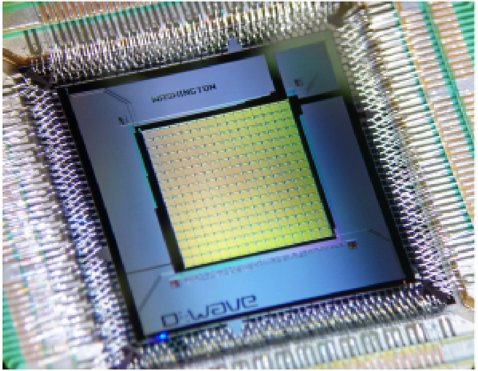
Quantum simulation of condensed matter in programmable qubit lattices

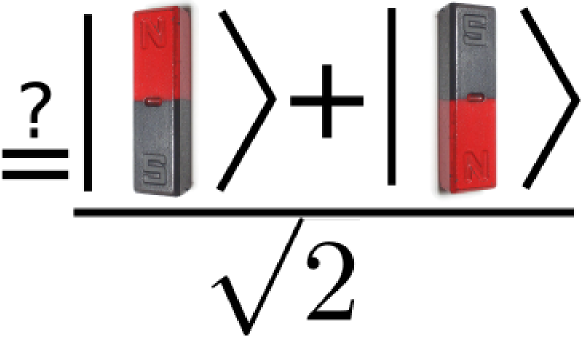
Jack Raymond, D-Wave Systems

Workshop IV: New Architectures and Algorithms
Science at Extreme Scales: Where Big Data Meets Large-Scale Computing
November 2018

D-Wave
The Quantum Computing Company™

How does one simulate a quantum magnet with a D-Wave processor?





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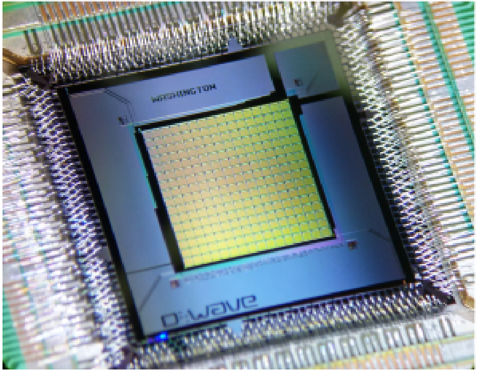
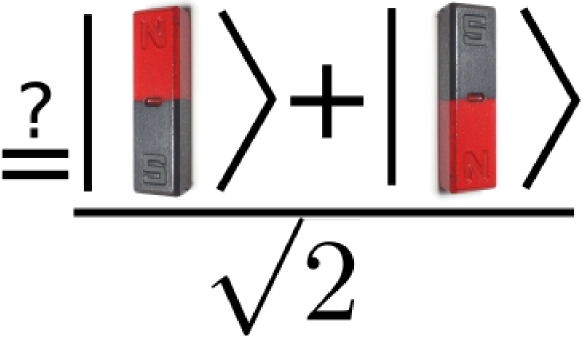




Experiments on single unit cells readily indicate quantum behaviour. Showing such behaviour over an entire processor is much more challenging.

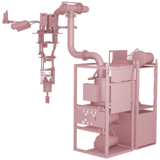
Outline

- Annealing for heuristic optimization
- Annealing for equilibrium sampling
- The anti-ferromagnetic, and spin-glass, phases on D-wave devices
- The Kosterlitz-Thouless phase (nuts and bolts)
- The Kosterlitz-Thouless phase on D-wave devices

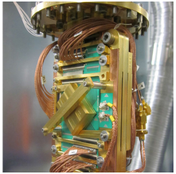
Annealing for heuristic optimization

D-Wave quantum annealing system in a clamshell

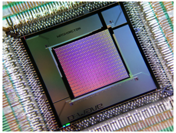
shielded room (1nT)



cryostat (10mK)



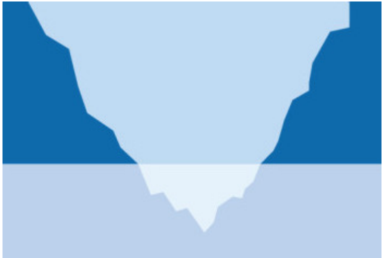
sample holder



processor (2048 qubits)

- Implementation of transverse field Ising model quantum annealing
- Prepare system of superconducting currents (± 1 spins) in a uniform superposition (flat potential)
- Evolve the physical system introducing interactions, default evolution time is 5 µs
- Finish in a low-energy state of the target model (complicated potential)

Initial plan: classical minimization 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

Hamiltonian: Transverse field Ising model

D:WAVE

Annealing parameter $0 \leq s \leq 1$

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

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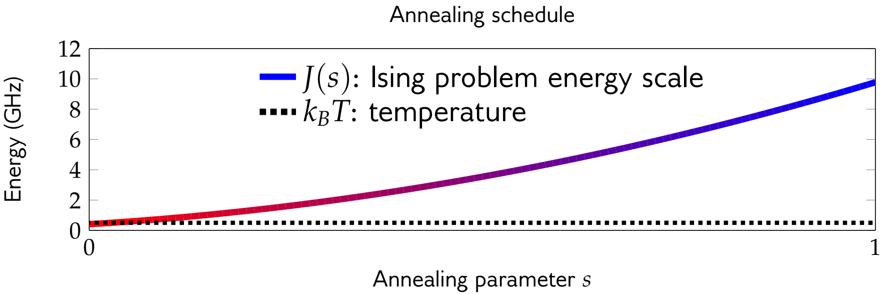
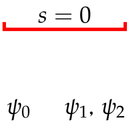
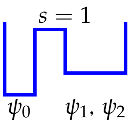
Two approaches to minimize the classical Ising Hamiltonian

- Classical thermal annealing, $\Gamma(s) = 0$ (Kirkpatrick, Gelatt, Vecchi, Science, 1983)
- Quantum annealing, $\Gamma(s) \to 0$ (Kadowaki+Nishimori, PRE, 1998)

Simulated (thermal) annealing







Bypass energy barriers: **hop over** (classical)

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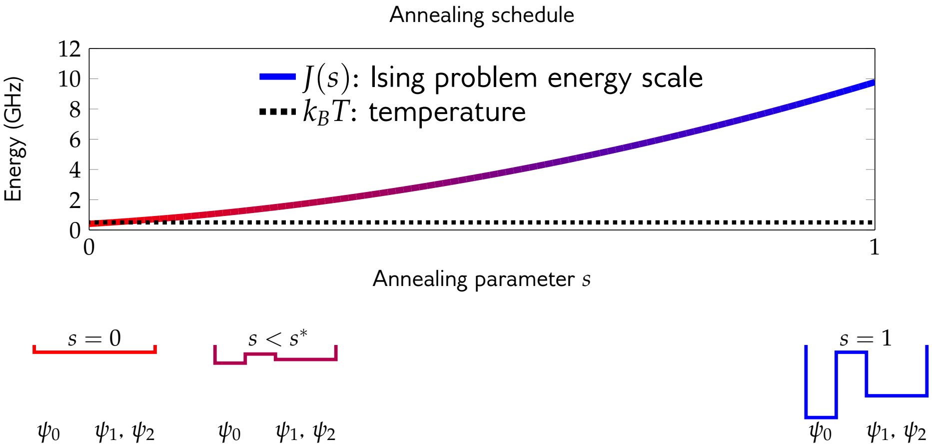

