Simulations of the Ising model on a Shastry-Sutherland lattice by quantum annealing

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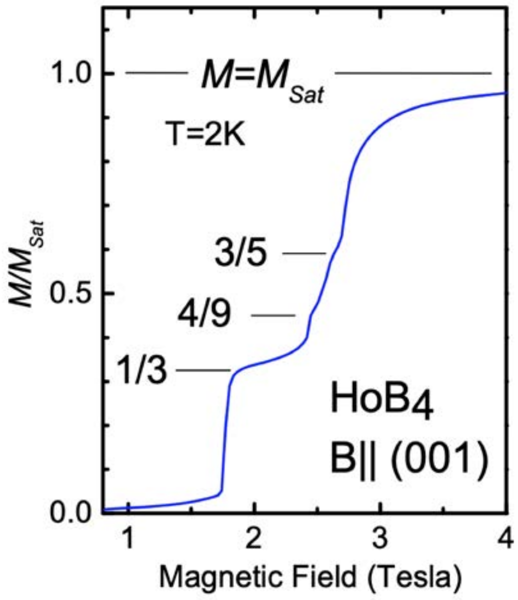
Outline

- Material science motivation
- Shastry-Sutherland lattice
- Embeddings
- Boundary conditions
- Information processing on D-Wave 2000Q
- Results and comparison to experimental data

We demonstrate how quantum annealing enables accurate simulations of many-particle Hamiltonian systems.

Rare-earth tetraboride materials

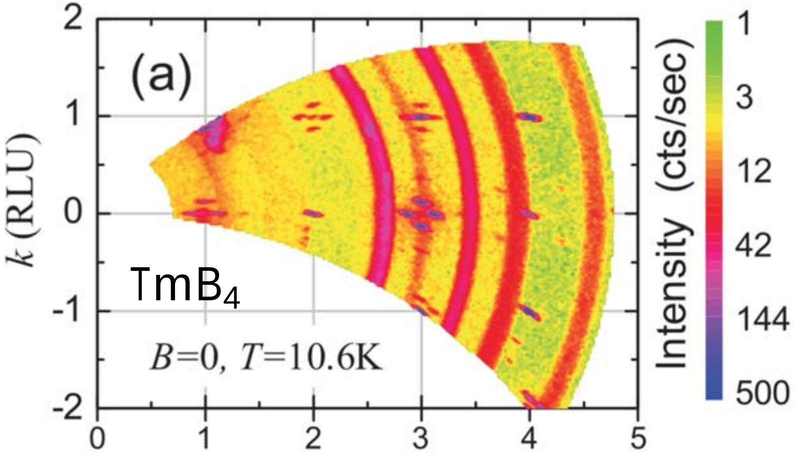
Magnetization



S Mat'as̆ et al. 2010

Structure Factor

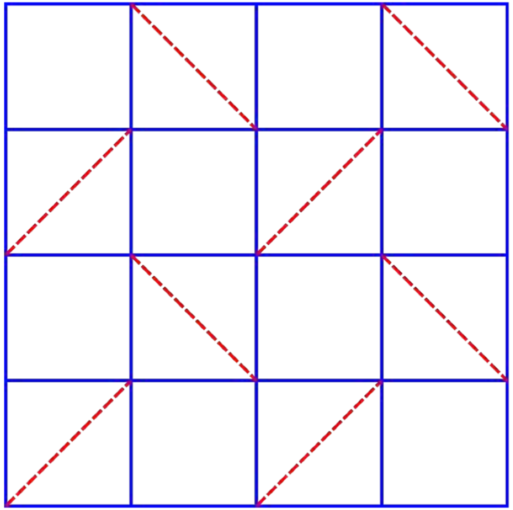
$$S(\vec{q}) = \sum_{\langle ij \rangle} \langle \sigma_i^z \sigma_j^z \rangle e^{i\vec{q}\cdot\vec{R}_{ij}}$$



Siemensmeyer et al. 2008

Can we simulate these behaviors using quantum annealing?

The Shastry-Sutherland lattice



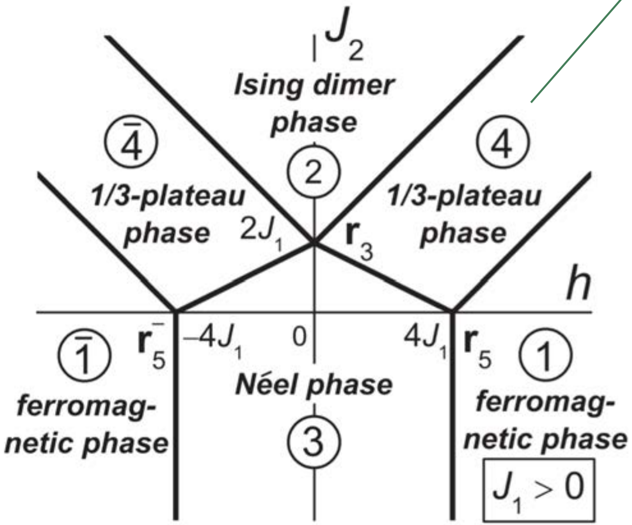
Ising magnet

$$H = J_1 \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z + J_2 \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \quad \longleftrightarrow \quad \mathrm{RB_4,\ R = La\text{-}Lu}$$

