



# Quantum Annealing

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# Outline & Goals

## Outline:

- Adiabatic theorem & quantum annealing algorithm
- Physical implementation of a quantum annealer
- Physics/materials simulation problem: KT phase transition

## Goals:

- Understand quantum annealing as a computational paradigm
- Introduce mathematical representation of the Ising model and corresponding hardware implementation
- Introduce an example of using a quantum annealer to model a complex physical system



# Recap – Schrödinger Equation

Wavefunction  $\psi$  describes the state of a quantum system. It can also be represented by a vector

The Schrödinger equation describes the energy of the system for a given state:

$$H\psi = E\psi$$

Hamiltonian  $H$  is an operator (matrix) that acts on the wavefunction of the system (represented by a vector) and returns the wavefunction multiplied by its energy

This is an example of an eigenvalue problem. In general, it's difficult to solve for the wavefunctions (eigenstates) of the system but evaluating the energy of a given state is much easier



# Spin-½ Systems

- Fundamental particles (and other quantum objects) have a type of angular momentum called *spin*
  - Quantized
  - Likes to align with applied magnetic field
- We can describe spin-1/2 systems using the Pauli matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



- Each of these defines a direction along which we can measure the spin. Usually we choose the *z*-direction
- Eigenvectors are the “spin up” and “spin down” states with eigenvalues 1 and -1

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- Eigenstates of the  $\sigma_x$  operator are superpositions of spin up and down:

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\rangle + |\downarrow\rangle)$$

$$|- \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\rangle - |\downarrow\rangle)$$



# Adiabatic Theorem

If a system is in the nth eigenstate  $\psi_n$  of the Hamiltonian  $H_i$  and  $H_i$  is transformed to  $H_f$ , the system will end in the nth eigenstate  $\psi'_n$  of Hamiltonian  $H_f$  as long as the evolution from  $H_i$  to  $H_f$  is slow



# Quantum Annealing

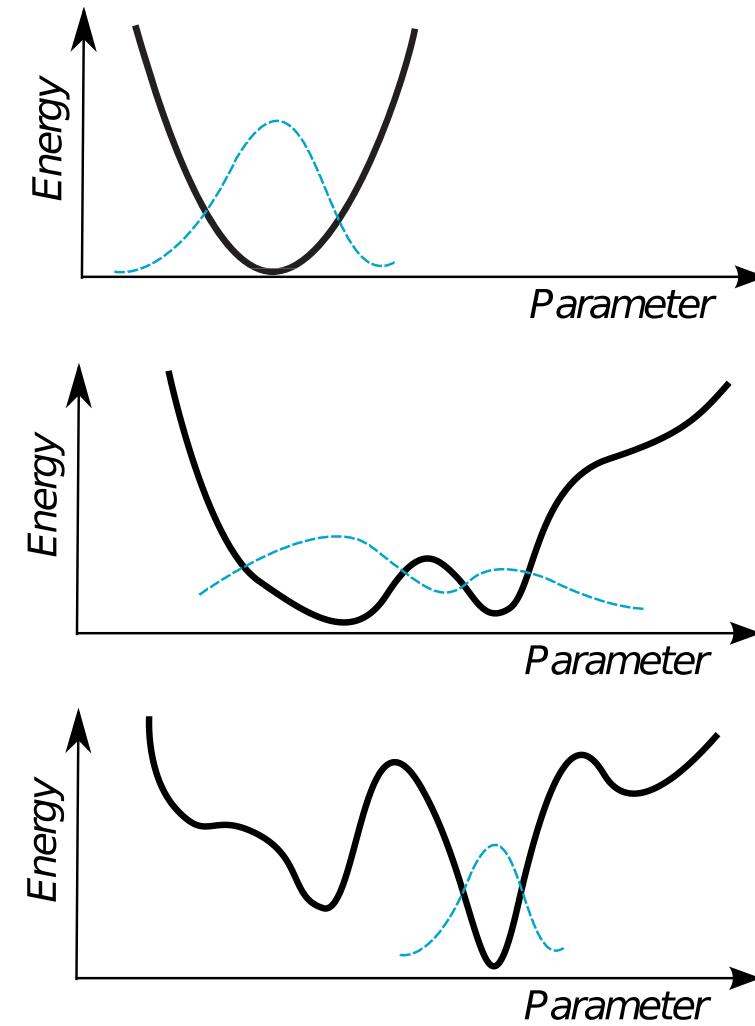
Start from  $H_i$  and anneal slowly to  $H_f$ :

$$H_i = - \sum_i \sigma_x^{(i)}$$

- The ground state of  $H_i$  will be superposition state of spin up and spin down
- This term drives quantum tunneling/spin flipping

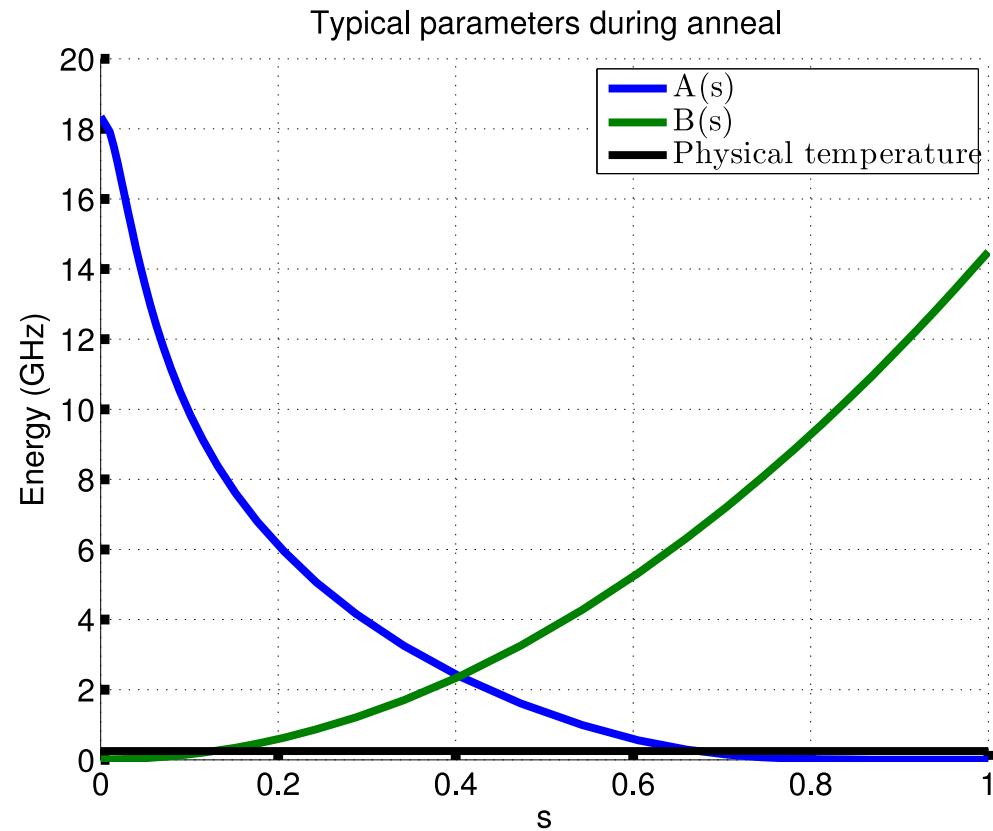
$$H_f = - \sum_i h_i \sigma_z^{(i)} + \sum_{i,j>i} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)}$$

Classical term representing the problem  
(ground state is the sol.)