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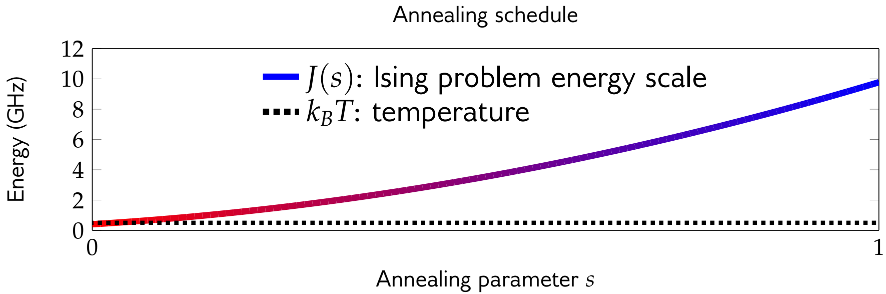

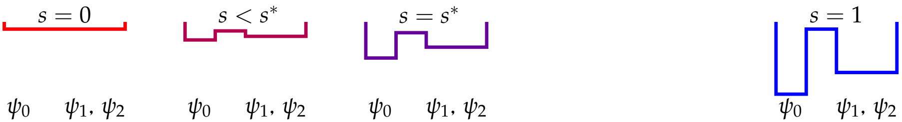

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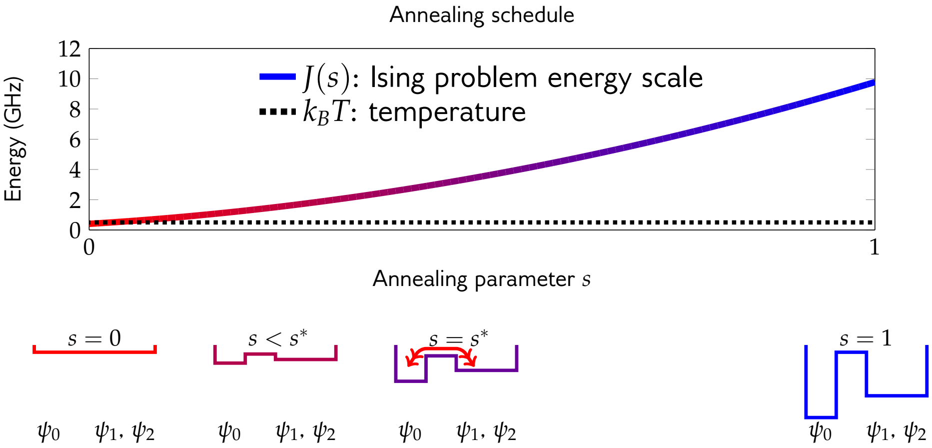
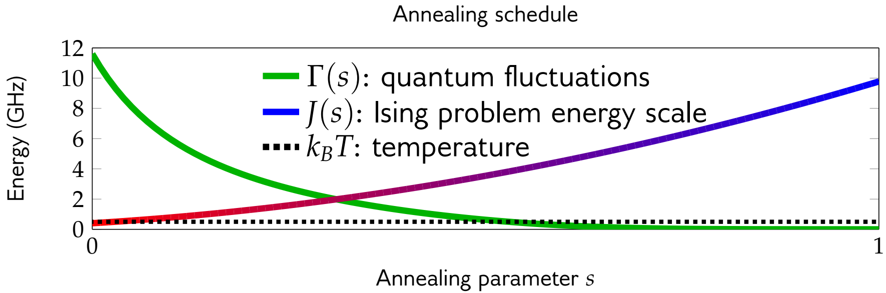
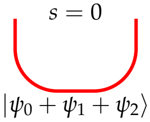
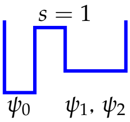


Bypass energy barriers: **hop over** (classical)

Quantum annealing



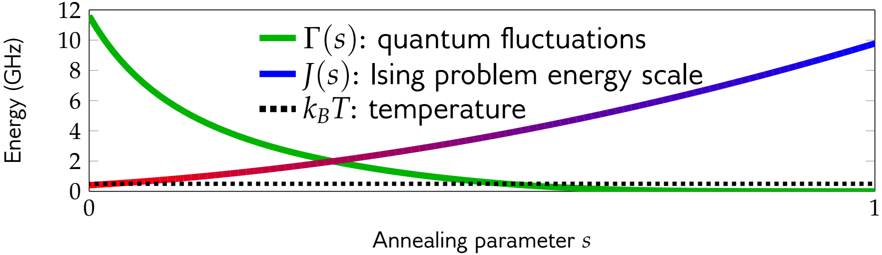




Bypass energy barriers: **tunnel through** (quantum) or **hop over** (classical)

Quantum annealing

Annealing schedule



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Quantum annealing

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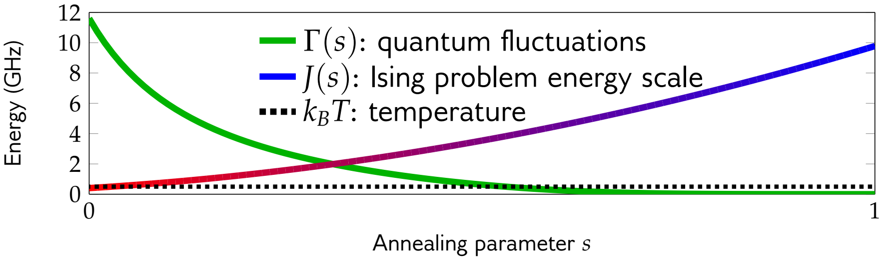

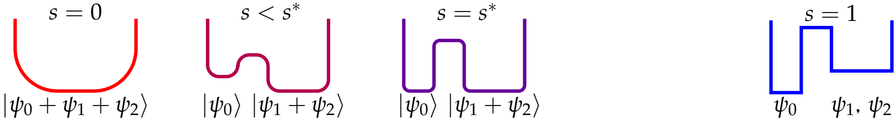

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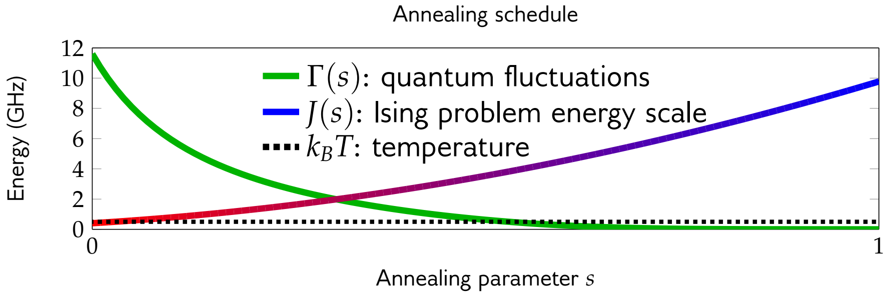

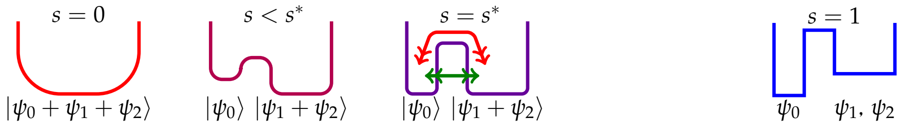

Bypass energy barriers: **tunnel through** (quantum) or **hop over** (classical)

Ising models can represent hard problems

frontiers in PHYSICS

REVIEW ARTICLE
published: 12 February 2014
doi: 10.3389/fphy.2014.00005

Ising formulations of many NP problems

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Mauro Faccin, ISI Foundation, Italy
Ryan Babbush, Harvard University, USA
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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

