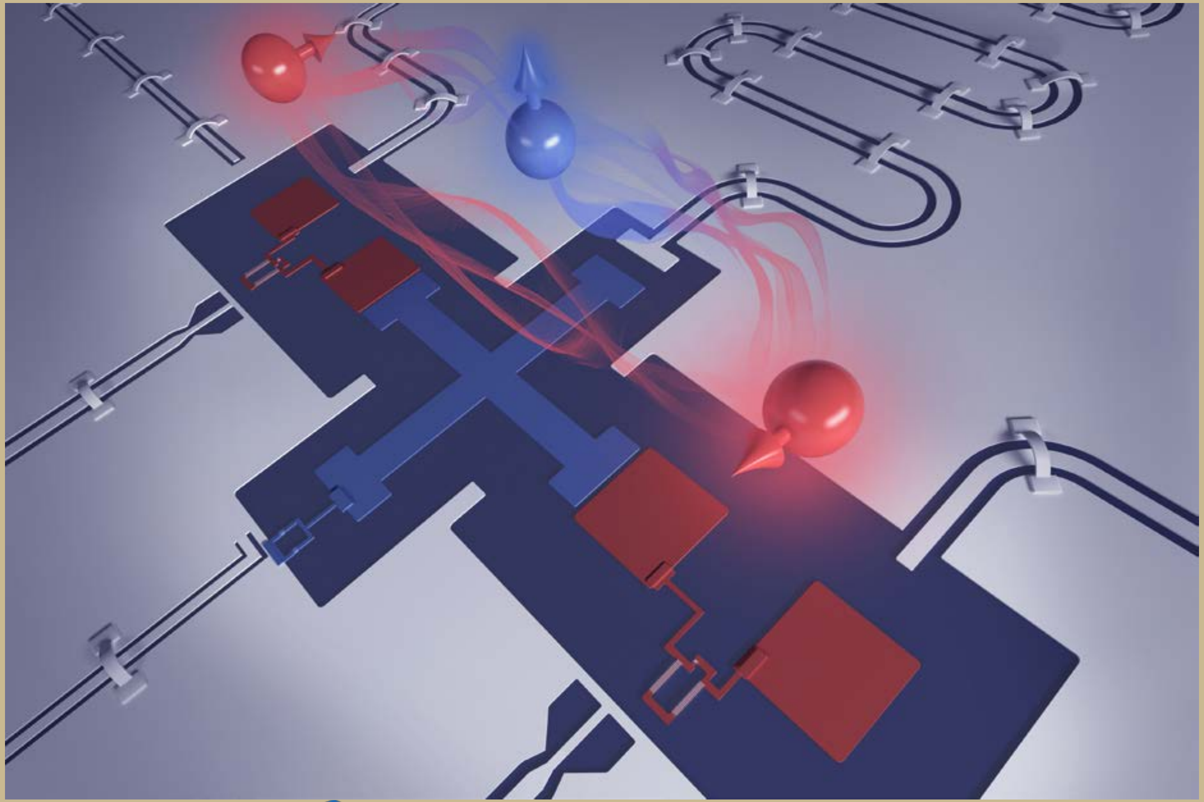
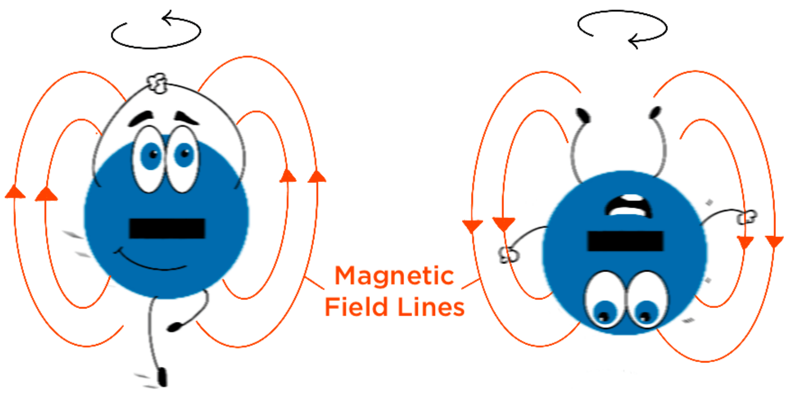
QUANTUM COMPUTATION ROUTE TO MAGNETIC PHASE DISCOVERY

Arnab Banerjee, Assistant Professor

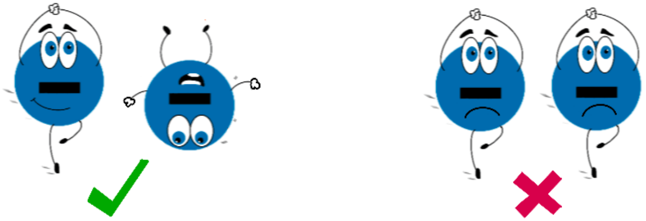


Electrons are like tiny bar magnets - Spins

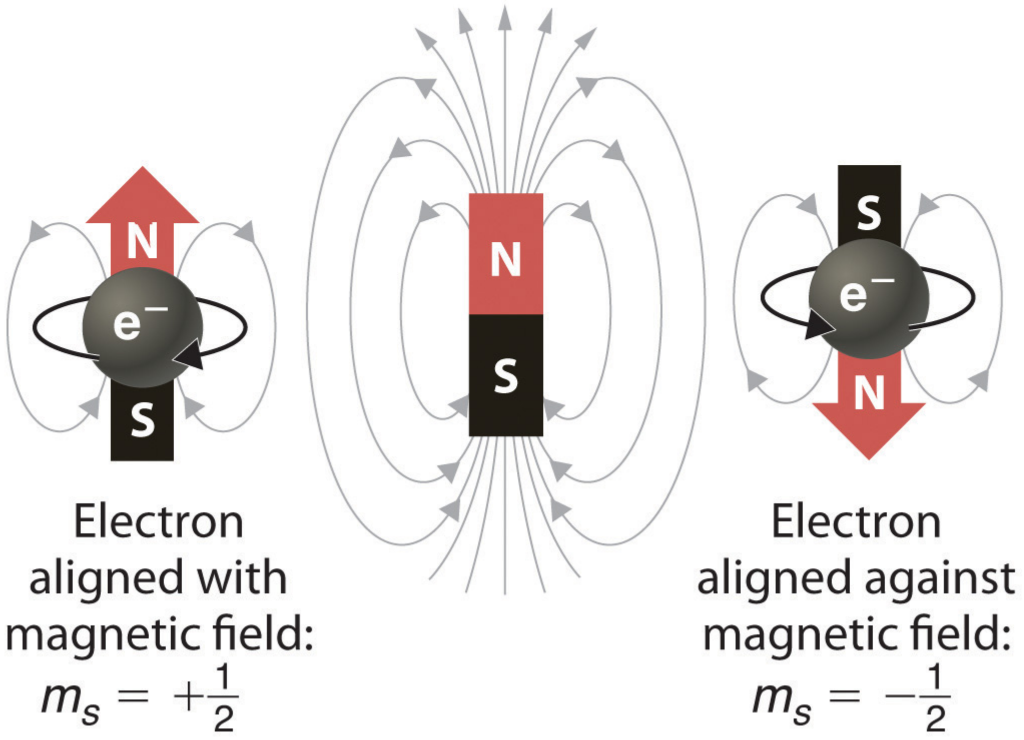
What are Electron Spins



Electrons can spin around their axis and create corresponding magnetic spin in the direction of the magnetic field lines



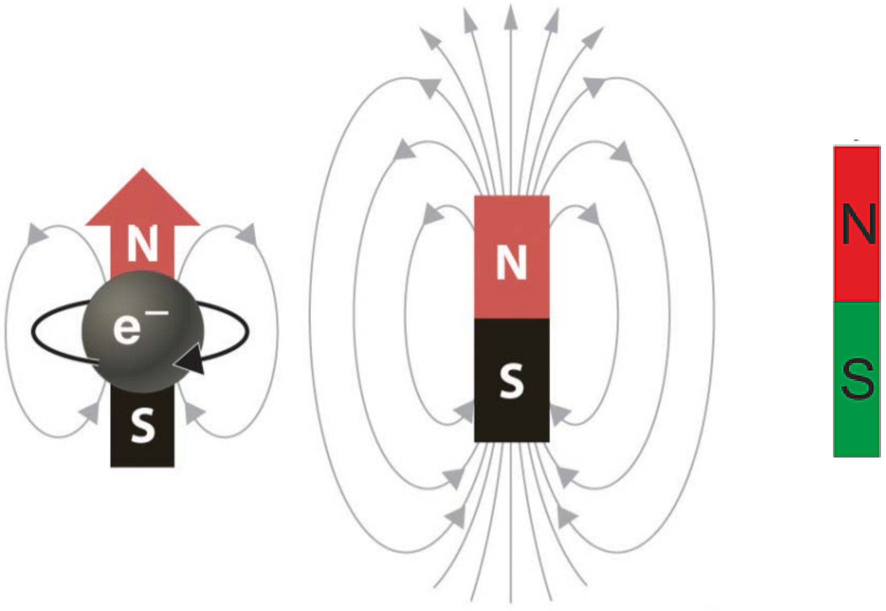
Each orbital of an atom can have two electrons, but they have to be in opposite spins



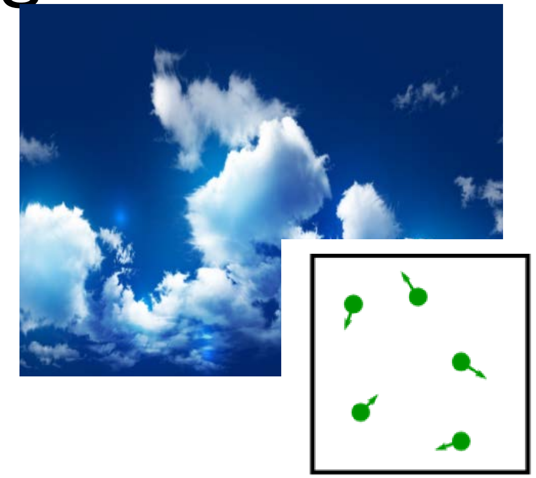
What are spins?

- Unpaired electron contributes a net spin moment of $S = \pm 1/2$.
- Orbital motion of electrons create a net angular moment L.

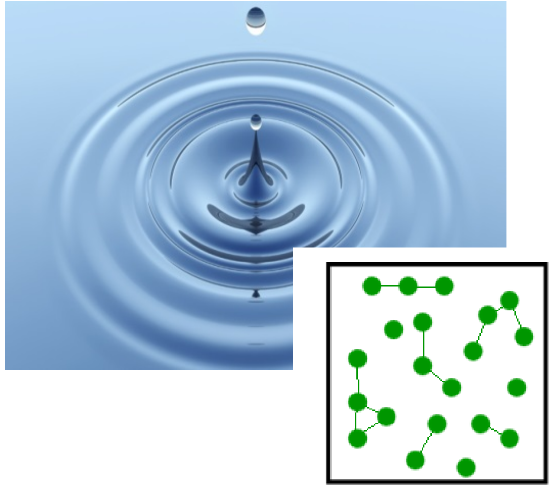
$$J = L + S$$



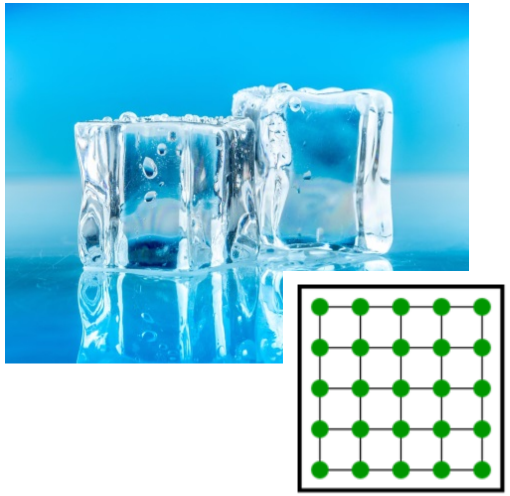
Spin phases



GAS



LIQUID

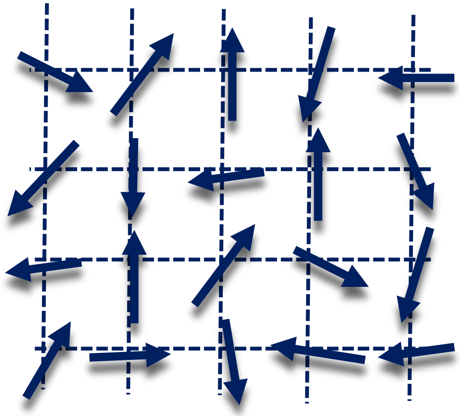


SOLID

REDUCE THERMAL FLUCTUATIONS

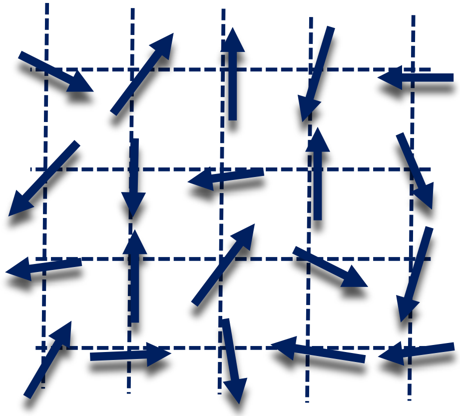
High Spin

SPIN GAS
(Paramagnet)

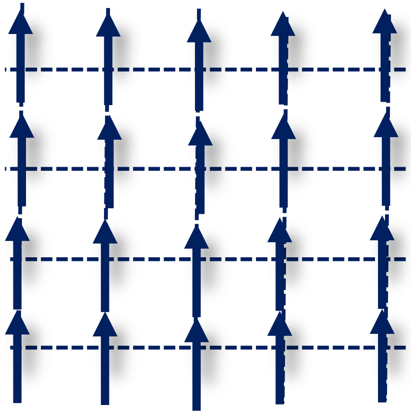


FULLY DISORDERED MOTIONS

LIQUID OR NEMATIC



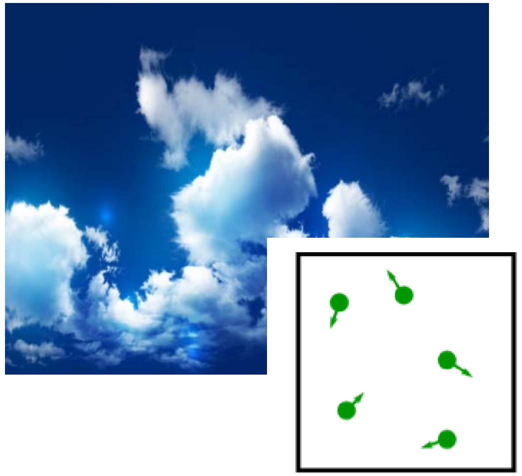
SPIN SOLID



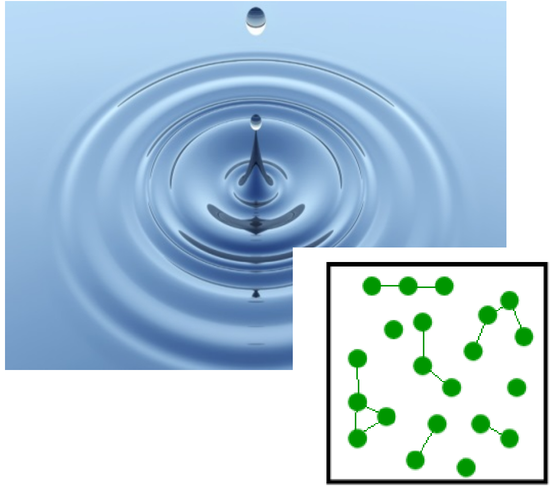
ORDERED

e.g.,
ferromagnet

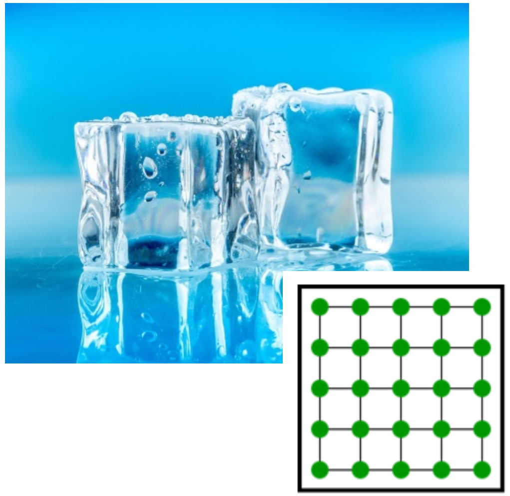
Spin Liquid



GAS



LIQUID



SOLID

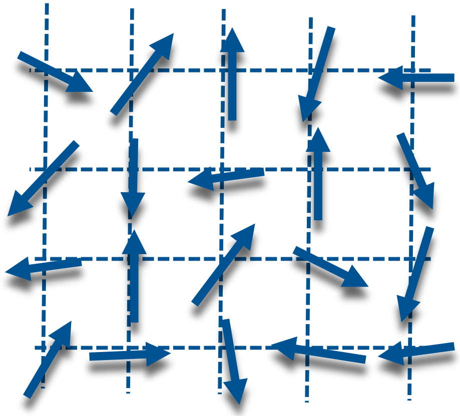
REDUCE THERMAL FLUCTUATIONS

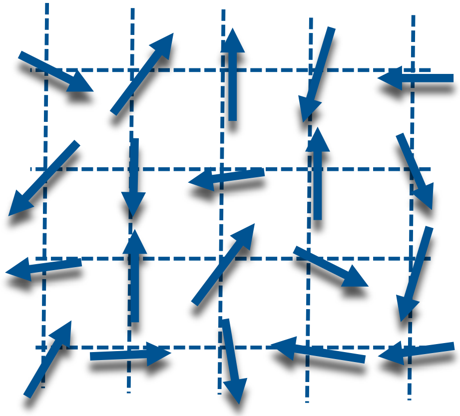
SPIN GAS
(Paramagnet)

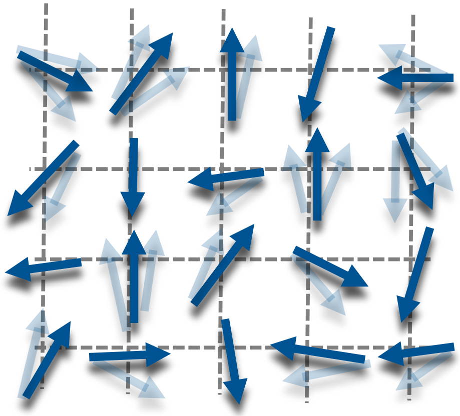
LIQUID

QUANTUM LIQUID

Low Spin







Quantum Fluctuations

Motions are entangled

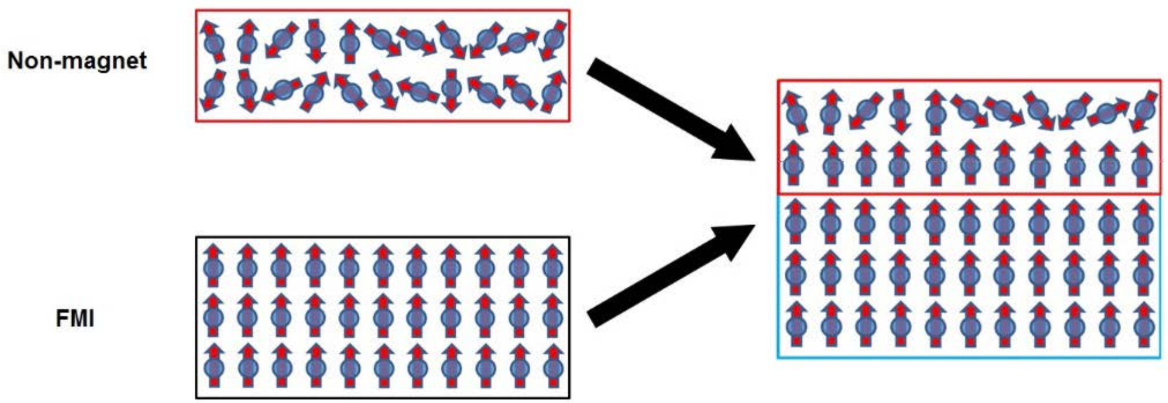
FULLY DISORDERED MOTIONS

ORDERLY MOTIONS

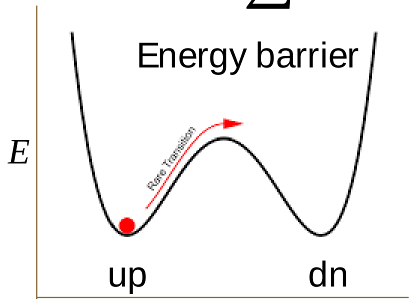
QUANTUM ZERO POINT MOTIONS

Applications of Magnetism

Spin Phases of Matter

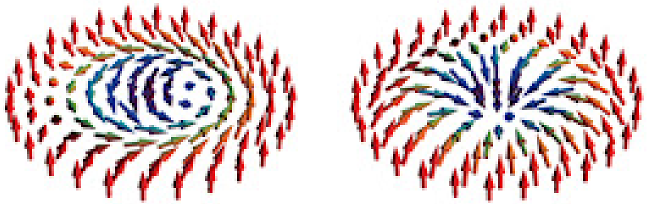


$$H = -J_{ij} \sum S_i^z . S_j^z$$

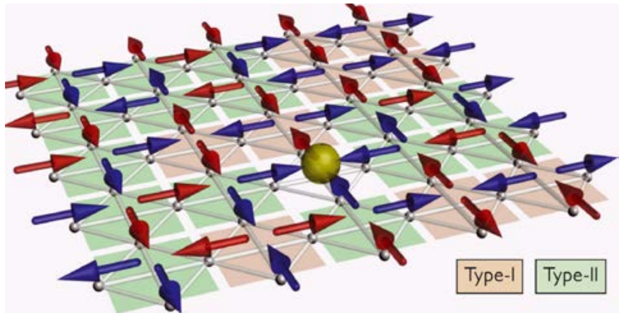


Ferromagnetism have led to magnetic memories. but many more states of magnetism are possible…

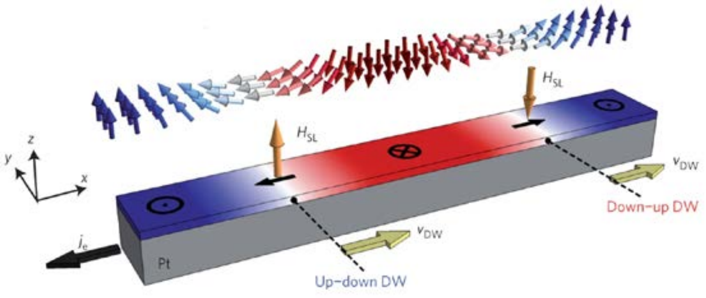
Topological phases, skyrmions



New phases, e.g. spin ice, spin glass



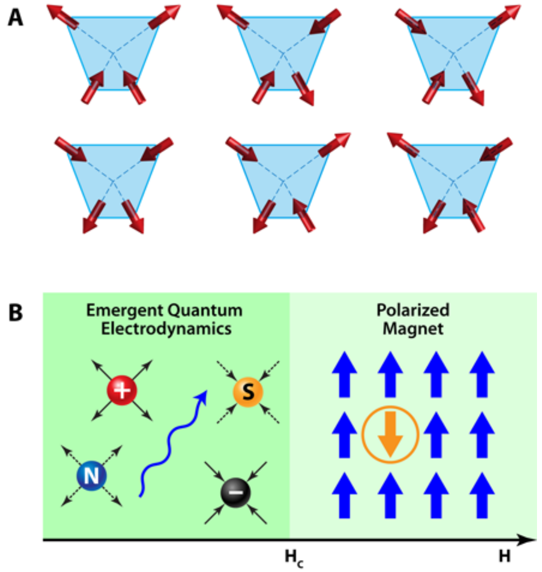
Emergent defects, domain walls



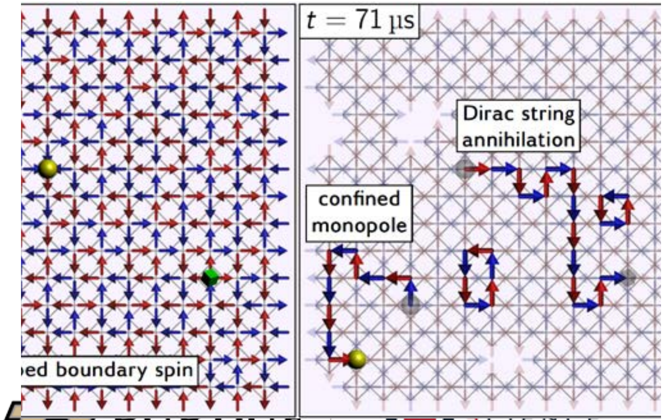
Discovery of new magnetic phases is important as it will lead to new applications in spintronics

Zoo of new magnetic phases of matter

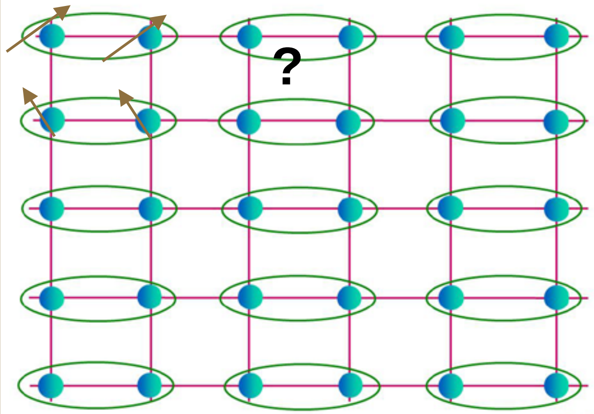
Spin Ice



Example: $DyTi_2O_7$



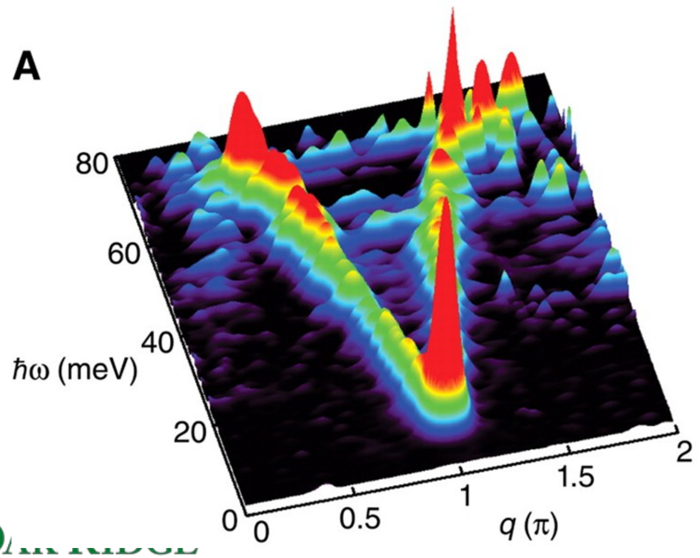
Valence Bond entanglement in quantum spin systems



$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

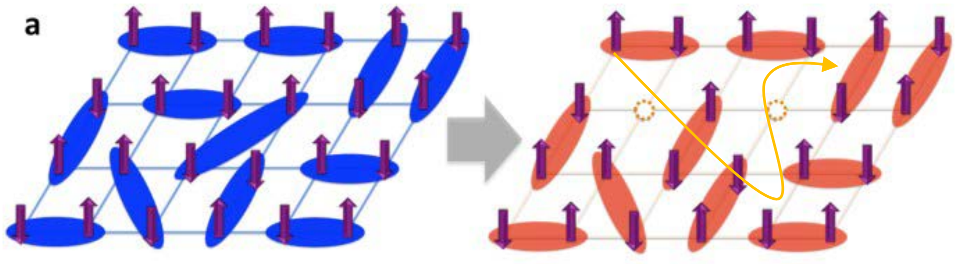
Valence Bond Solid (VBS)

N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).
R. Moessner and S. L. Sondhi, *Phys. Rev.* B **63**, 224401 (2001).