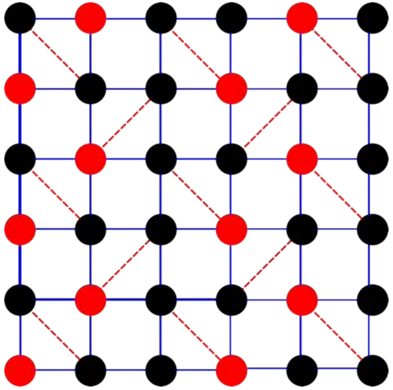
$J_2 = \mathrm{Dimer}$

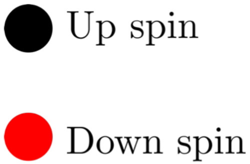
$J_1 = \mathrm{Square}$

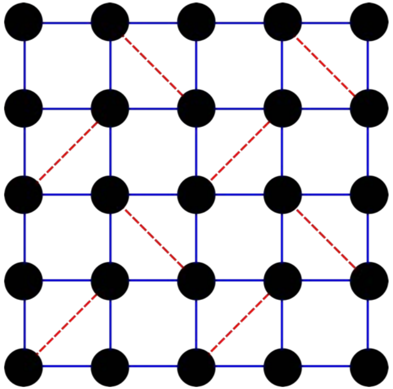
Phase diagram

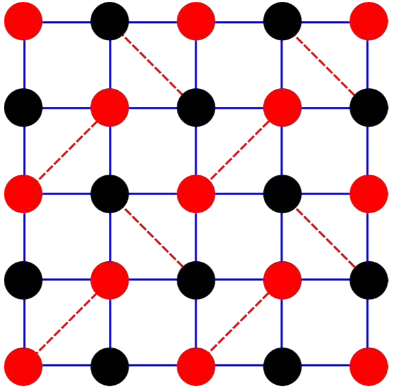


Dublenych 2012









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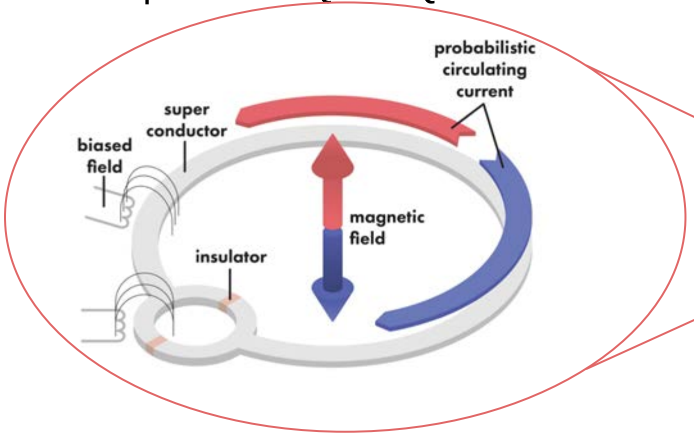
D-Wave 2000Q Processor

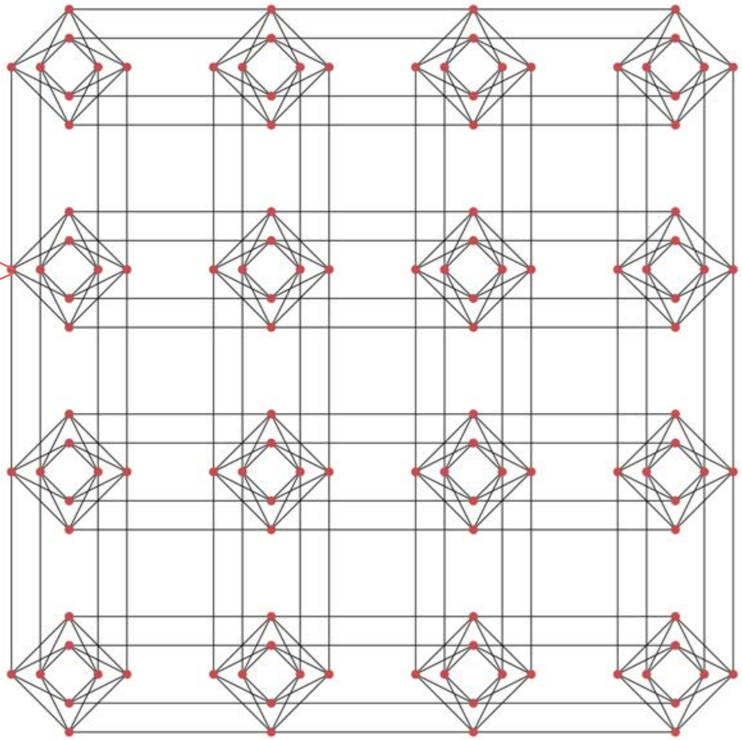
Coupled RF-SQUID Qubits



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

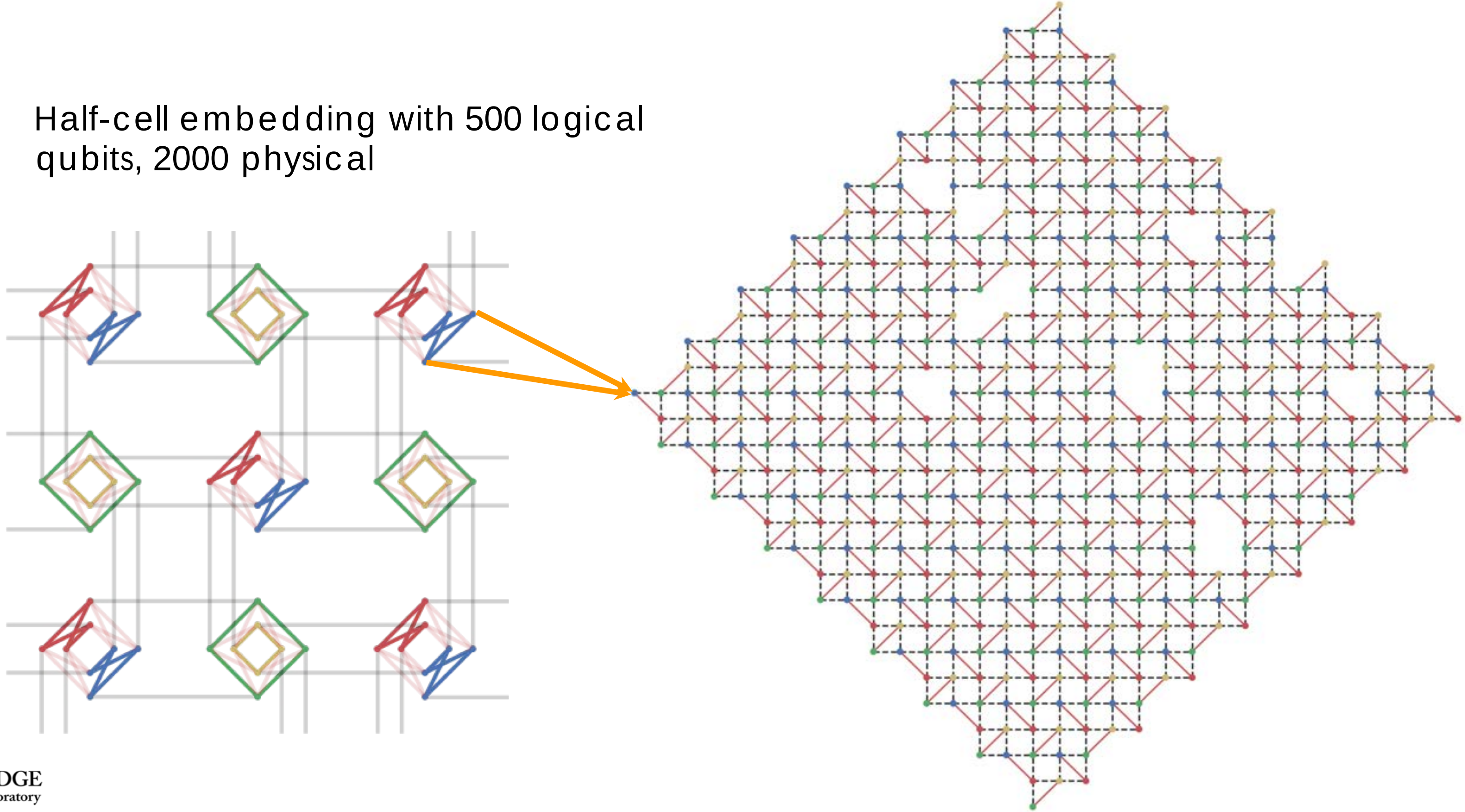
Independently tunable biases and couplers