Quantuma annealing can yield an exponential speedup

PRL **109,** 050501 (2012) PHYSICAL REVIEW LETTERS week ending 3 AUGUST 2012

Quantum Speedup by Quantum Annealing

Rolando D. Somma,[1] Daniel Nagaj,[2] and Mária Kieferová[2]
[1]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Research Center for Quantum Information, Slovak Academy of Sciences, Bratislava, Slovakia*
(Received 9 March 2012; revised manuscript received 17 May 2012; published 31 July 2012)

We study the glued-trees problem from A. M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D. Spielman, in *Proceedings of the 35th Annual ACM Symposium on Theory of Computing* (ACM, San Diego, CA, 2003), p. 59. in the adiabatic model of quantum computing and provide an annealing schedule to solve an oracular problem exponentially faster than classically possible. The Hamiltonians involved in the quantum annealing do not suffer from the so-called sign problem. Unlike the typical scenario, our schedule is efficient even though the minimum energy gap of the Hamiltonians is exponentially small in the problem size. We discuss generalizations based on initial-state randomization to avoid some slowdowns in adiabatic quantum computing due to small gaps.

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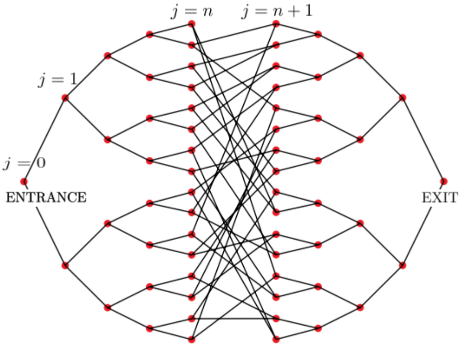
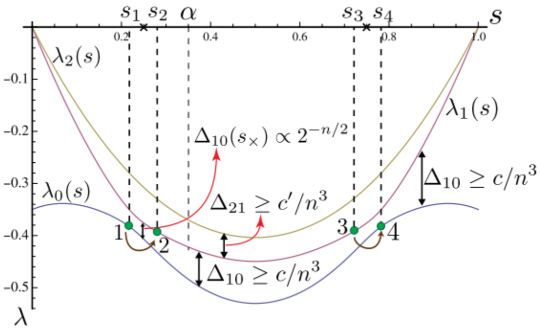




Some scientific milestones

2010 Demonstration of quantum annealing
(Johnson et al., *Nature*)

2013 First benchmarking study, 3000x faster than CPLEX
(McGeoch + Wang, *ACM CF'13*)

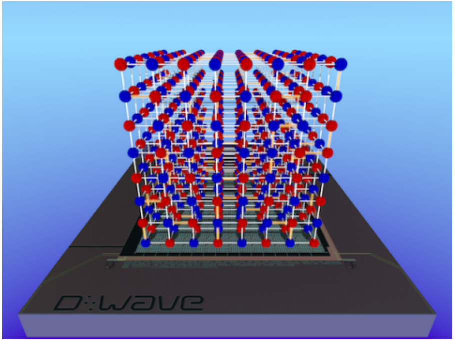
2015 Entanglement demonstrated in D-Wave processor
(Lanting et al., *PRX*)

2016 Multiqubit cotunneling confers scaling advantage over SA
(Denchev et al., *PRX*)

2018 Scaling advantage over simulated annealing
(Albash + Lidar, *PRX*)

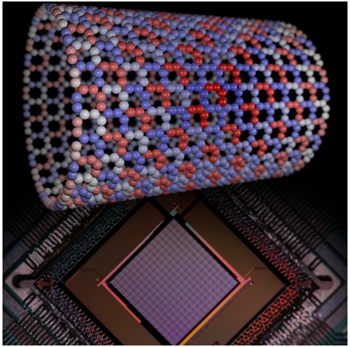
Annealing for equilibrium sampling

New demonstrations: Quantum simulation



Harris et al., Phase transitions in a programmable quantum spin glass simulator

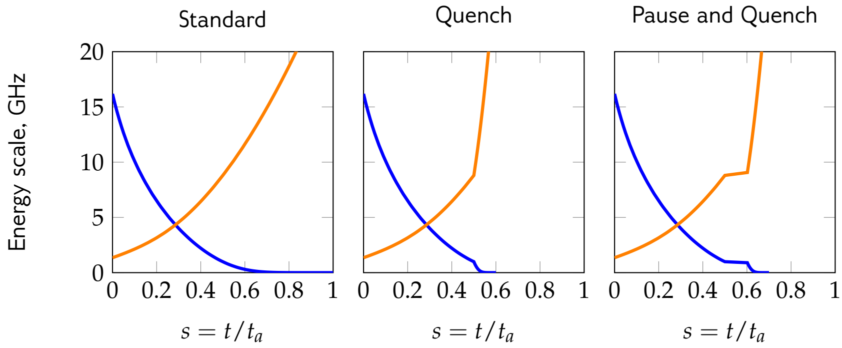
Science **361** 6398 162-165 (2018)



King et al., Observation of topological phenomena in a programmable lattice of 1,800 qubits

Nature **560** 7719 (2018)

Annealing protocols for equilibrium sampling

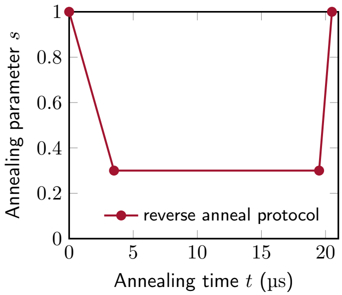


- **Pause** beyond the equilibration time, then **quench** faster than physical dynamics
- Allows access to non-classical distributions, where superposition is non-trivial

Success requires both equilibration up to s, and fast quench

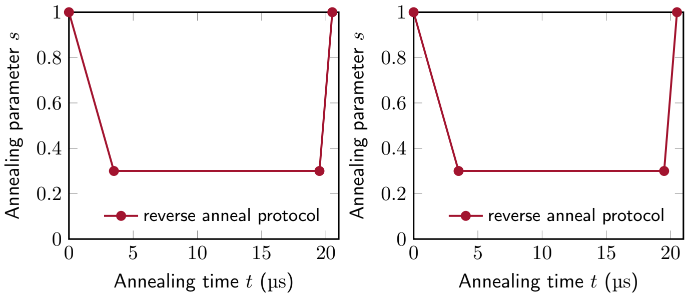
We access quantum distributions projected on the classical space

Annealing protocols for equilibrium sampling



- We can also start from a classical initial condition (reverse annealing)
- We can check escape from controlled subspaces
- and potentially avoid dynamical obstacles

Annealing protocols for equilibrium sampling



- We can also start from a classical initial condition (reverse annealing)
- We can check escape from controlled subspaces
- and potentially avoid dynamical obstacles
- and processes can be daisy-chained together to access long time scales

Success requires that the quench does not set us back to zero knowledge

What is the alternative?