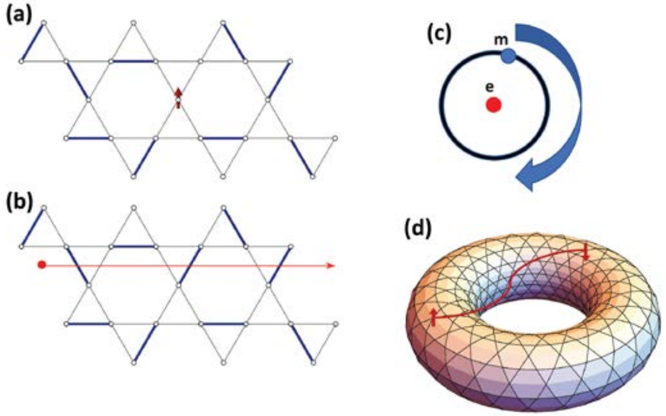


Quantum Spin Liquids

Spin liquids have a long-range entanglement and short-range correlation.

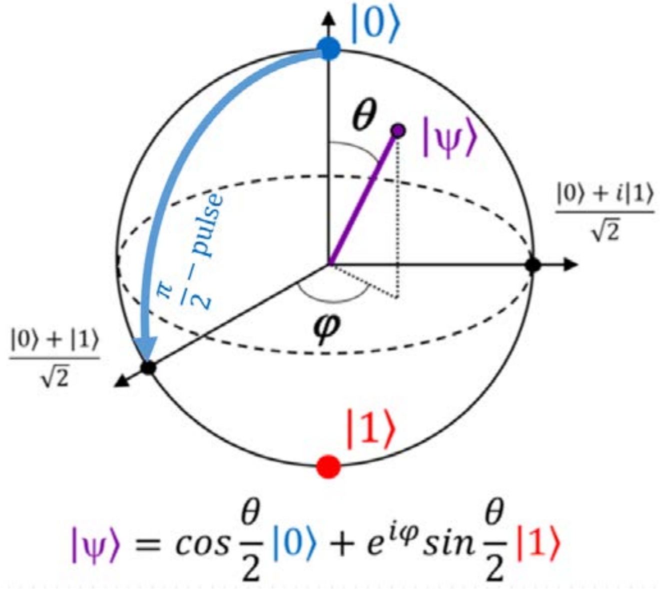


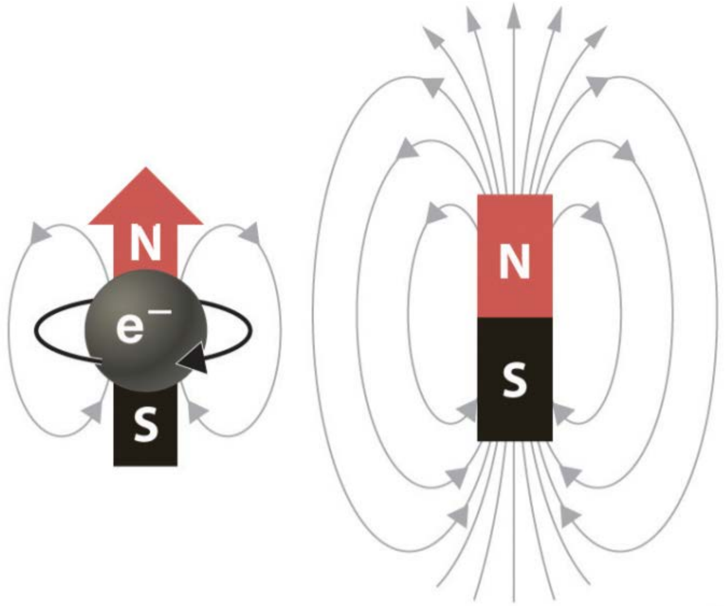
Motion (breaking of bonds) can be topological and depends on the symmetry of the system



Qubits

Spin

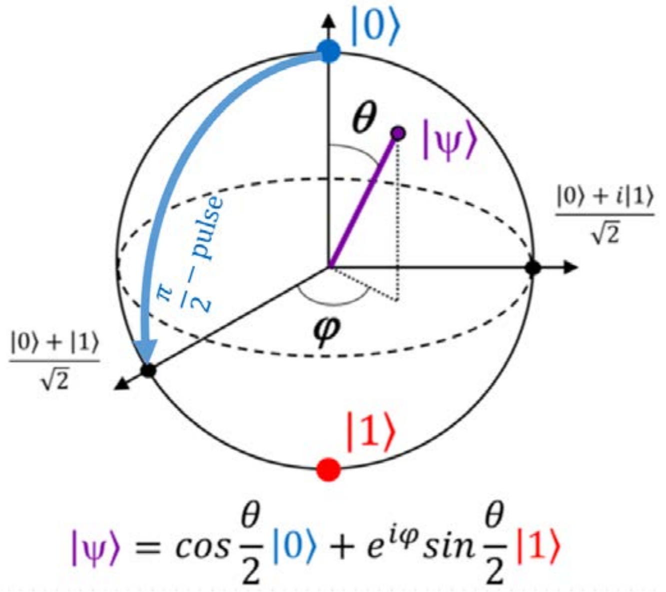


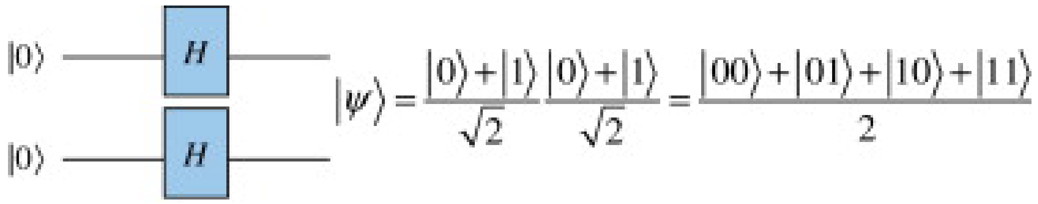


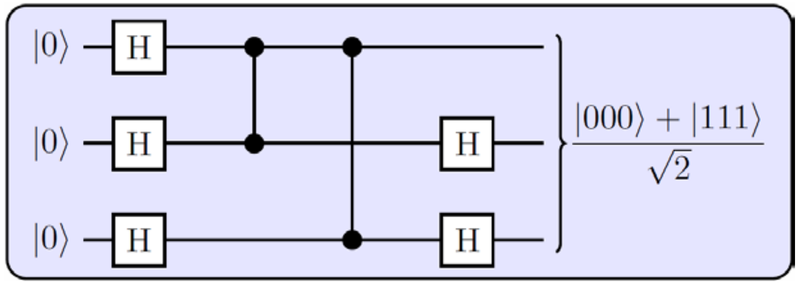
Bloch spins have a direct correspondence with qubit states and phase gates

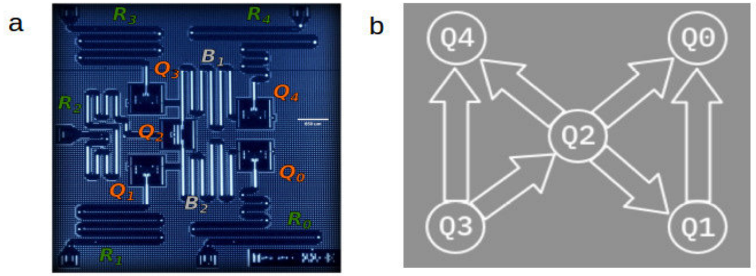
Spin and Qubits

Easy to entangle



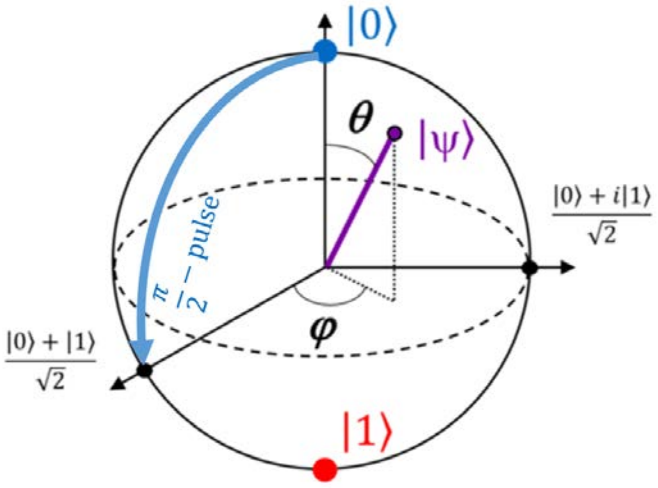






Bloch spins have a direct correspondence with qubit states and phase gates

Spin and Qubits



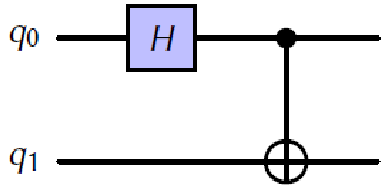
$$|\psi\rangle = cos\frac{\theta}{2}|0\rangle + e^{i\varphi}sin\frac{\theta}{2}|1\rangle$$

Bloch spins have a direct correspondence with qubit states and phase gates

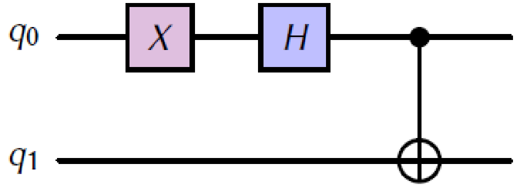
Easy to entangle

We can create quantum circuits that represent quantum states. the Bell states:

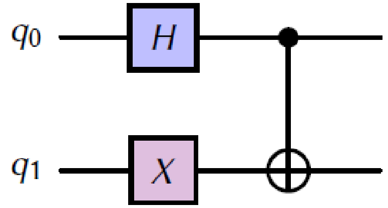
- $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$:



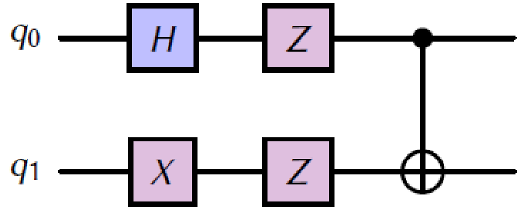
- $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$:



- $|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$:

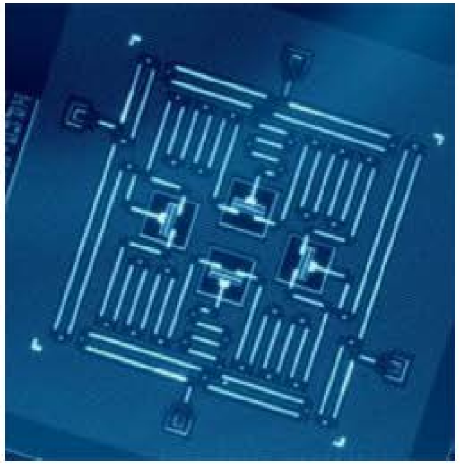


- $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$:

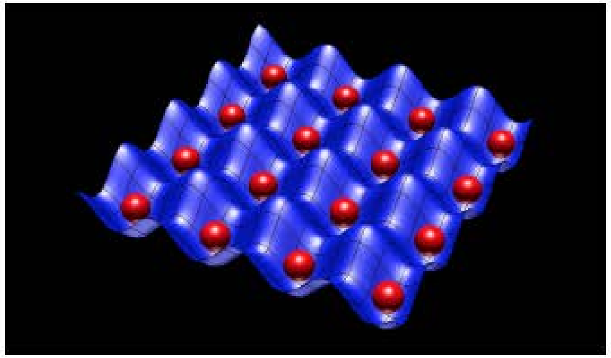


NISQ

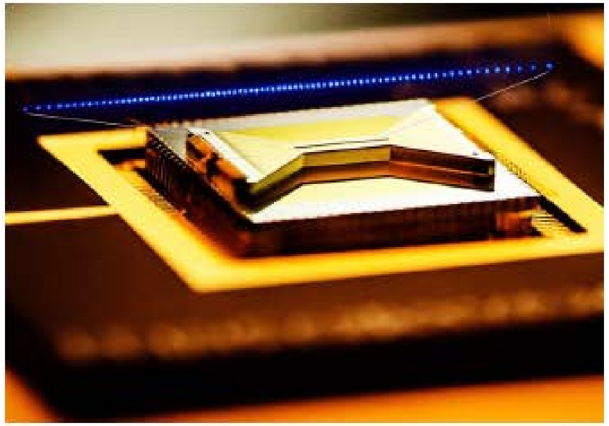
- In the current era of **noisy intermediate-scale quantum (NISQ)** devices, it is very intriguing to explore the possibilities they provide for simulating quantum systems.



(a) Superconductors

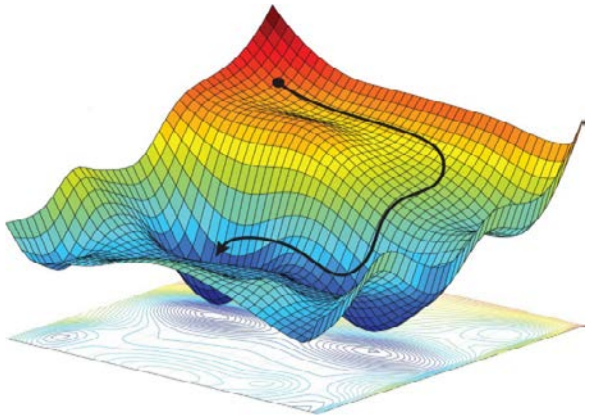


(b) Rydberg atoms



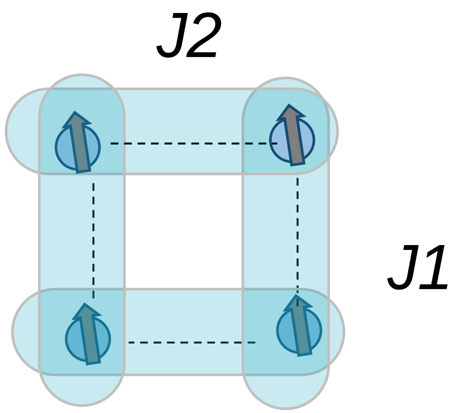
(c) Trapped ions

Optimization



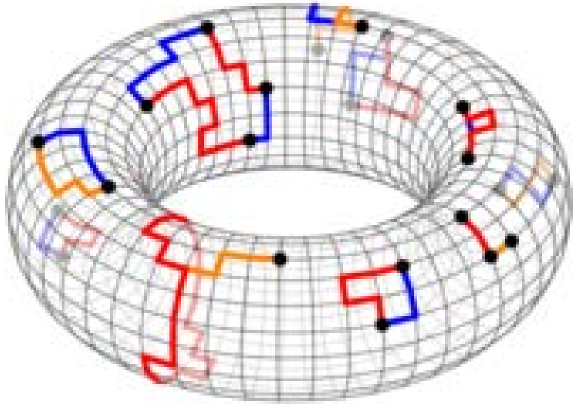
- Find the objective function
- Applications in various industrial and societal and design problems
- Find the ground state of quantum Hamiltonians

Hamiltonian Engineering



- Design dynamics of Hamiltonians using quantum hardware
- Study how to beat noise
- Study how to scale up simple building blocks to complex circuits
- Get to materials co-design and experiments

Topological Phases



- Design topologically relevant models
- Study how environmental and device parameters affect state
- Understand quasiparticles and protection
- Get to materials co-design and experiments.

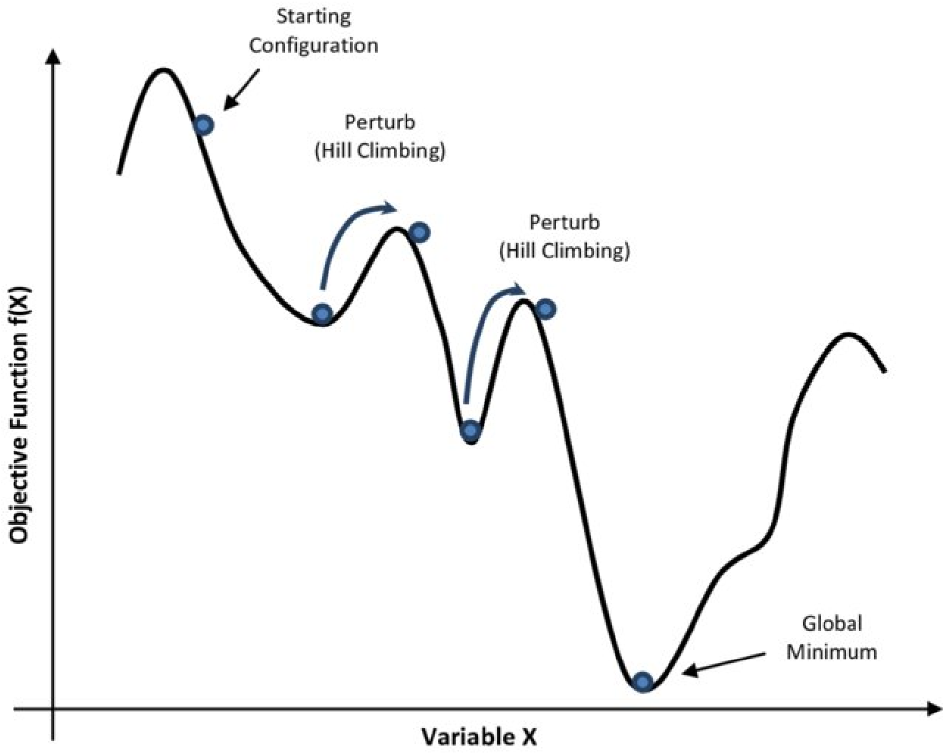
Quantum Optimization

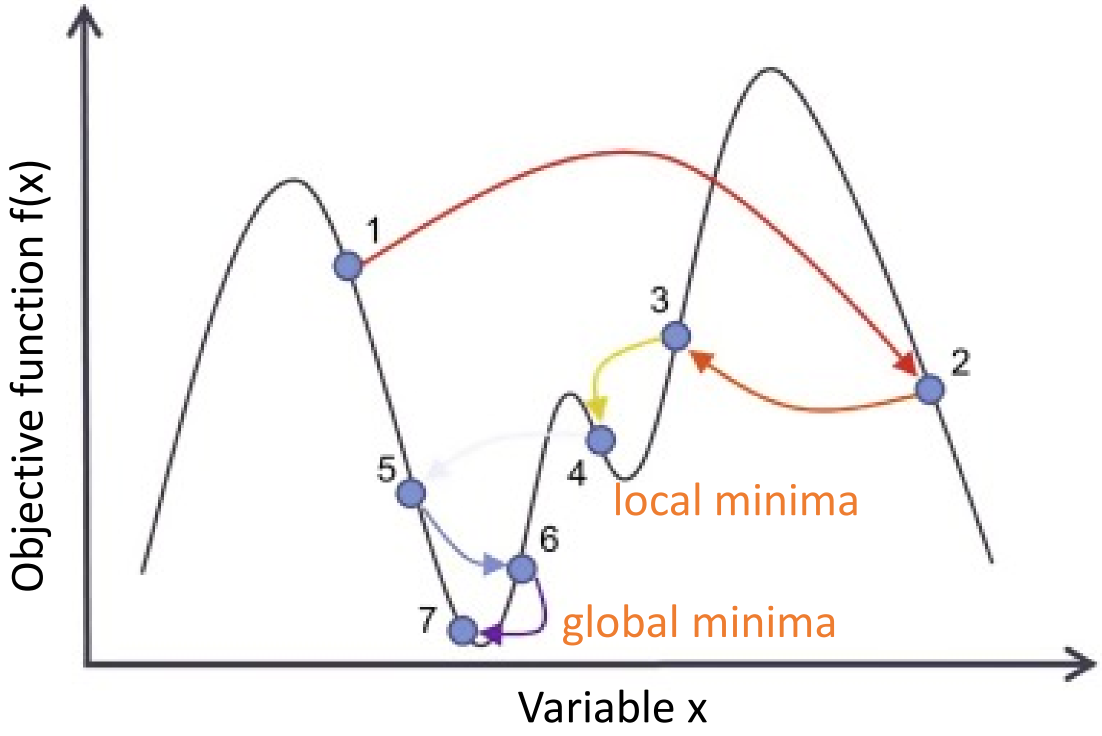
$$Minimize\ an\ Objective\ Function\ f(x)$$

$$x = (\mathrm{x}_1, \mathrm{x}_2, \ldots, \mathrm{x}_\mathrm{n}),$$

where x = discrete or continuous variables

$$e^{-\frac{E}{kT}}$$

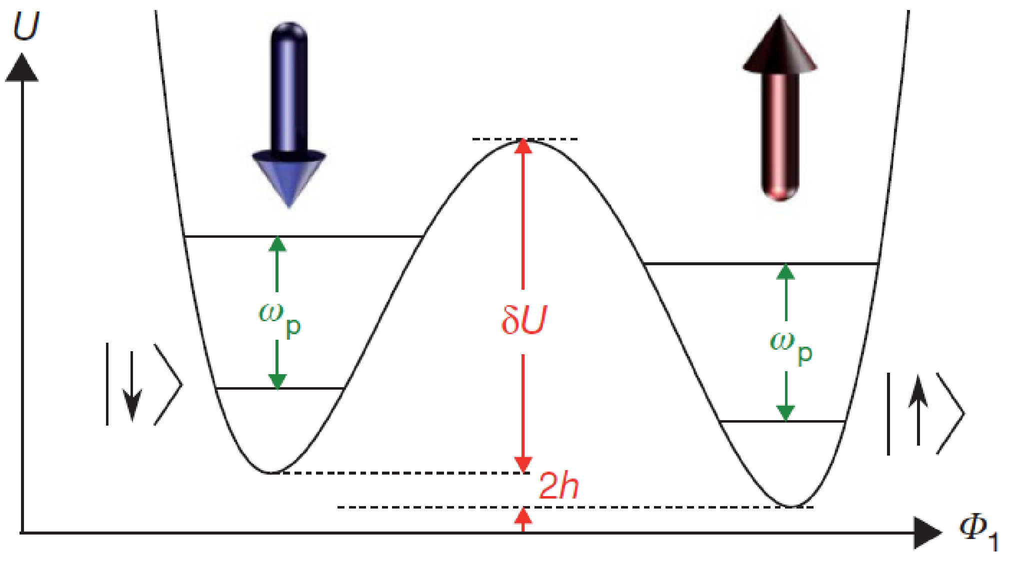


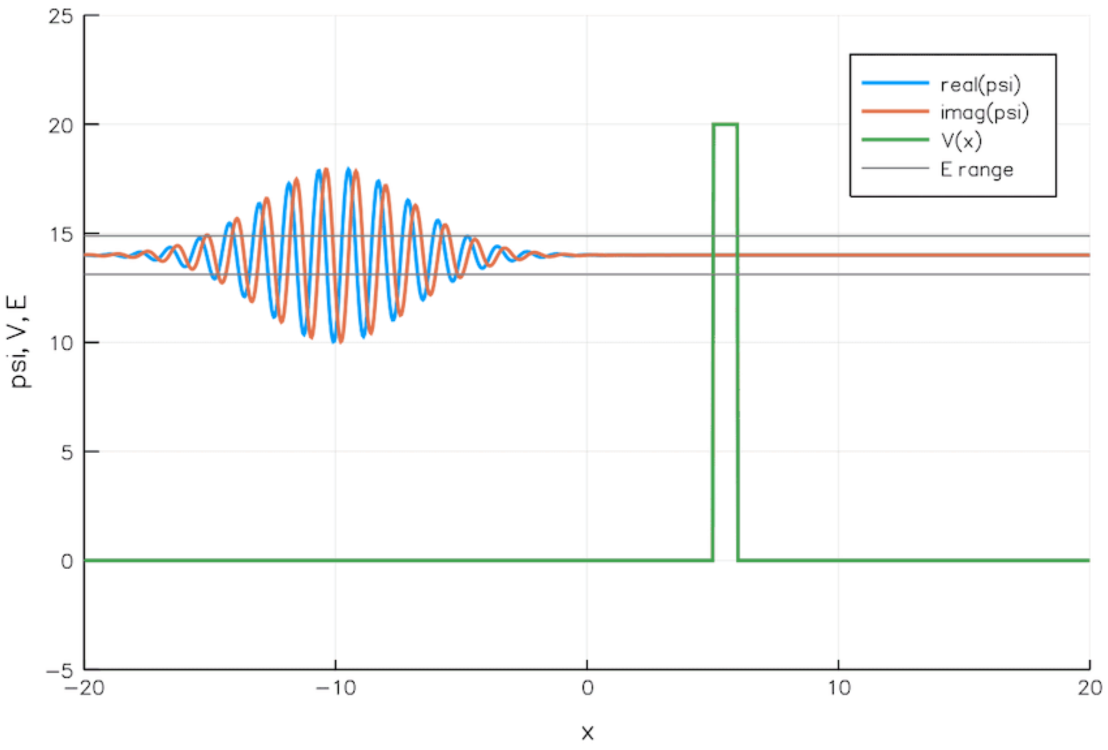


SLOW AND UNCERTAIN PROCESS

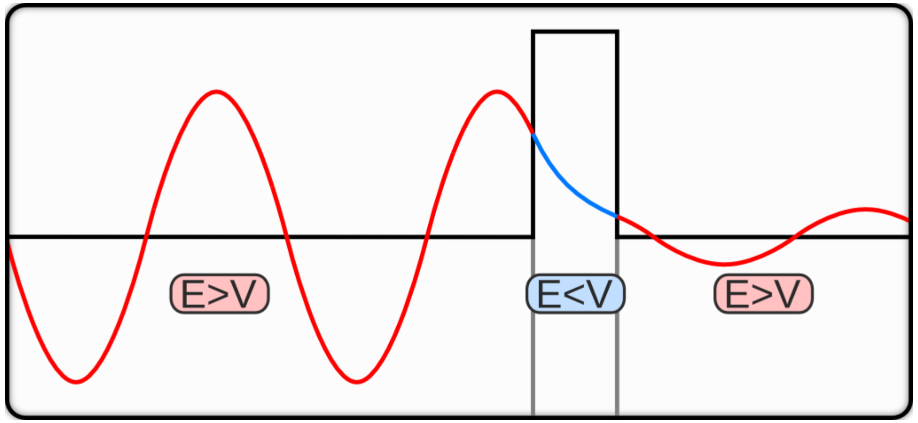
Ghasemalizadeh et al., A Review of Optimization Techniques in Artificial Networks International Journal of Advanced Research 4(9):1668-1686