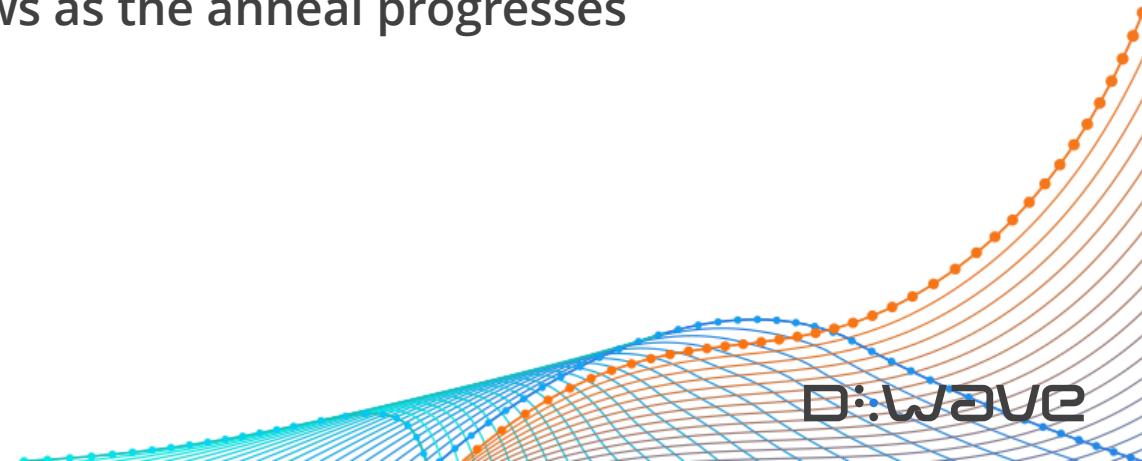


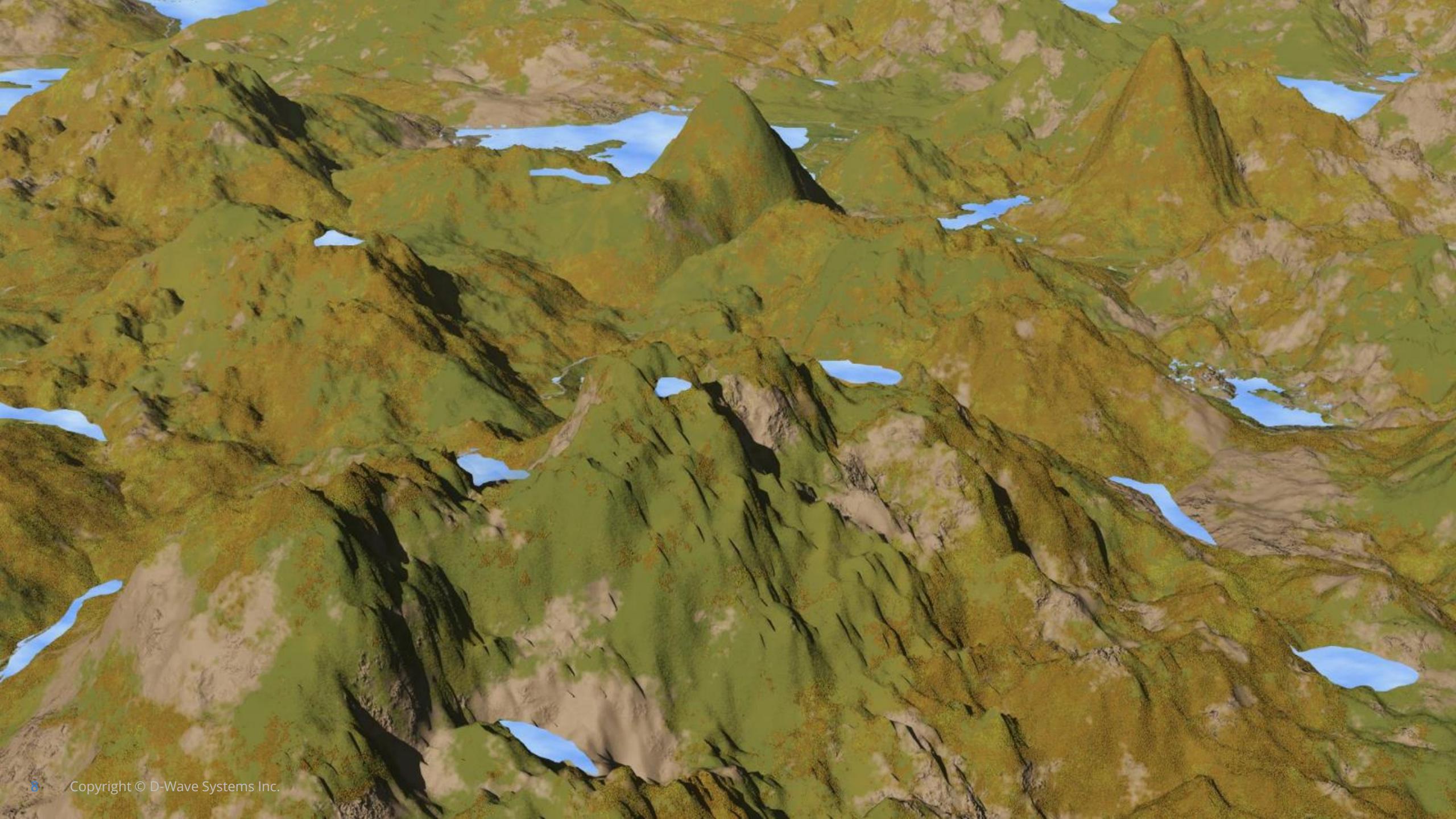
# Quantum Annealing



$$H(s) = A(s)H_i + B(s)H_f$$
$$0 \leq s = t/t_{anneal} \leq 1$$

B(s) is the problem energy scale, which grows as the anneal progresses

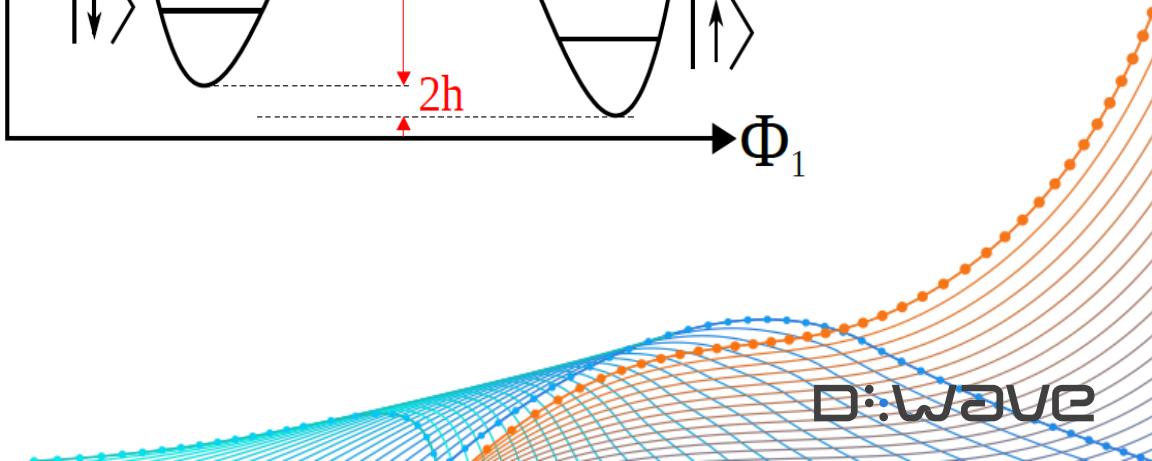
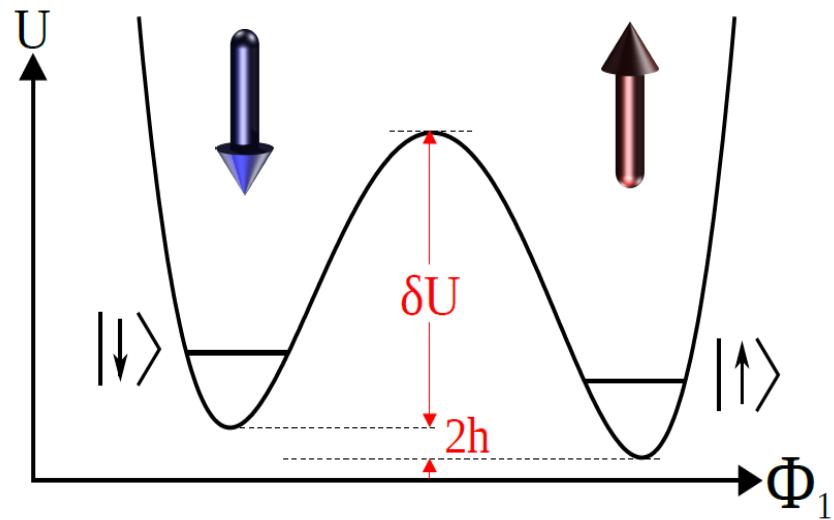
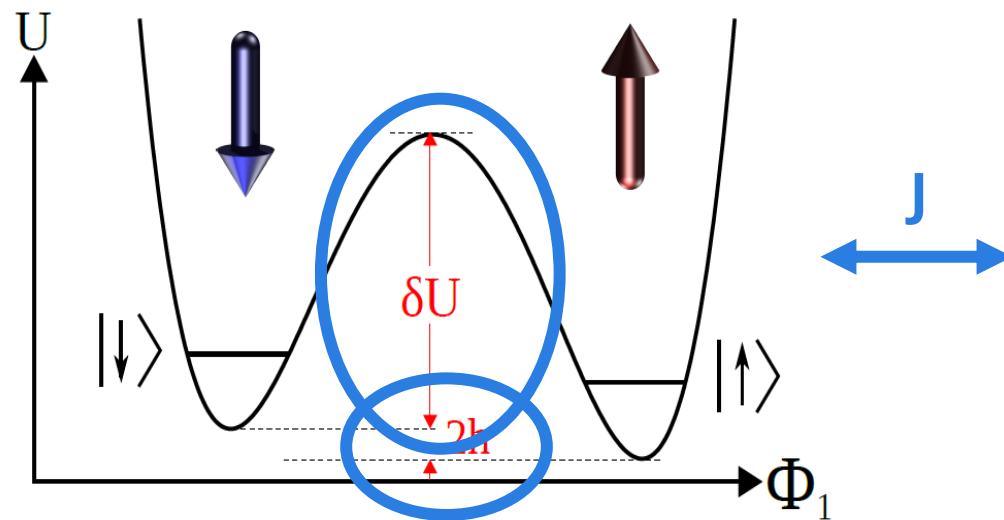






# Transverse Field Ising Hamiltonian

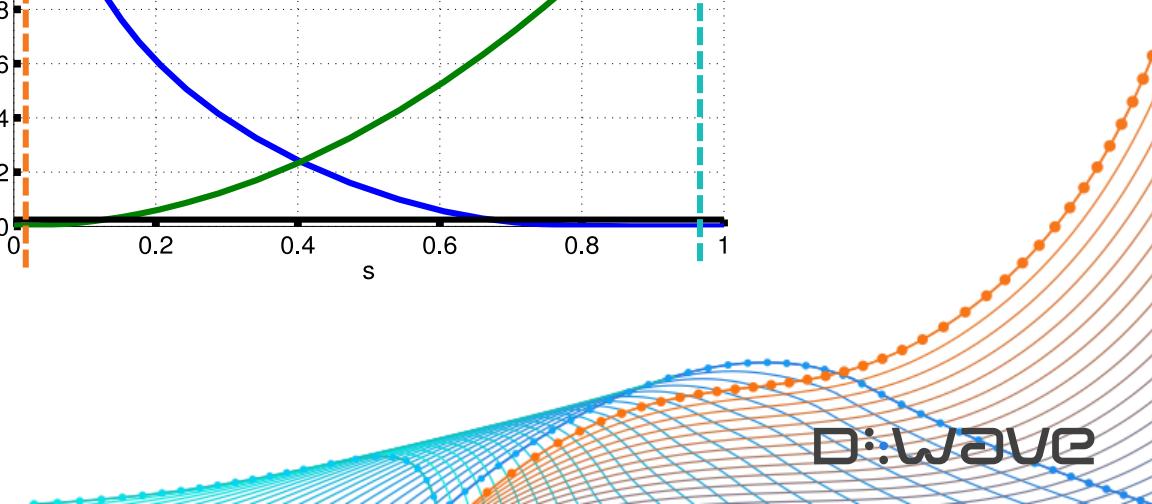
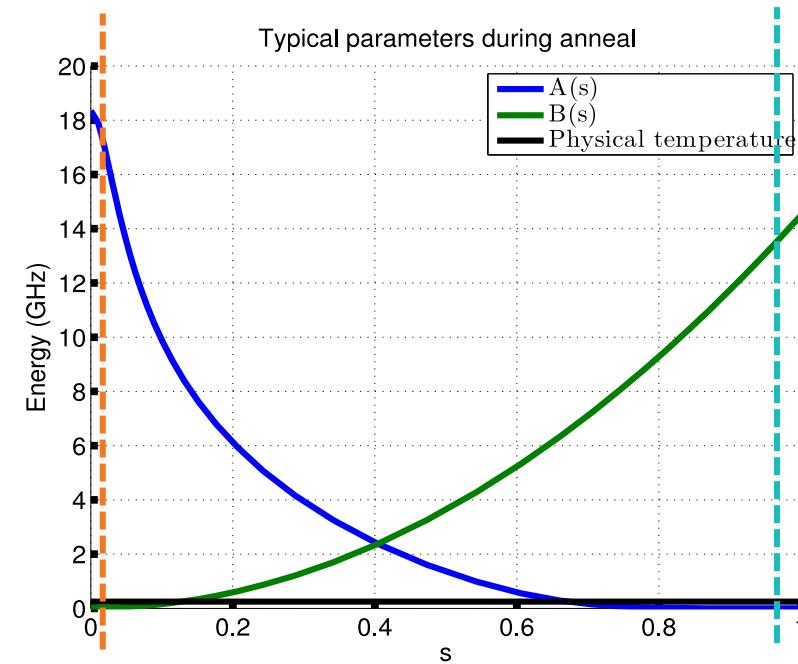
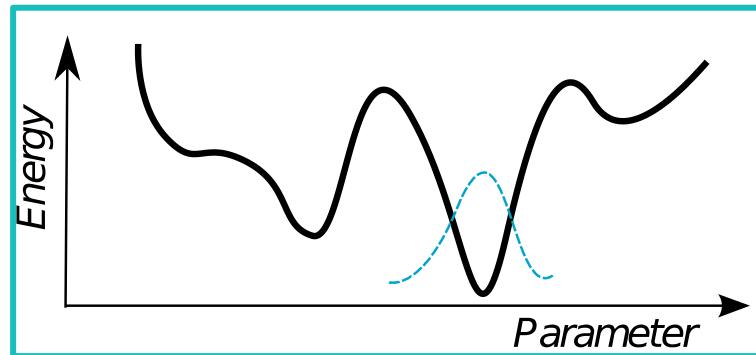
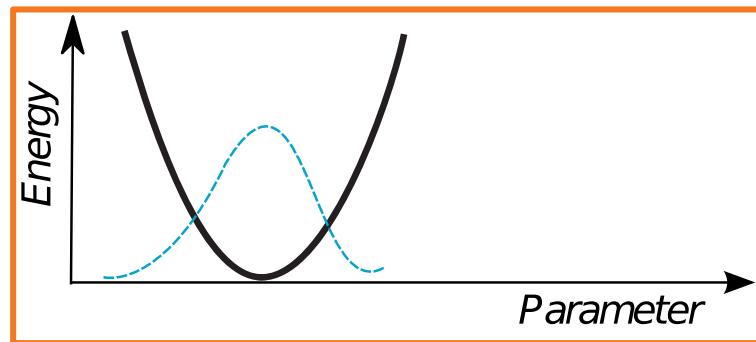
$$H(s) = -A(s) \left[ \sum_i \sigma_x^{(i)} \right] + B(s) \left[ -\sum_i h_i \sigma_z^{(i)} + \sum_{i,j>i} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} \right]$$





# Transverse Field Ising Hamiltonian

$$H(s) = -A(s) \left[ \sum_i \sigma_x^{(i)} \right] + B(s) \left[ -\sum_i h_i \sigma_z^{(i)} + \sum_{i,j>i} J_{ij} \sigma_z^{(i)} \sigma_z^{(j)} \right]$$



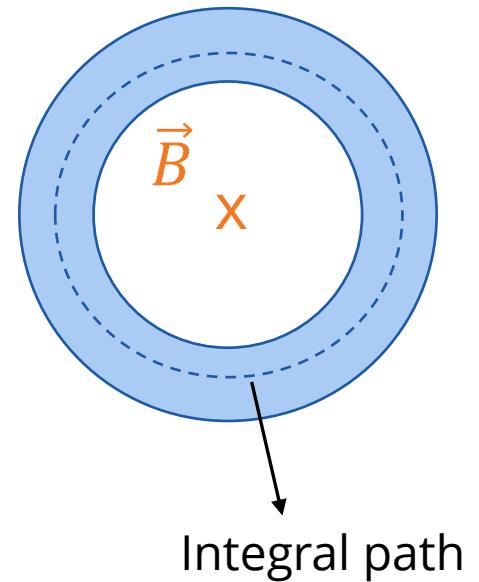
# Physical Implementation

# Superconducting Wavefunction

Macroscopic quantum state (many pairs of electrons)  
governed by a global wavefunction

$$\psi = \sqrt{n_s} e^{i\varphi(\vec{r},t)}$$

Continuity of the wavefunction in a loop results in  
quantization of the flux within the loop



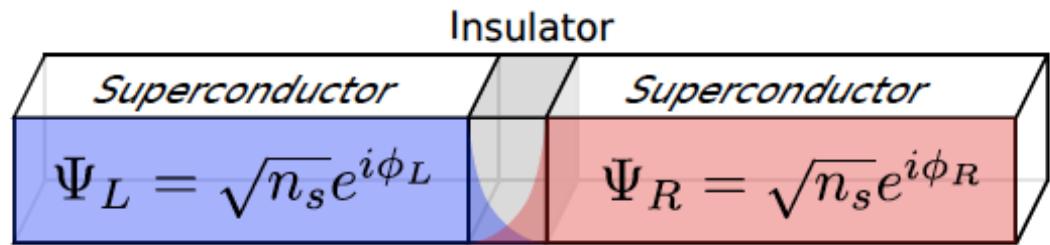
$$\Phi = n\Phi_0$$
$$\Phi_0 = \frac{h}{2e} = 2.067 \times 10^{-15} \text{ Wb (Flux quantum)}$$

The flux of earth's magnetic field through a human red blood cell

# Josephson Junction

Thin non-superconducting barrier between two superconductors

Cooper pairs of electrons tunnel across the barrier

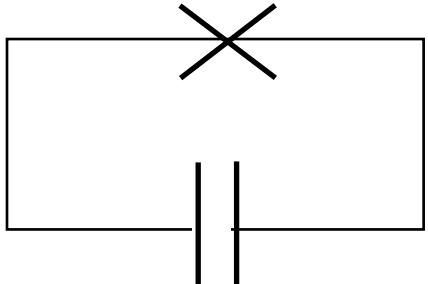


Phase difference across JJ:  
 $\phi = \phi_L - \phi_R$

**Josephson Equations:**  $I = I_c \sin \phi$  (DC)

$$\frac{d\phi}{dt} = \frac{2\pi}{\Phi_0} V \text{ (AC)}$$

Governed by  $I_c$ , the critical current; JJ acts as a nonlinear inductor

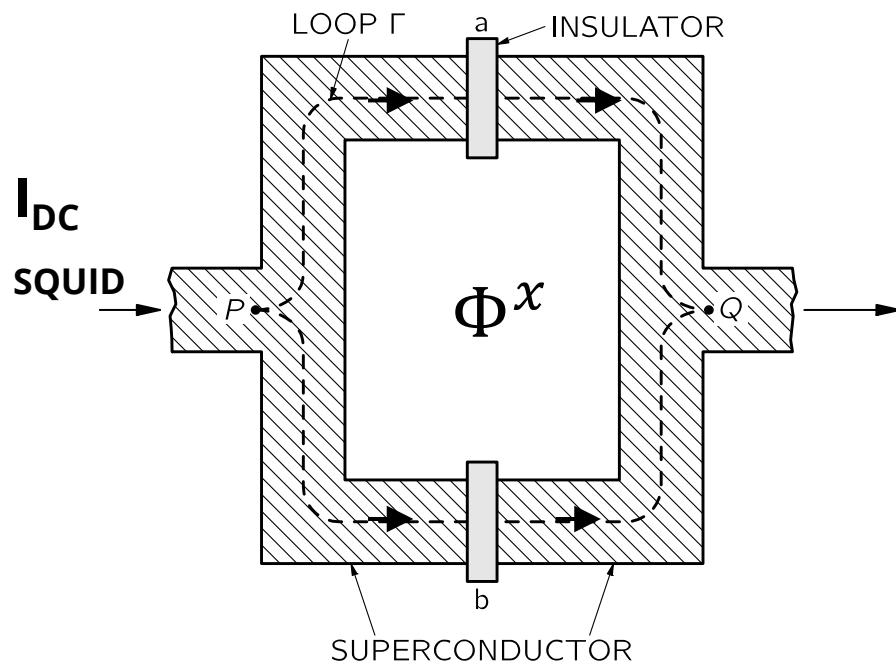


$$L_J = V \left( \frac{dI}{dt} \right)^{-1} = \frac{\Phi_0}{2\pi I_c \sin \phi}$$