Chimera Topology



Embedding the Shastry-Sutherland Lattice

- Half-cell embedding with 500 logical qubits, 2000 physical

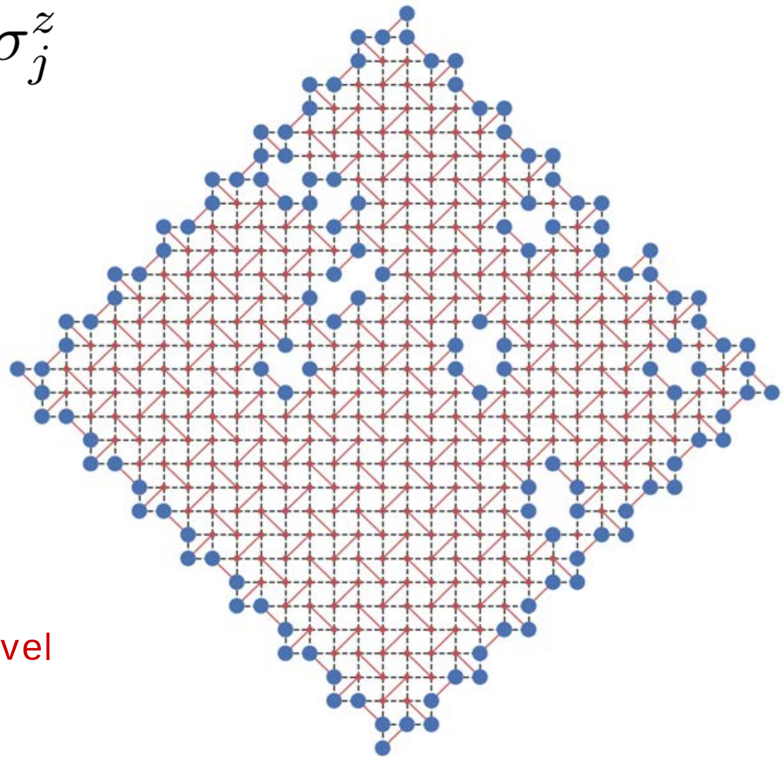


Self-consistent mean-field boundary conditions

$$H = \sum_i h_i^z \sigma_i^z + h^z \sum_i \sigma_i^z + \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$

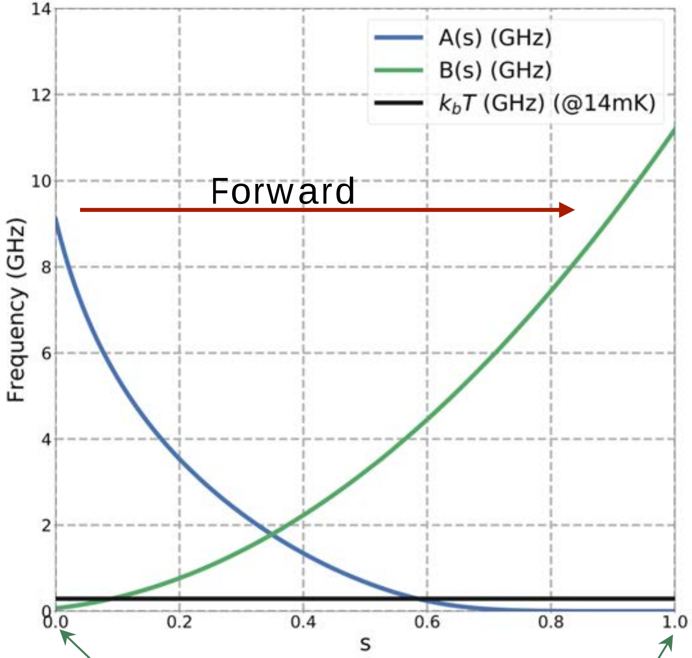
$$\underset{\vec{h}}{\text{minimize}} \quad \langle m \rangle - \langle m \rangle$$