Quantum tunnelling

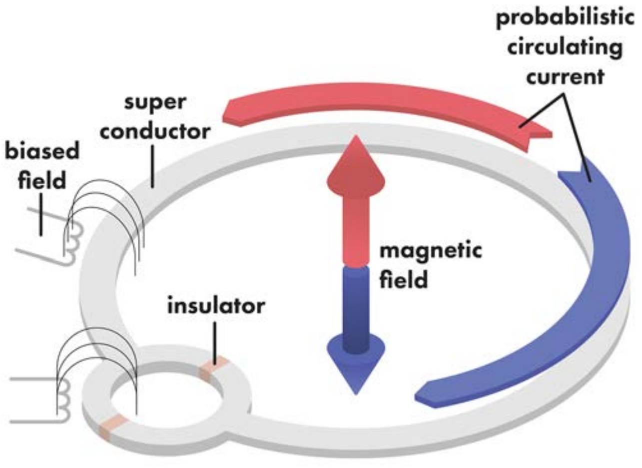




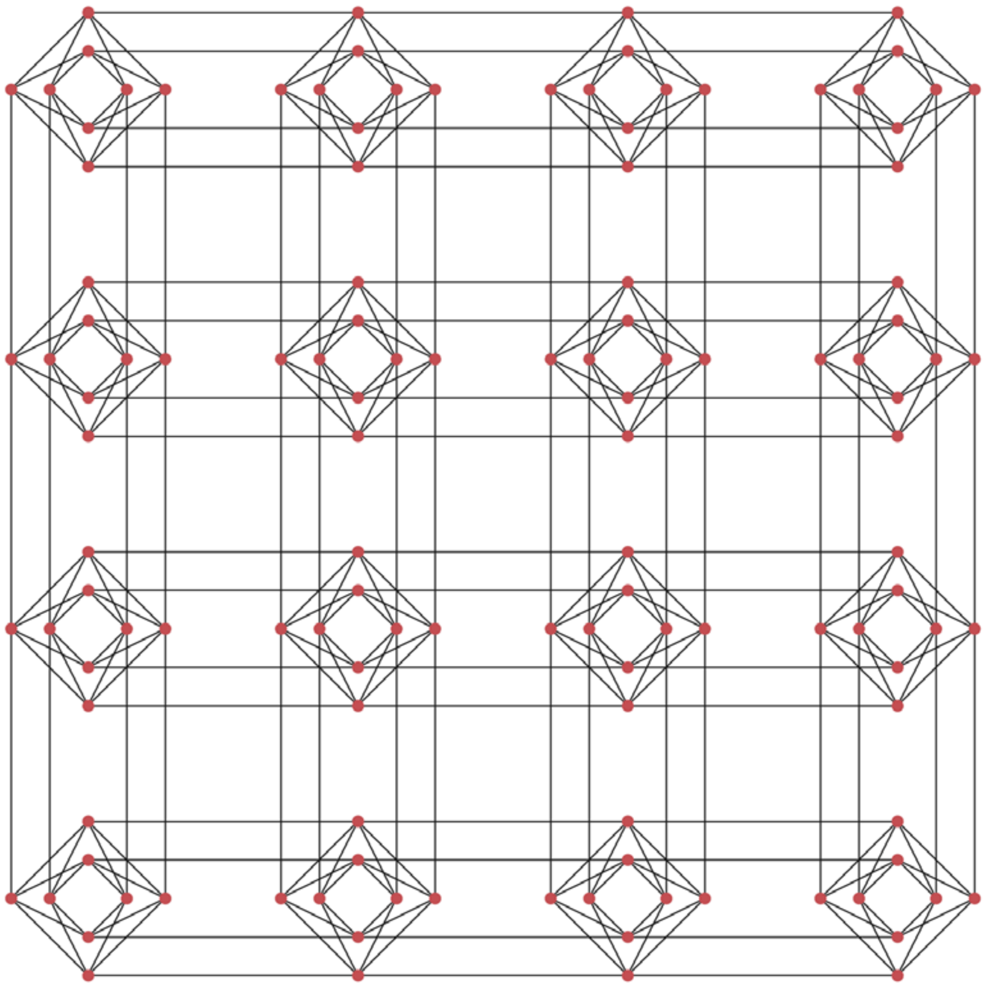
If one can find a means to change δU then the states can controllably tunnel into the minima.



D-Wave 2000Q Annealer : 'Chimera architecture'



Coupled RF-SQUID Qubits



Transverse magnetic field (quantum annealing)

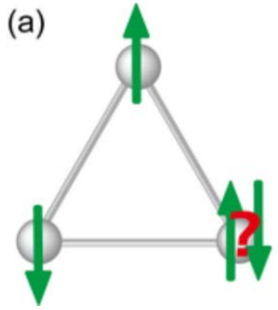
$$H = B(s)\left[\sum_i h_i \sigma_i^z + \sum_{\langle ij \rangle} J_{ij}\sigma_i^z \sigma_j^z\right] + A(s)\sum_i \sigma_i^x$$

Hamiltonian to solve

Each term can be independently tuned

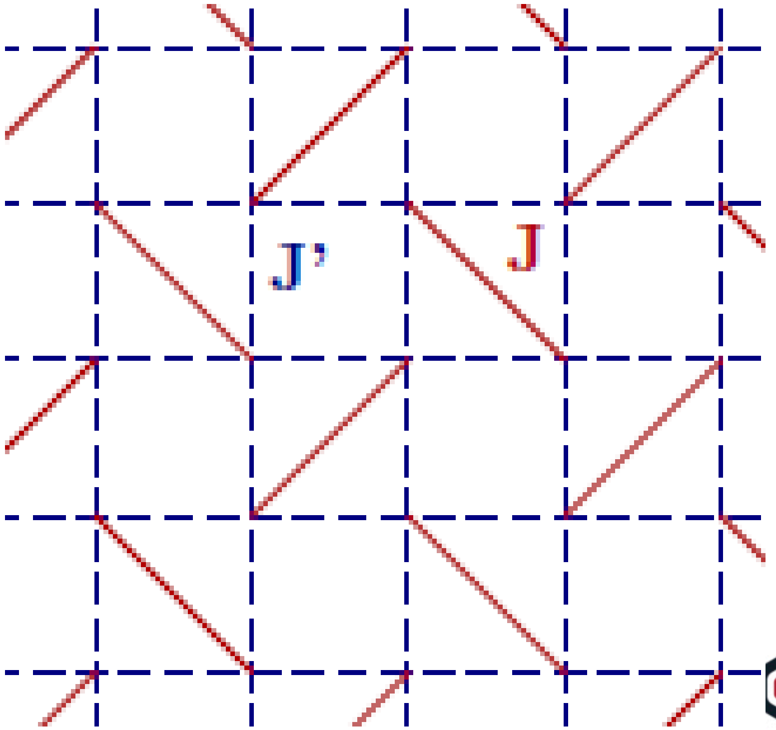
Frustrated Magnets

Competition between spins can give rise to highly degenerate and complex states of matter



Shastry-Sutherland model is an example of such a system

$$H = J \sum_{nn} \vec{S}_i \vec{S}_j + J' \sum_{nnn} \vec{S}_i \vec{S}_j$$

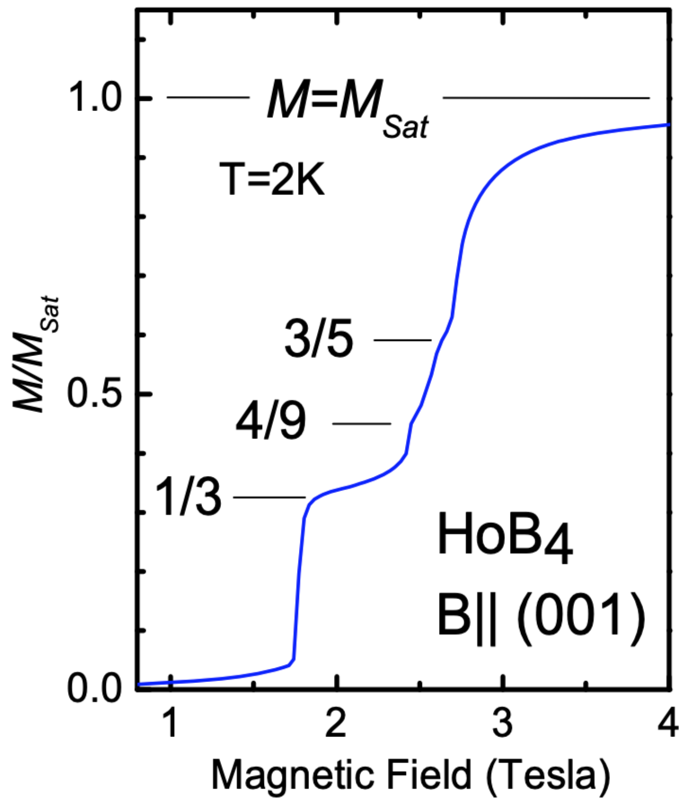


Has physical and material realizations, e.g. rare-earth tetraborides, Yb_2Pt_2Pb

Can be exactly solved.

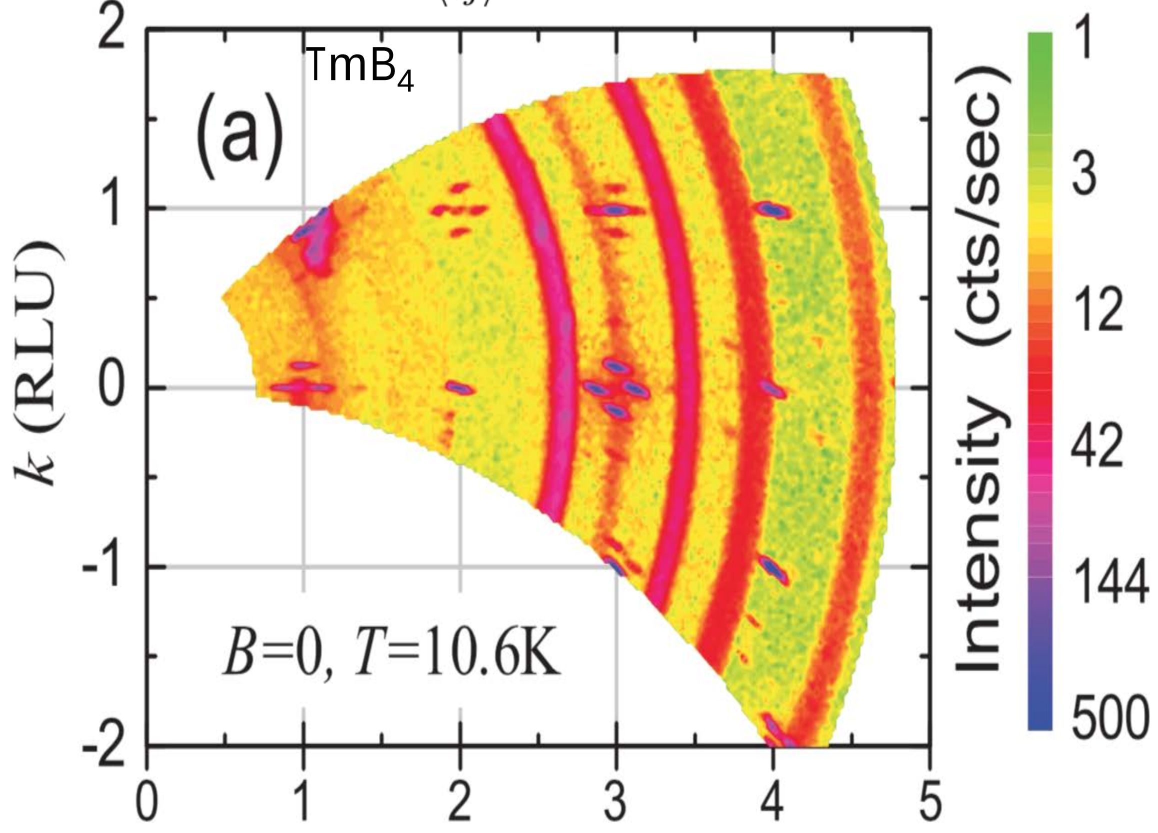
Ising Shastry-Sutherland: RB_4 materials

$$M = \left| \frac{1}{N} \sum_{i}^{N} S_i \right|$$



S Mat'as̆ et al. 2010

$$S(\vec{q}) = \sum_{\langle ij \rangle} \langle \sigma_i^z \sigma_j^z \rangle e^{i\vec{q}\cdot\vec{R}_{ij}}$$

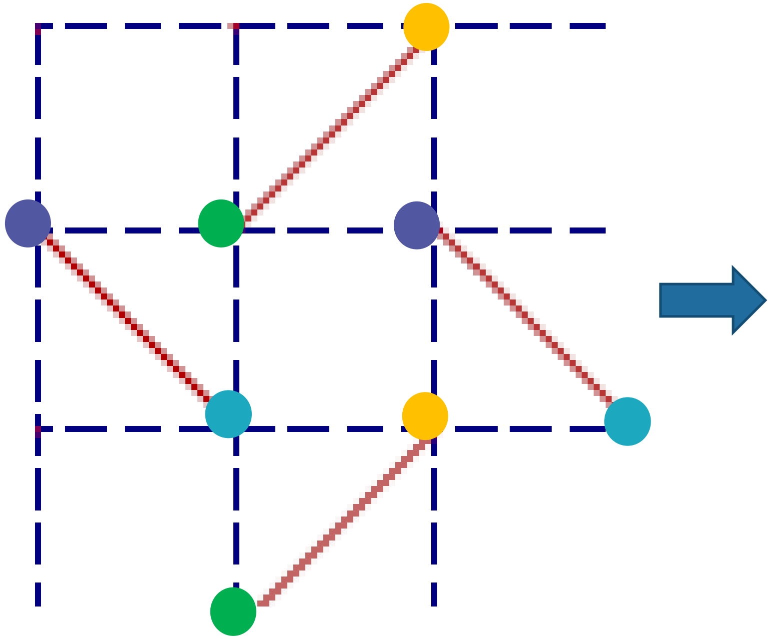


Siemensmeyer et al. 2008

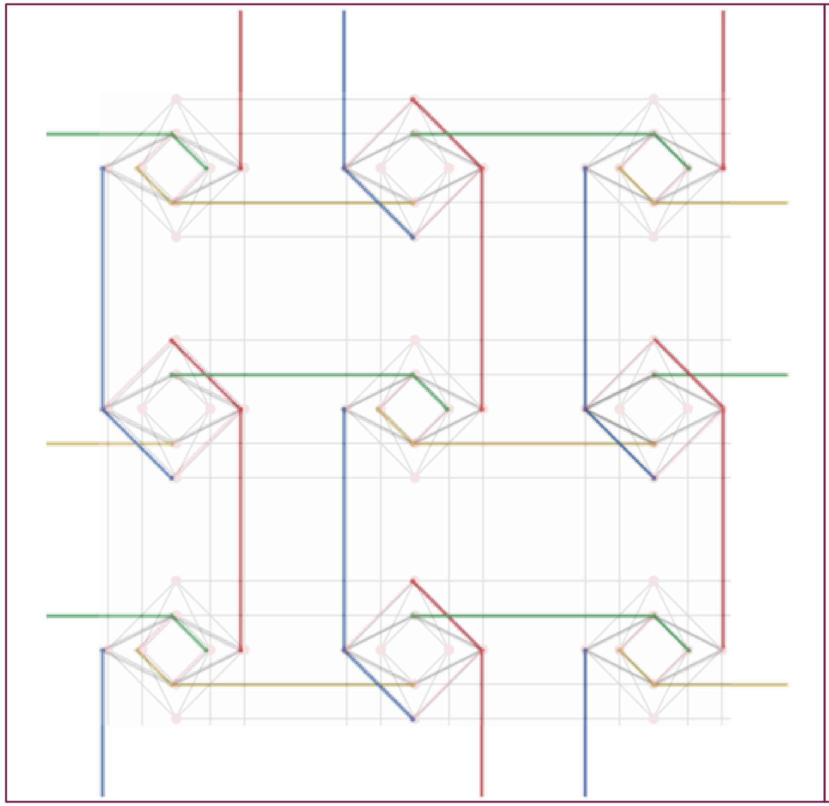
Can we achieve these results from a quantum device (such as an annealer)?

Ways to embed Shastry-Sutherland Lattice:

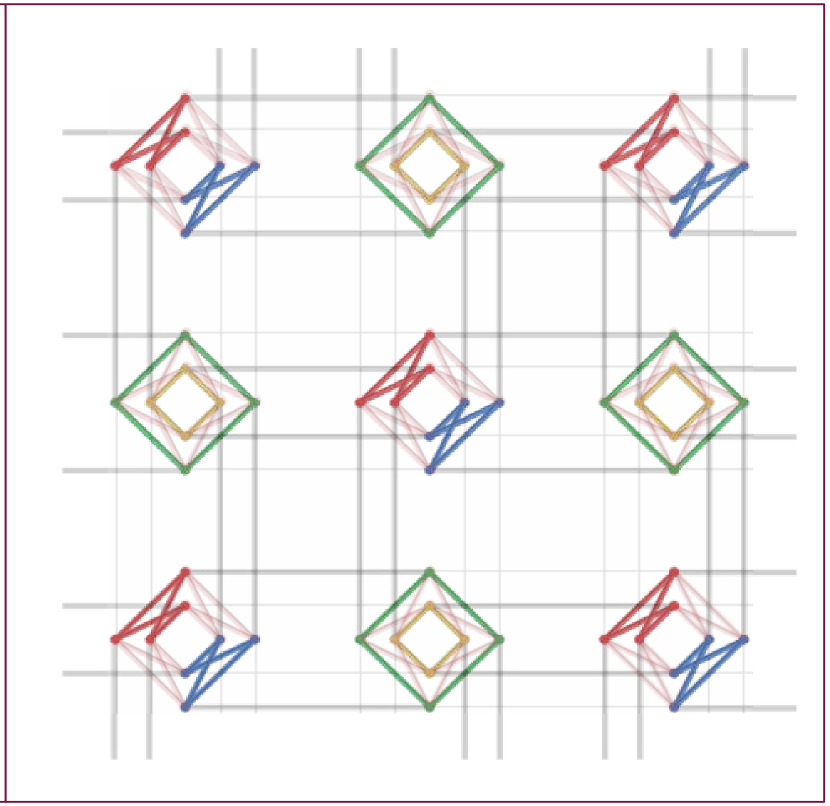
Unit Cell for
Shastry-Sutherland



Tilt Embedding



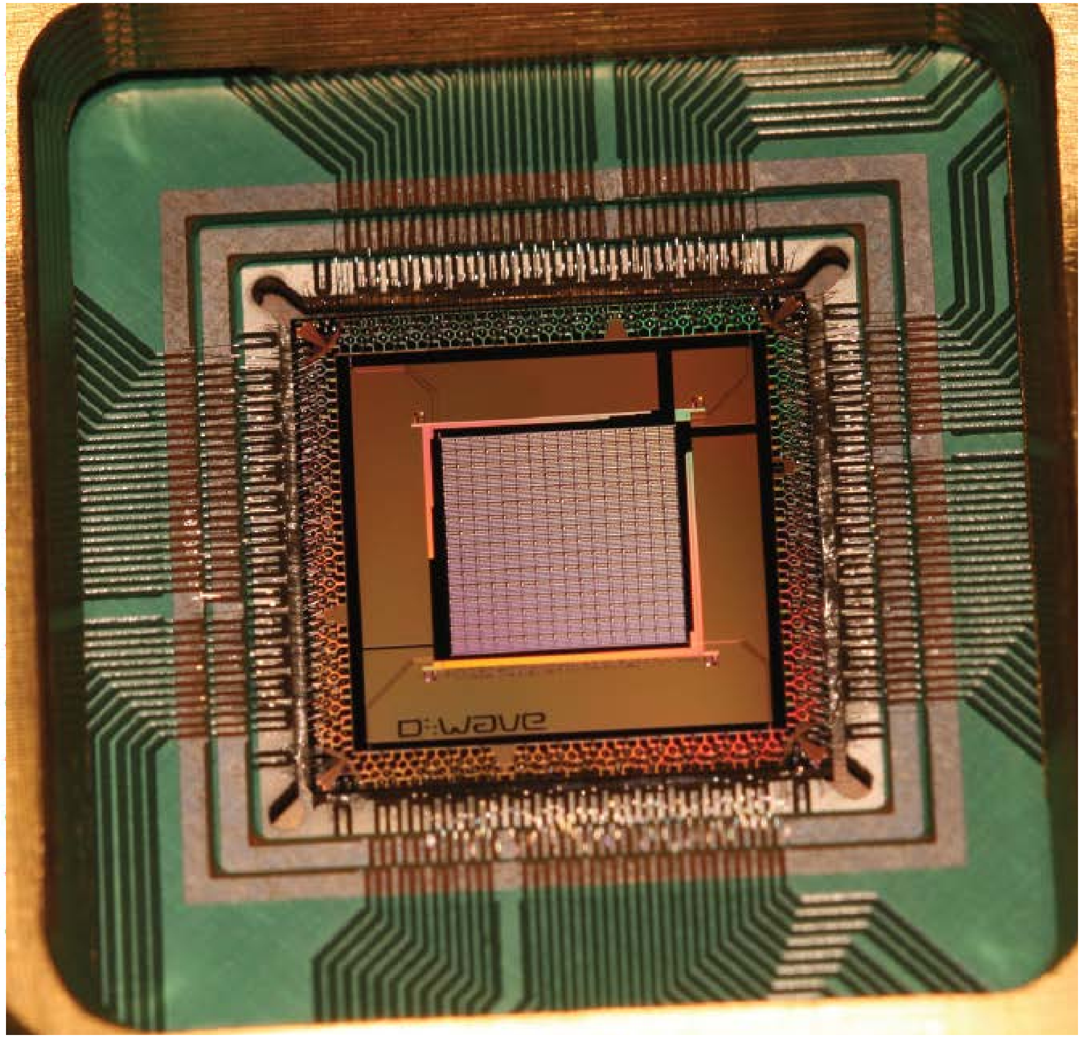
Half-Cell Embedding



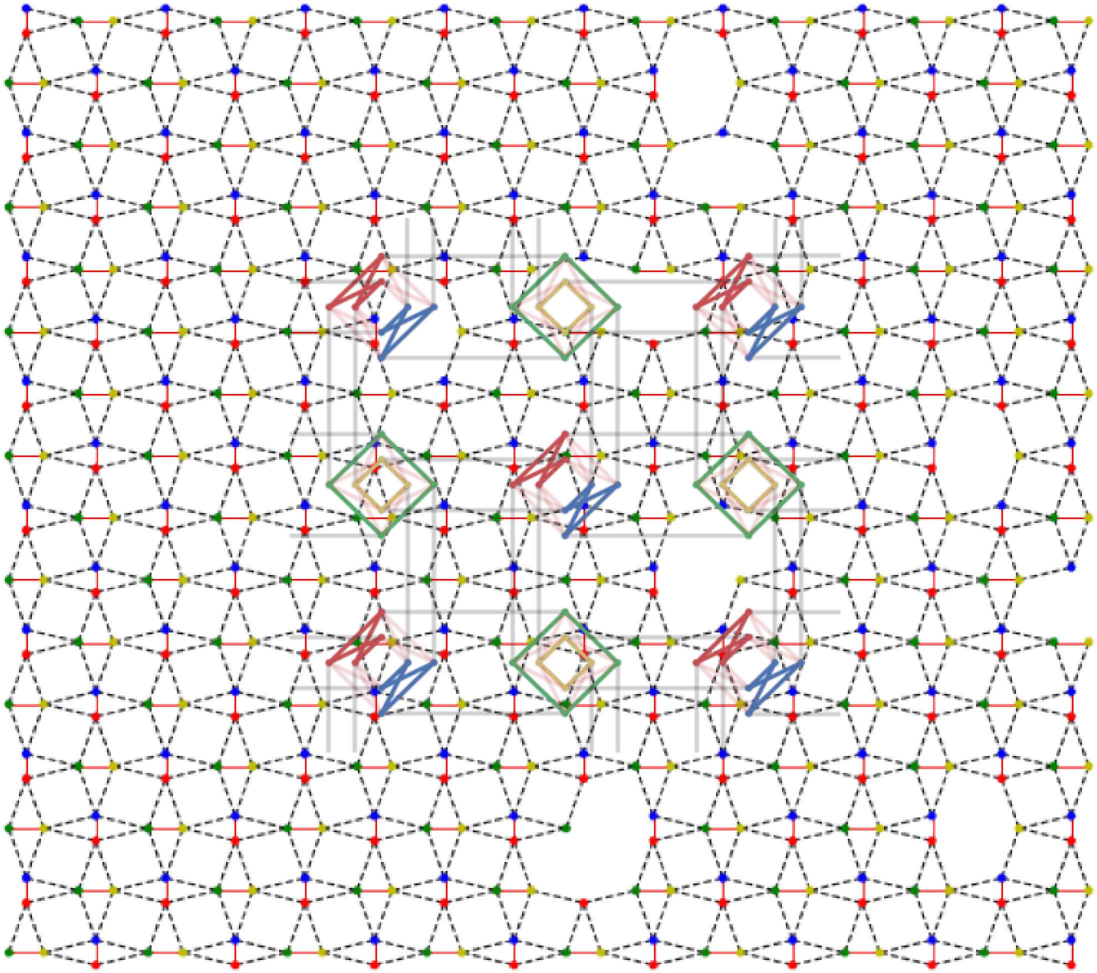
We only pursue the half-cell embedding as more symmetric graph in an imperfect lattice

