

AFM couplers have $J_{ij} = 1$, FM couplers have $J_{ij} = -1.8$

Square Octagonal Lattice: An Embedded Triangular Lattice



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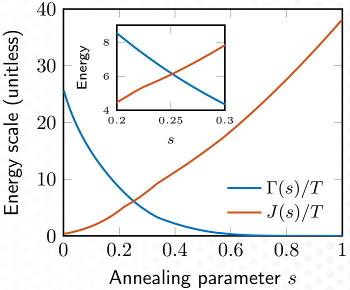
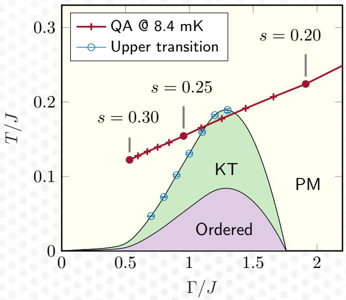
AFM couplers have $J_{ij} = 1$, FM couplers have $J_{ij} = -1.8$

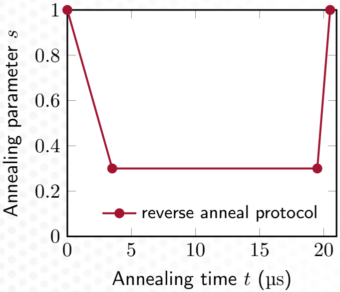
Fully-frustrated square-octagonal $\approx$ triangular AFM

- Similar low-energy theory (equivalent as $T \to 0, \Gamma \to 0$)
- Statistically very different

Square Octagonal Lattice: sampling protocol

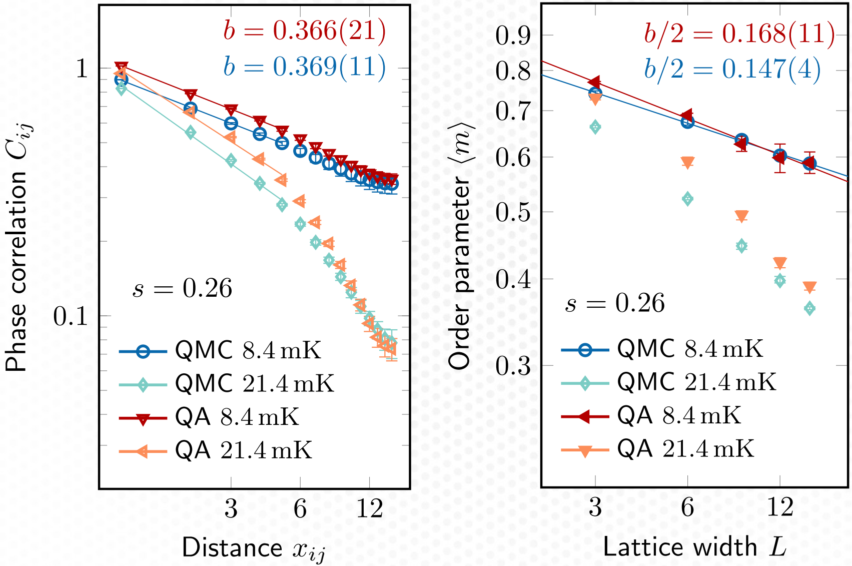




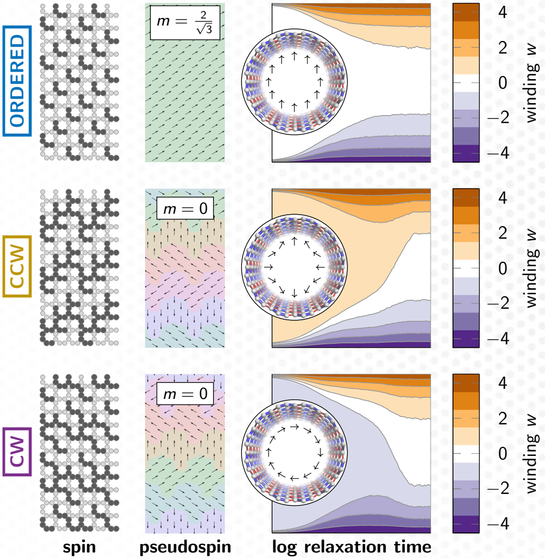


- QA schedule: Sequence of Hamiltonians, annealing parameter s
- **Pause** allows long relaxation at fixed Hamiltonians
- **Quench** allows "projective" readout
- **Reverse anneal** allows initialization in classical state at $s = 1$

Square Octagonal Lattice: Onset of power-law correlation decay



Square Octagonal Lattice: Convergence from three initial conditions



Unwinding

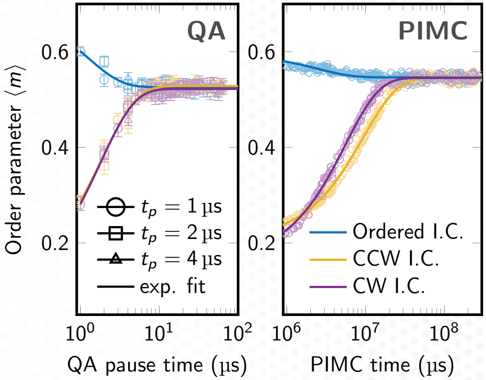
- Clear relaxation
- Based on Fourier transform of pseudospin vector field