$$\text{subject to} \quad \text{sgn}(h_i^z) = \text{sgn}(h^z) \ \forall i$$



Independent tunability of biases allows us to explore novel boundary conditions

Forward Annealing



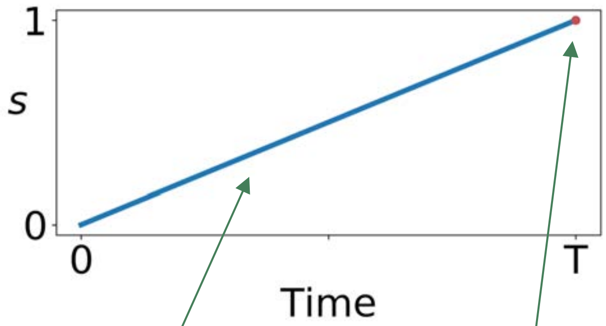
Begin

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

End

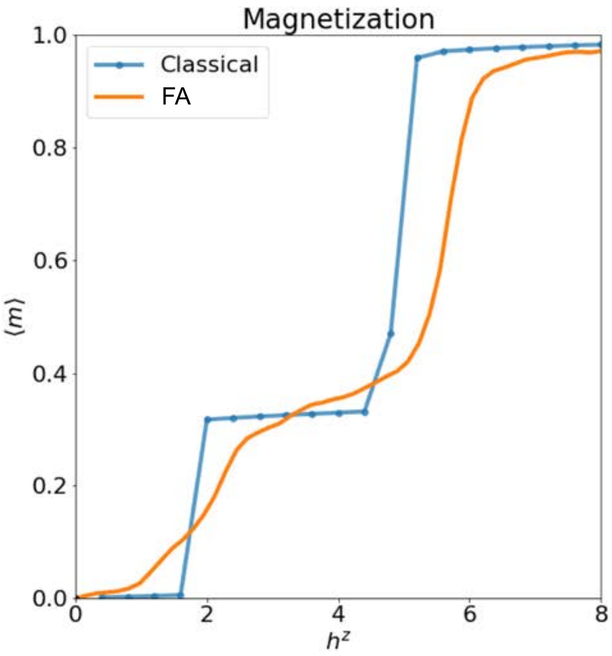
$A(s) << B(s)$

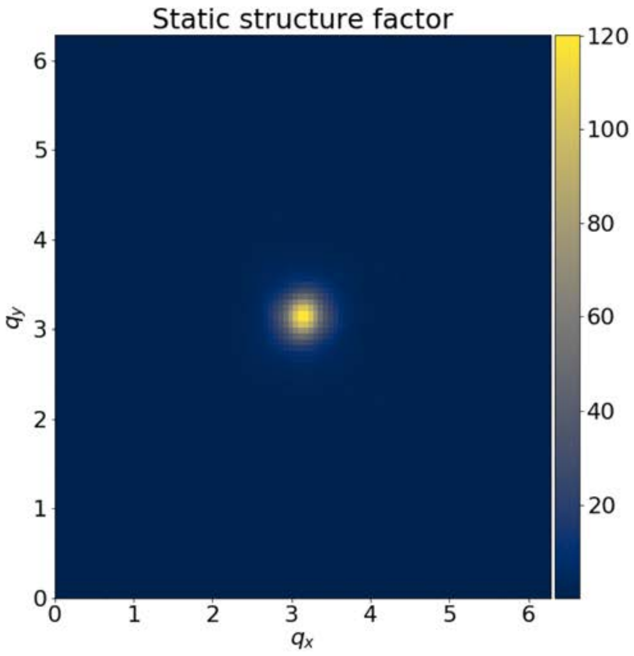
$$H = A(s)\sum_i \sigma_i^x + B(s)\left[\sum_i h_i\sigma_i^z + \sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z\right]$$

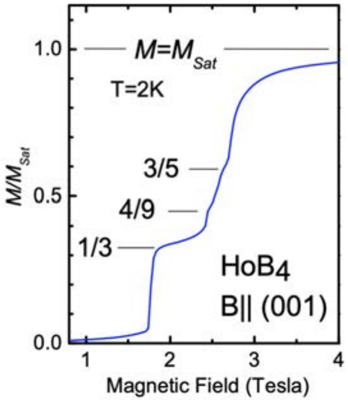


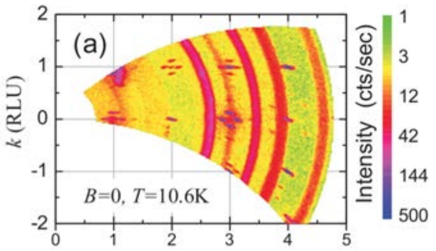
Adiabatic evolution and readout

Forward Anneal with the half-cell embedding



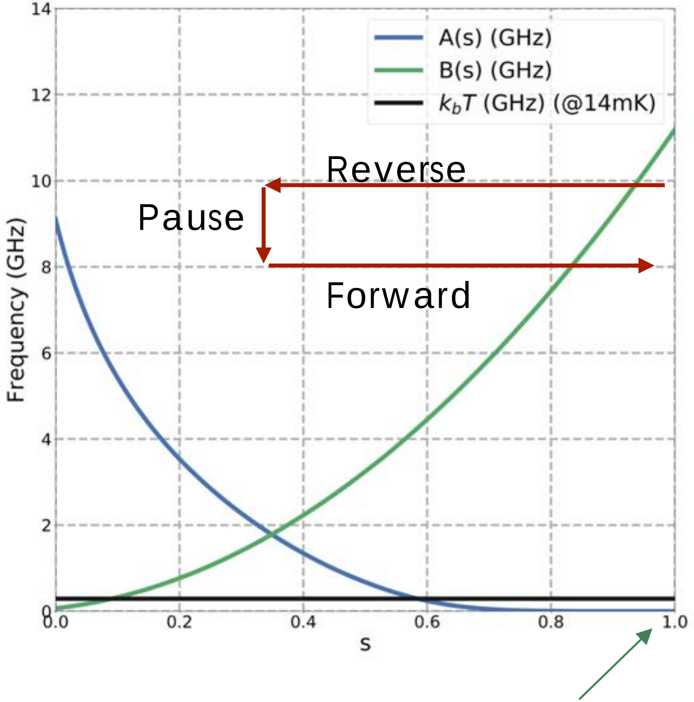






Reverse Annealing

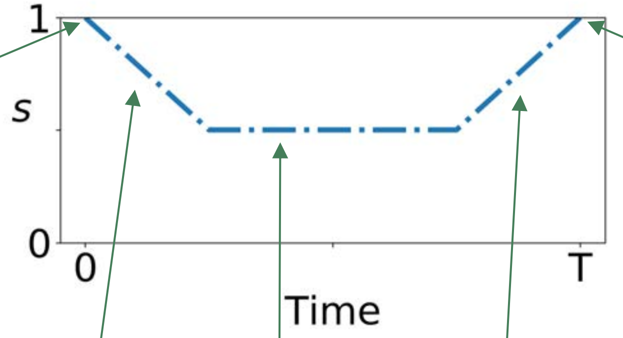
$$H = A(s)\sum_i \sigma_i^x + B(s)\left[\sum_i h_i\sigma_i^z + \sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z\right]$$