The defective D Wave Lattice: 2048 qubits → 496 logical spins

D-Wave lattice



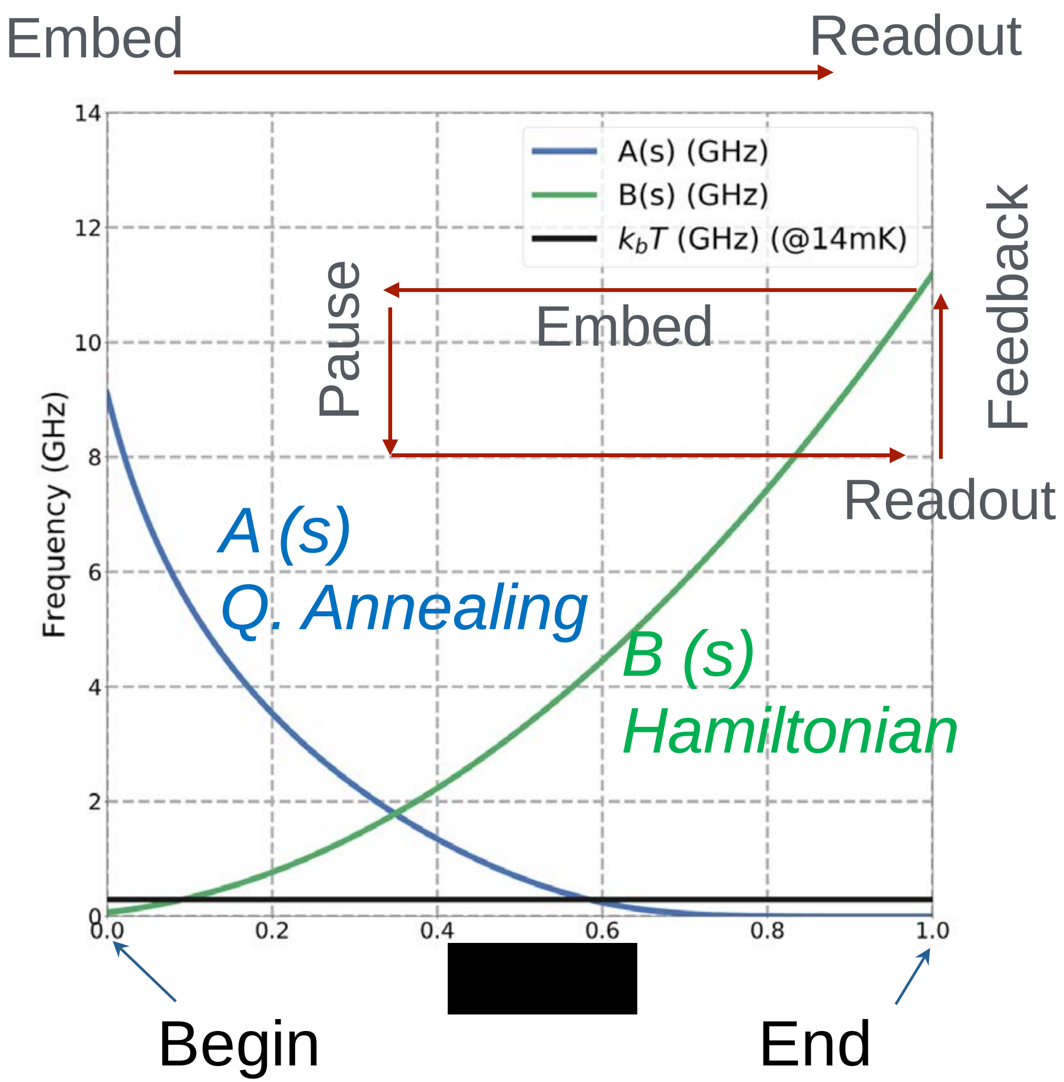
Interesting spin lattice



Has defects!

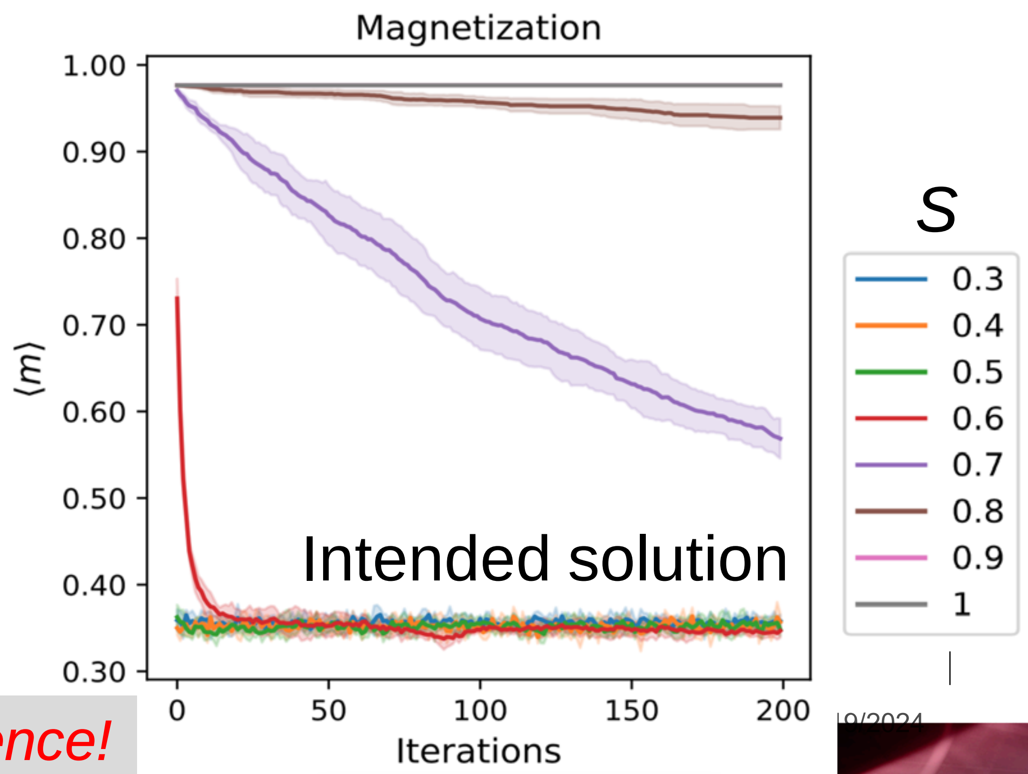
Annealing Routines

$$H = A(s)\sum_i \sigma_i^x + B(s)\left[\sum_i h_i\sigma_i^z + \sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z\right]$$



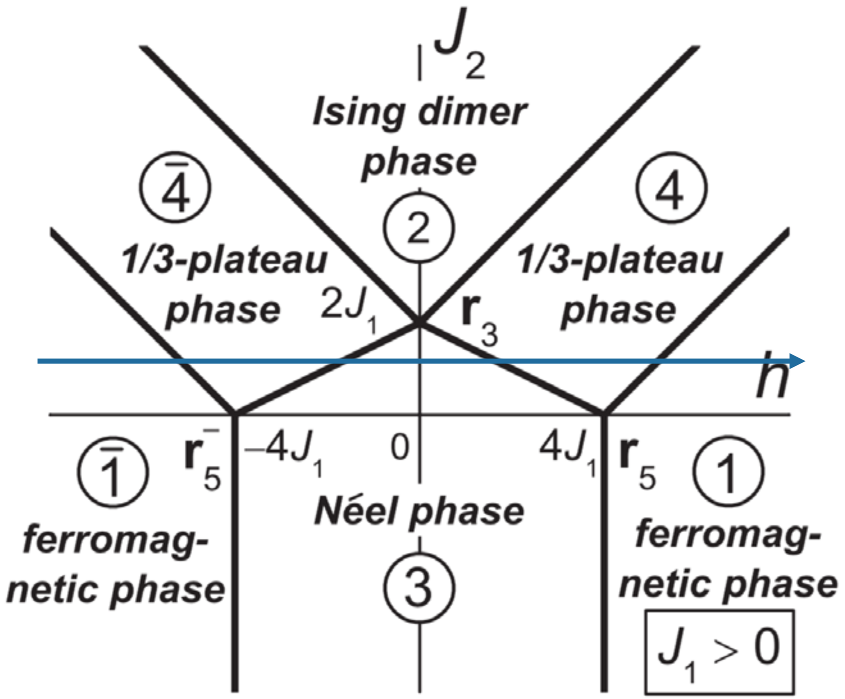
$A(s) >> B(s)$ $A(s) << B(s)$

- Forward annealing
- Reverse annealing
- Markov Chain quantum annealing(!)



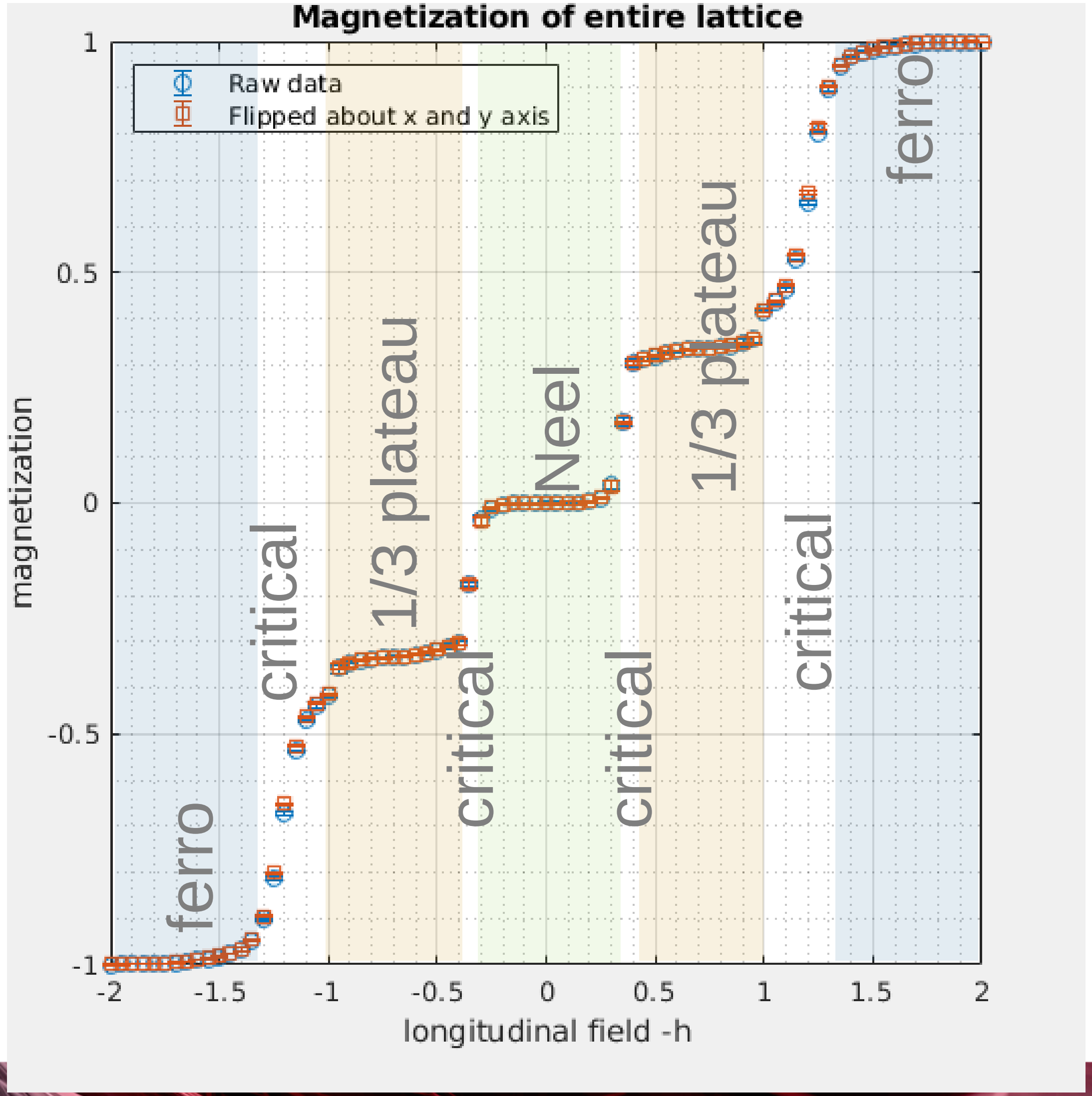
Quick convergence!

Can we see the phase diagram?



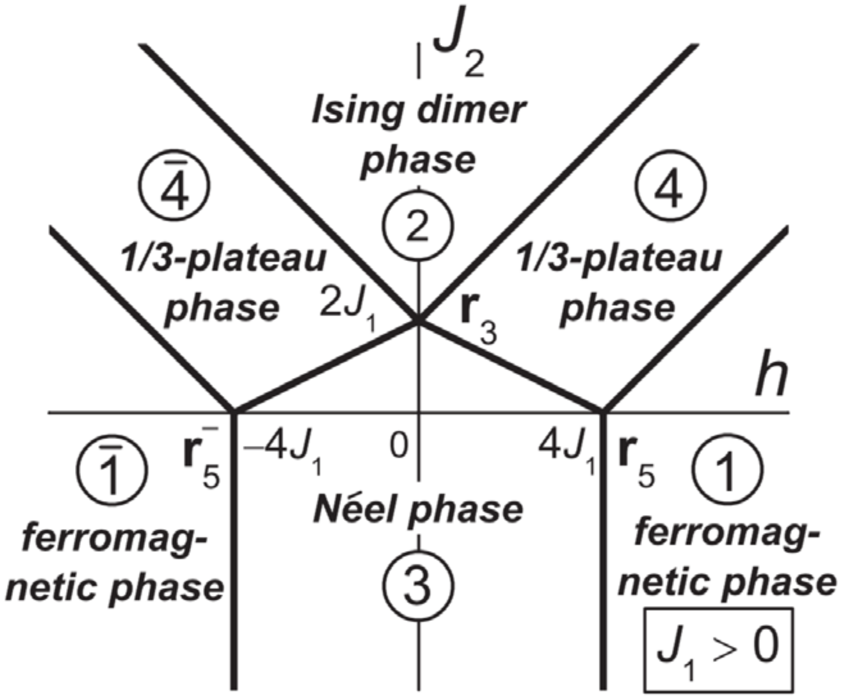
Liu & Sachdev, PRL, 101, 177201 (2008)
Dublenych et al., PRL 109, 167202 (2012)

Result on D-Wave Chip

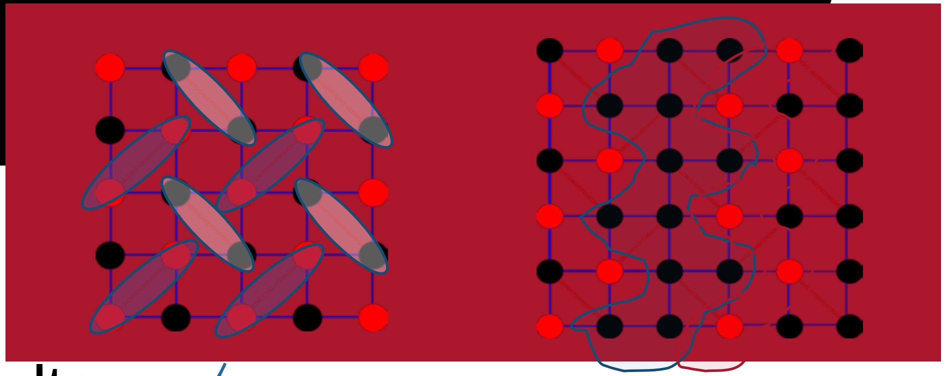


D-Wave results, phase diagram

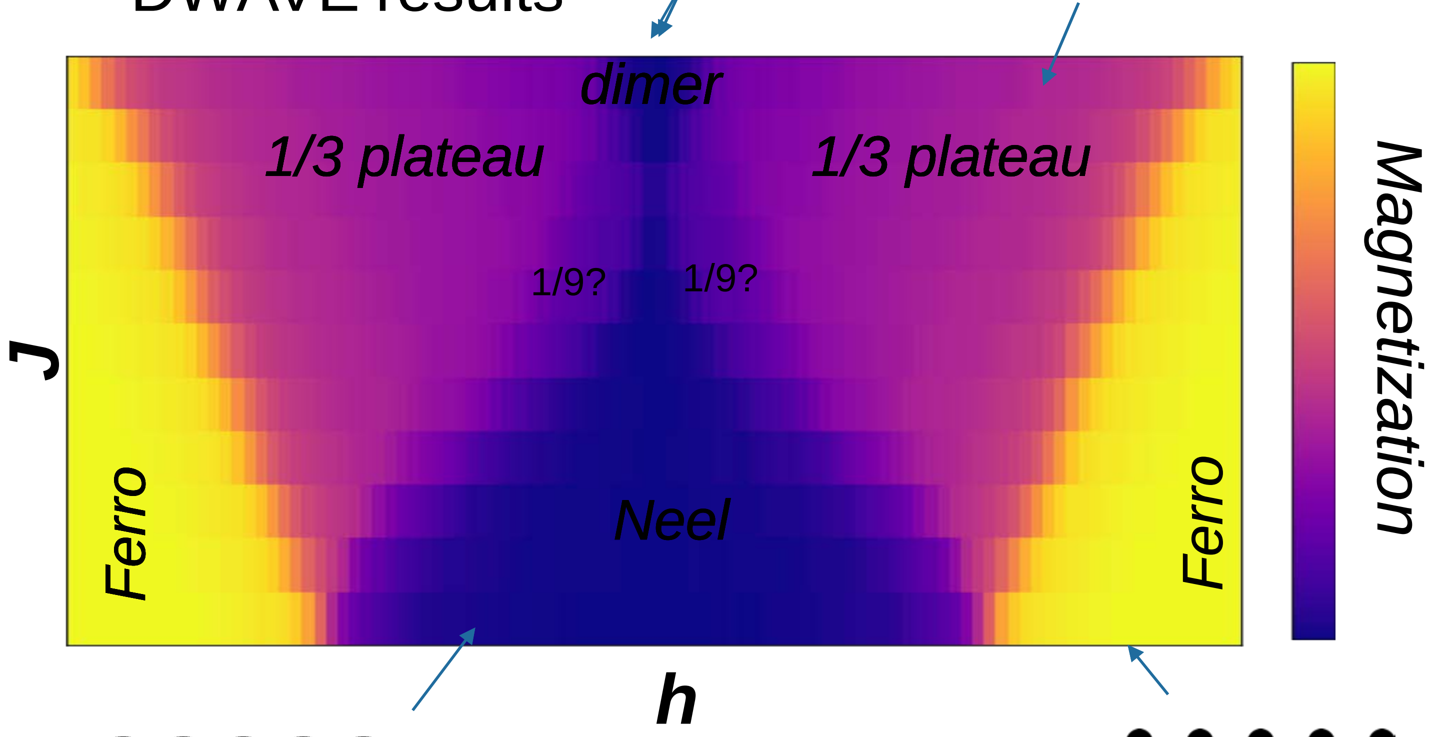
Theory

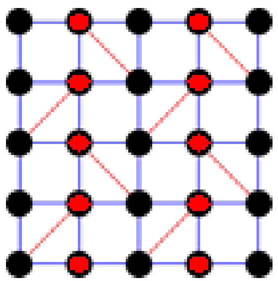


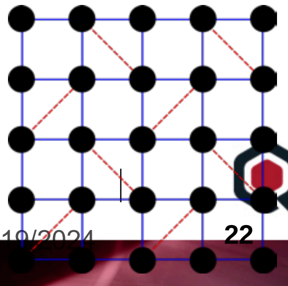
Liu & Sachdev, PRL, 101, 177201 (2008)
Dublenych et al., PRL 109, 167202 (2012)



DWAVE results







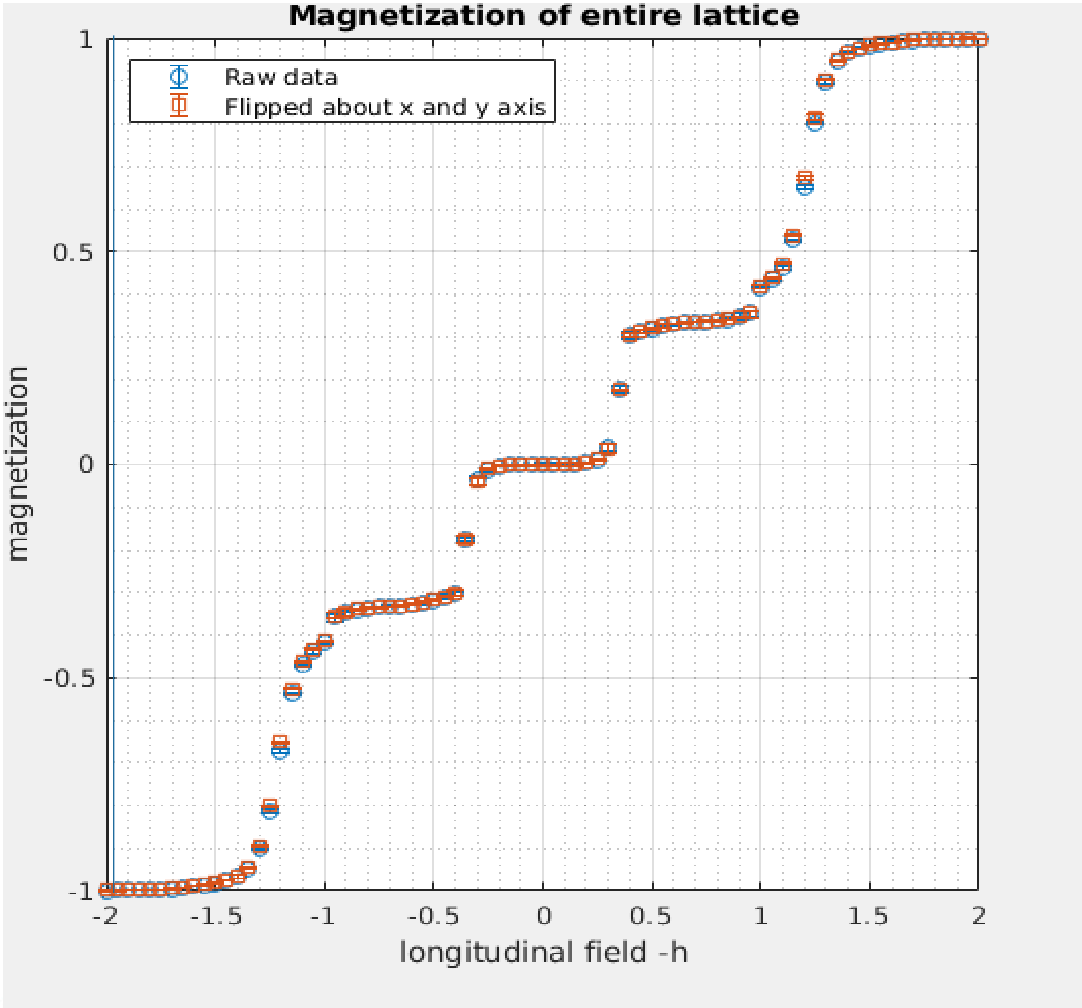
Up Spin

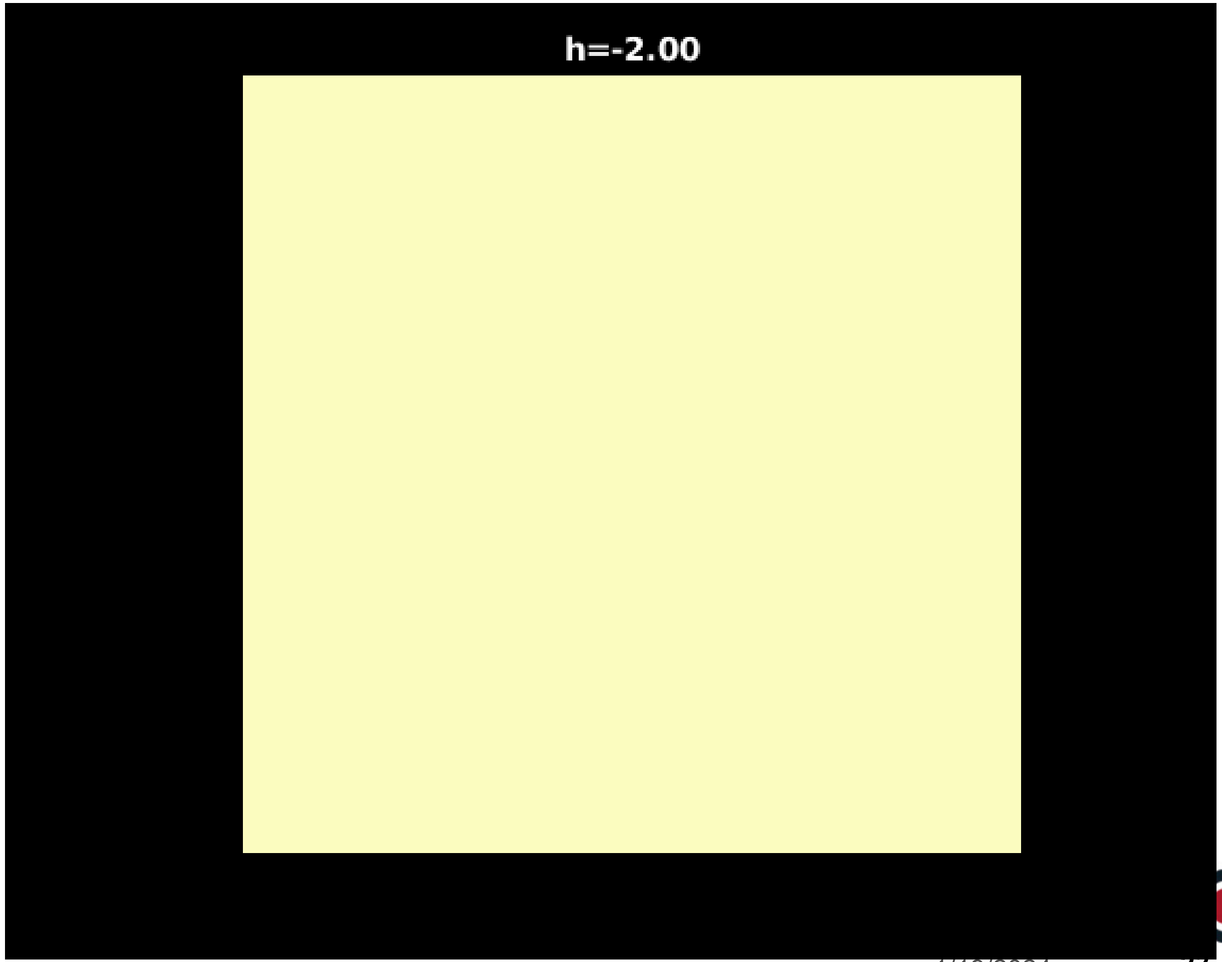
Down Spin

Structure factor

1/3rd Bragg peak

$$S(\vec{q}) = \sum_{\langle ij \rangle} \langle \sigma_i^z \sigma_j^z \rangle e^{i\vec{q}\cdot\vec{R}_{ij}}$$