- Quantum equilibria and dynamics require exponential resources to simulate
- Spin glass and KT phases are relatively resilient to approximation methods
- However, quantum equilibria of the transverse field Ising model allow a path-integral representation

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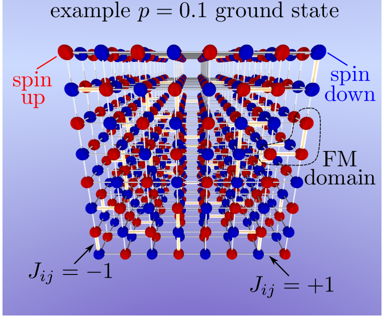
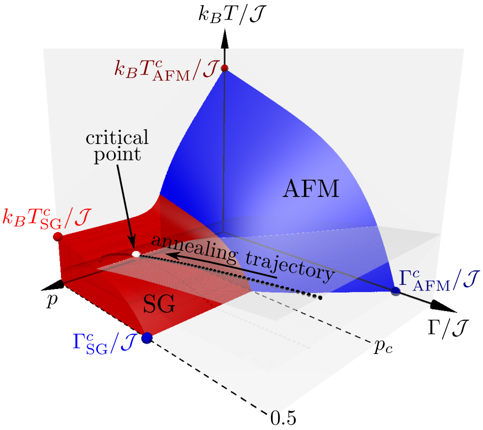
- Quantum equilibria and dynamics require exponential resources to simulate
- Spin glass and KT phases are relatively resilient to approximation methods
- However, quantum equilibria of the transverse field Ising model allow a path-integral representation
  - Sampling by Markov chain Monte Carlo methods (QMC, PIMC)
  - Allows a check on results at scale
  - Local path dynamics are not equivalent to physical dynamics of wavefunctions

The anti-ferromagnetic, and spin-glass, phases on D-wave devices

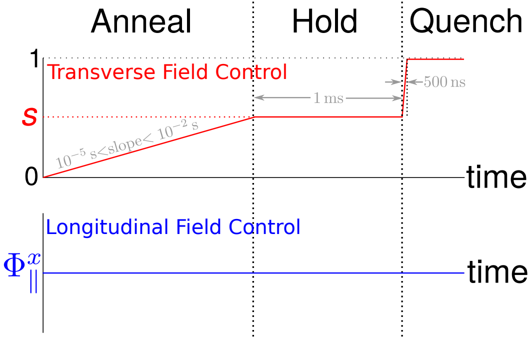
The 3D AFM lattice (Harris et al.)

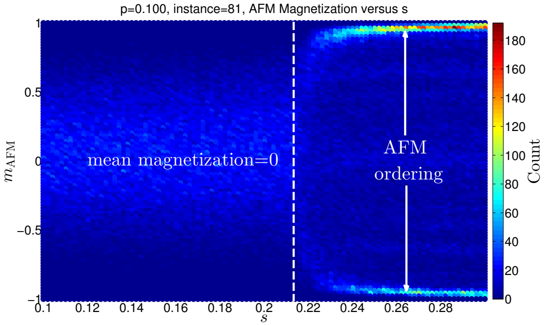
- First large-scale quantum simulation result on a QA processor
- Simulate quantum phase transition of doped AFM lattice
- Parameters T/J, Γ/J, doping probability p.



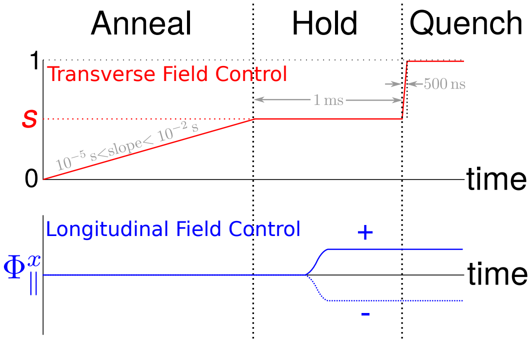


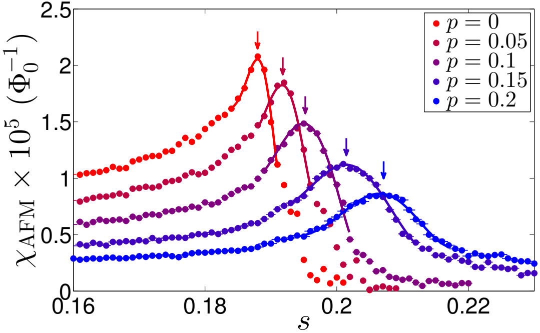
Magnetization measurement



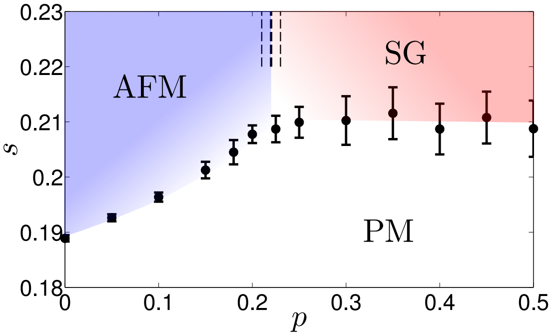


Susceptibility measurement





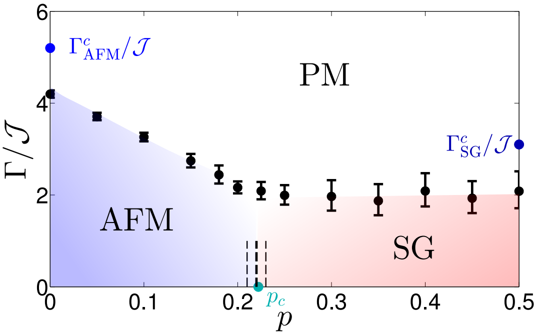
The Phase diagram



Sketching out the phase diagram

- Binder cumulant crossings give p_c
- Susceptibility peak gives Γ_c
- Deviations consistent with finite temperature/size effects

The Phase diagram



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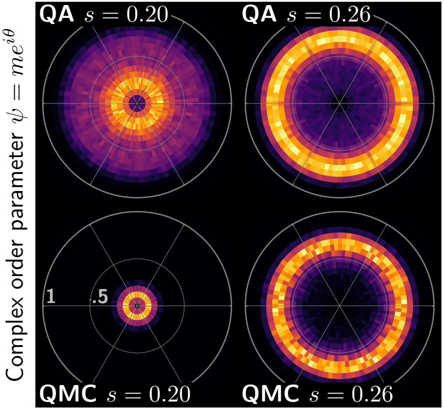
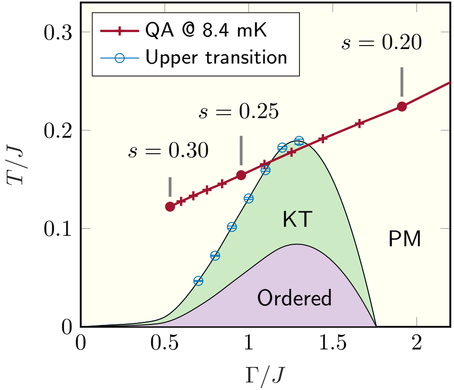
The Kosterlitz-Thouless phase (nuts and bolts)

The Fully Frustrated Square-octagonal lattice (King et al.)

- First physical lattice demonstration the transverse field Ising model KT phase
- Simulation of the KT phase transition
- Parameters T/J and Γ/J





The Kosterlitz-Thouless phase transition

2016 Nobel for theoretical discoveries of topological phase transitions and topological phases of matter

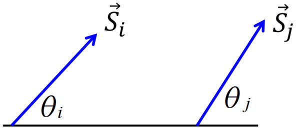
Vadim Berezinskii

J. Michael Kosterlitz

David Thouless

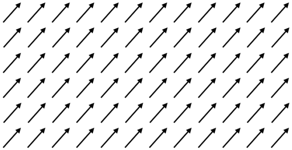
- Most easily described in 2D XY model.
- Finite-temperature phase transition, but does not exist in 2D Ising model without quantum fluctuations.