Begin + End

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

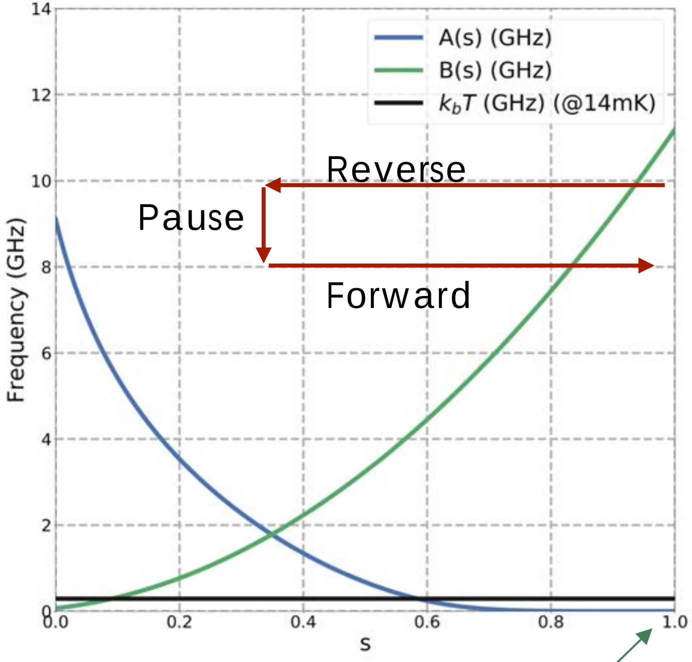
initialize



readout

Reverse evolution , pause, forward evolution

Quantum Evolution Markov Chain



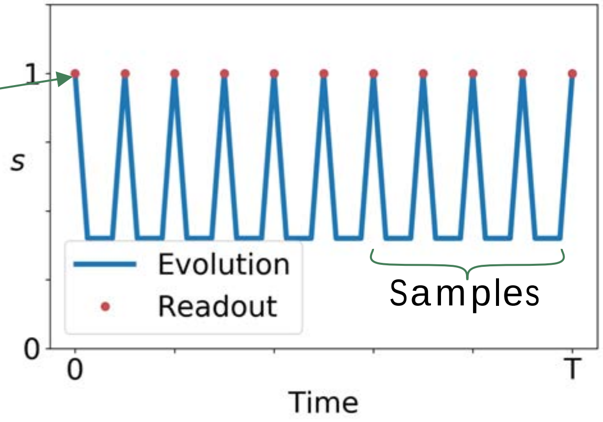
Begin + End

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

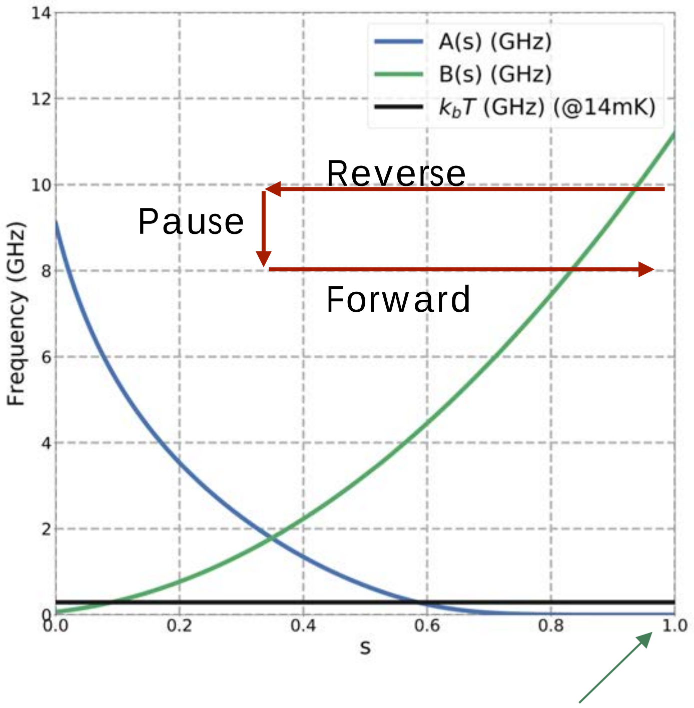
$$H = A(s)\sum_i \sigma_i^x + B(s)\left[\sum_i h_i\sigma_i^z + \sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z\right]$$

- Iterative reverse annealing schedule

initialize



Quantum evolution Markov chain

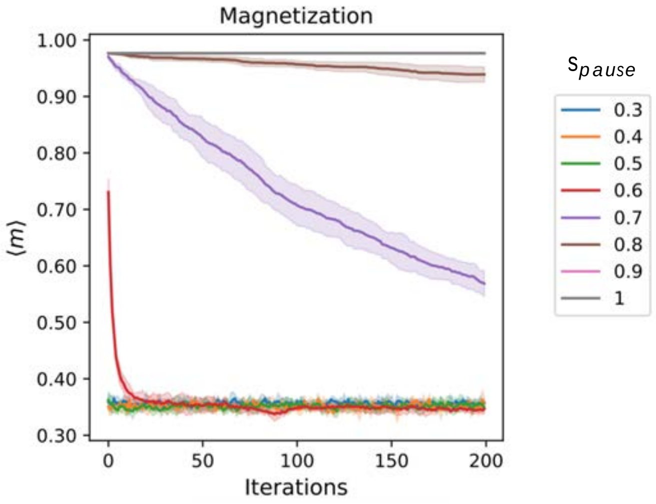


Begin + End

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

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

- Iterative reverse annealing schedule



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QEMC Motif Convergence

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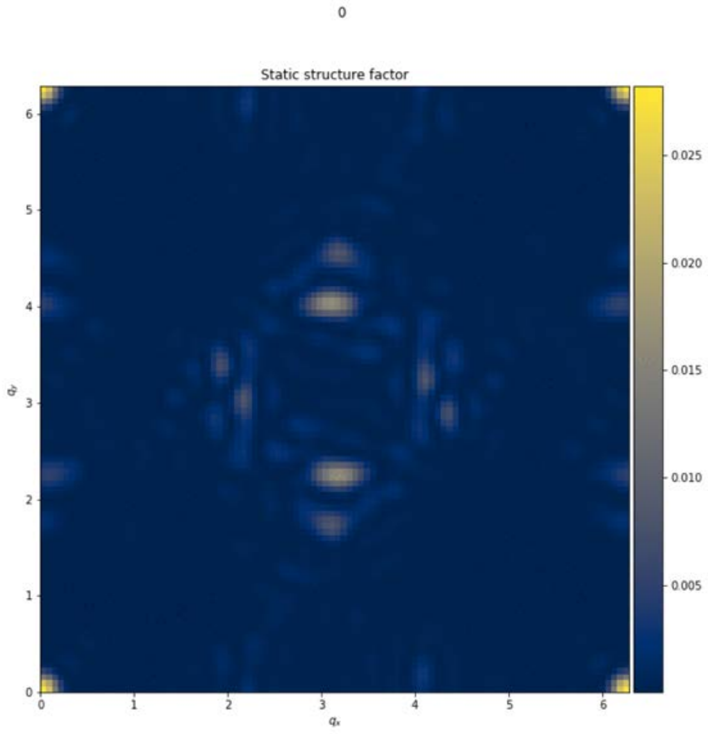
QEMC Structure Factor convergence