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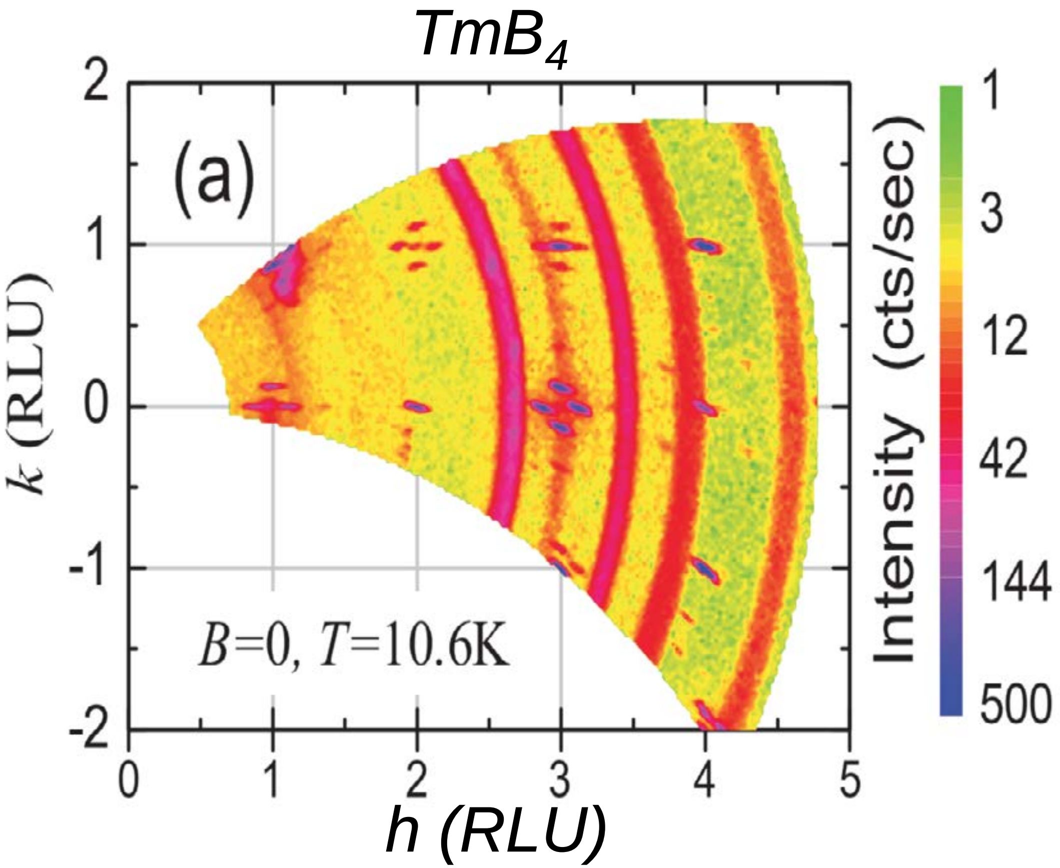
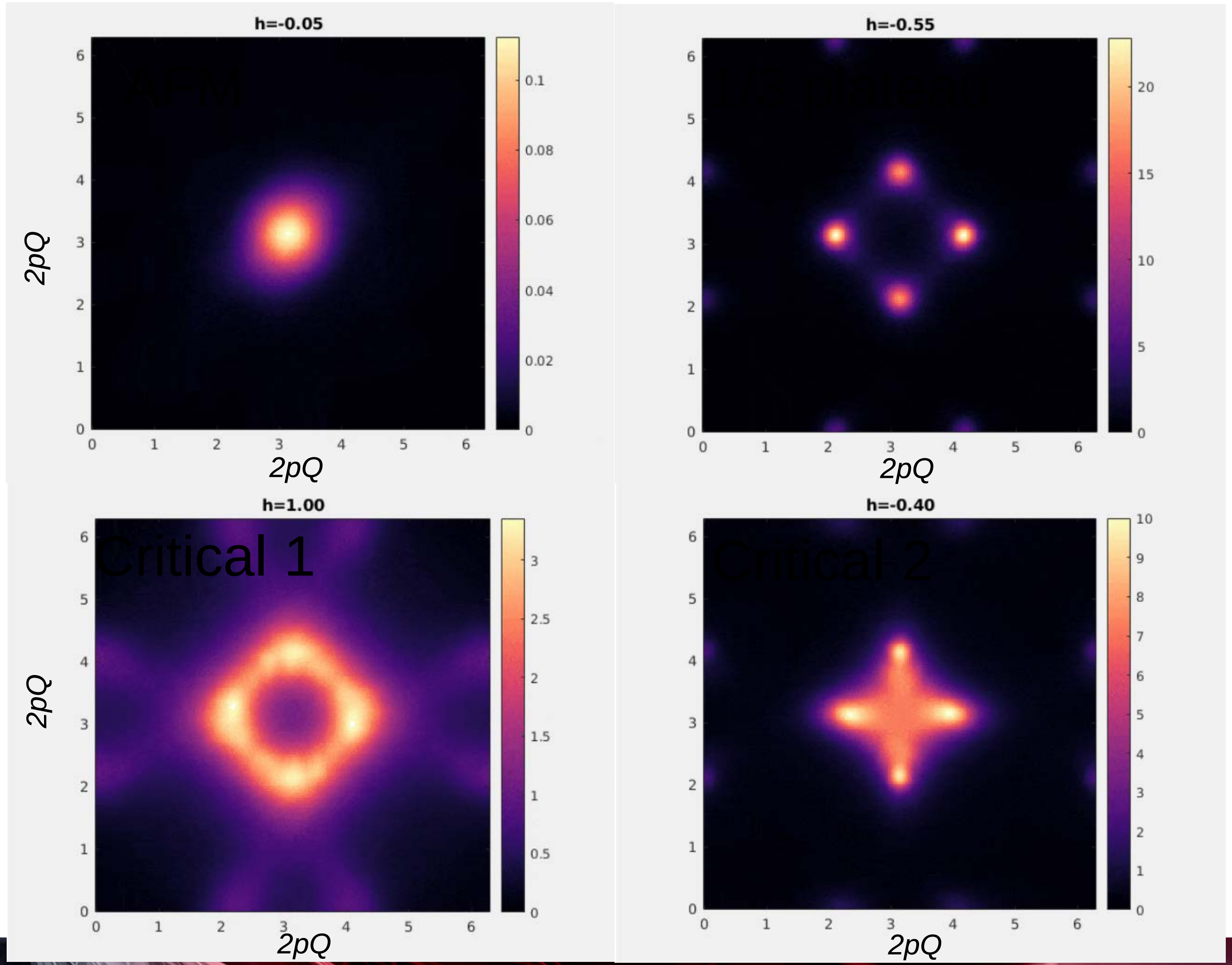
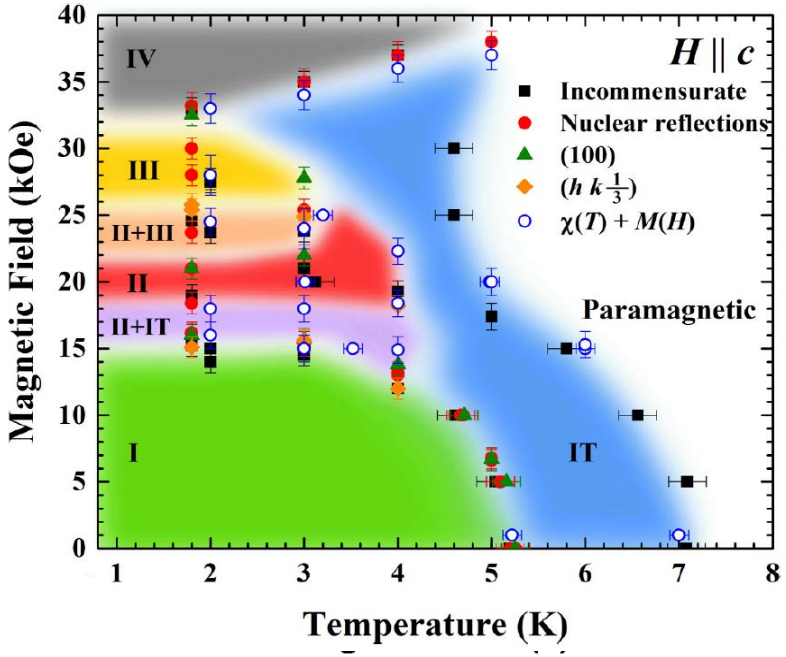
Structure factor

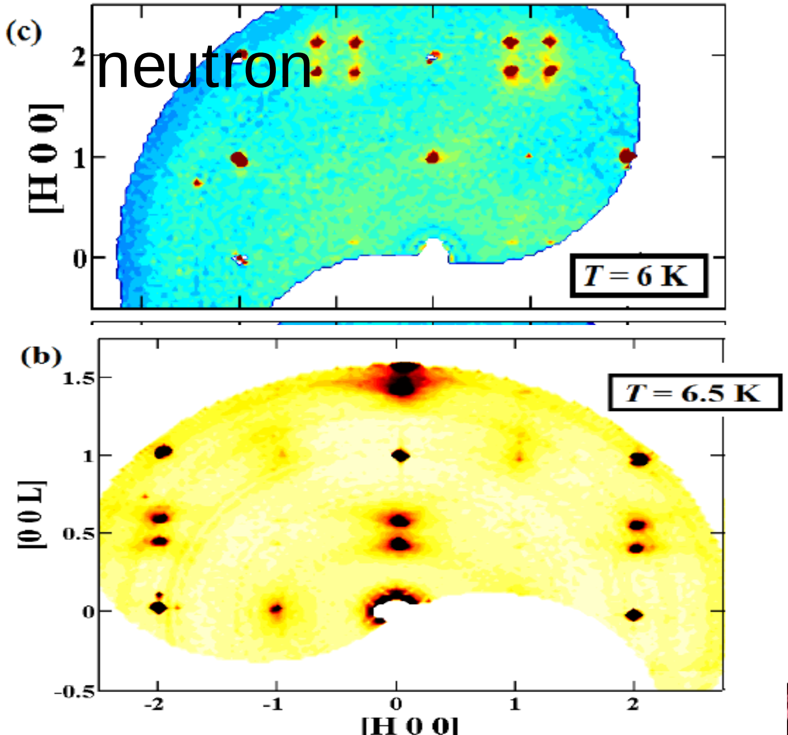
$$S(\vec{q}) = \sum_{\langle ij \rangle} \langle \sigma_i^z \sigma_j^z \rangle e^{i\vec{q}\cdot\vec{R}_{ij}}$$

- The 1/3 Bragg peaks









- What is the Hamiltonian?
  - What is the phase diagram of a material

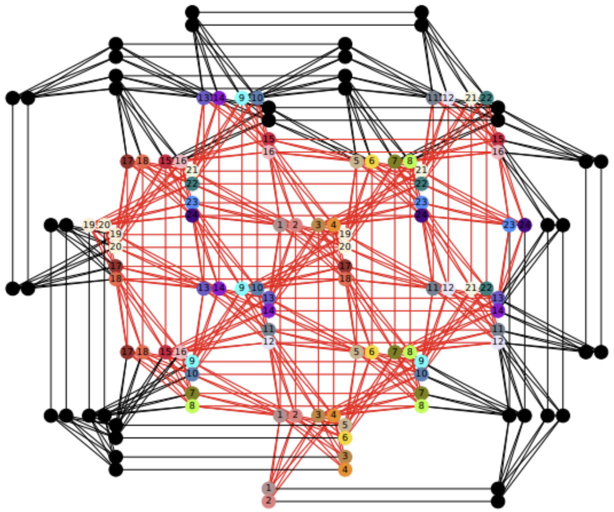
- How do we understand criticality?
  - Critical phases lend new states of matter
  - Thermal and Quantum fluctuations?

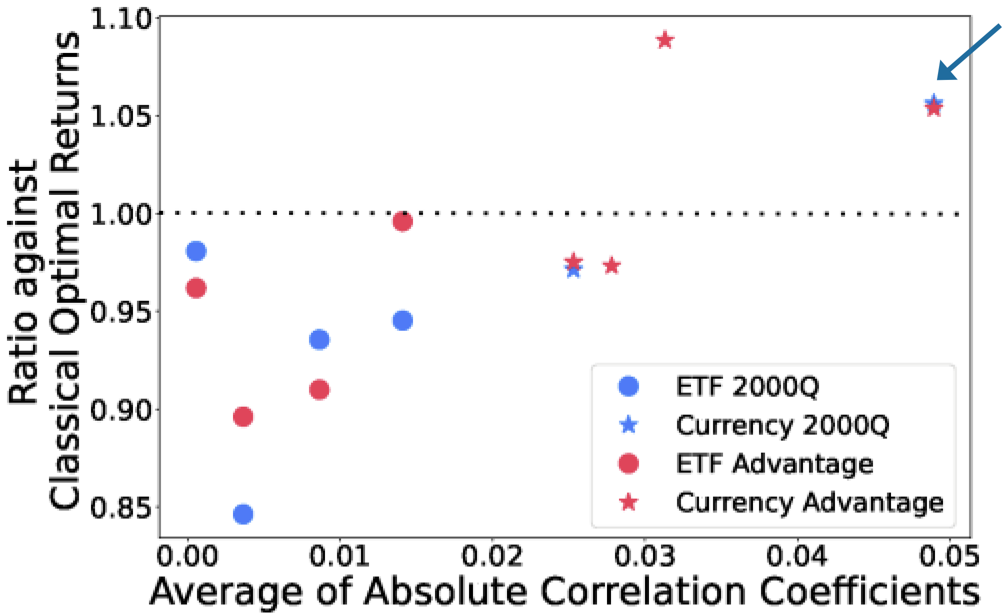
- What is the role of defects in the material?
  - Size of defects,
  - Type of defects (point, domains)
  - Density of defects.
  - Does it change the Hamiltonian?

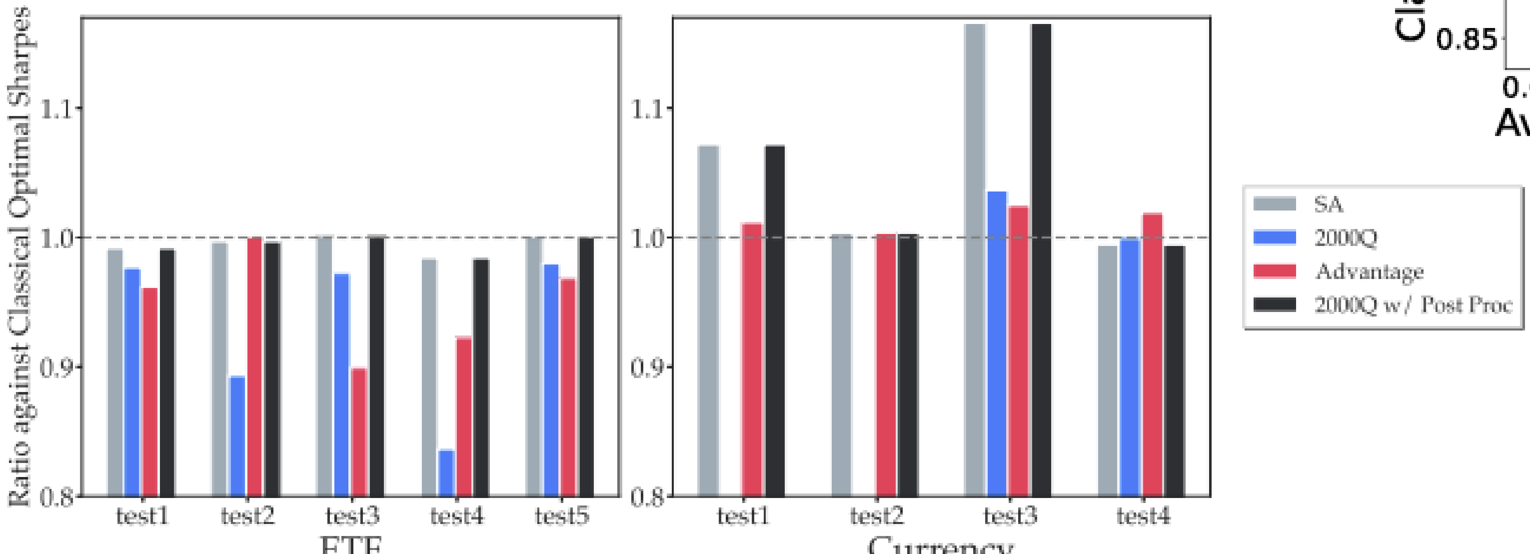
Applications in various fields

An example: Applications in finance

Better solution than classical computers





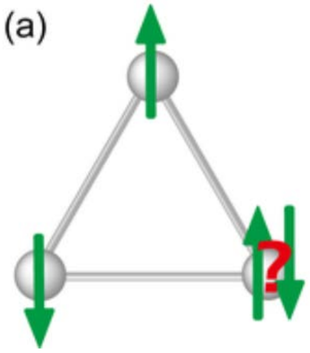


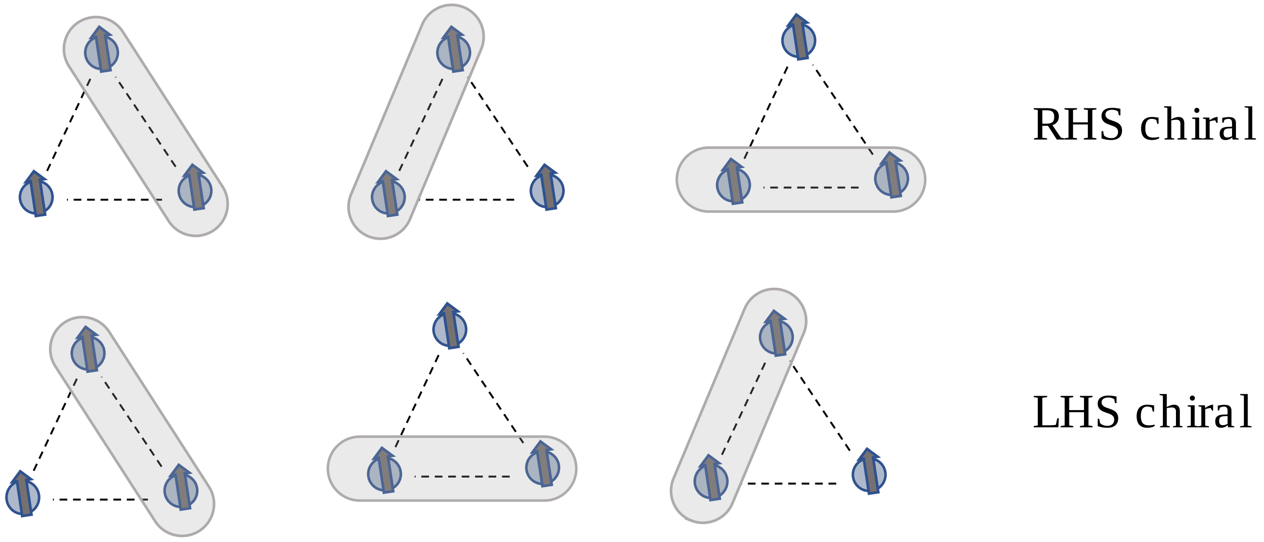
Published in *Entropy*

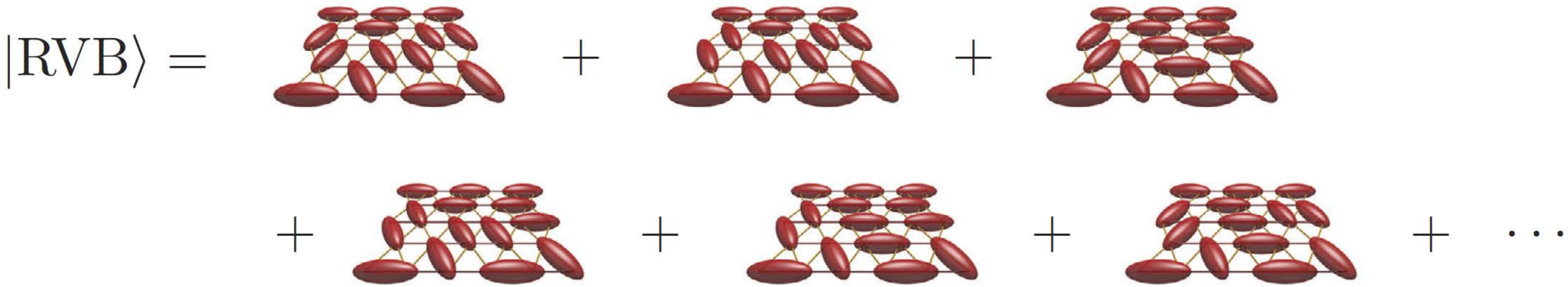
Hamiltonian design and dynamics using universal quantum computers

Frustration and Chirality

Chirality

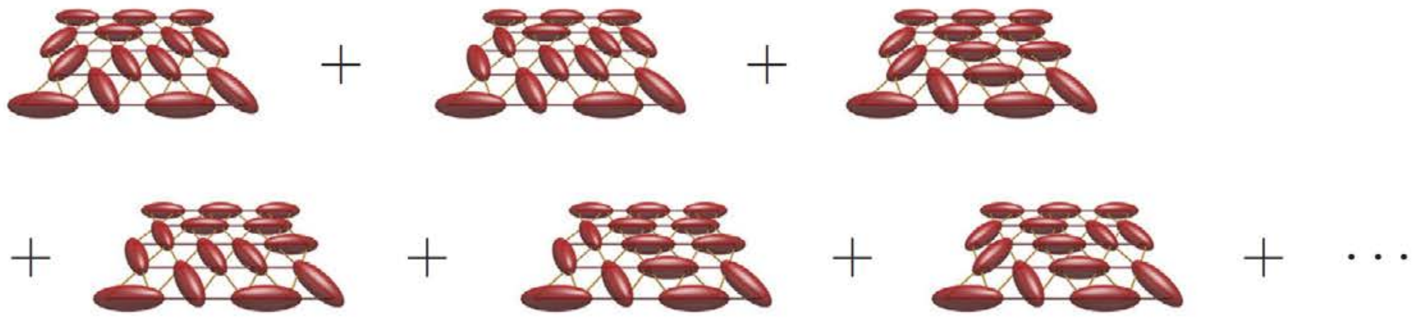




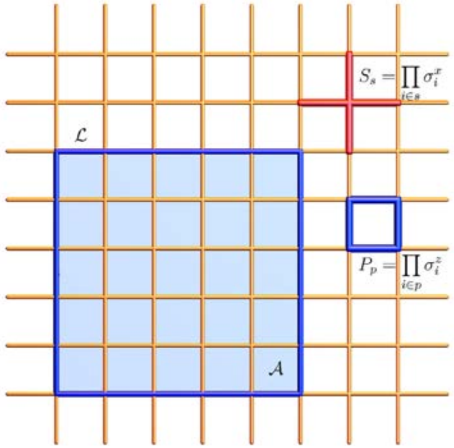


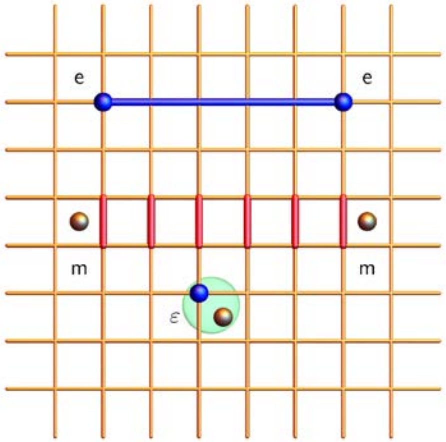
New quantum physics can emerge from geometric frustration