With  $C$ , have an anharmonic oscillator



# DC SQUID



Feynman Lectures Vol III, Ch 21

$$\Delta \text{Phase}_{p \rightarrow Q} = \phi_a + \frac{2\pi}{\Phi_0} \int_{upper} \vec{A} \cdot d\vec{l}$$

$$\Delta \text{Phase}_{p \rightarrow Q} = \phi_b + \frac{2\pi}{\Phi_0} \int_{lower} \vec{A} \cdot d\vec{l}$$

$$\phi_b - \phi_a = \frac{2\pi}{\Phi_0} \oint \vec{A} \cdot d\vec{l}$$

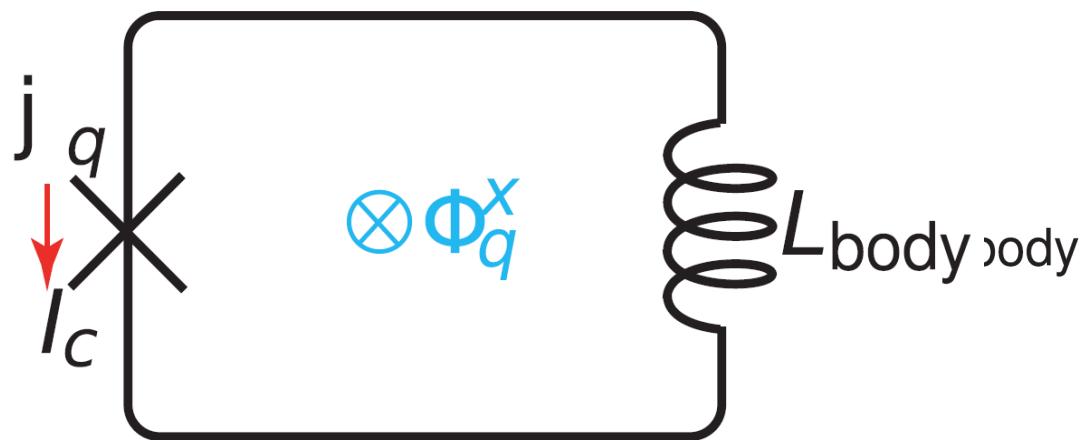
$$\phi_b - \phi_a = \frac{2\pi}{\Phi_0} \Phi^x$$

$$I_{C_{SQUID}} = 2I_c \left| \cos \frac{\pi \Phi^x}{\Phi_0} \right|$$

→ Tunable critical current

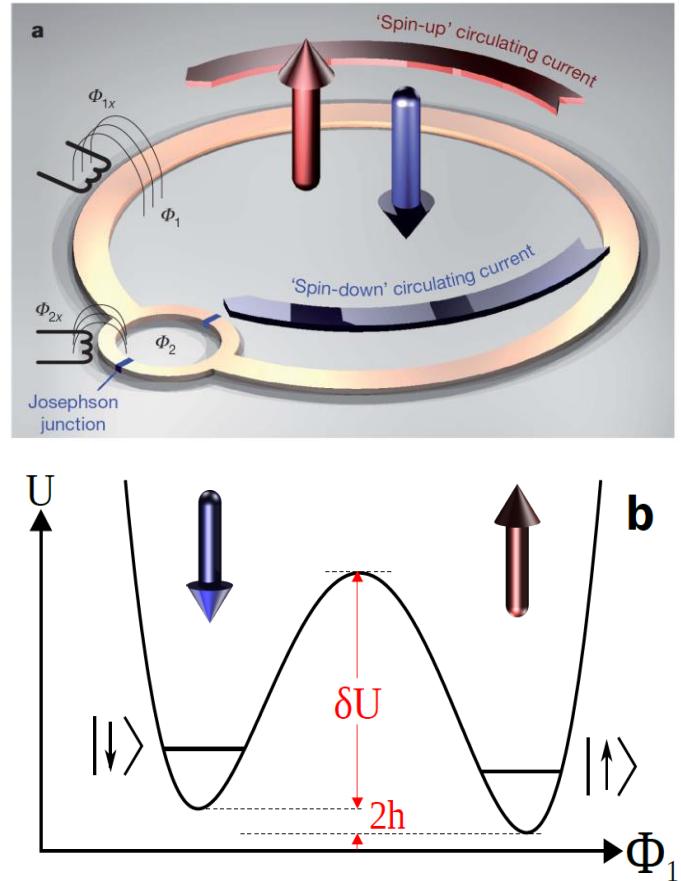
# CJJ RF SQUID Qubit

Computational states: current flowing CW or CCW around superconducting loop



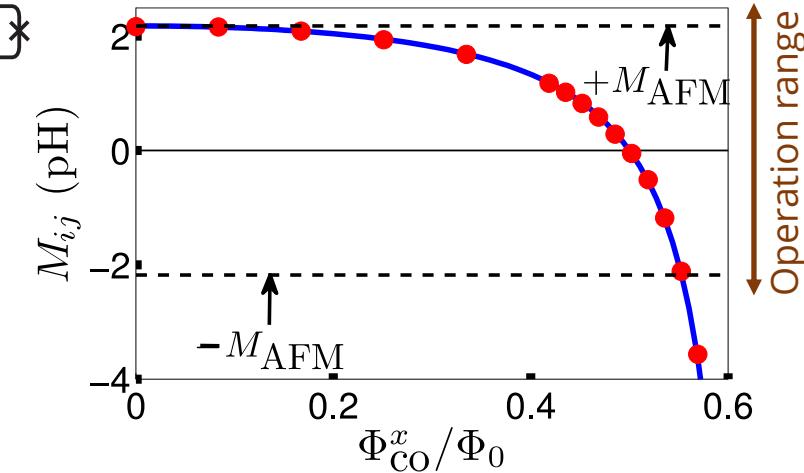
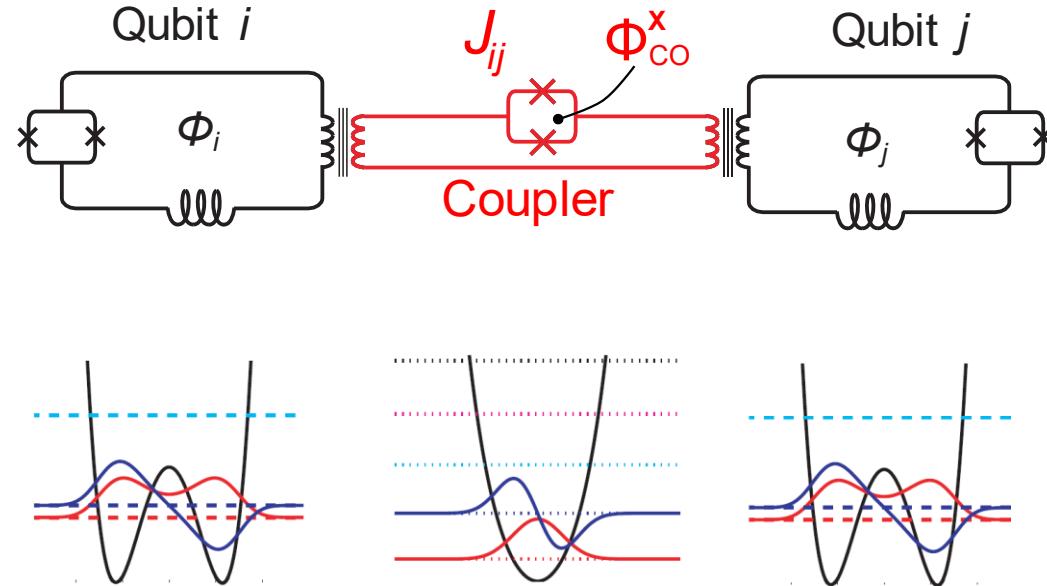
Josephson junction creates barrier in potential

*Compound* Josephson junction (DC SQUID) creates *tunable* barrier in potential





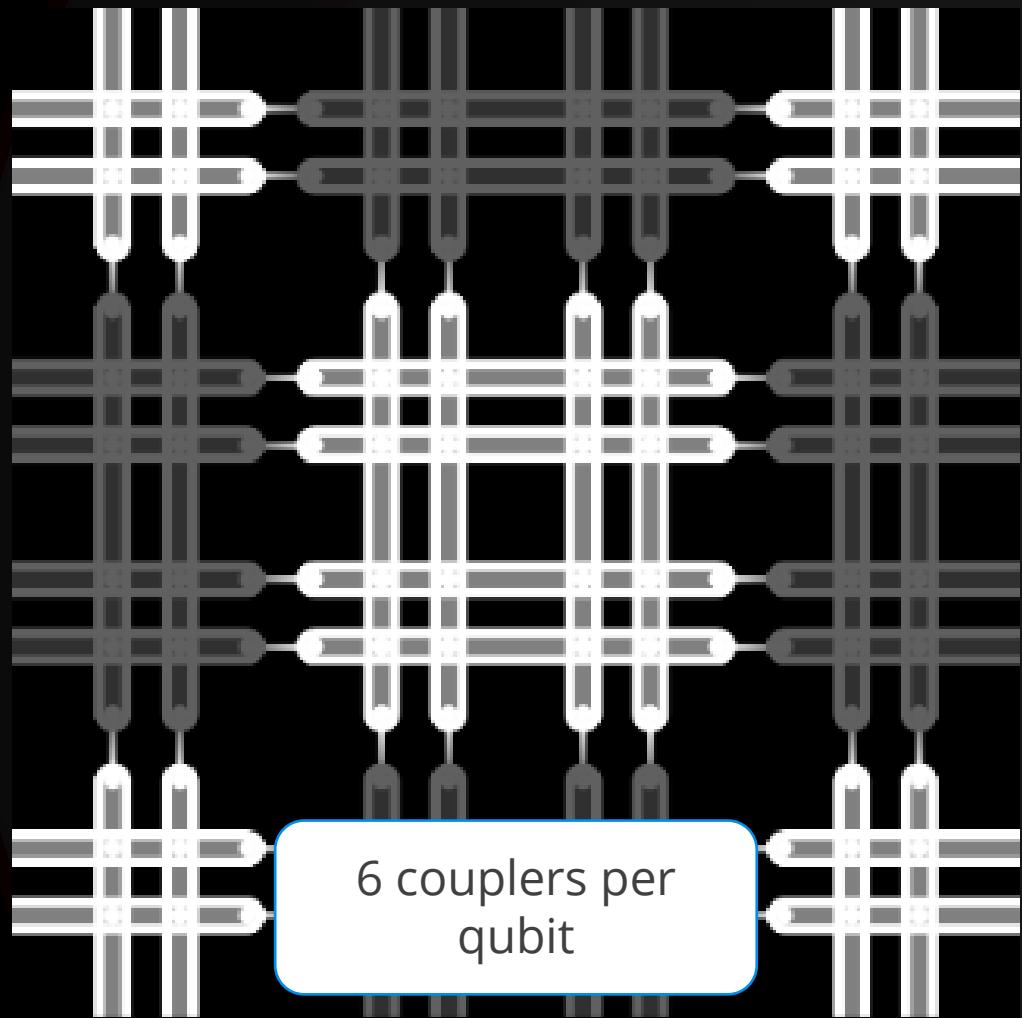
# Coupling Qubits



A mono-stable two-junction rf-squid provides a tunable mutual inductance

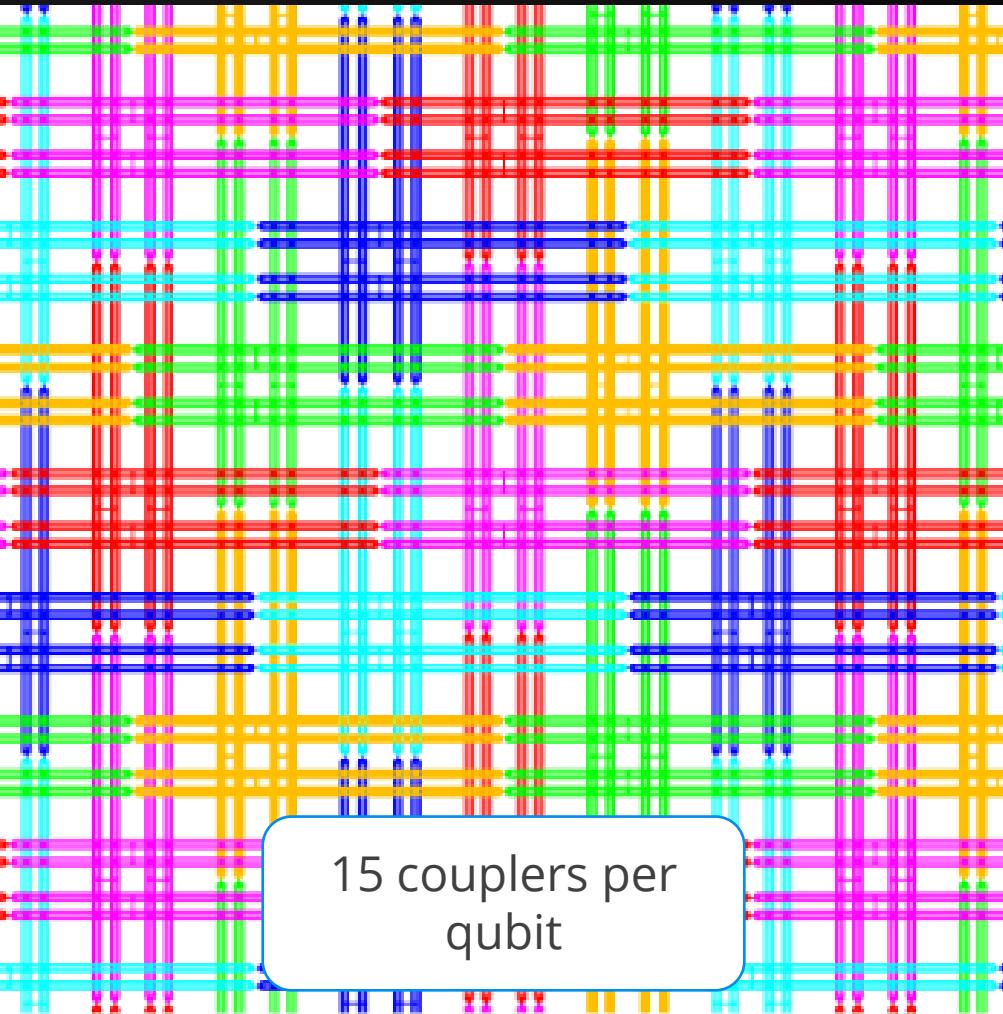
$$H_{ij} = -J_{ij}\sigma_z^{(i)}\sigma_z^{(j)}$$