2D XY model

Classical 2D spin: 

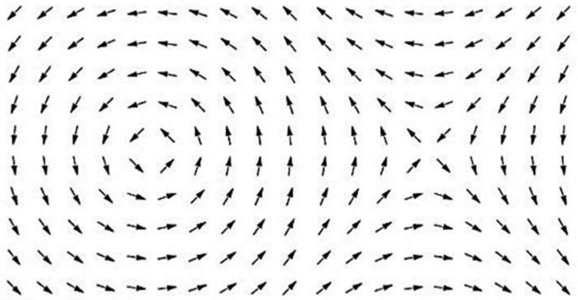
XY-Hamiltonian $H = -J_{\text{XY}} \sum_{i,j} \vec{S}_i \cdot \vec{S}_j = -J_{\text{XY}} \sum_{i,j} \cos\left(\theta_i - \theta_j\right)$

Ground state:
all spins aligned



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

Topological excitations



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

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

Experimental Observation of KT Phase Transition

Ordering, metastability and phase transitions in two-dimensional systems
JM Kosterlitz, DJ Thouless - Journal of Physics C: Solid State …, 1973 - iopscience.iop.org
A new definition of order called topological order is proposed for two-dimensional systems in which no long-range order of the conventional type exists. The possibility of a phase transition characterized by a change in the response of the system to an external …
☆ 99 Cited by 10047 Related articles All 15 versions

As observed physically in. . .

- superfluid ^{4}He films, 1978
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- trapped atoms, 2006
- graphene-tin hybrid JJ arrays, 2014

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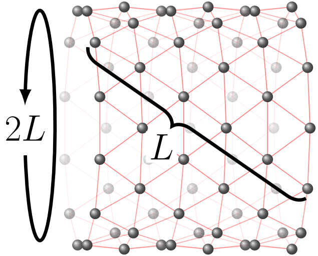
As theorized/simulated in. . .

- Triangular AFM transverse field Ising model



KT phase transition in TAFM TFIM

Theoretical predictions / Monte Carlo

- Blankschtein, Ma, Berker, Grest & Soukoulis, PRB 29, 5250 (1984)
- Jalabert & Sachdev, PRB 44, 686 (1991)
- Moessner & Sondhi, PRB 63, 224401 (2001)
- Isakov & Moessner, PRB 68, 104409 (2003)
- Wenzel, Coletta, Korshunov & Mila, PRL 109, 187202(2012)

No experimental demonstration to date

Simulation or observation? Both!
Programmable superconducting qubits $\approx$ Ising model

AFM triangle: Order by disorder (transverse field Γ)

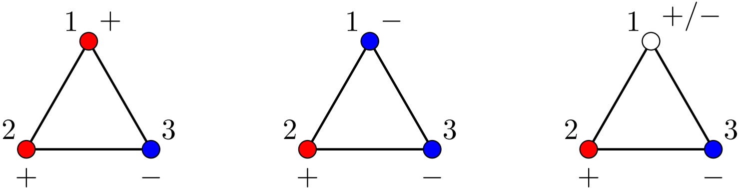
Hamiltonian

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

6-degenerate frustrated ground state

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

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



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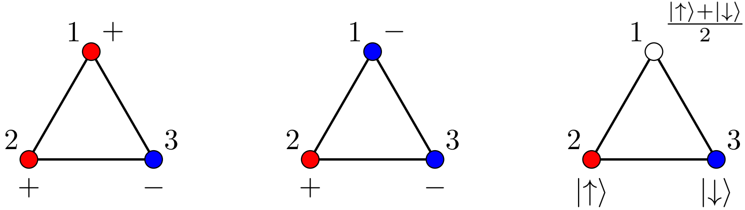


$E = -J$ $E = -J$ $E = -J - \Gamma$

Perturbative picture

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

AFM triangle: Order by disorder (transverse field Γ)

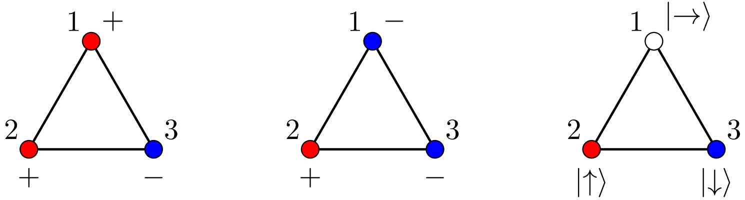
Hamiltonian

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

6-degenerate frustrated ground state

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

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



$E = -J$ $E = -J$ $E = -J - \Gamma$

Perturbative picture

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

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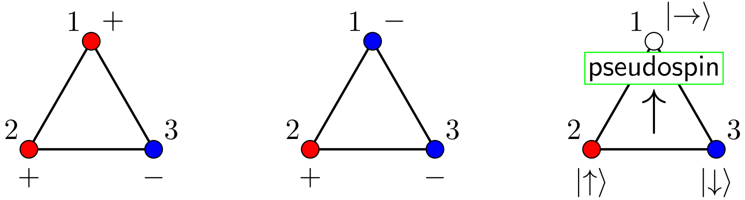

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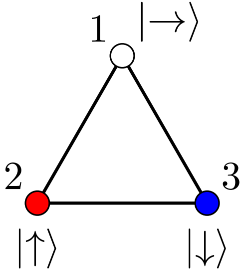
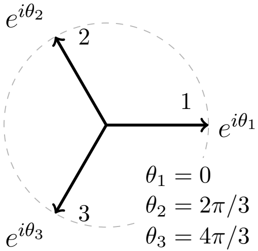
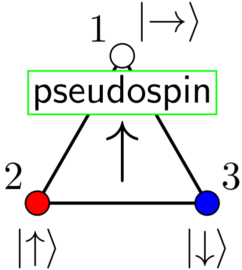
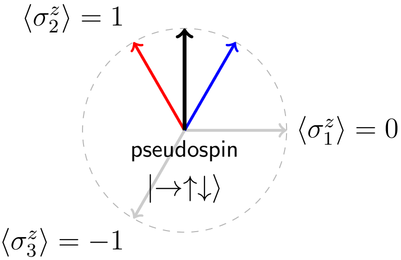
Pseudospin = linear combination of 3 basis vectors



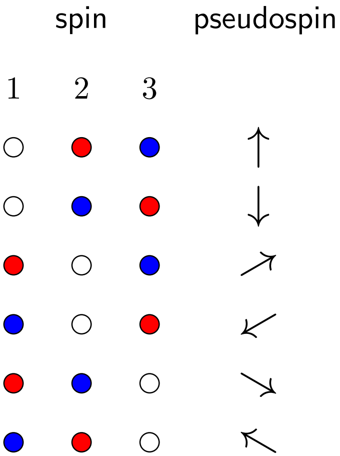


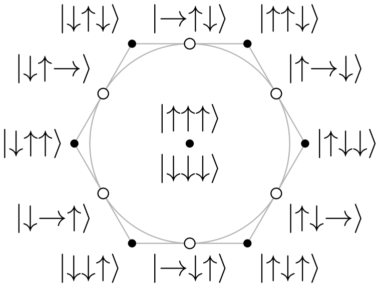
Pseudospin = linear combination of 3 basis vectors





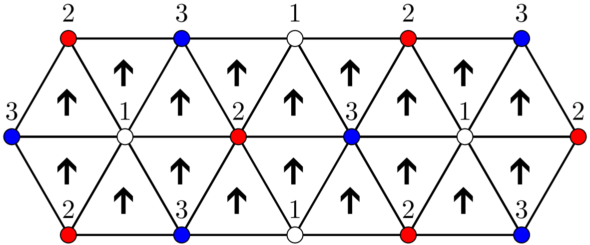
Pseudospin ⇒ 6 clock states (in perturbative picture)