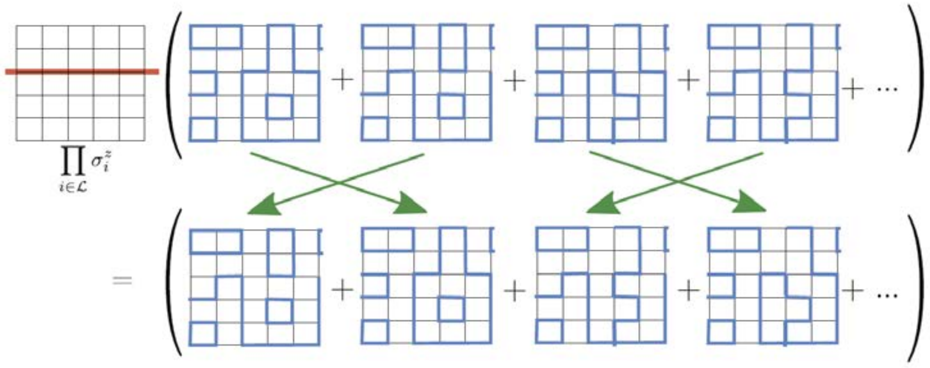
The RVB Liquid

$|\mathrm{RVB}\rangle =$ 

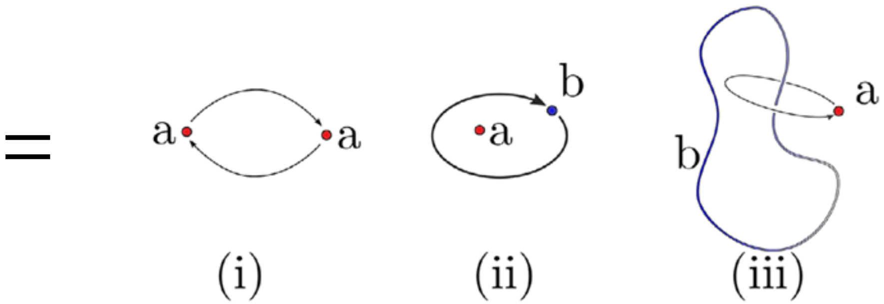
Breeding ground for emergent quasiparticles, scaling laws, physical properties







Loops and braiding

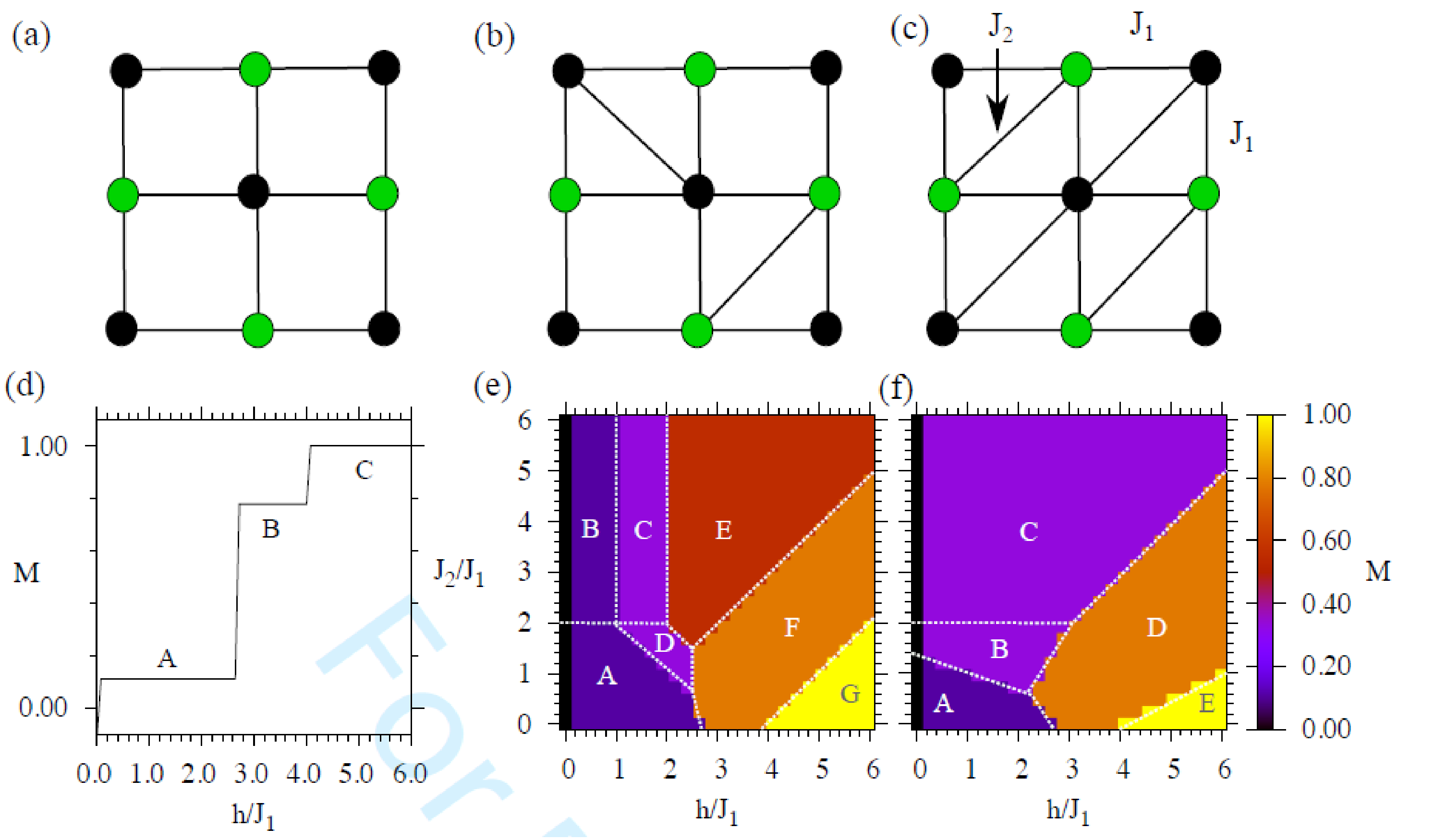


Ground State - Quantum Approximate Optimization

Simulations of Frustrated Ising Hamiltonians using Quantum Approximate Optimization

Phillip C. Lotshaw[1], Hanjing Xu[2], Bilal Khalid[2,3], Gilles Buchs[1,3], Travis S. Humble[1,3] and Arnab Banerjee[2,3]

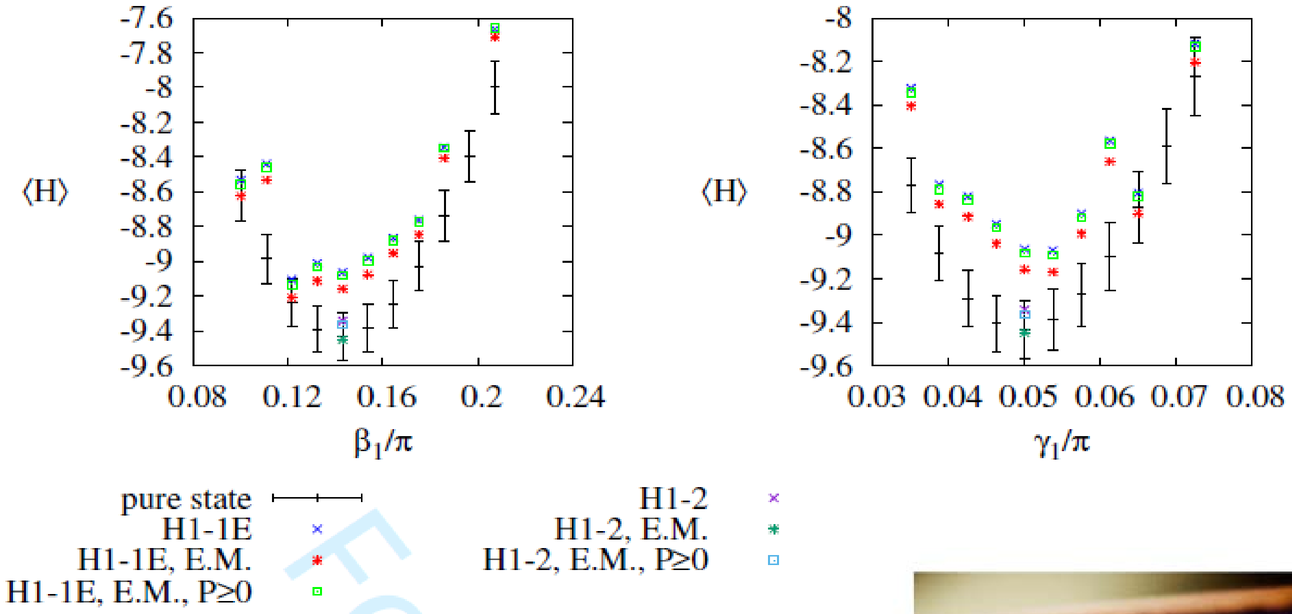
No frustration | SS Lattice | Triangular Lattice



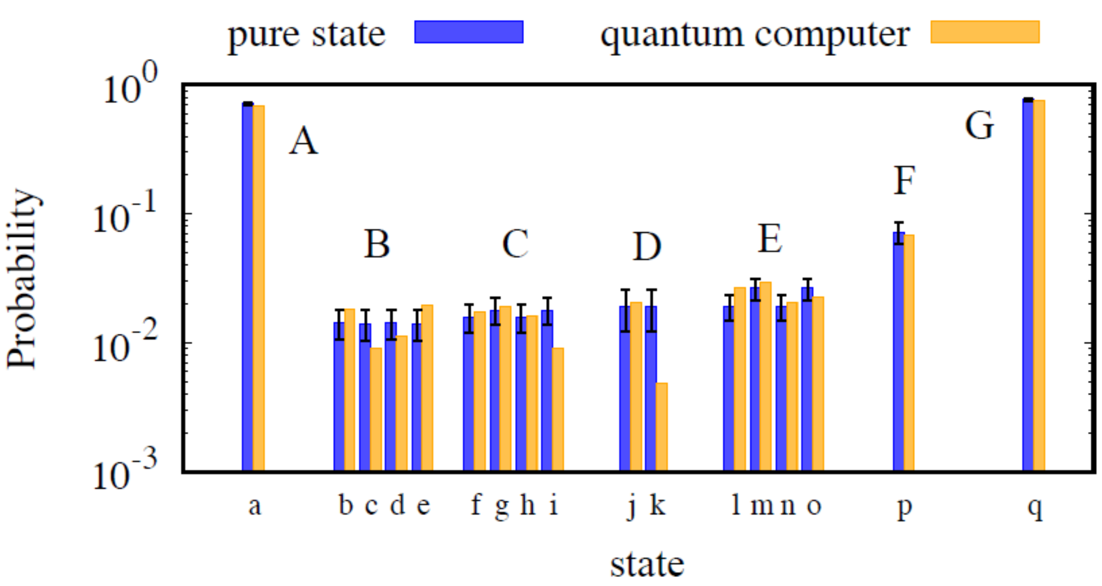
Annealing to the Quantum ground states – a start

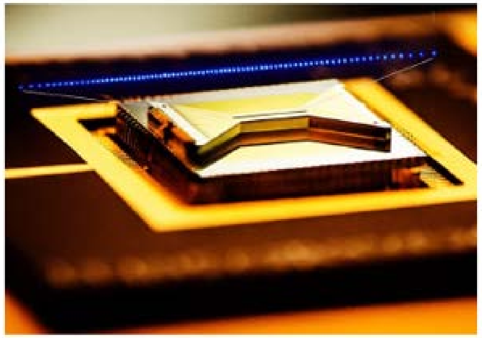
QAOA Frustrated Lattice

$$|\psi_p(\gamma,\beta)\rangle = \left(\prod_{l=1}^{p} e^{-i\beta_l B} e^{-i\gamma_l H}\right)|\psi_0\rangle$$

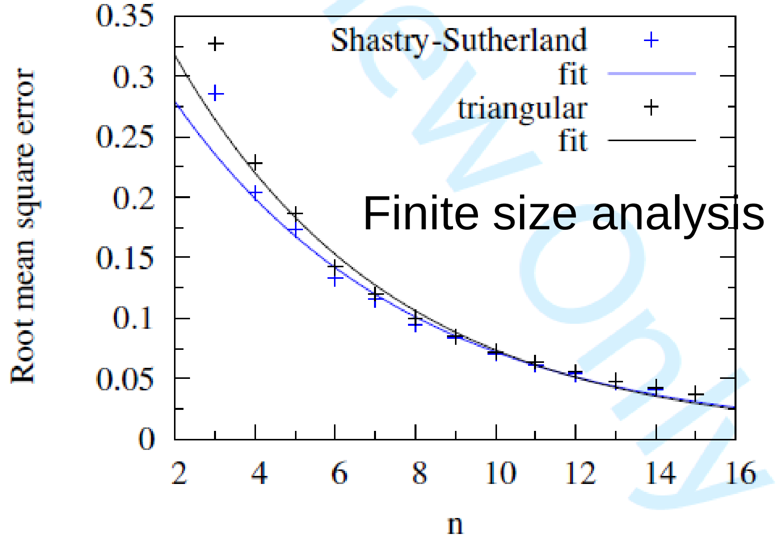


(a)





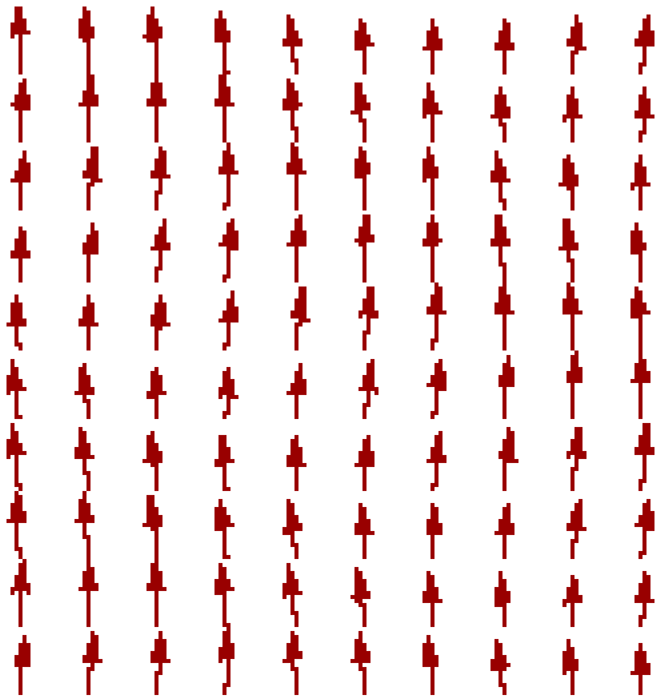
(c) Trapped ions



Finite size analysis

Honeywell H1 device

How do we measure spin dynamics in real life?



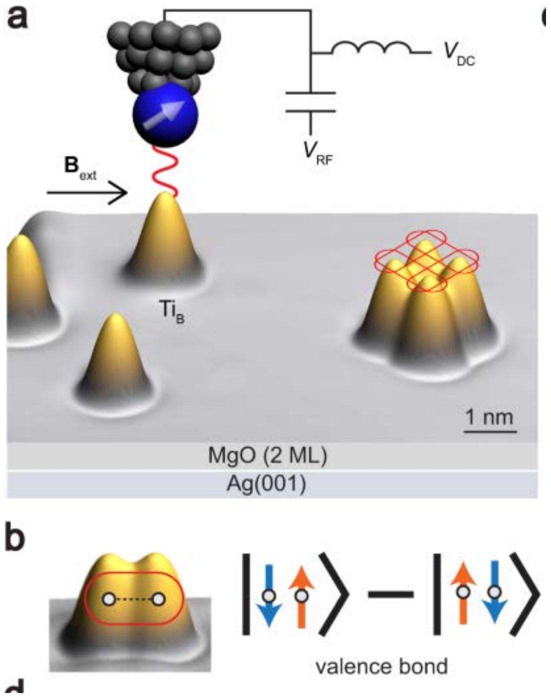
Measure the dynamic spin-spin correlation $\langle S^{\alpha}(r,t) | S^{\beta}(r',t') \rangle$

Fourier transform of dynamic 2-spin correlation is measured by:

Neutron scattering, Inelastic X-Ray, Raman Spectroscopy, NMR, THz …

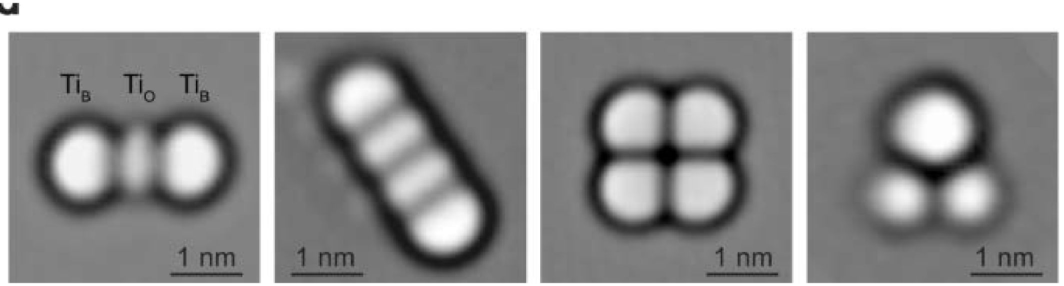
No way to (yet) measure sophisticated quantum observables in real materials:
Multi-spin correlators? Loop operators? Entanglement Entropy?

STM tip moves Ti (S = ½) and entangles them



Move
Ti nano-dots on
MgO/Ag

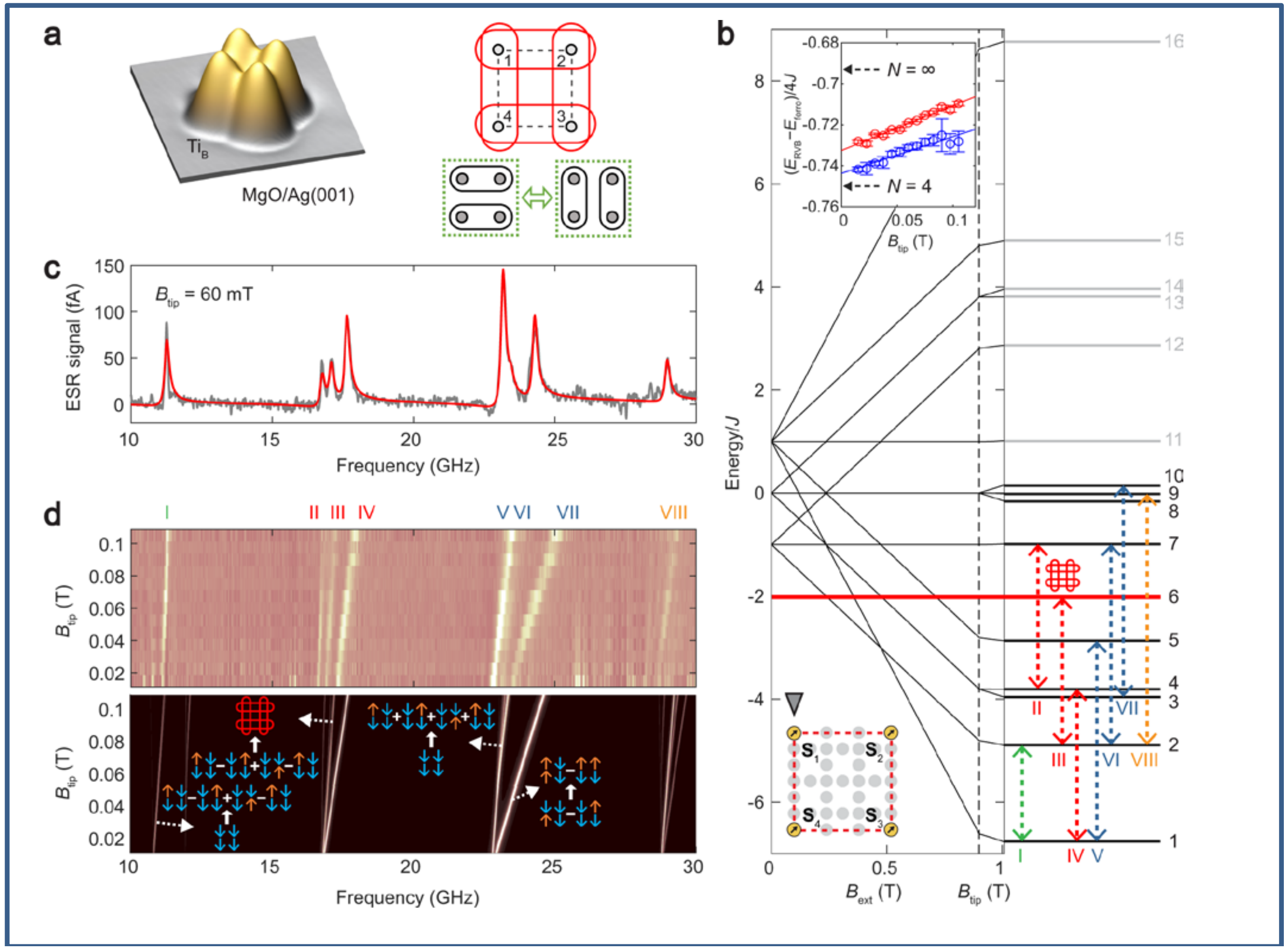
Arbitrarily entangle several spins



ARTICLE

https://doi.org/10.1038/s41467-021-21274-5 OPEN

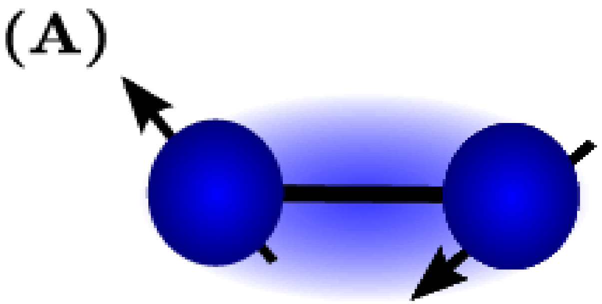
Probing resonating valence bond states in artificial quantum magnets

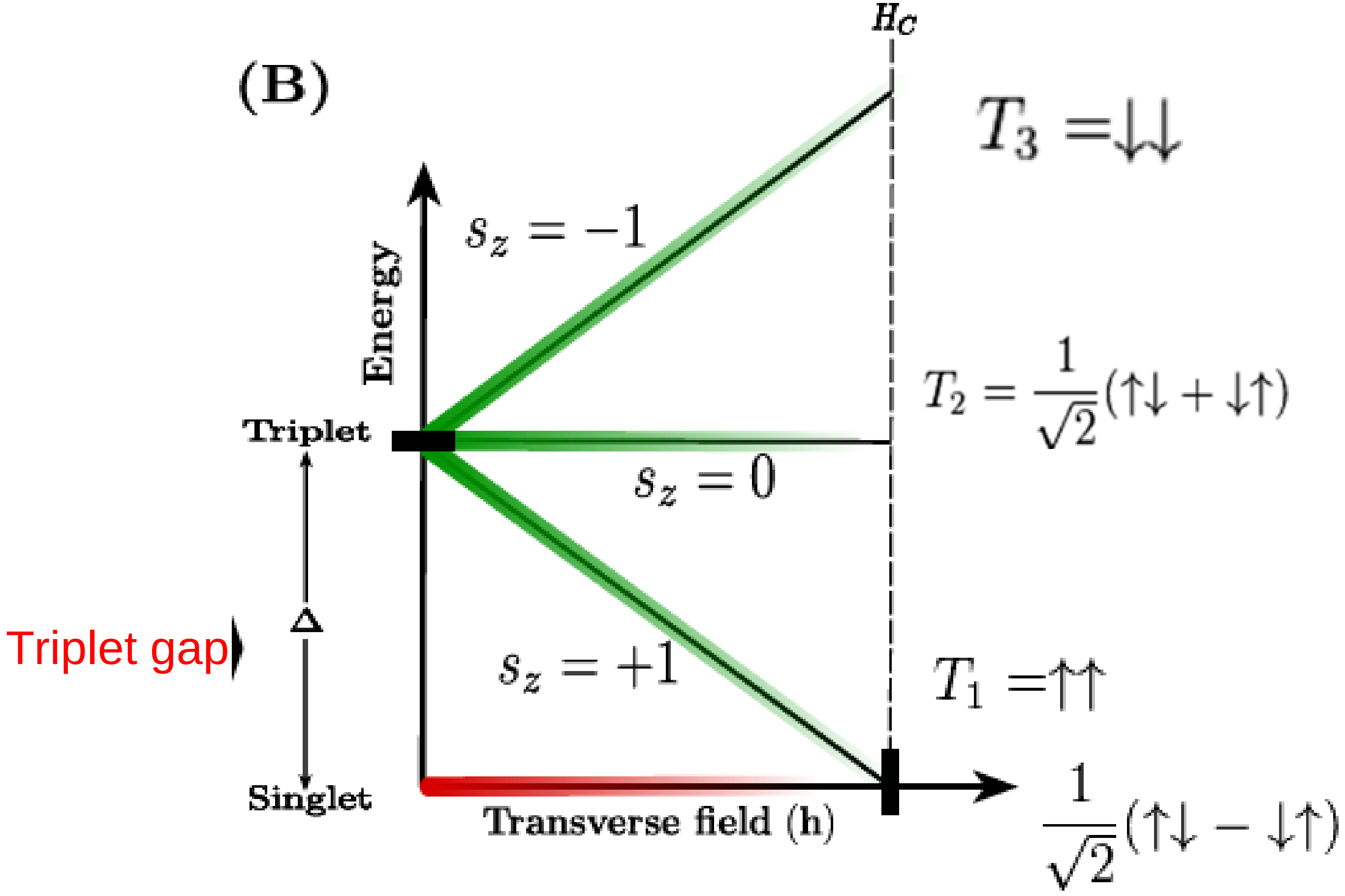


Realize dimers and a quantum spin liquid state to achieve lossless information tunneling (superfluidity)