# Processor Architecture



Chimera

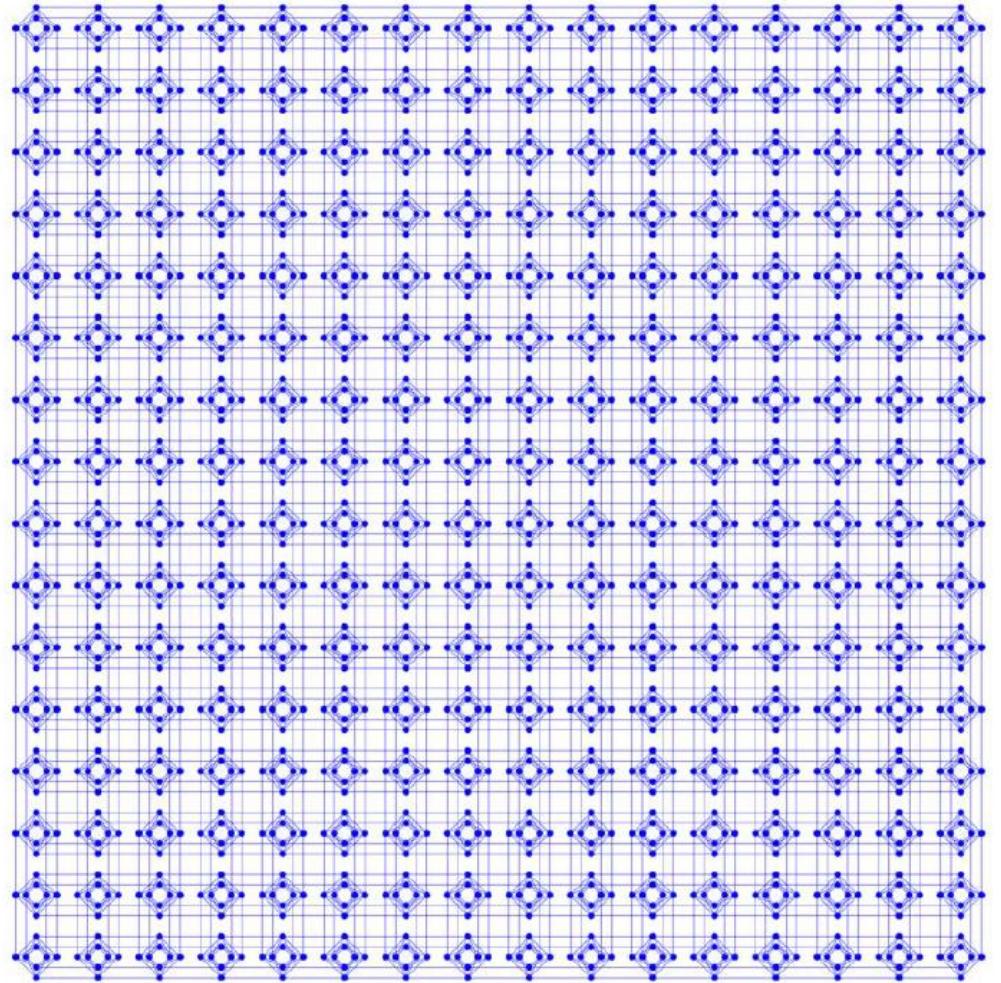
D-WAVE



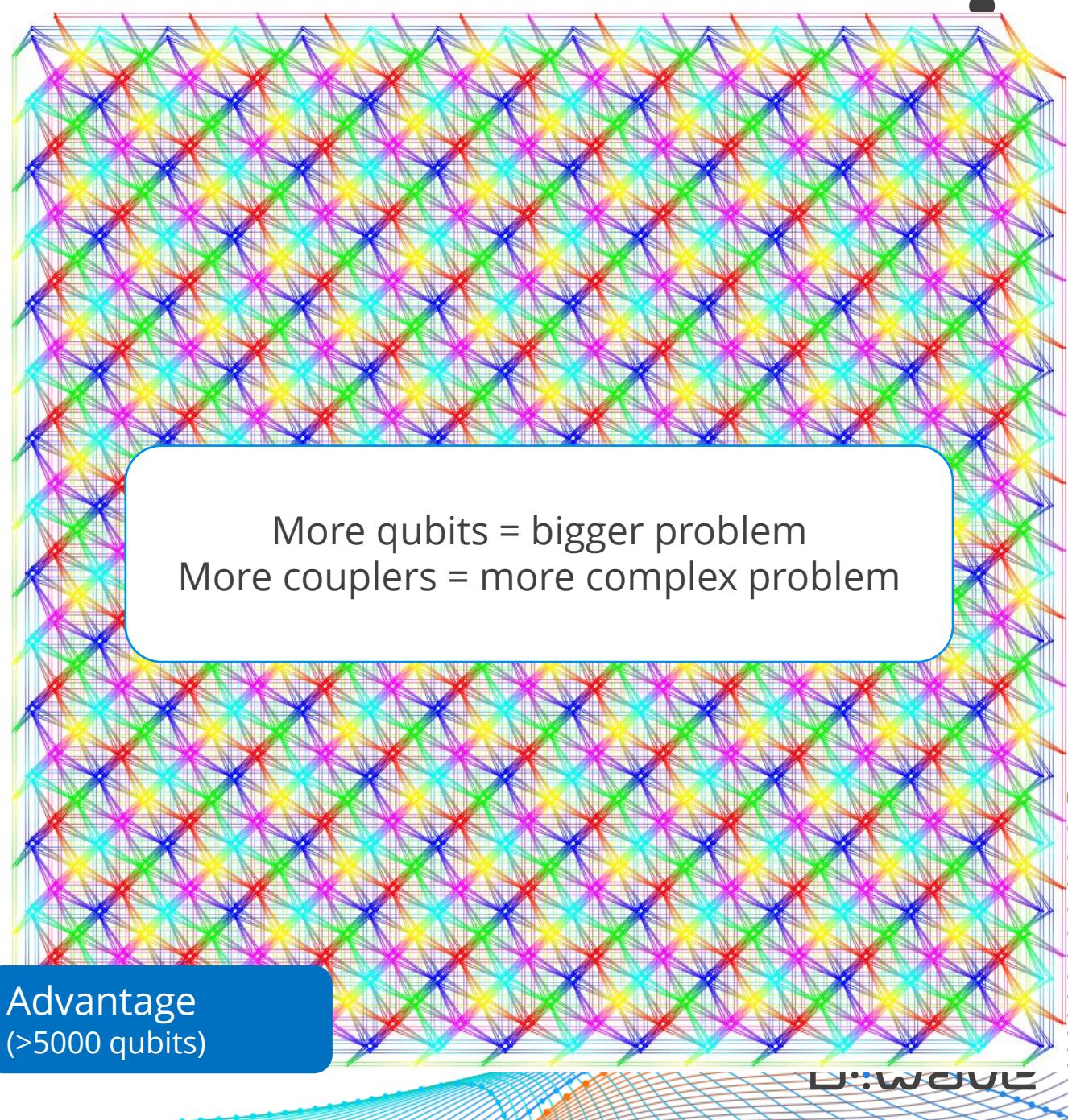
Pegasus

D-WAVE

# Processor Architecture



2000Q



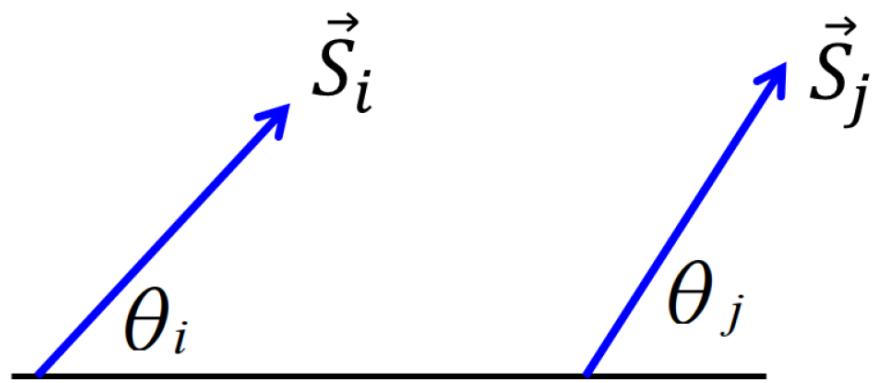
# KT Phase Transition

A. King *et al*, Nature **560**, 456 (2018)

A. King *et al*, Nature Communications **12**:1113 (2021)

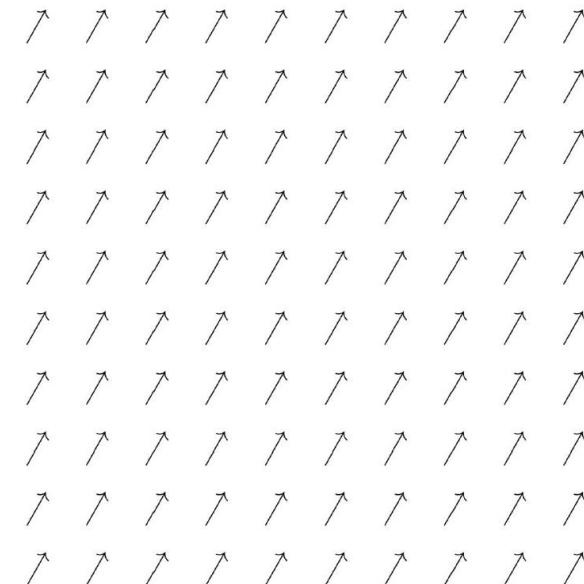


# 2d XY Model



$$H = -J_{xy} \sum_{i,j} \vec{S}_i \cdot \vec{S}_j = -J_{xy} \sum_{i,j} \cos(\theta_i - \theta_j)$$

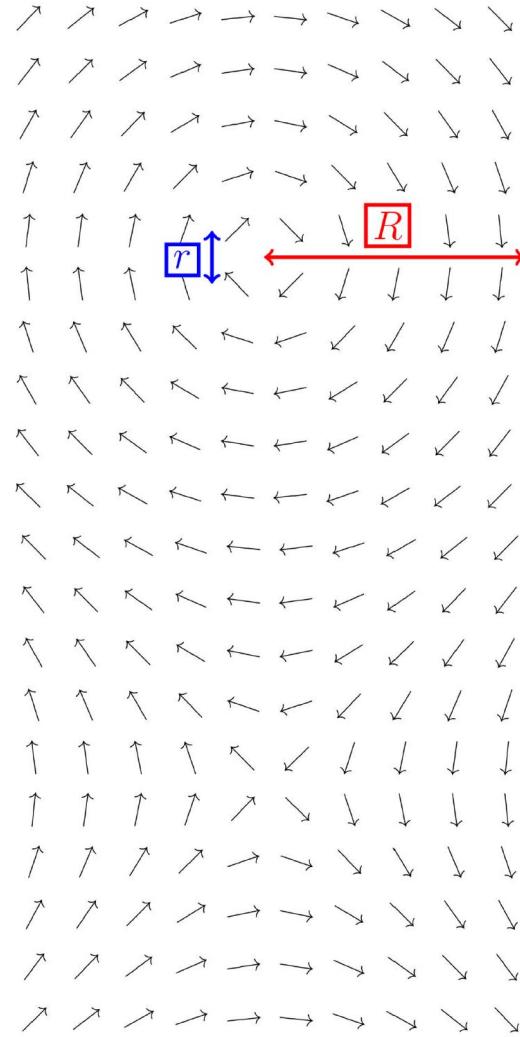
Classical ground state → all spins aligned



A. King *et al*, 2018

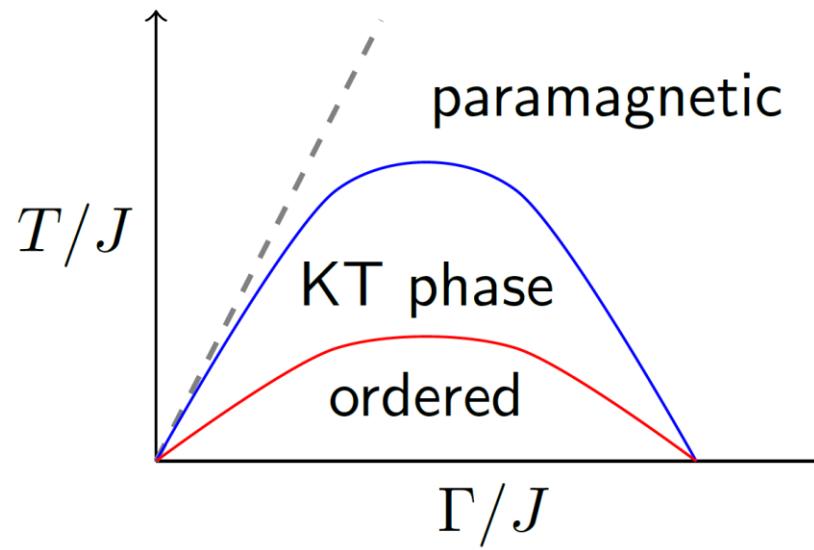


# Vortices & Anti-Vortices



A. King *et al*, 2018

- Vortex: clockwise winding of the spin angle
- Anti-vortex: counter-clockwise winding
- Energy diverges with size  $R$
- Become bound below critical temperature according to free energy minimization