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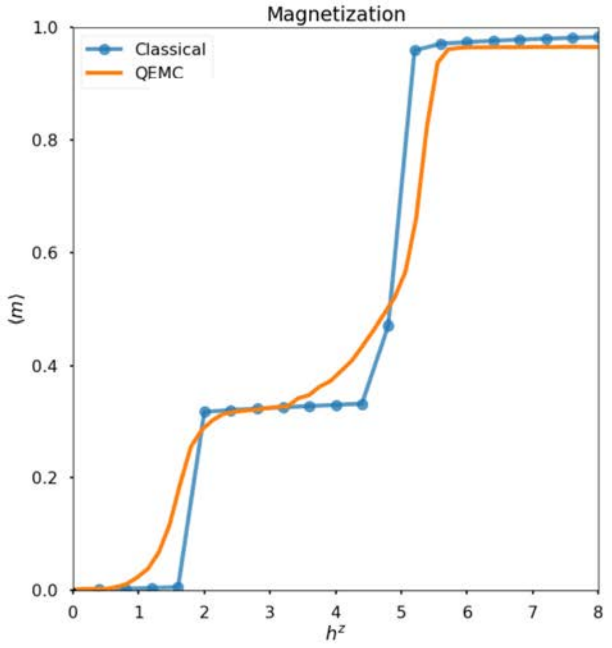
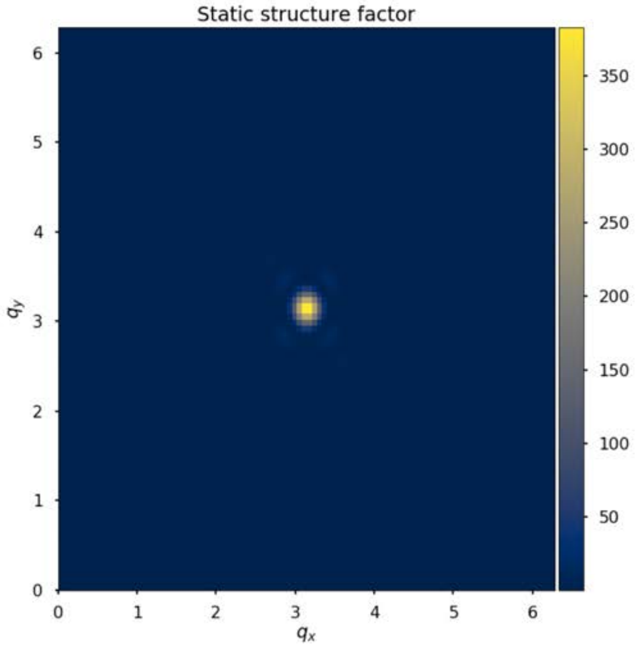
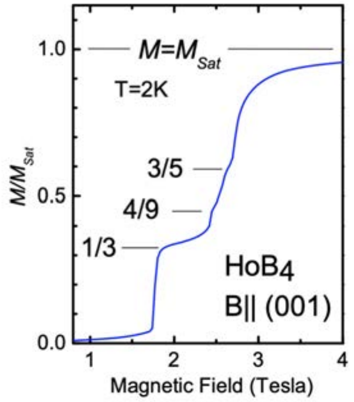
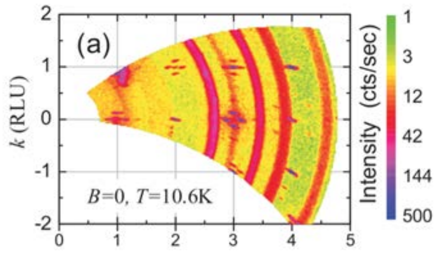
Quantum evolution Markov chain: half-cell embedding









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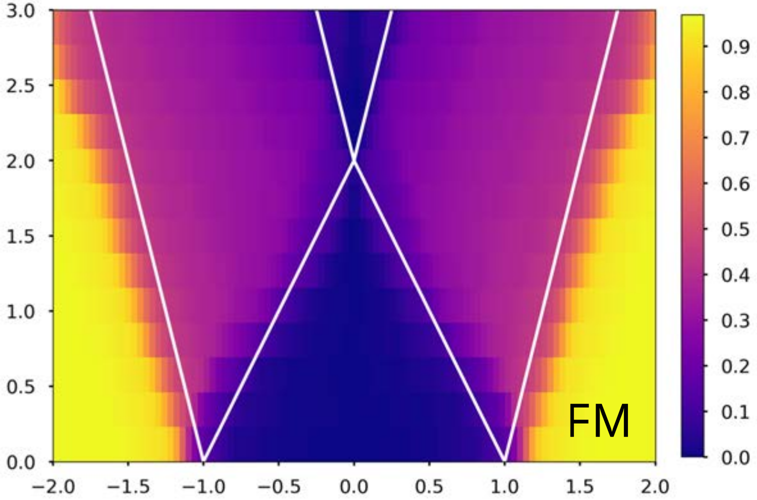
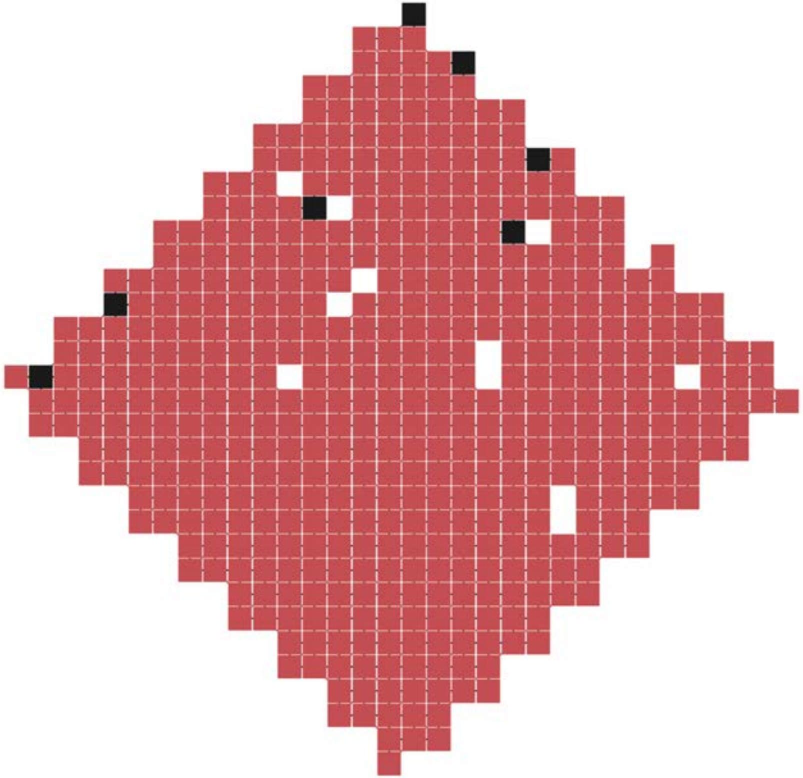
Quantum evolution Markov chain: half-cell embedding