Pseudospin phase = XY model

Spin alignment $\Rightarrow$ sublattice ordering $\Rightarrow$ $|\psi| = 1$

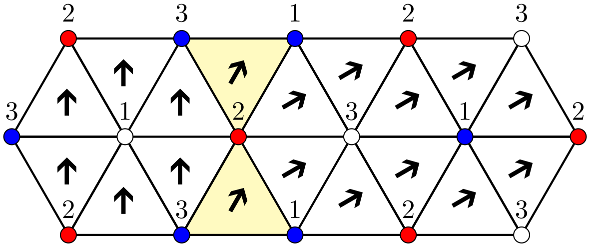


Order parameter ψ = average pseudospin

Real order parameter $m = |\psi|$

Pseudospin phase = XY model

Spin alignment ⇒ sublattice ordering ⇒ $|\psi| = 1$



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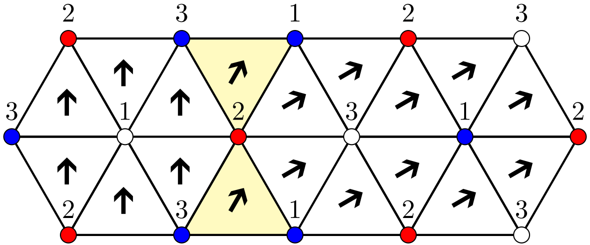


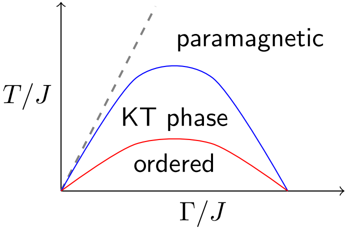
Twisting pseudospin phase ⇒ triangles with no floppy qubit

Exactly like the XY model! Except T_c depends on Γ.

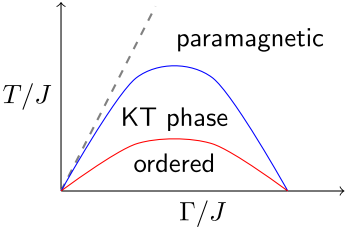
$$T_c = J_{\mathrm{XY}} \frac{\pi}{2} = \Gamma \frac{\pi}{12(2-\sqrt{3})}$$

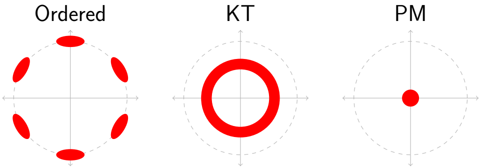
Only applies in perturbative regime.

Triangular AFM phase diagram



Triangular AFM phase diagram





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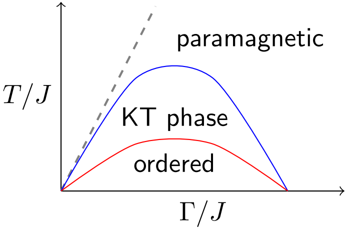
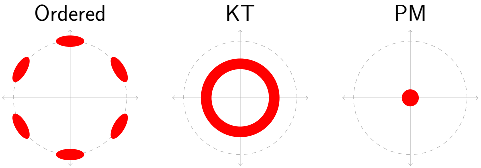
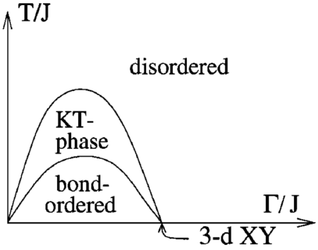
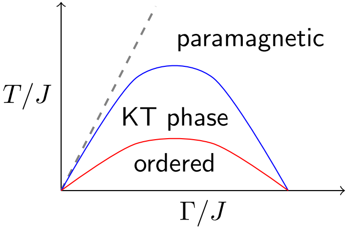


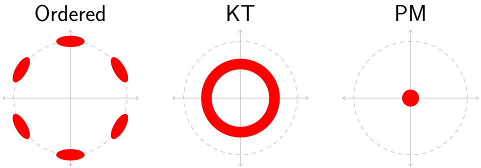


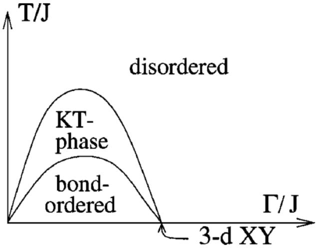


Moessner & Sondhi, 2001

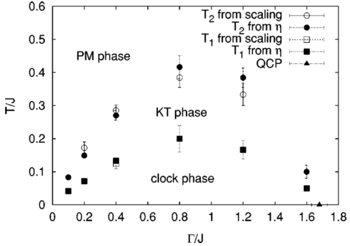
Triangular AFM phase diagram







Moessner & Sondhi, 2001



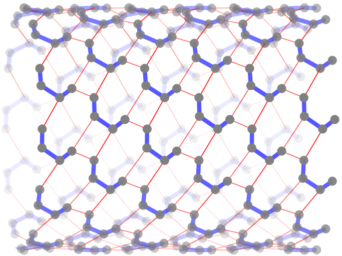
Isakov & Moessner, 2003

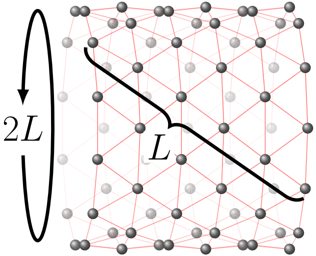
The Kosterlitz-Thouless phase on D-wave devices

Geometrically frustrated lattices

Fully-frustrated square-octagonal ≈ triangular AFM

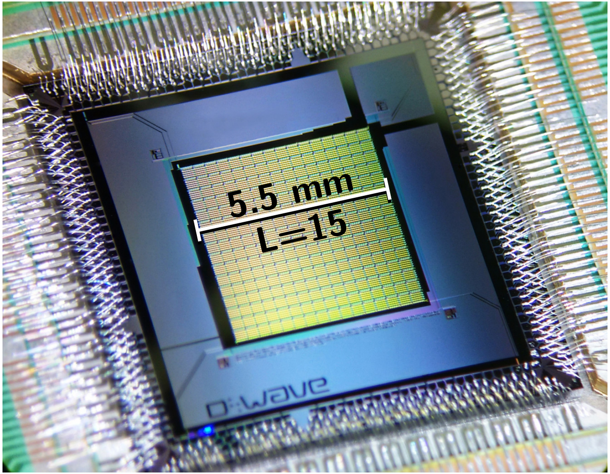
- Same theoretical understanding in one perturbative limit ($T \to 0$, $\Gamma/\mathcal{J} \to 0$)
- Different elsewhere, including non-universal phase transition properties
- Differs from classical XY, and standard incoherent quantum (rotor) models



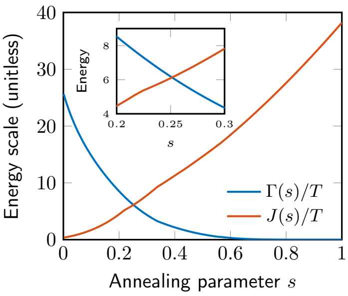


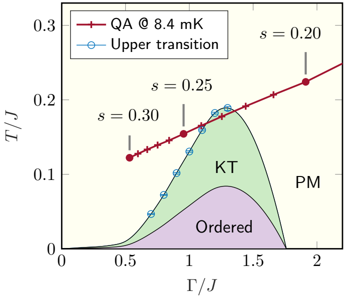
- AFM couplers have $J_{ij} = 1$; FM couplers have $J_{ij} = -1.8$