Entangled Valence bond – Dimer states

Smallest unit of entangled spin (qubit) pair



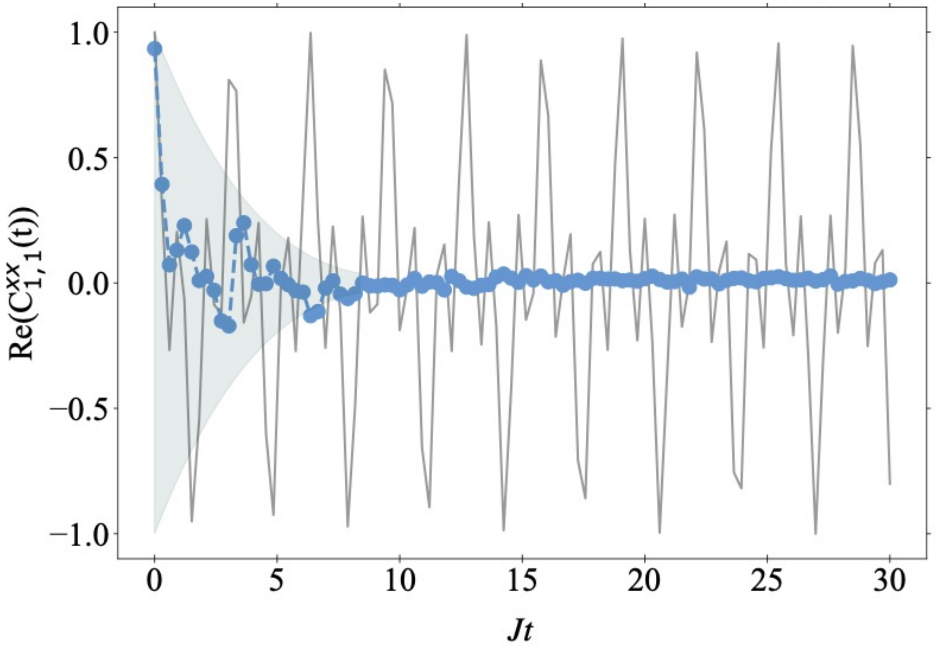


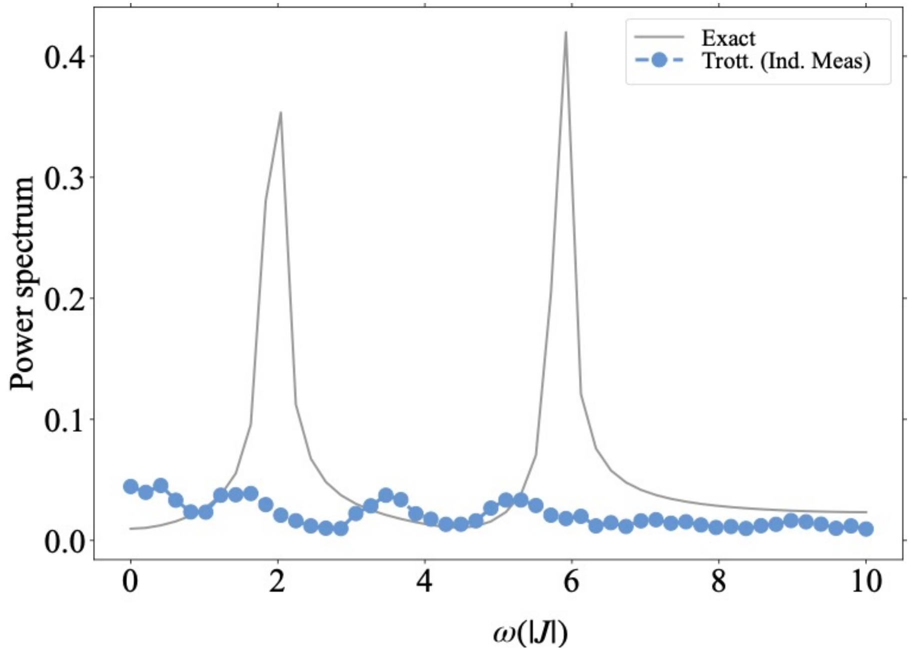
$$H = \sum_{j=1}^{N-1} J_{xx}\sigma_j^x\sigma_{j+1}^x + J_{yy}\sigma_j^y\sigma_{j+1}^y + J_{zz}\sigma_j^z\sigma_{j+1}^z + h\sum_{j=1}^{N}\sigma_j^z$$

Methods of Time Evolution Simulation: Trotterization

$\alpha, \beta = x, y, z$
$i, j =$ index for spin

$$H = \sum_{j=1}^{N-1} J_{xx}\sigma_j^x\sigma_{j+1}^x + J_{yy}\sigma_j^y\sigma_{j+1}^y + J_{zz}\sigma_j^z\sigma_{j+1}^z + h\sum^{N}\sigma_j^z$$





$$C_{ij}^{\alpha\beta}(t) = \langle s_i^\alpha(t) s_j^\beta \rangle_0 = \sum_p \langle 0|s_i^\alpha|p\rangle \langle p|s_j^\beta|0\rangle\, e^{-iE_p t}$$

$$U(t) = e^{-iHN\Delta t} = \left(\prod_{j=1}^{k} e^{-iH_j\Delta t}\right)^N + \mathcal{O}(\Delta t^2)$$

Hopeless on NISQ . Is there a way to avoid this?

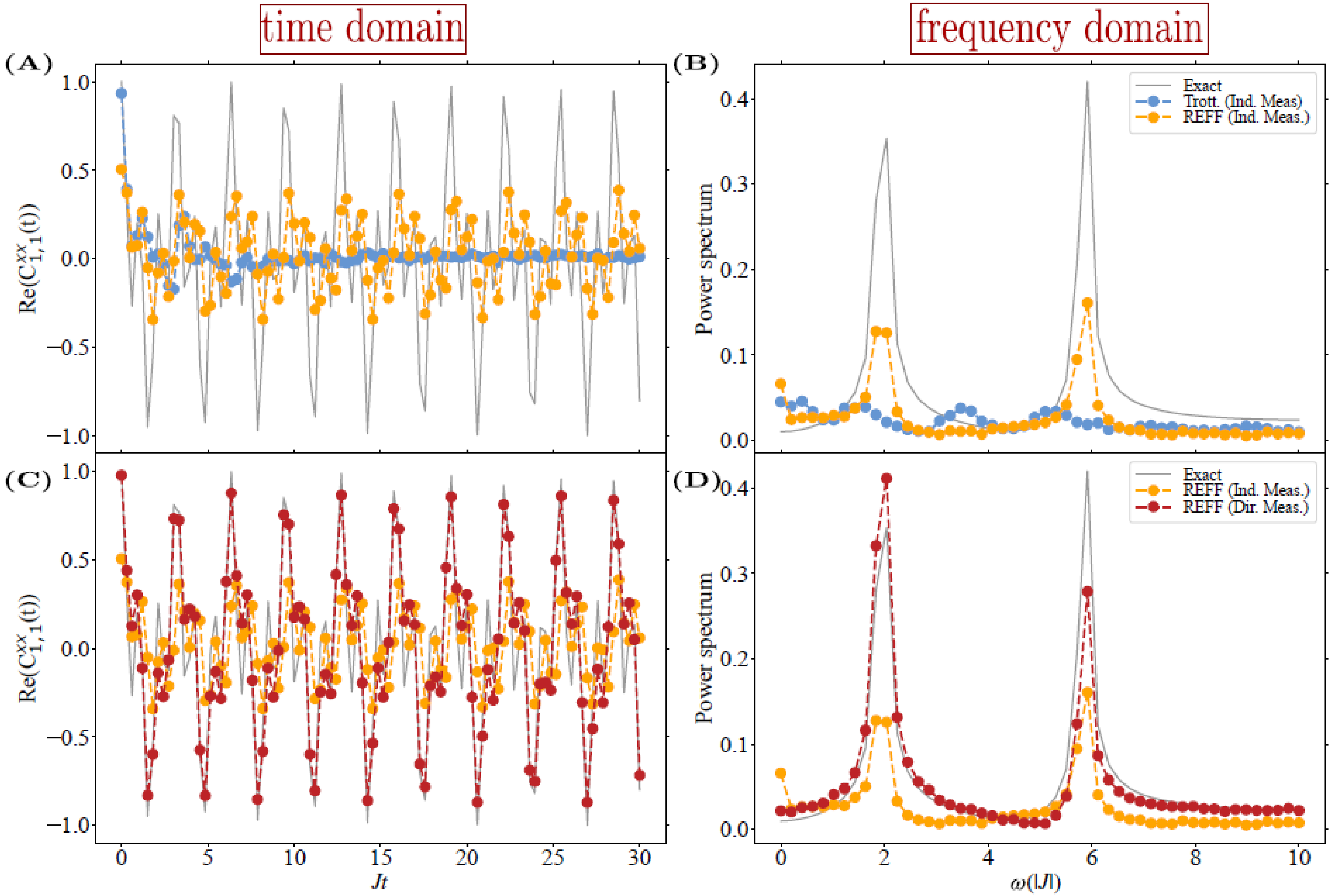
2+2 qubits, Fast Forwarding Algorithm: XY+h Hamiltonian

$$H = J_{xx} \sum s_x s_x + J_{yy} \sum s_y s_y + h \sum s_z$$

Neutron Scattering Cross Section using Circuits
Purdue, LANL, IBM

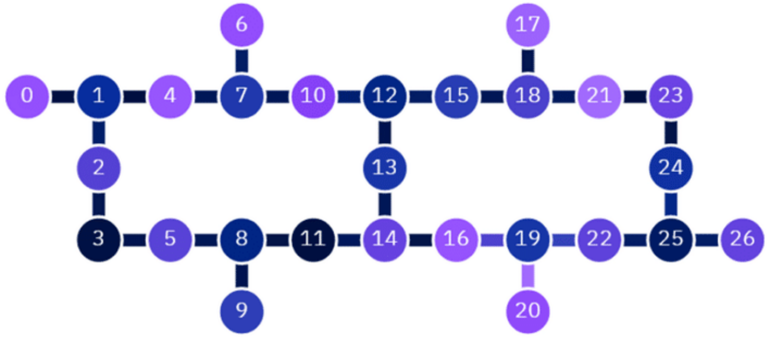
Norhan Eassa (PU, IBM)

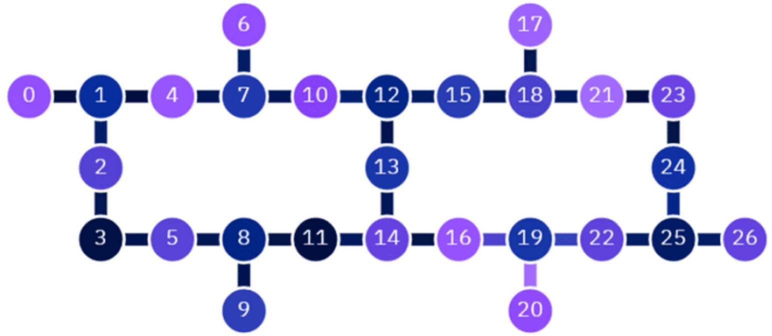
Zoe Holmes (LANL)



- $J = 1, h = 1.$

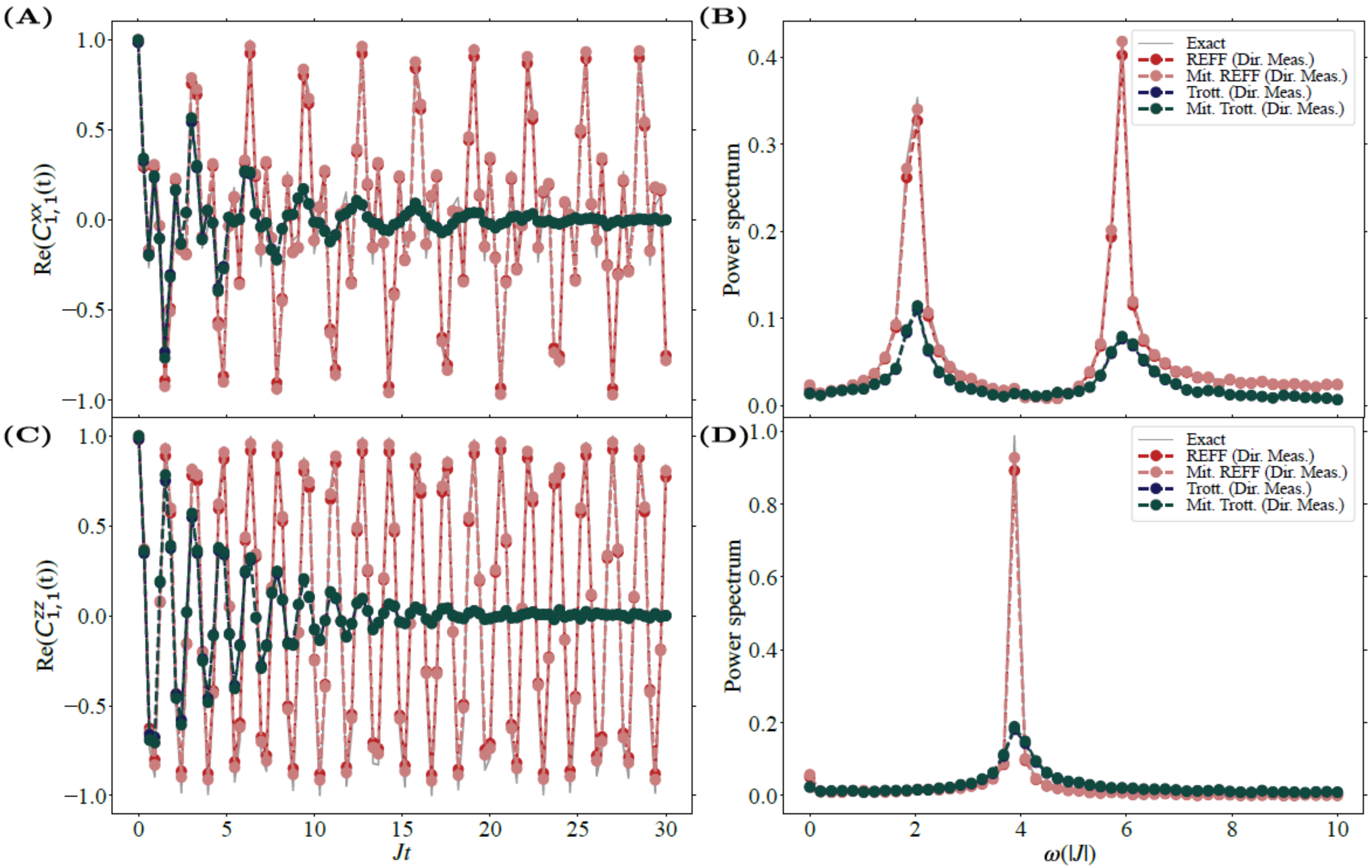
Understanding the crosstalk among several qubit pairs towards scale-up to a VBS state





Correlation function plotted for VFF results for the XY model: The hardware results were obtained using ibmq_kolkata

Results: Final (64 such coefficients)



$$H = \sum_{j=1}^{N-1} J_{xx}\sigma_j^x\sigma_{j+1}^x + J_{yy}\sigma_j^y\sigma_{j+1}^y + J_{zz}\sigma_j^z\sigma_{j+1}^z + h\sum_{j=1}^{N}\sigma_j^z$$

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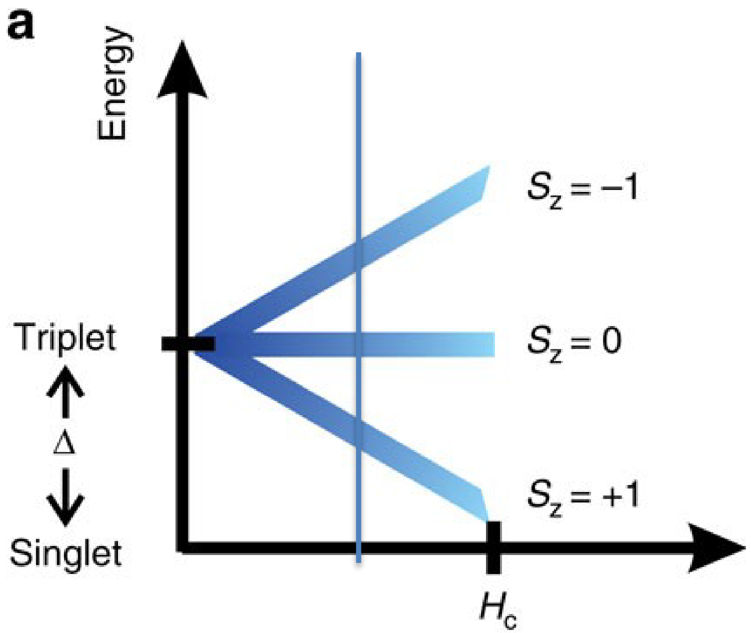
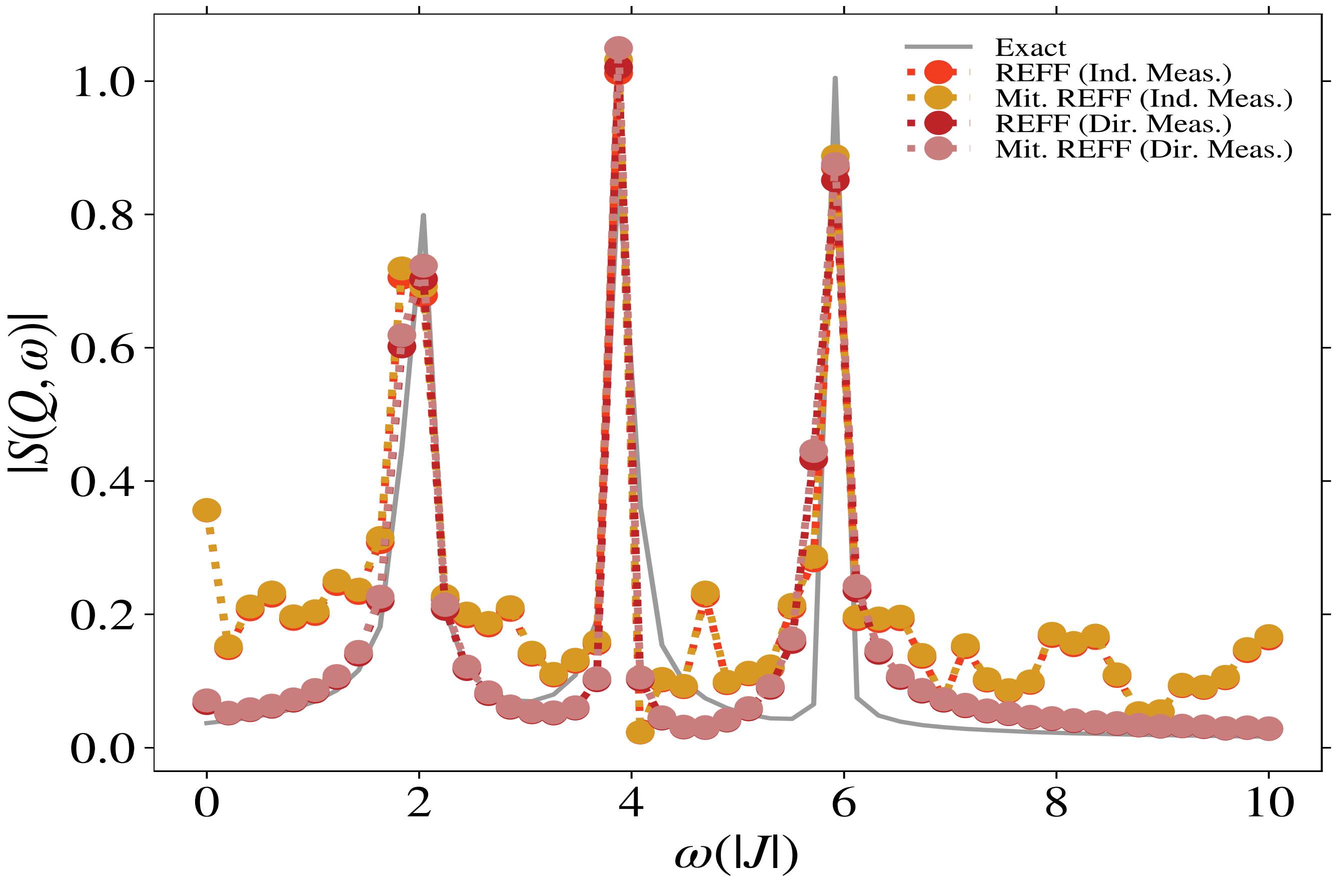
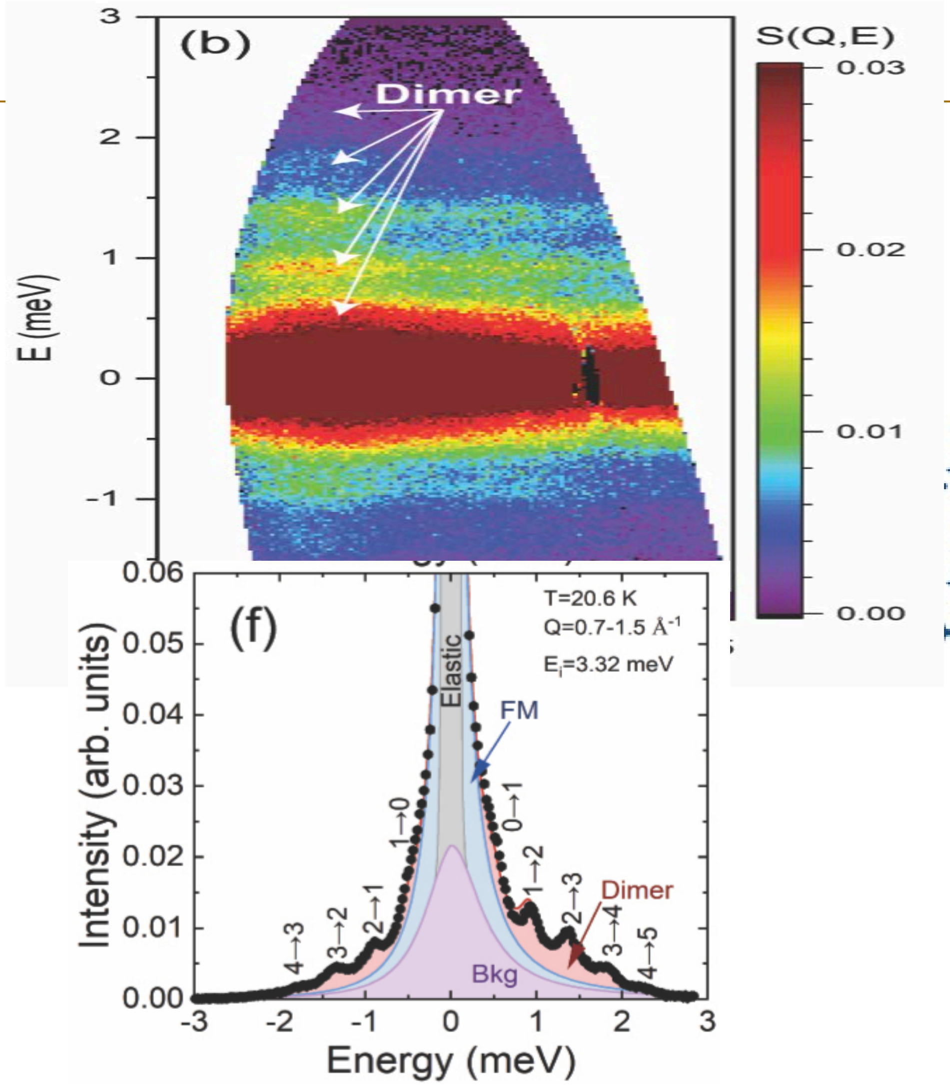
Results: The Triplet States with high fidelity

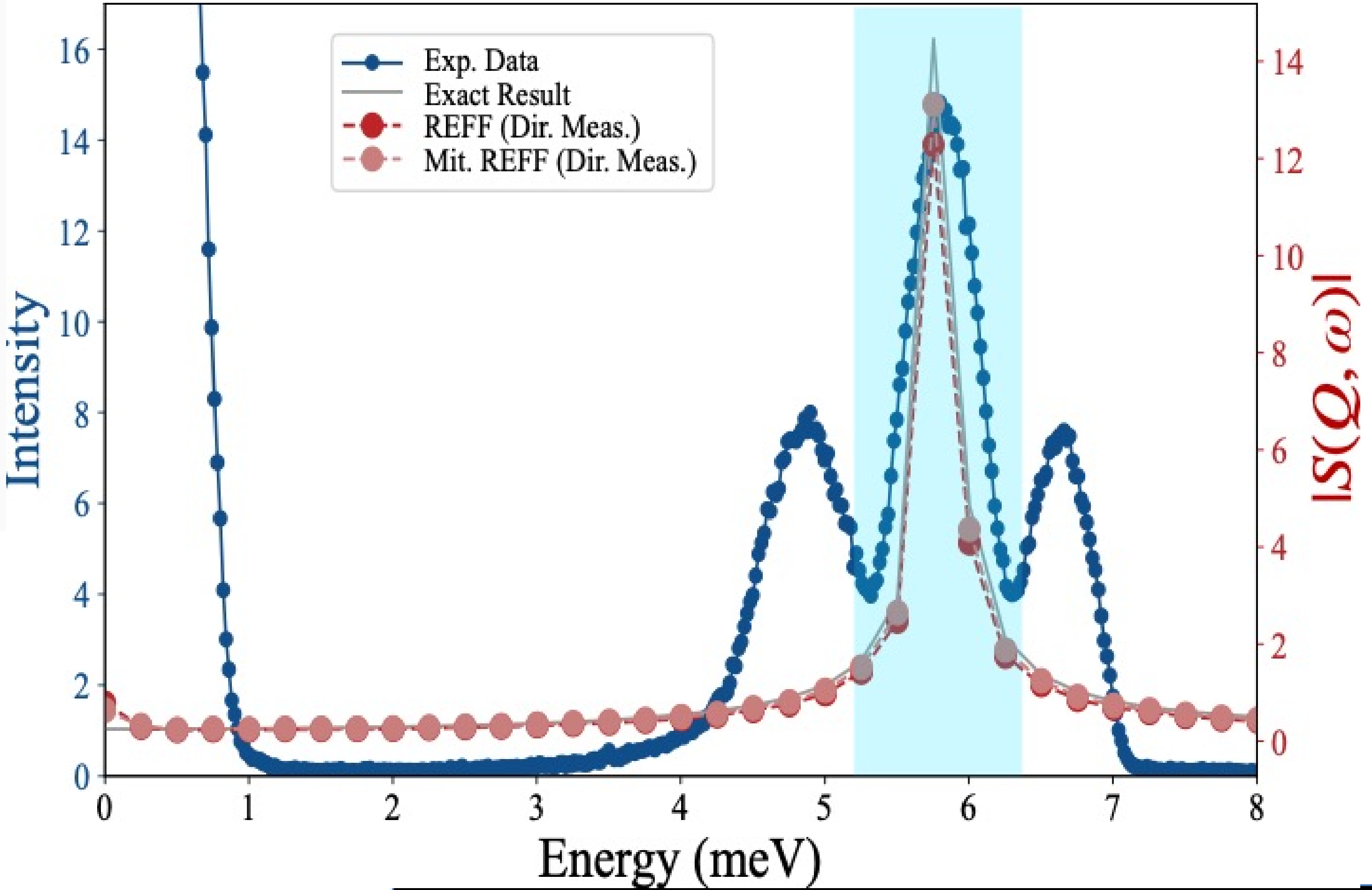




$$H = \sum_{j=1}^{N-1} J_{xx}\sigma_j^x\sigma_{j+1}^x + J_{yy}\sigma_j^y\sigma_{j+1}^y + J_{zz}\sigma_j^z\sigma_{j+1}^z + h\sum_{j=1}^{N}\sigma_j^z$$

Results: Experimental Data Simulation





Kurita, N., et al. (2019). Localized Magnetic Excitations in the Fully Frustrated Dimerized Magnet $Ba_2CoSi_2O_6Cl_2$. *Physical Review Letters*, *123*(2), 027206.