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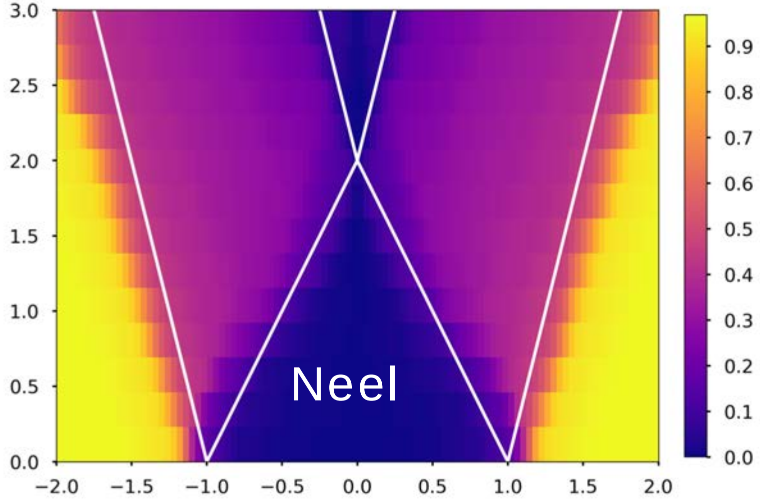
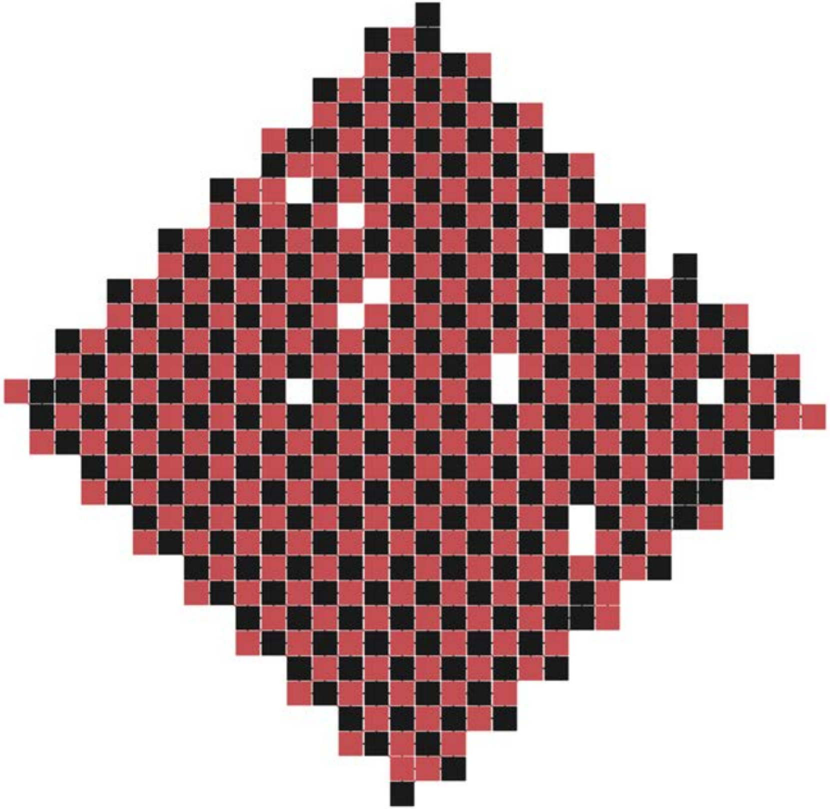
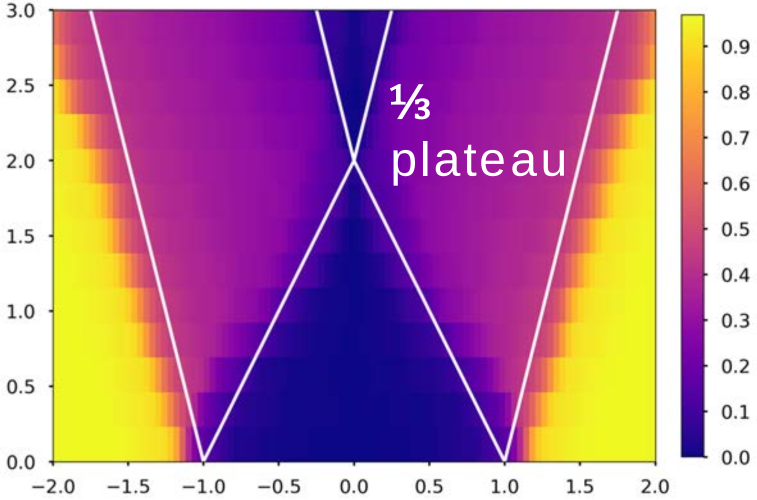
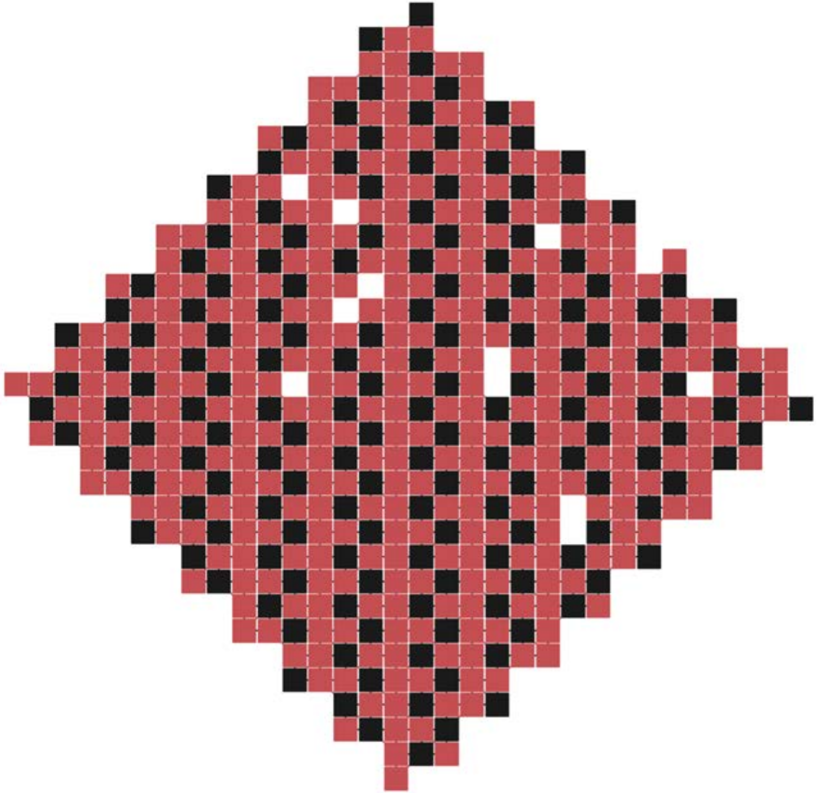
Quantum evolution Markov chain: half-cell embedding