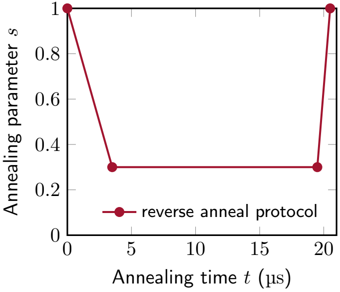
Demonstration in D-Wave 2000Q



Sampling with Reverse anneal, pause and quench

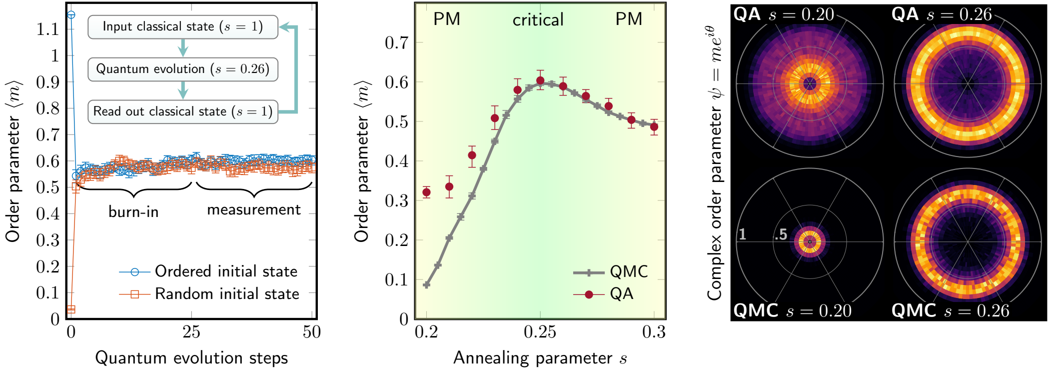






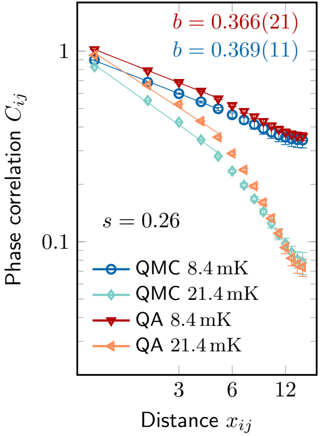
- QA schedule: Sequence of Hamiltonians, annealing parameter s
- **Pause** allows long relaxation at fixed Hamiltonians
- **Quench** allows “projective” readout
- **Reverse anneal** allows initialization in classical state at $s = 1$

Quantum evolution Monte Carlo



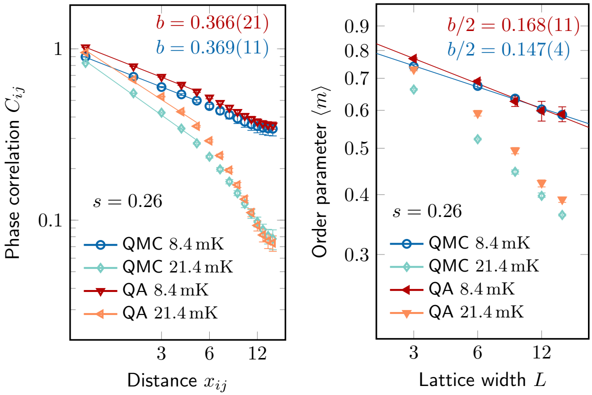
- Reverse annealing "Markov" chain
- Start from random and ordered state. Bound $\langle m \rangle$ above/below
- Peak in $\langle m \rangle$ near KT phase
- $U(1)$ symmetry in complex order parameter
- Agreement with QMC

Onset of power-law correlation decay



- **HOT** PM region: Exponential decay
- **COLD** KT region: Power-law decay

Onset of power-law correlation decay



- HOT PM region: Exponential decay
- COLD KT region: Power-law decay

Quantum simulation with D-Wave

New features, new possibilities

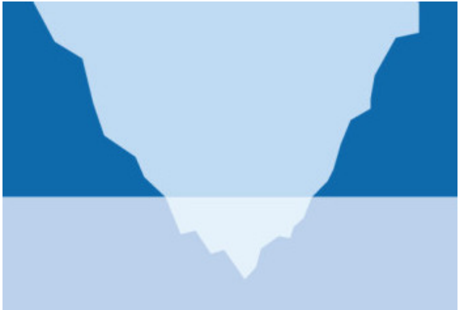
- Anneal features allow previously unreachable experiments

Phase transitions and critical phenomena

- Kosterlitz-Thouless, ferromagnetic and spin glass transitions studied

Programmable magnetic material

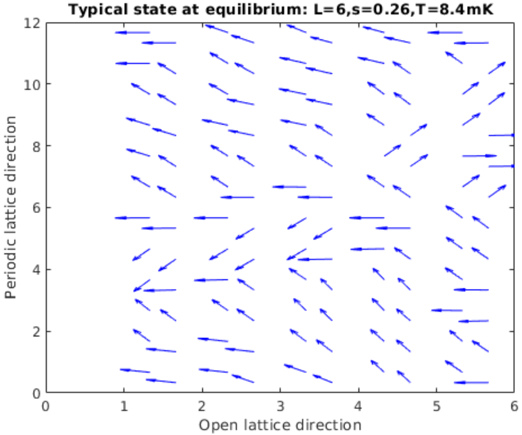
- Feynman's vision for quantum computing…to a point: Simulate a quantum system with a programmable quantum system.



Thanks for your attention

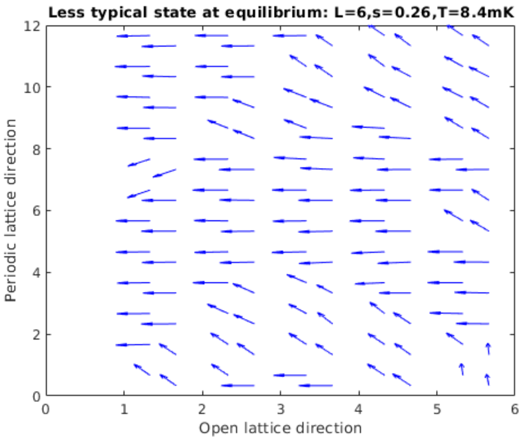
Extra material

Typical Pseudospin field at equilibrium



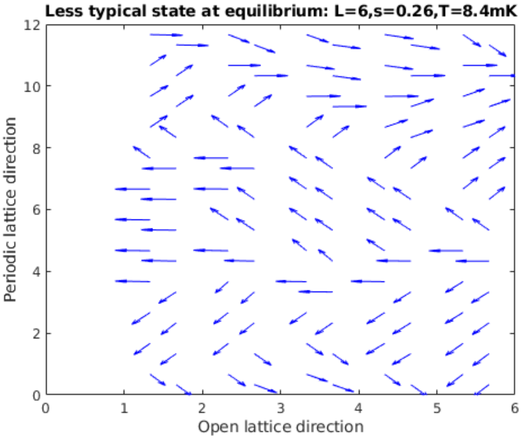
Typical state (L=6, Γ/J=0.842 , T/J=0.146 [s=0.26, T=8.4mK]).