Easier just to track order parameter m

- Single statistic
- Convergence from above and below

Square Octagonal Lattice: Equilibration dynamics

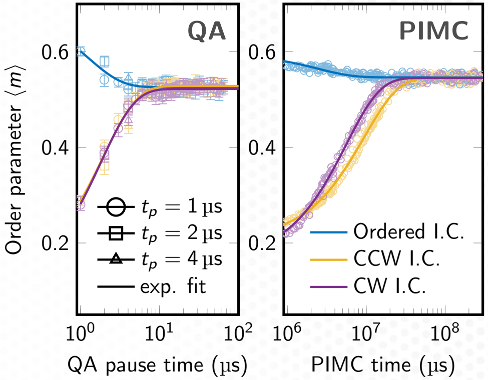
$s = 0.38, \ \ T = 13.7$ mK



- Path Integral Monte Carlo (a standard spatially local classical dynamics over worldlines, a form of Quantum Monte Carlo)
- Obeys detailed balance, converges to correct equilibria on some time scale

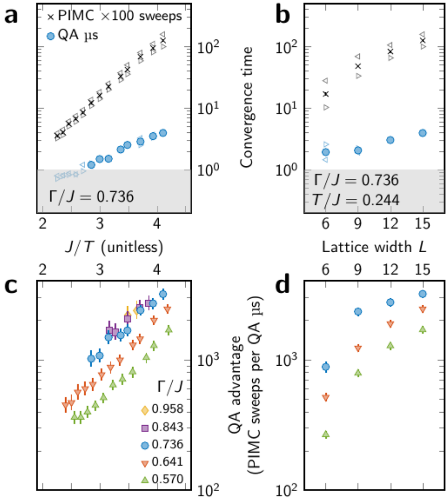
Square Octagonal Lattice: Equilibration dynamics

$s = 0.38, \;\; T = 13.7$ mK



- Path Integral Monte Carlo (a standard spatially local classical dynamics over worldlines, a form of Quantum Monte Carlo)
- Obeys detailed balance, converges to correct equilibria on some time scale
- Significantly slower in CPU and GPU implementations compared to anneal time

Square Octagonal Lattice: Time scale dependence on parameters



Inferior scaling in interesting regimes:

- Temperature decreases
- Transverse field increases
- System size increases

Quo Vadis? **Advantage^{TM} (2020)**

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Improved Pegasus topology (connectivity 15 replaces 6 in bulk)

Lower noise fabrication

Lower latency

Leap^{TM} and Ocean^{TM} integration

Support for hybrid applications

Conclusions

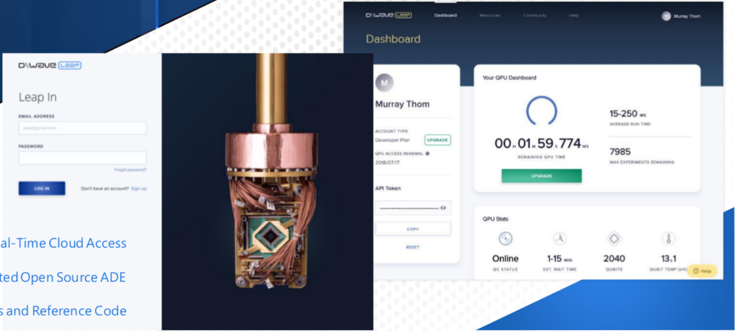
- D-Wave processors are well suited for material simulation
- Many models of interest are programmable
- Flexible protocols allow studies of equilibria, and dynamics

Thanks for your attention!

You can try it!

D-Wave Leap™
The *Only* Real-Time
Quantum Application Environment

Enabling a New Developer Community



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Extras: Exponential Time scale dependence on parameters

FIG. 4. **Scaling of convergence time and QA speedup.** **a–b**, Convergence time for both QA and PIMC as a function of inverse temperature J/T (**a**) and lattice width L (**b**). Triangles $\triangleleft$ and $\triangleright$ indicate times for CCW and CW initial states respectively; other markers indicate geometric mean. QA data is discarded if the estimate of $\langle m \rangle$ is not accurate to within 0.03, or either CCW or CW convergence time is $< 1\,\mu s$ (shaded region). **c–d**, QA advantage over PIMC, given as the ratio of convergence times, increases as T decreases (**c**), as quantum fluctuations increase (**c**), and as system size increases (**d**). Temperatures shown in **d** are minimum for which QA results are accurate ($J/T \approx 4.2$ in each case). Scaling in L (**b**, **d**) is given in terms of PIMC sweeps to show relaxation dynamics rather than computation time. All filled data points have 95% CI bootstrap error bars, often smaller than the marker. At $\Gamma/J = 0.736$, $T/J = 0.244$, QA relaxation is three million times faster than PIMC on a CPU (Methods).