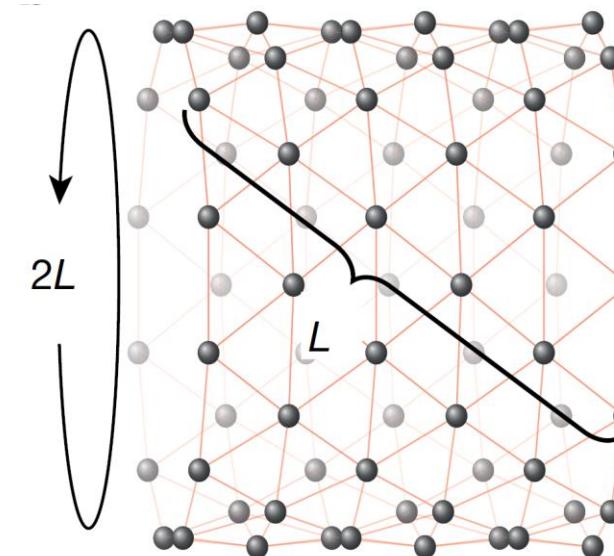


A. King *et al*, 2018



# Kosterlitz-Thouless Phase Transition

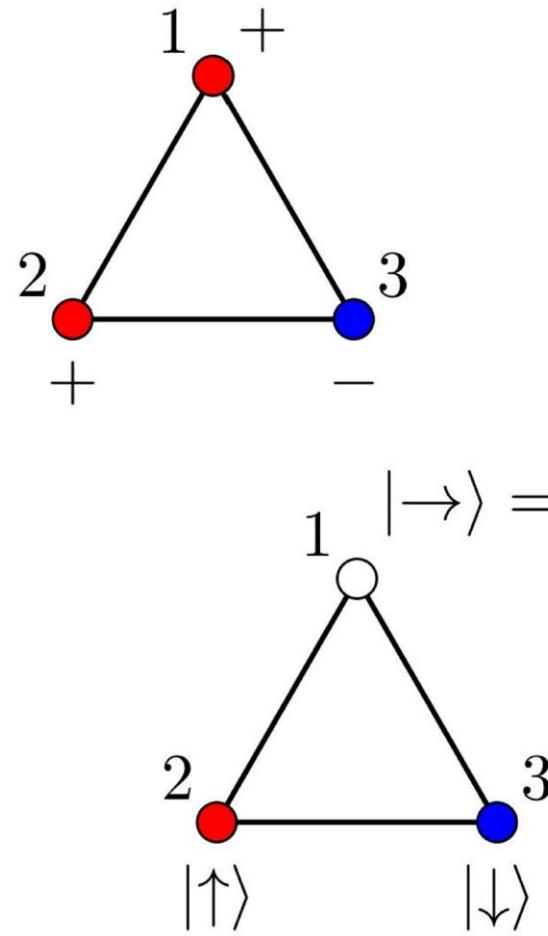
- Subject of the 2016 Nobel prize in physics
- Observed experimentally in
  - Superfluid He films
  - Superconducting films
  - JJ arrays
  - BEC in cold gases
- Theorized in triangular lattices of the transverse field Ising model



A. King *et al*, 2018



# Ising Spins on an AFM Triangle



A. King *et al*, 2018

Can't satisfy all couplings  $\rightarrow$  frustration  
6 degenerate classical ground states with energy  $-J$

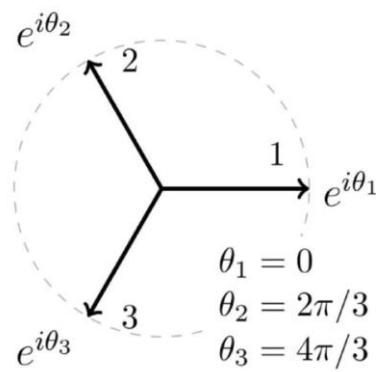
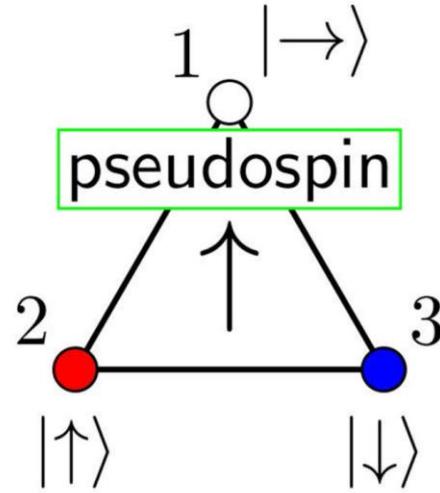
$$H = \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z$$

Add a perturbative transverse field  $-\Gamma$   
Ground state energy becomes  $E = -J - \Gamma$

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

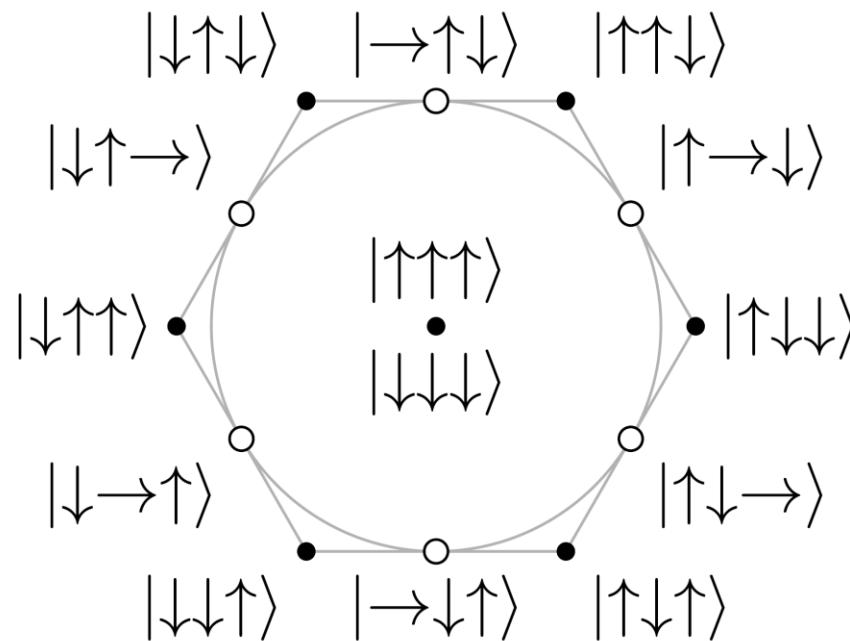


# Pseudospin



A. King *et al*, 2018

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



A. King *et al*, 2018

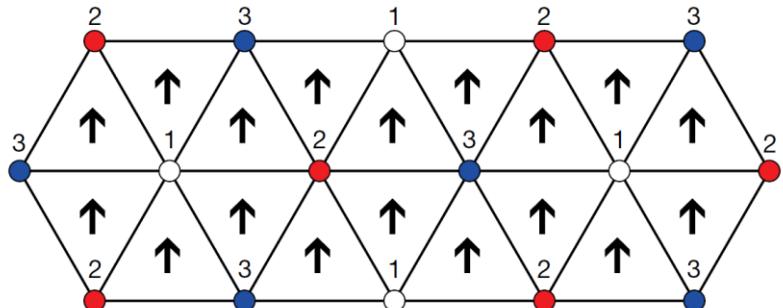
12 “clock” states  
(6 quantum, 6 classical)

2 excited states with  $\psi = 0$

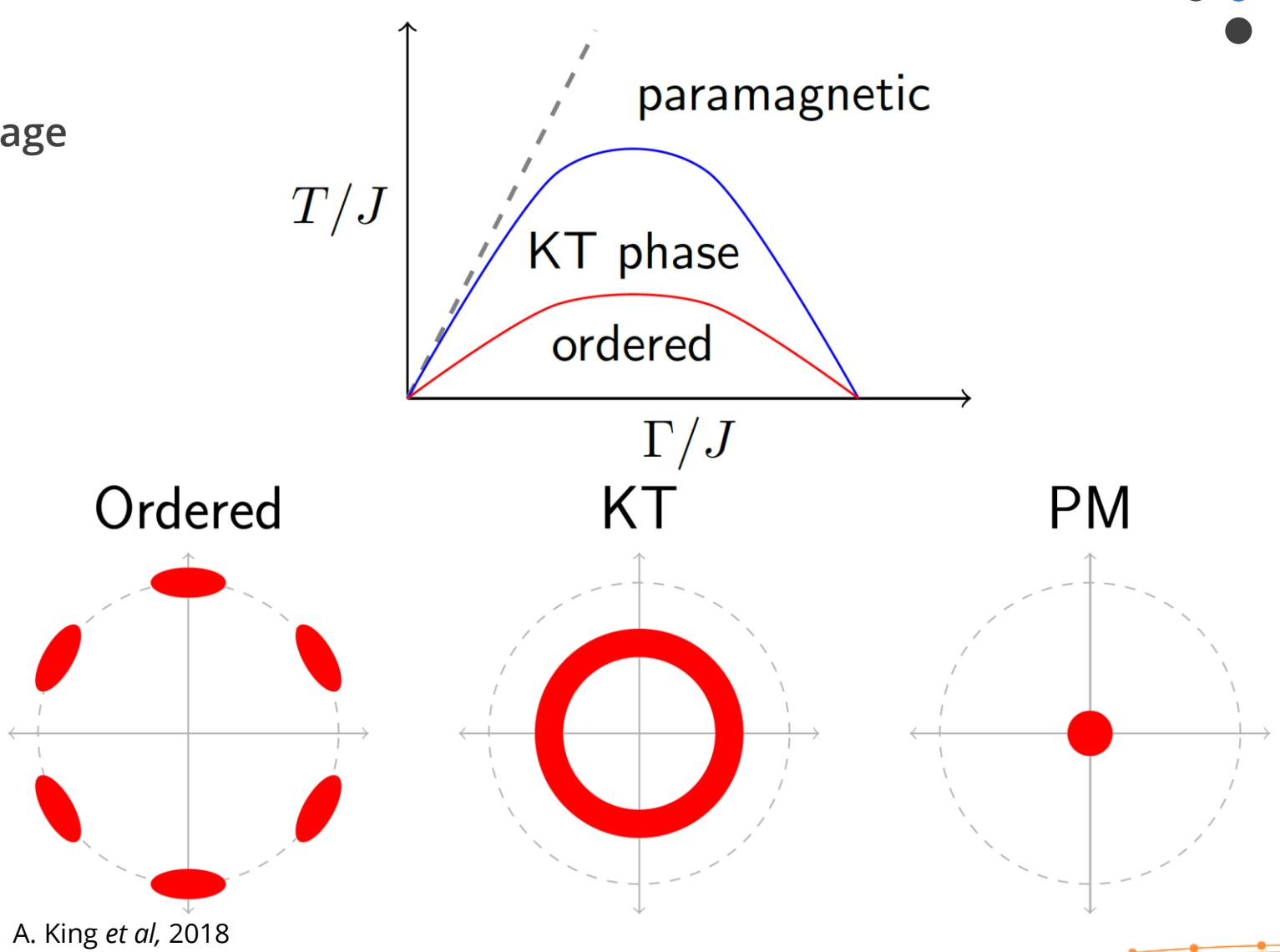
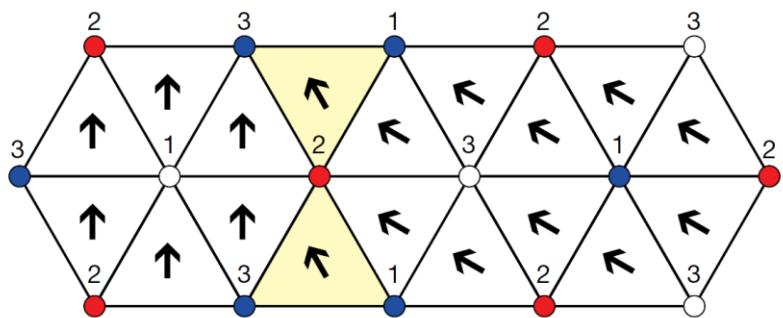