More-ordered pseudospin field

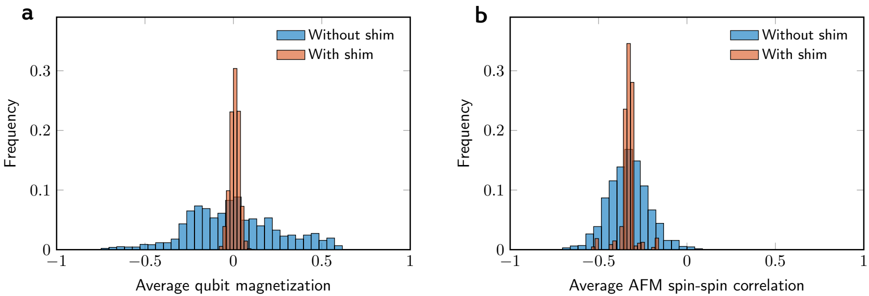


Similar to perturbative ground state (L=6, Γ/J=0.842 , T/J=0.146 [s=0.26, T=8.4mK])

Less-ordered pseudospin field



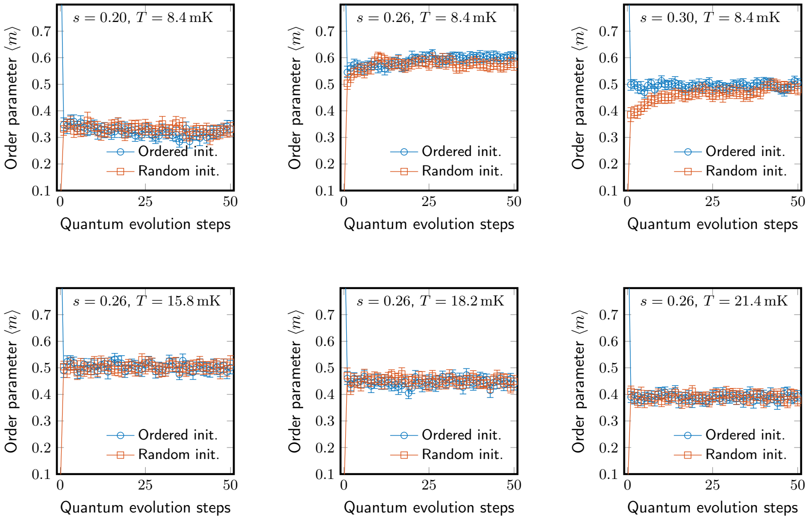
Dissimilar to perturbative ground state (L=6, Γ/J=0.842 , T/J=0.146 [s=0.26, T=8.4mK]).



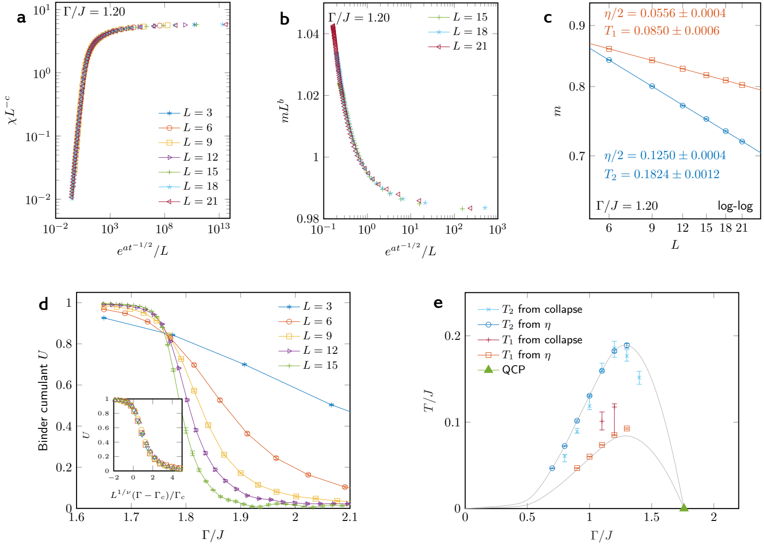
Use lattice symmetries to refine calibration

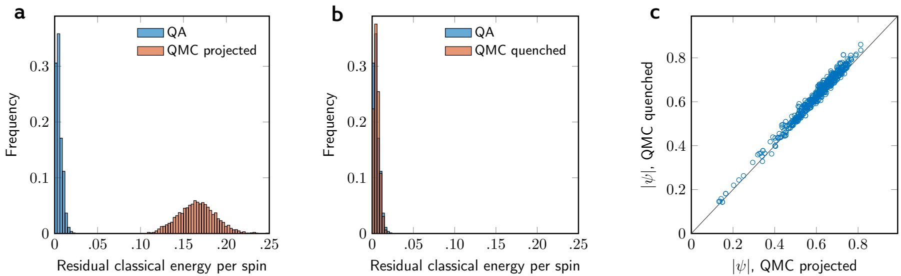
- Each qubit has average magnetization 0.
- Coupler frustration probabilities obey rotational symmetry.

Extras: "Markov" chain convergence



Extras: Phase diagram

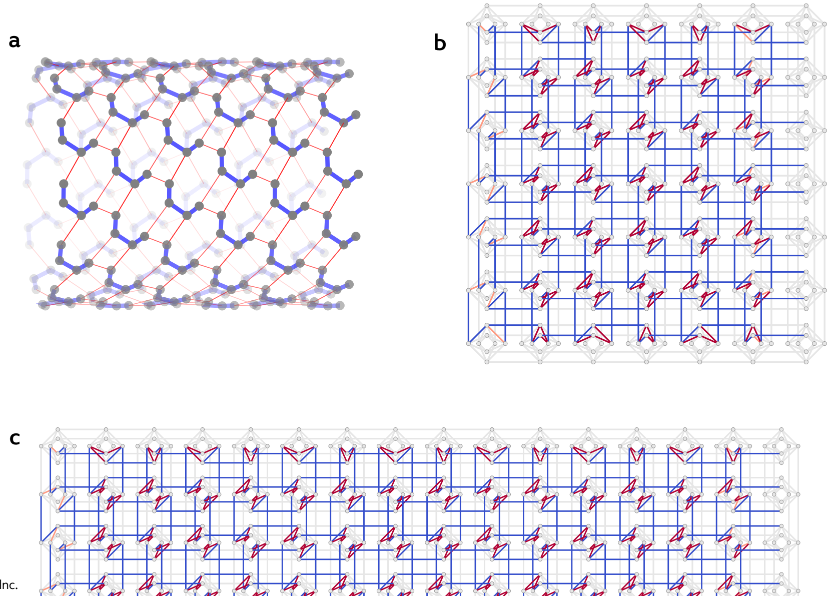




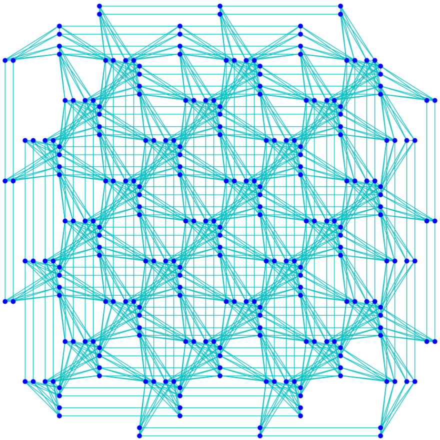
QA evolves during 1 µs quench.

- Huge difference between QMC and QA classical energies.
- Classical quench erases the difference
- ψ mostly unchanged.

Extras: Embedding into qubit lattice



Extras: Next-gen Pegasus topology



Planned Pegasus topology, shown at P4 scale.