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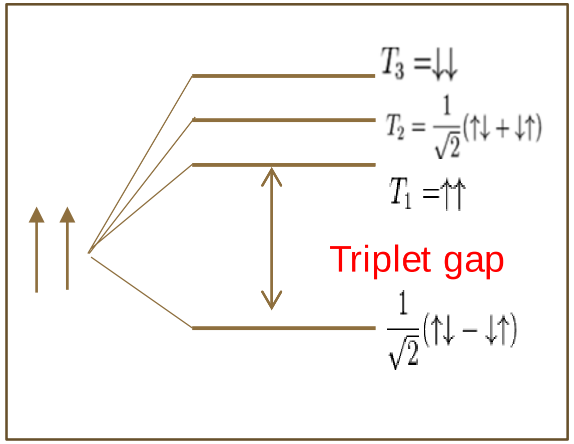
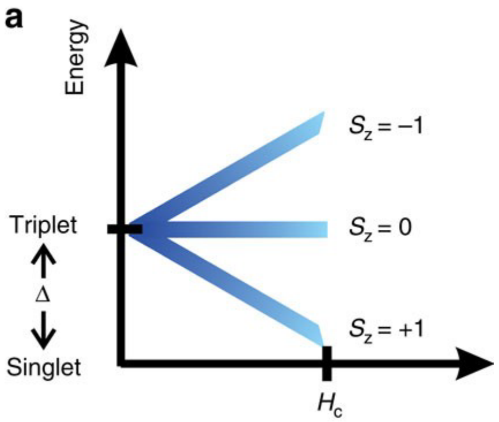
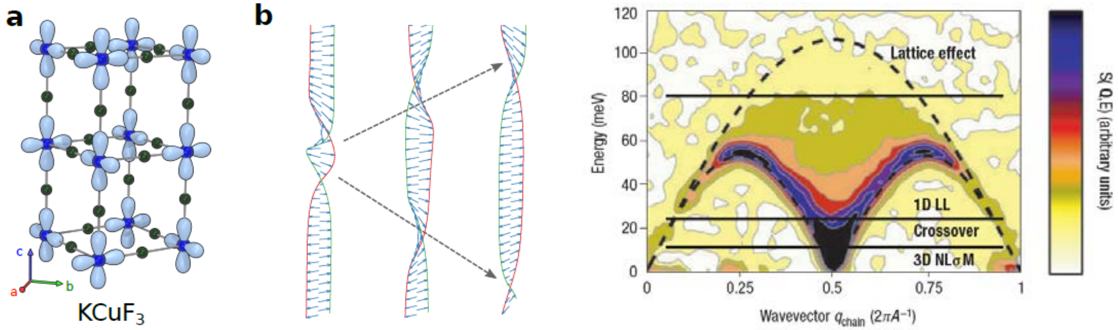
Hamiltonian Engineering:

Make a good noise-corrected spin dimer, Ising, Heisenberg, XY



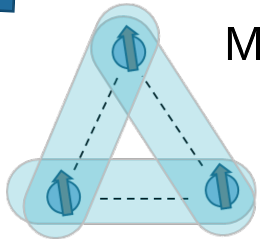


Make it into a good Spin – ½ chain, match to DMRG

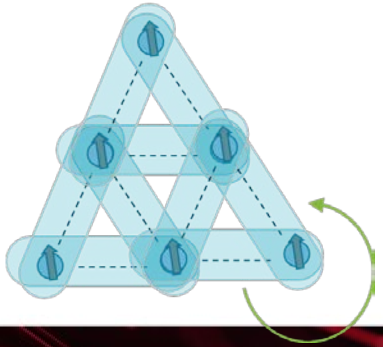


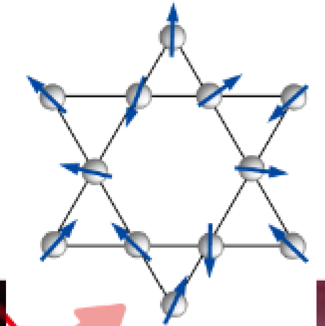
KPZ hydrodynamics, spin ladders, neutron data, etc…

Magnetic frustration, chirality



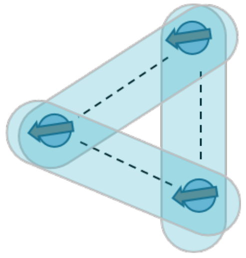
Spin Liquids





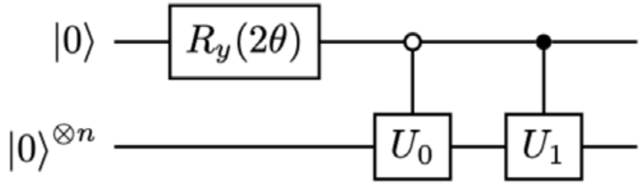
Quantum Spin Eigenfunctions at IBM

P. Carbone, Mario Motta, Barbara Jones, Quantum Circuits for the Preparation of Spin Eigenfunctions on Quantum Computers, *Symmetry* **2022**, *14*(3), 624

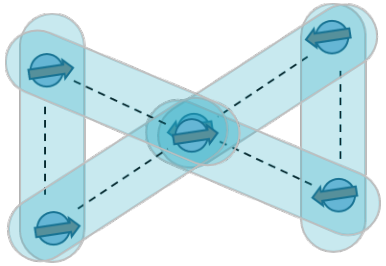


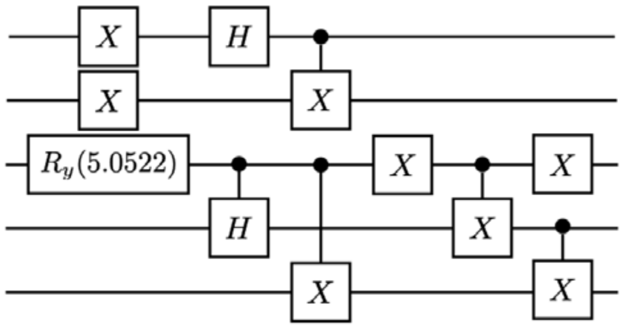
strategies: exact recursive construction (based on addition of angular momenta) accurate but expensive

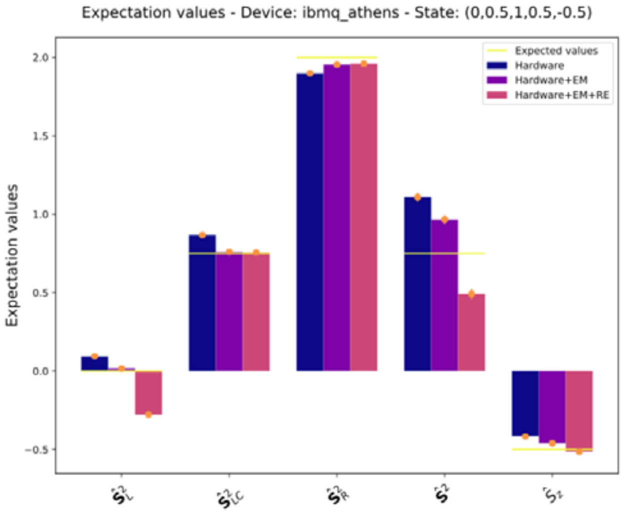
$$|\ell_1,\ell_2,\ell,m\rangle = \sum_{m_1,m_2} C^{\ell m}_{\ell_1 m_1,\ell_2 m_2} |\ell_1,m_1\rangle \otimes |\ell_2,m_2\rangle \rightarrow$$

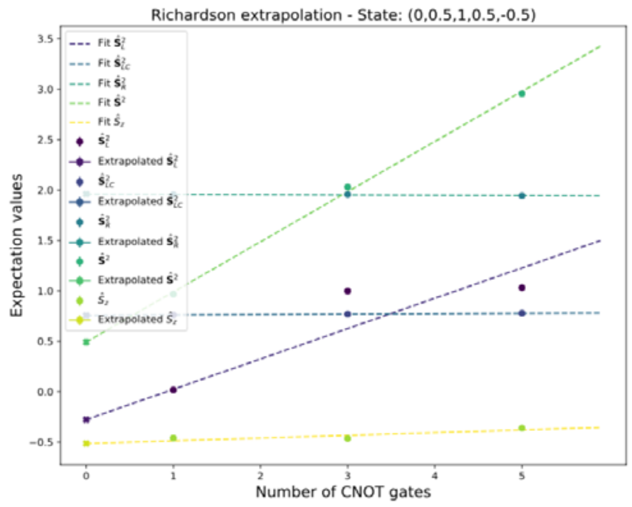


results: simulated on IBMQ hardware (3,5 spins) deploying error mitigation techniques









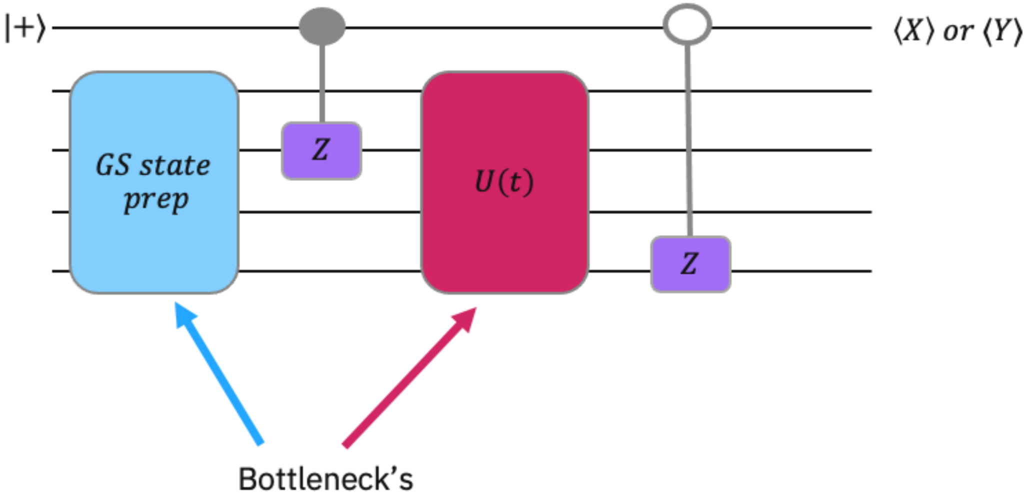
perspectives: use to support research in frustrated spin systems, exploration of tailored variational Ansatz, reduction of computational cost

Macro Project: States on 2D defective Honeycomb and Kagome lattices

$$H = \sum_{<i,j>,\alpha,\beta} J_{ij}^{\alpha,\beta}\, S_i^{\alpha} S_j^{\beta} + h \sum_i \vec{B} \cdot \vec{S}_j$$

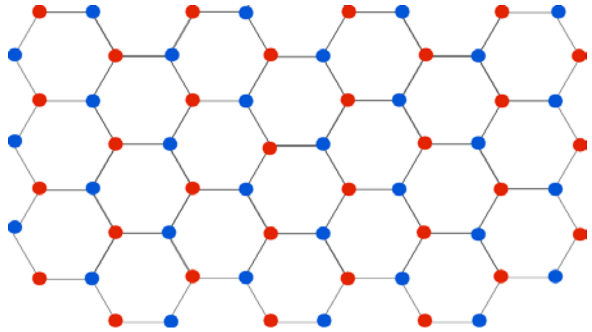
$$\mathcal{S}(\vec{q},\omega) = \frac{1}{N} \sum_{ij} \int_{-\infty}^{\infty} e^{-i\vec{q}\cdot(\vec{x}_i - \vec{x}_j)} e^{i\omega t} \mathcal{C}_{ij}^{\alpha\beta}(t)$$

$$\mathcal{C}_{ij}^{zz}(t) = \langle gs | Z_i(0) Z_j(t) | gs \rangle$$

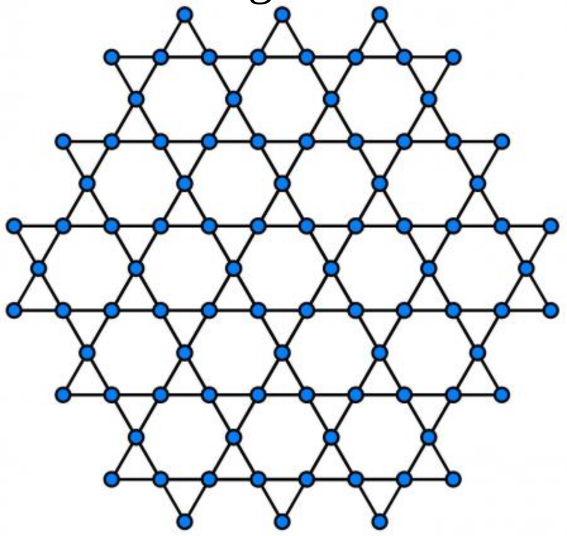


Smart Algorithms
Transpilation + Error Mitigation

Honeycomb



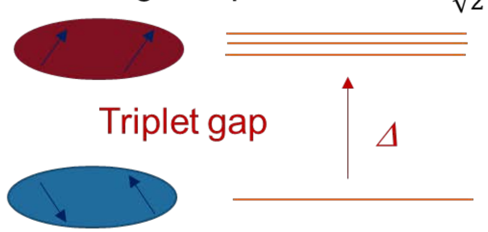
Kagome



Hamiltonian Engineering

Spins, to Spin chains to Spin plaquettes:

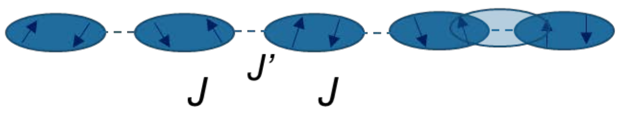
Two entangled spins. $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) + |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$



$S_{tot} = 1$ (triplet)

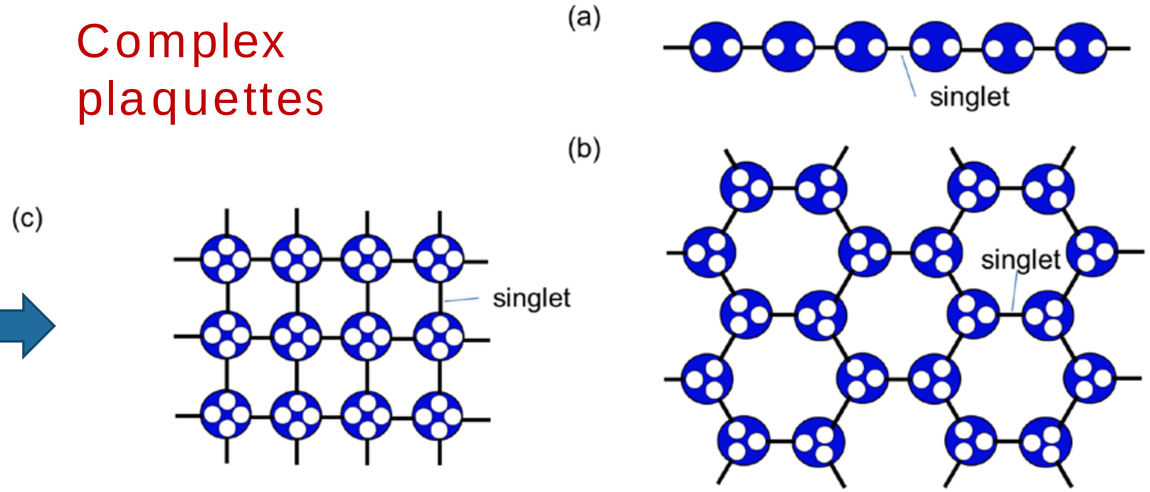
$S_{tot} = 0$ (singlet) $\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$

Consider a system of entangled spin chain:

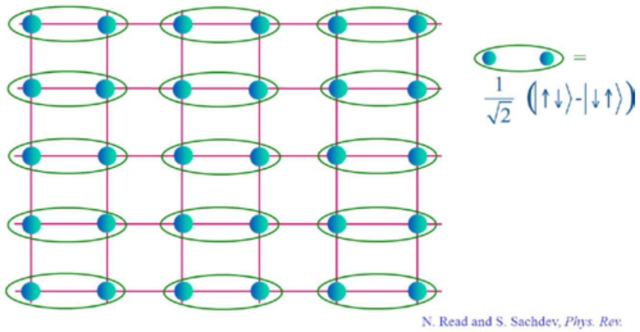


(AKLT model)
Haldane model

Complex plaquettes

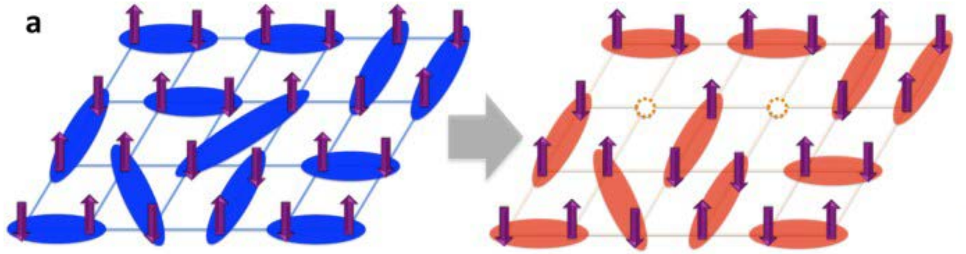


Emergent structures from long-range entanglement



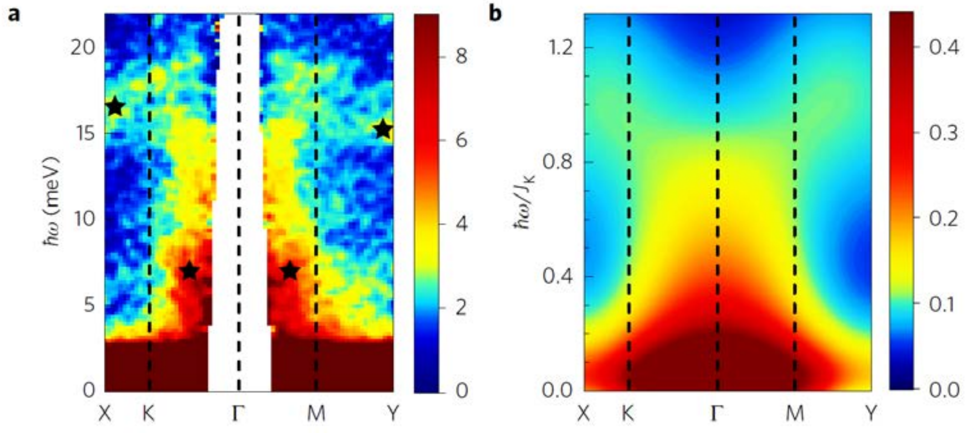
Valence Bond Solid (VBS)

N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).
R. Moessner and S. L. Sondhi, *Phys. Rev. B* **63**, 224401 (2001).

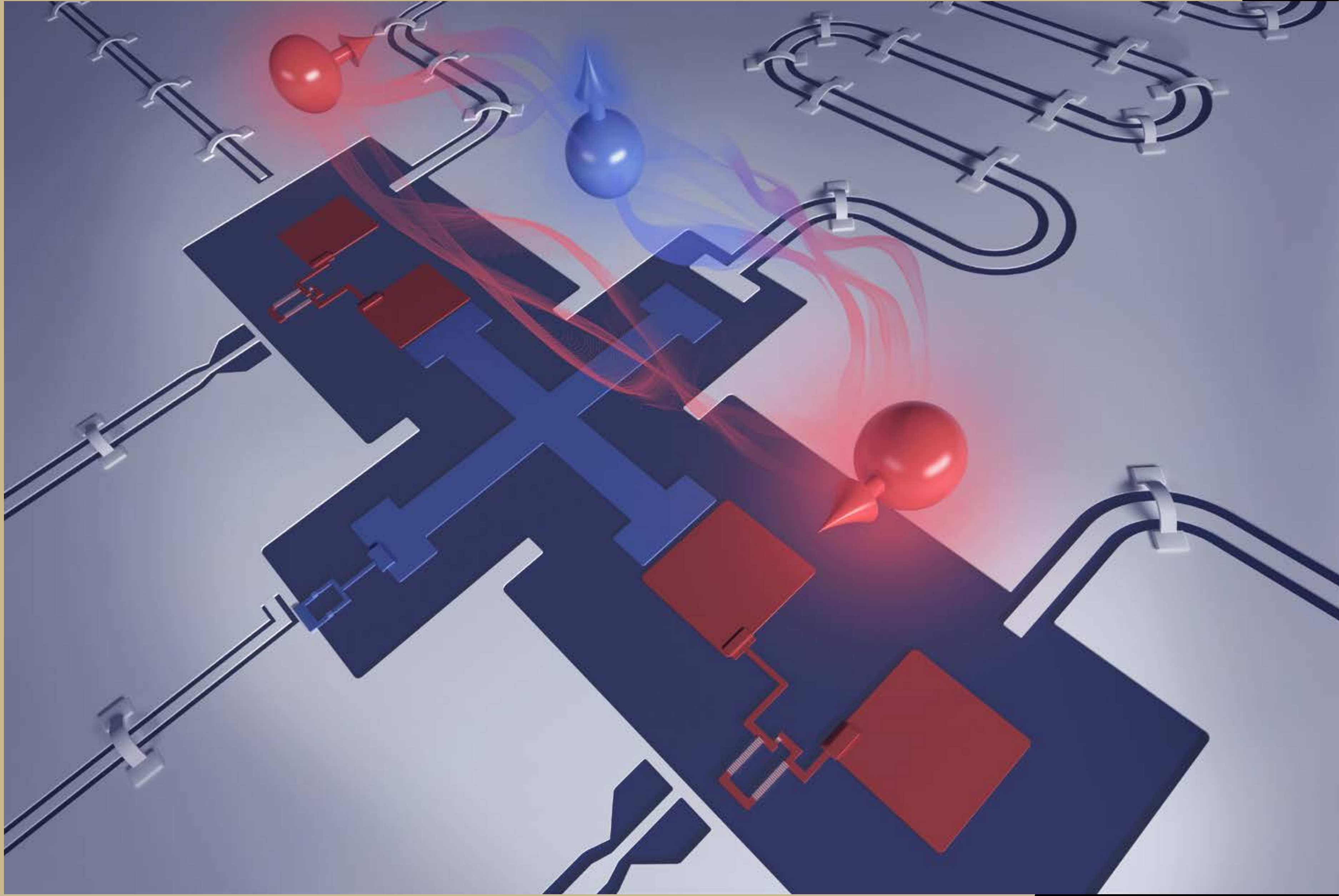


Dynamic data

Data | Model



THANK YOU



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