# Order Parameter

Define the order parameter as the average pseudospin across the lattice



A. King *et al.*, 2018

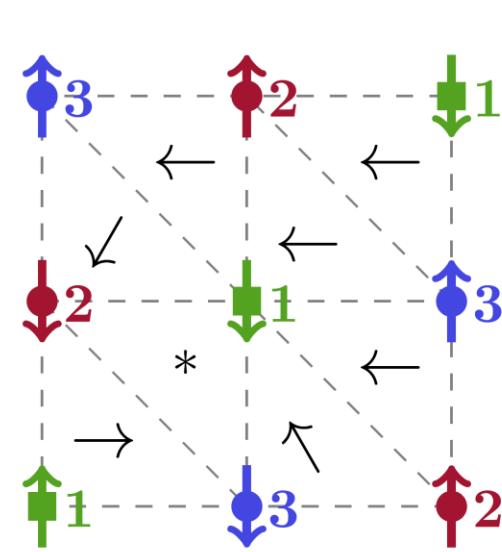


A. King *et al.*, 2018

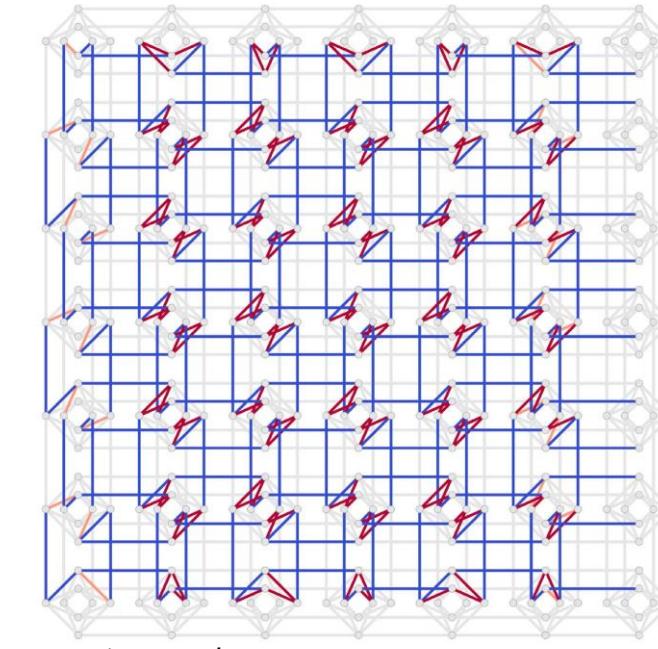
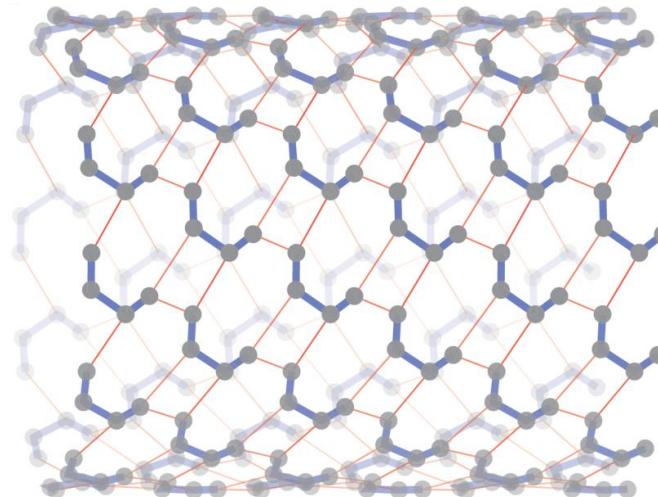
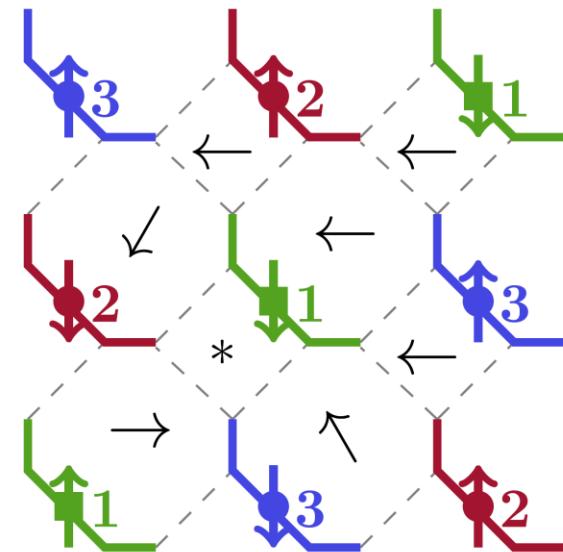


# Mapping to the QPU

- Can't intrinsically solve triangular lattice on 200Q chip
- Embed as a square-octagonal lattice
  - Expect qualitatively the same behaviour
- Chains of 4 qubits strongly FM coupled ( $J = -1.8$ )
- AFM coupling between the chains ( $J = +1$ )



A. King *et al.*, 2018

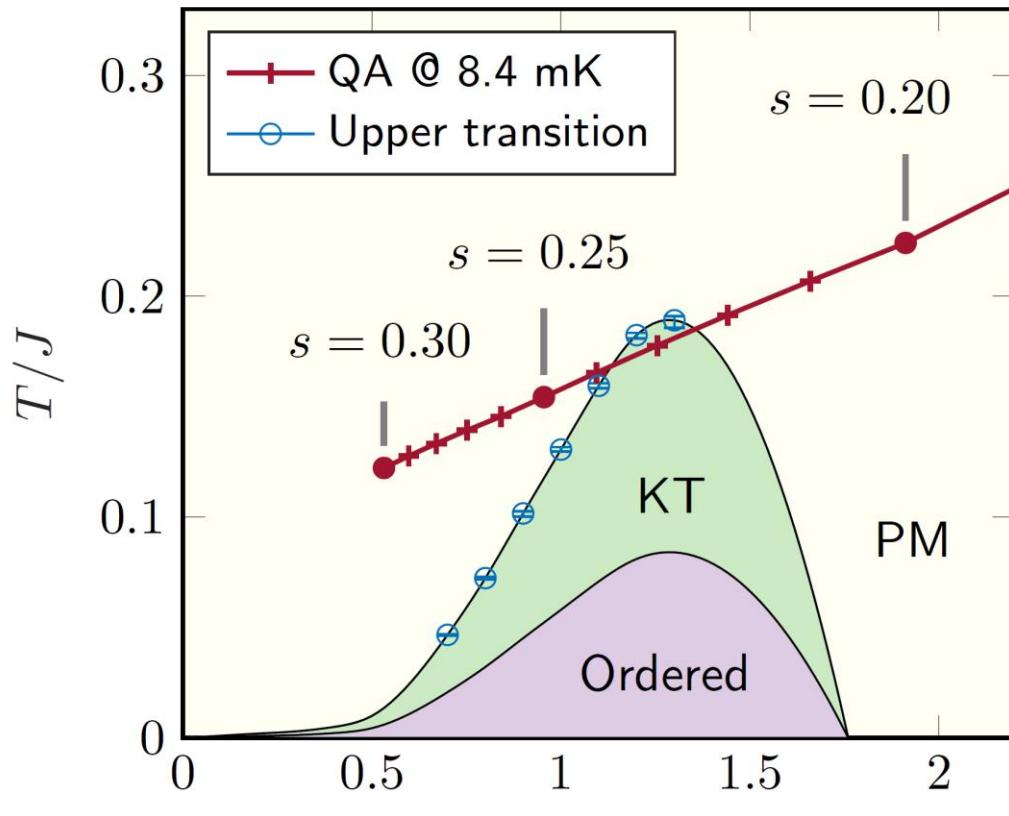


A. King *et al.*, 2018



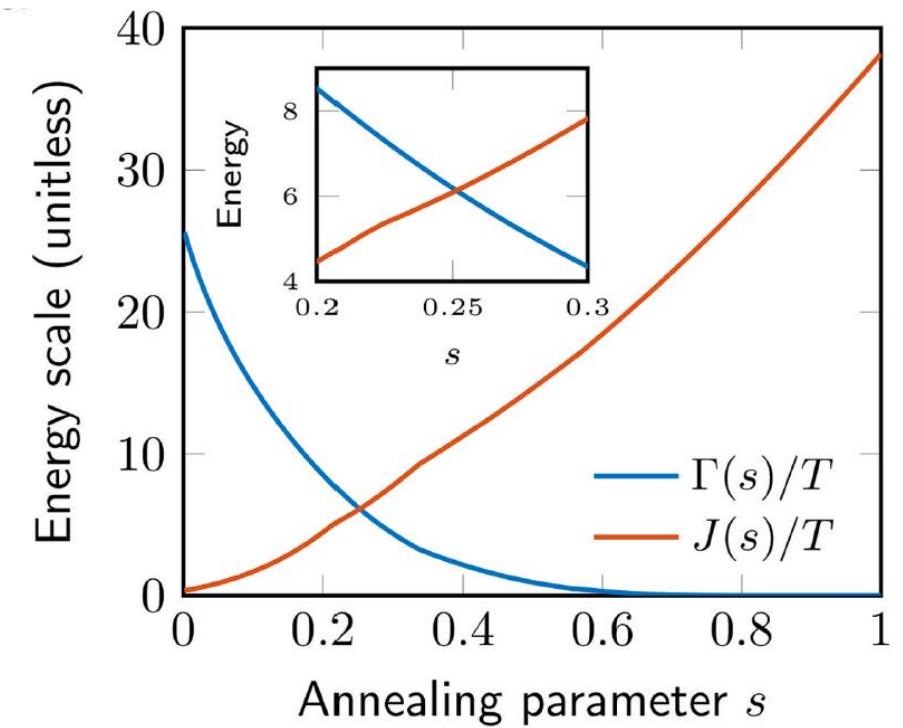
# Annealing Schedule

Annealing trajectory cuts through the phase transition



A. King et al, 2018

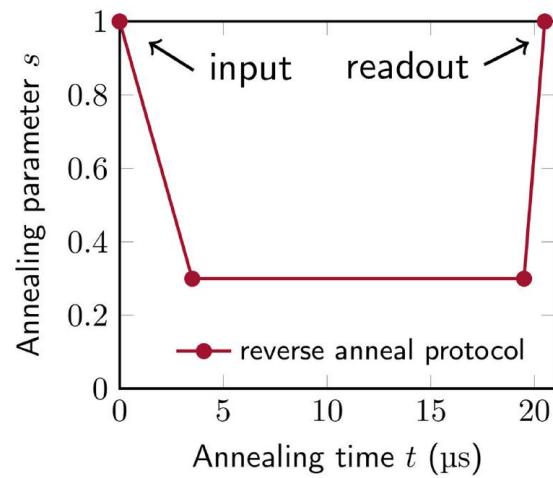
$\Gamma/J$



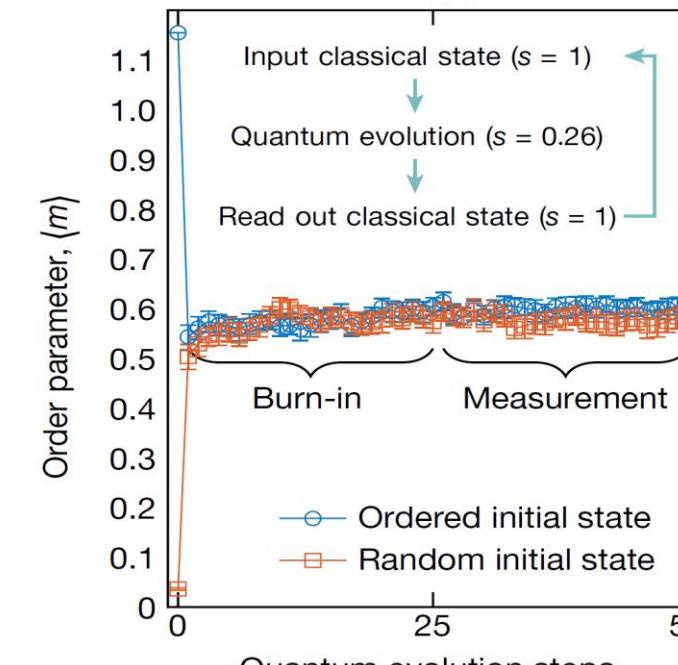
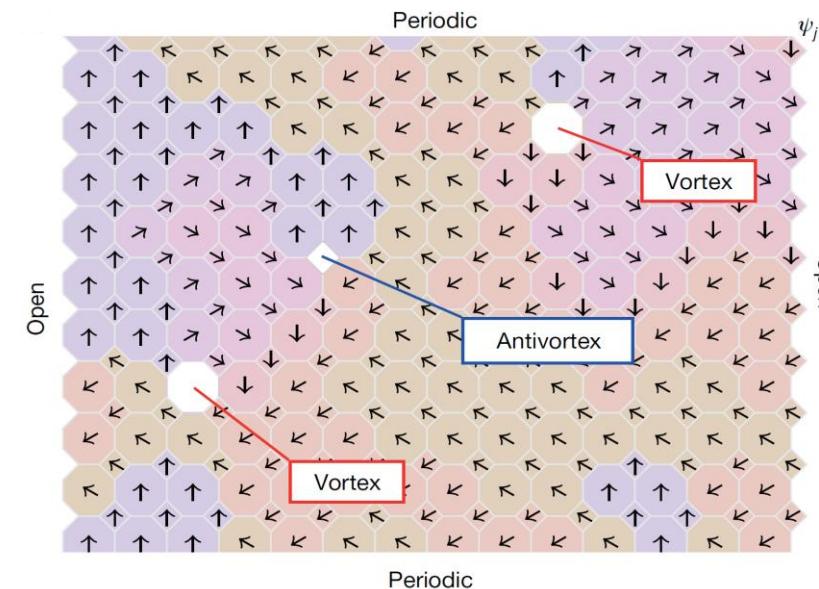
A. King et al, 2018

# Measurement Protocol

- Initialize the lattice in either an ordered clock state or random state
- Reverse anneal to the  $s$  of interest
- Allow the system to evolve for 65 ms
- Quench the system over 1  $\mu\text{s}$  and readout
- Repeat the reverse anneal, quench and readout



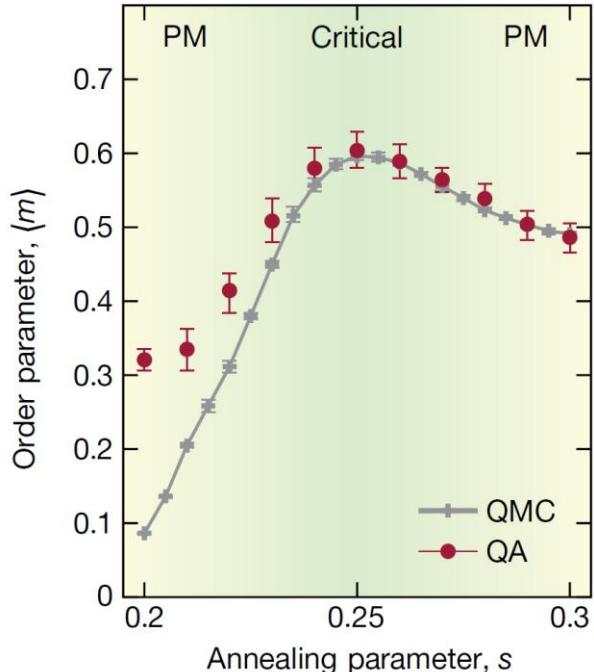
A. King et al, 2018



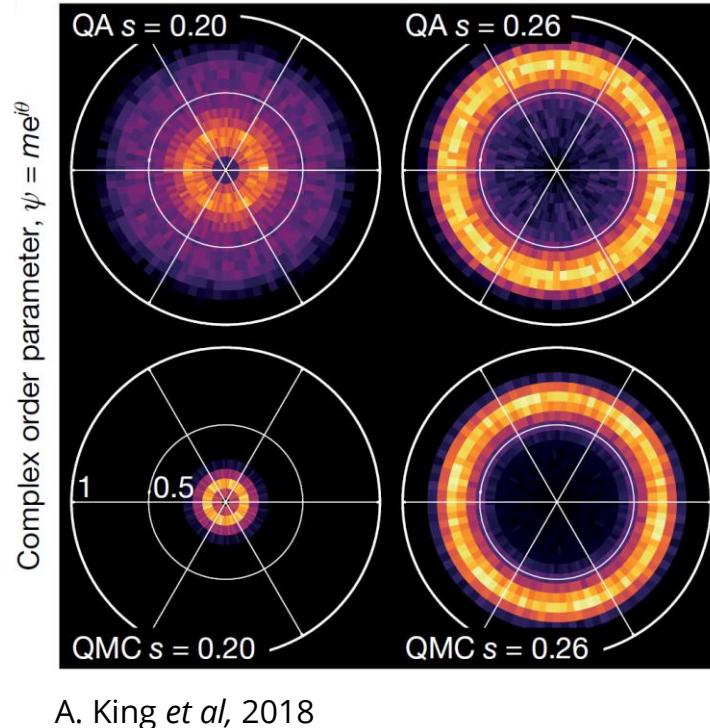
A. King et al, 2018



# Order Parameter



A. King *et al*, 2018

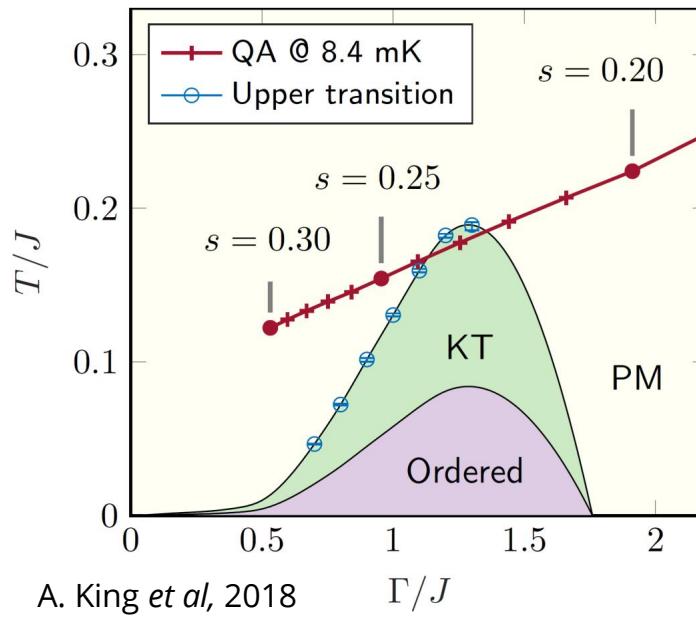


A. King *et al*, 2018

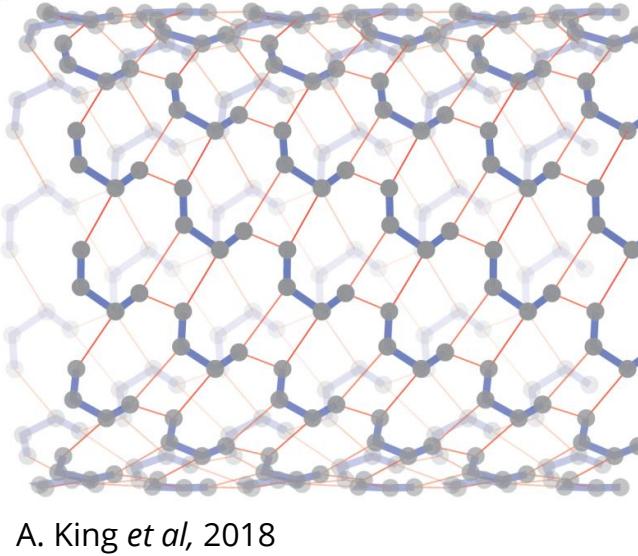
- Good agreement between QA and quantum Monte Carlo (QMC)
- Deviation at small  $s$  due to evolution of the processor during the quench

# Scaling of Phase Correlations

- Look at the correlations between plaquettes in the processor along the periodic dimension
- High (low) temperature  $\rightarrow$  exponential (power law) decay of correlations

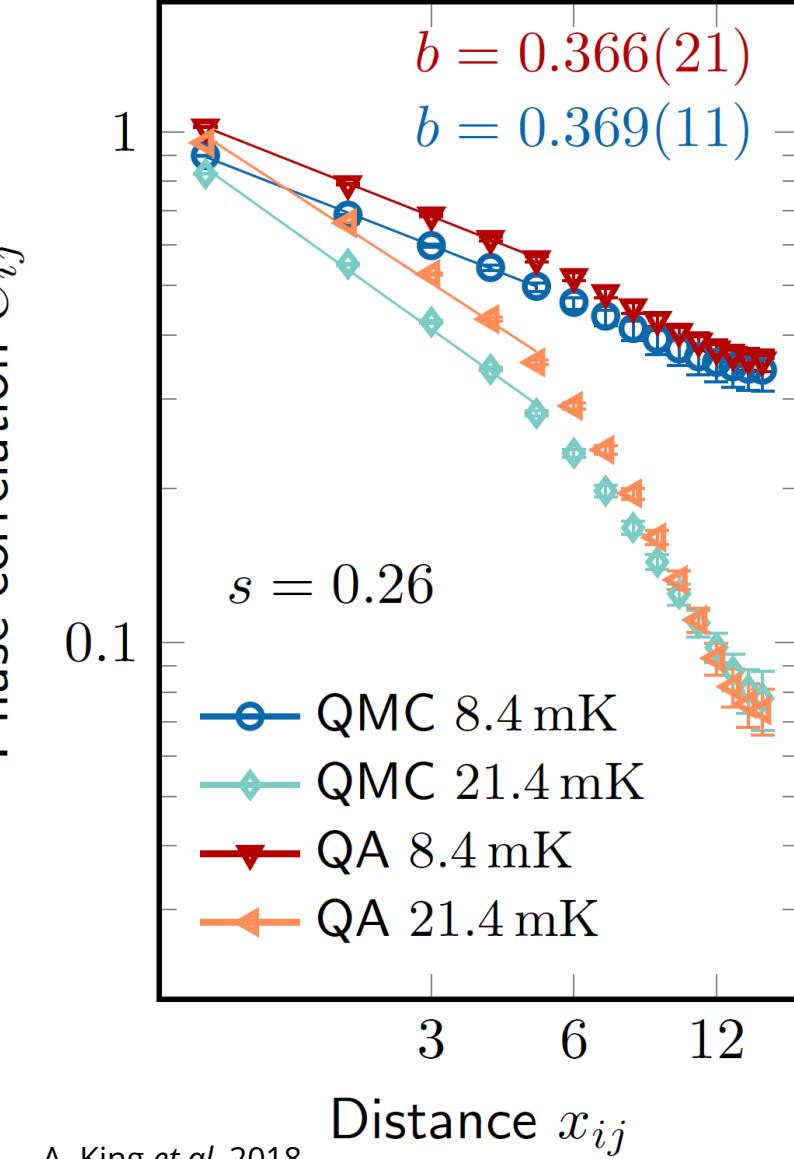


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A. King *et al*, 2018

Phase correlation  $C_{ij}$



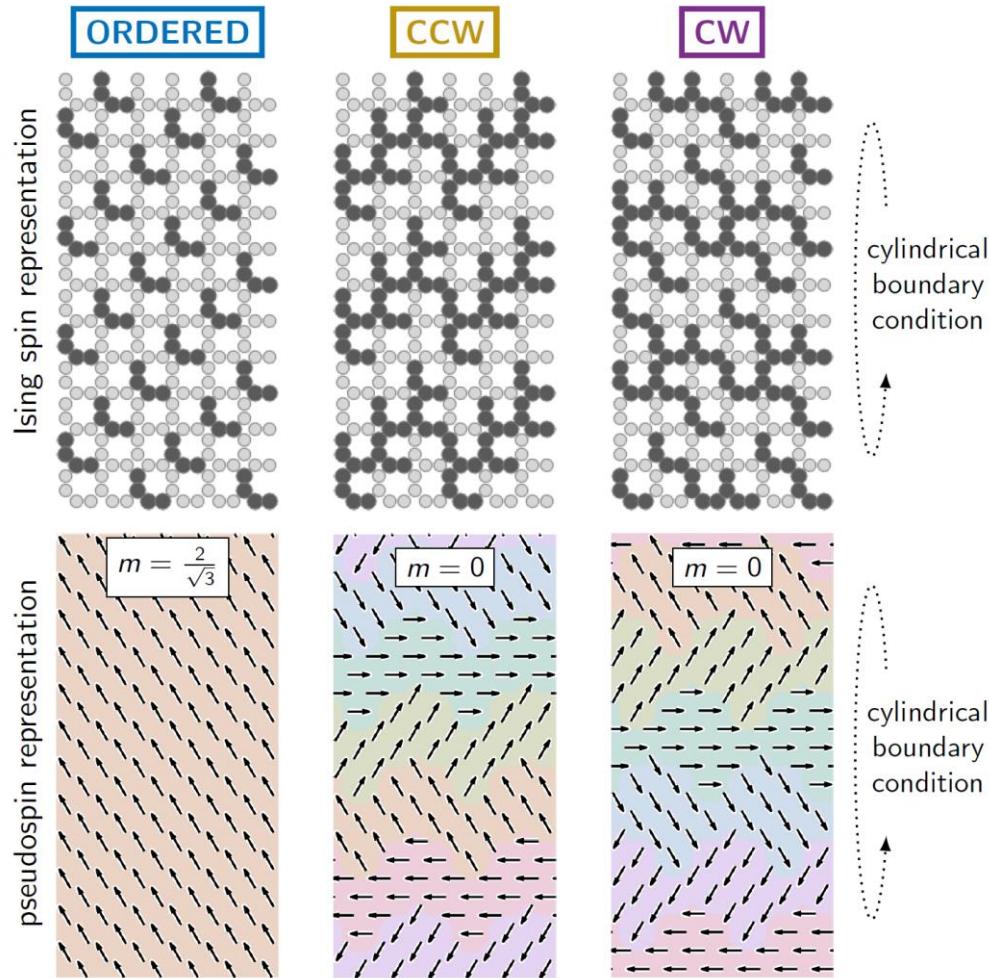
A. King *et al*, 2018

D-WAVE





# How Fast Is It?



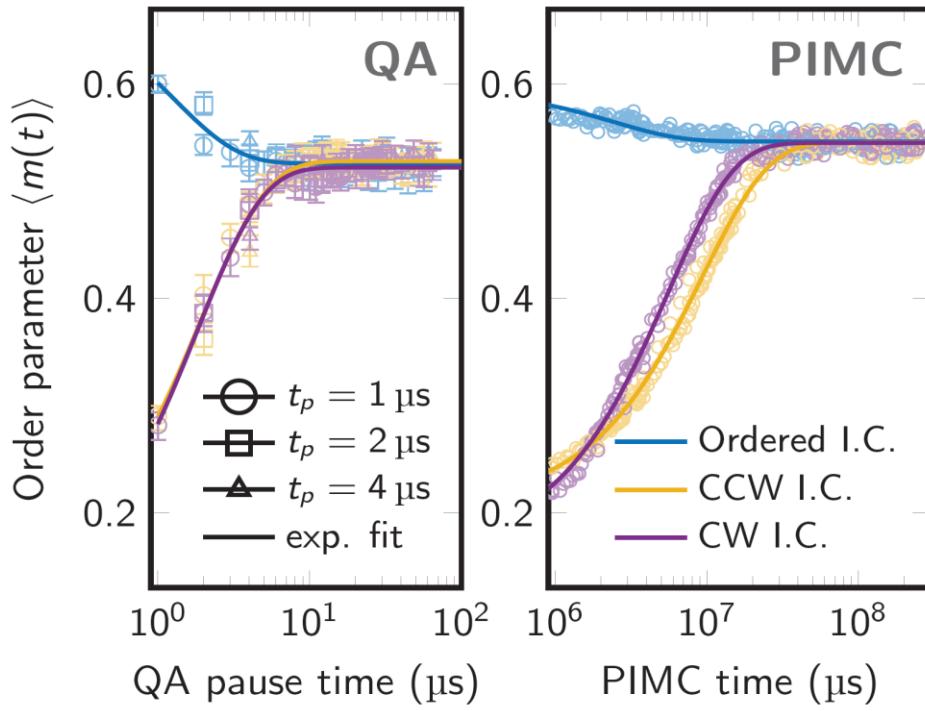
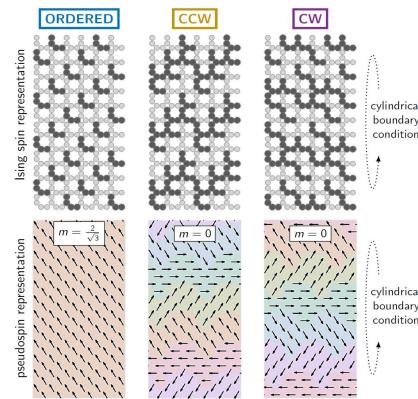
A. King *et al*, 2021

- CW or CCW winding of the pseudospin around the lattice adds a topological obstruction

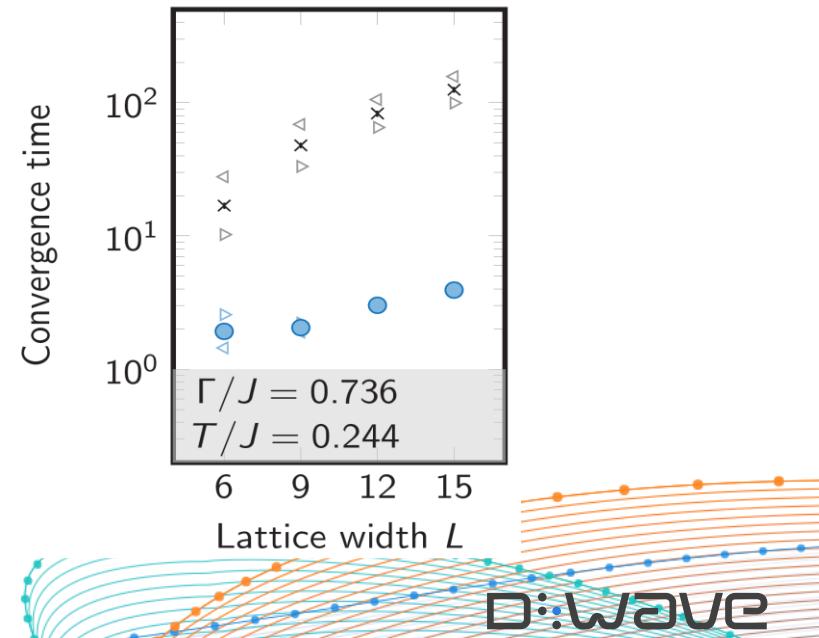
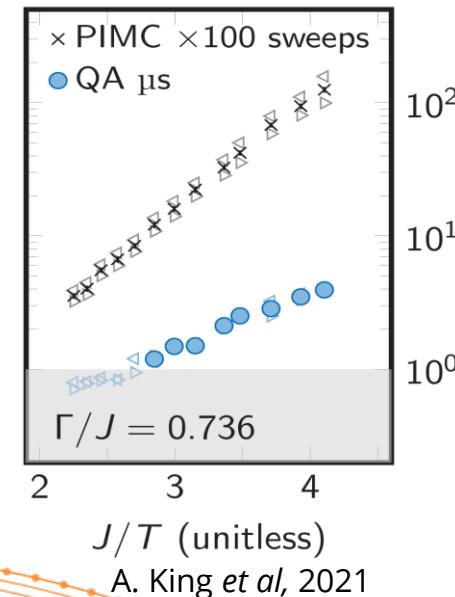
- Slows down the dynamics so that we can more easily measure the speed



# How Fast Is It?



- CW or CCW winding of the pseudospin around the lattice adds a topological obstruction
  - Slows down the dynamics so that we can more easily measure the speed
- Measure the time it takes for the order parameter to converge
- Compare PIMC and QA while making problem harder:
  - increase lattice size or increase  $J/T$





# Summary

- Quantum annealing relies on the adiabatic theorem → ground state computation
  - Implement a transverse field Ising model with superconducting flux qubits
  - Computational basis is direction of circulating current
- 
- KT work is an example of materials/quantum simulation using annealing
  - Demonstration of scaling advantage of QA over classical Monte Carlo
- 
- This problem well-suited to the hardware, but so are lots of others! Alex will tell you more in the next 3 lectures

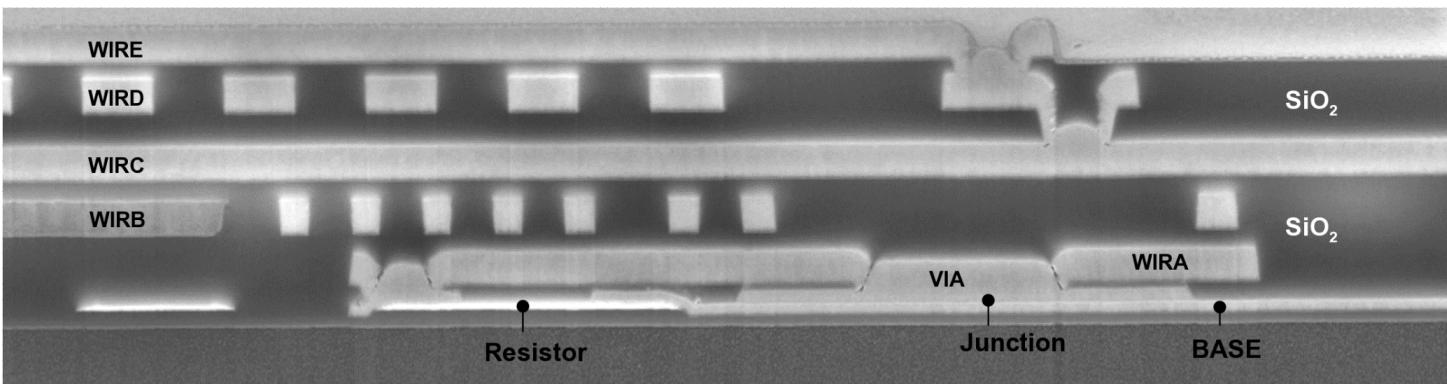
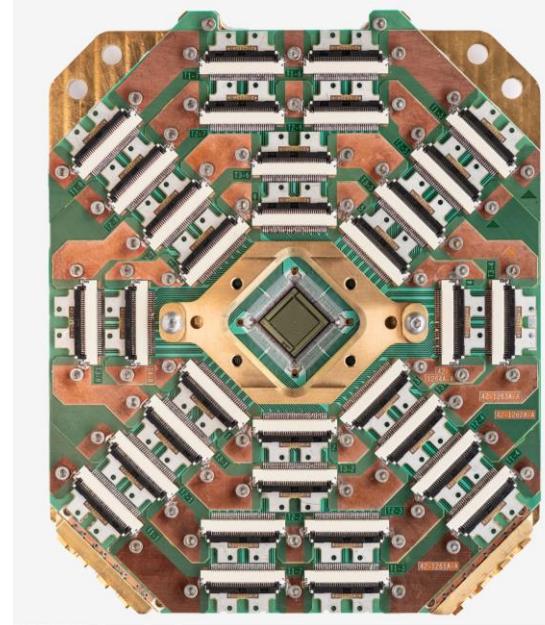
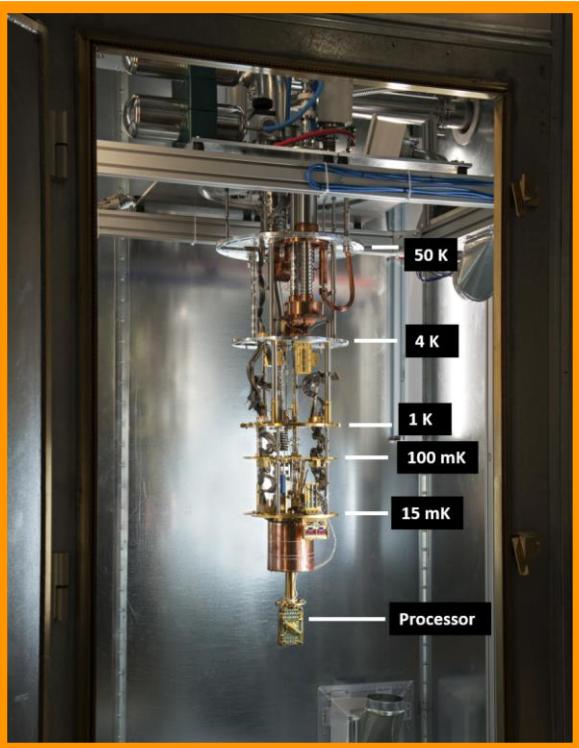


# Questions?

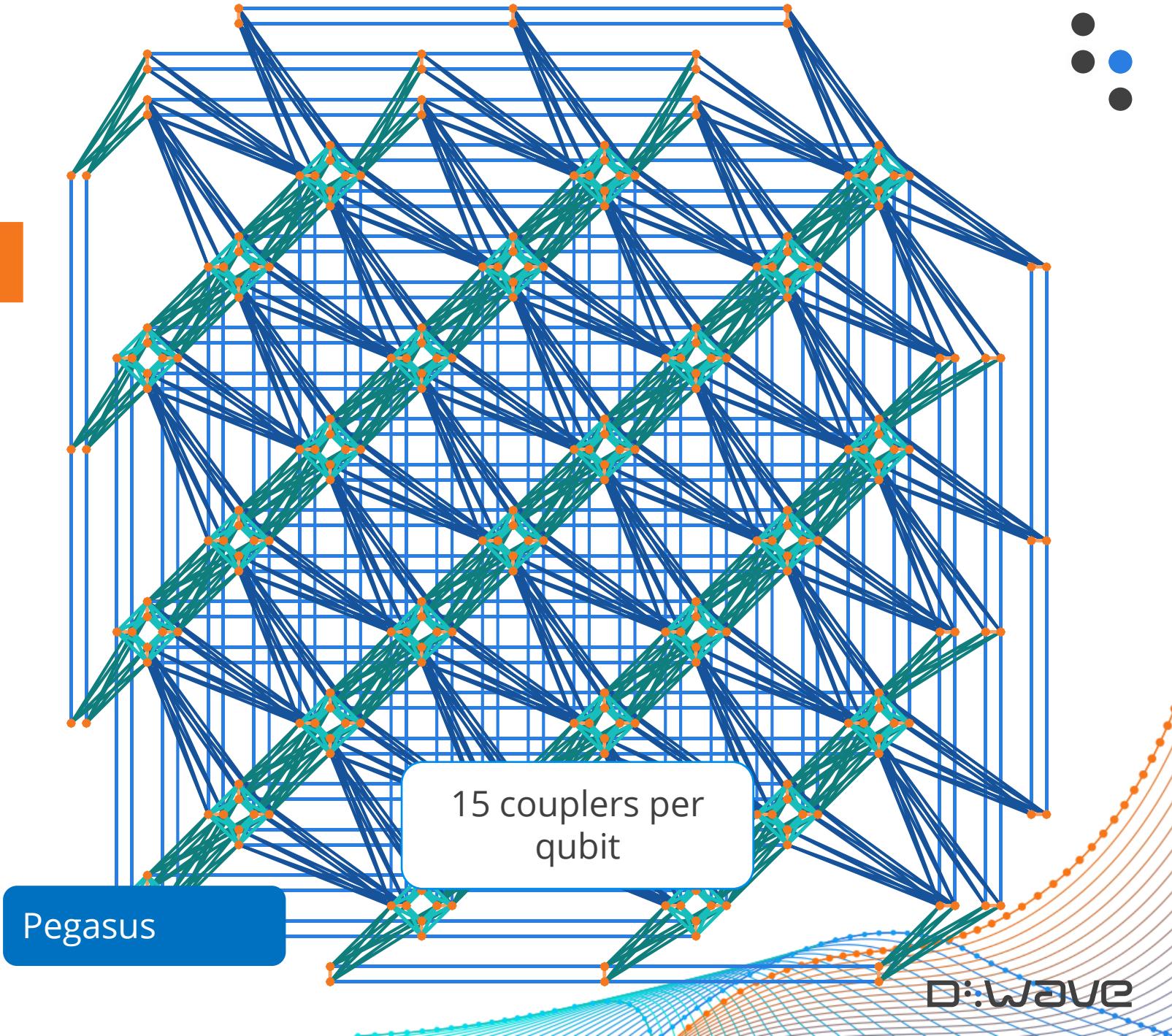
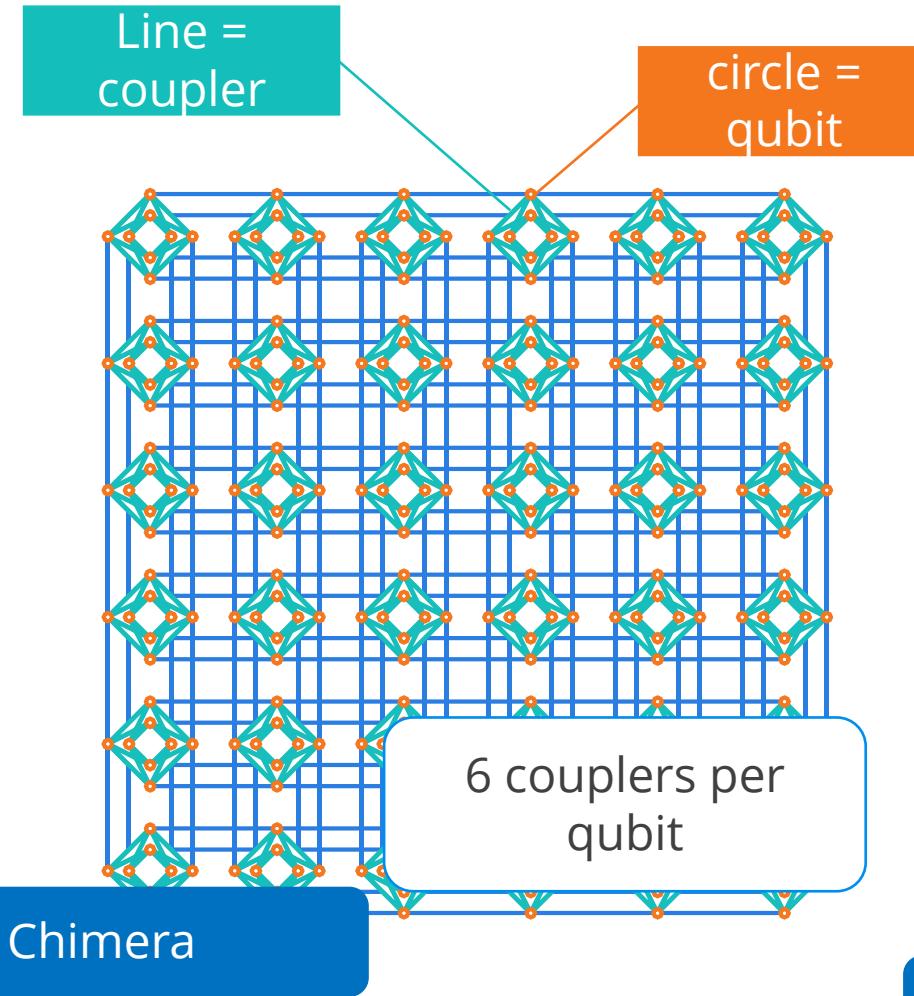
# More on Hardware



$T \sim 15 \text{ mK}$   
 $P \sim 25 \text{ kW}$   
 $B \lesssim 1 \text{ nT}$



# Processor Architecture



Qubits + Couplers

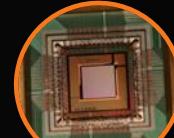
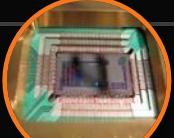
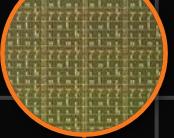
10,000  
1,000  
100  
10

2008

2012

2016

2020



Advantage

2000Q

D-Wave Two

D-Wave One