Quantum evolution Markov chain: half-cell embedding





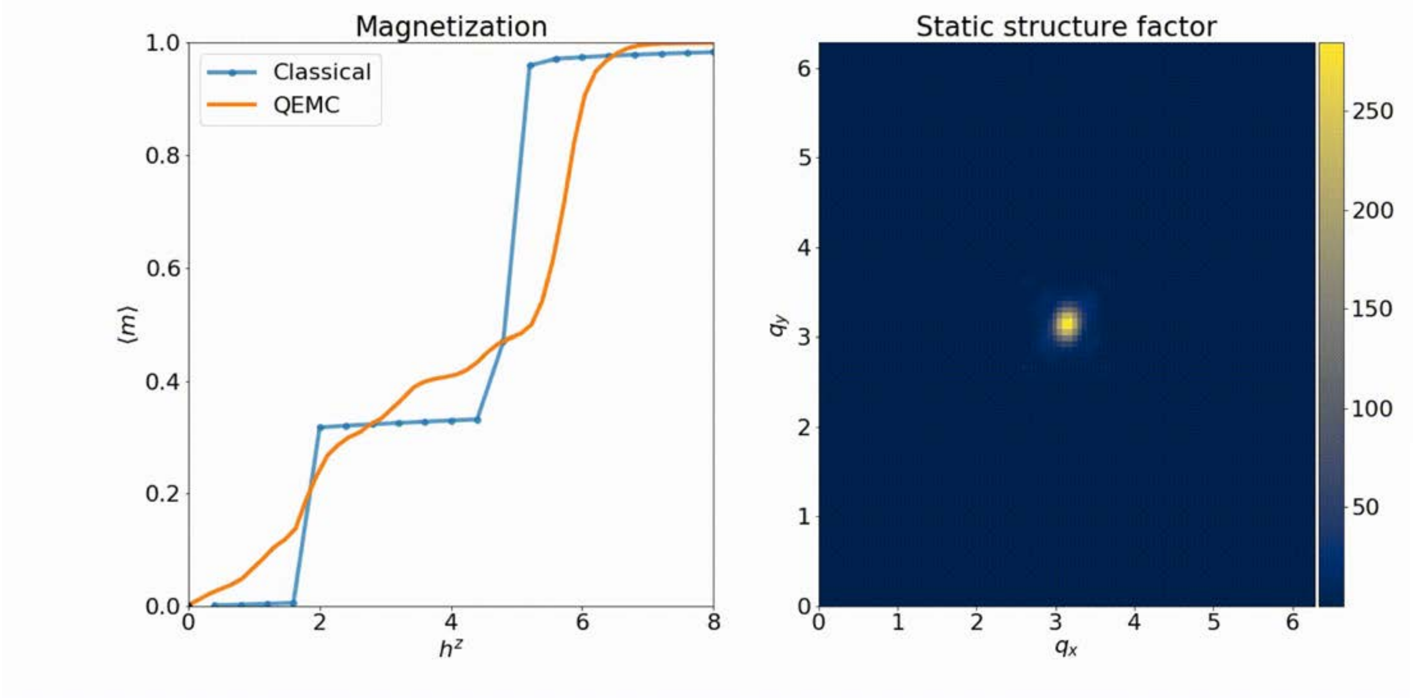
Simulations of the Ising model on a Shastry-Sutherland lattice by quantum annealing

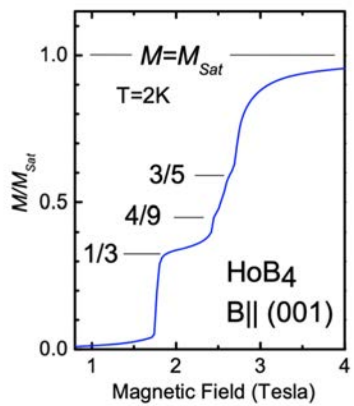
- We demonstrate how quantum annealing enables accurate simulations of many-particle Hamiltonian systems.
- We sample the ground state energy configurations of the the SS Ising model to calculate the structure factor
- We develop a novel method for mitigating finite size and defects.
- We observe good agreement between the observed and expected material behaviors
- We can now explore defect physics and temperature effects in this model.

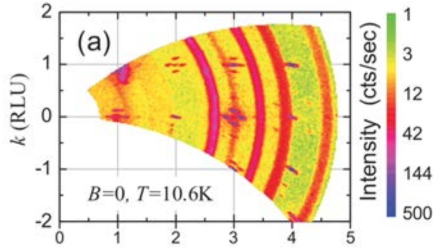
References

1. Mat'aš, S, K Siemensmeyer, E Wheeler, E Wulf, R Beyer, Th Hermannsdörfer, O Ignatchik, et al. "Magnetism of Rare Earth Tetraborides." Journal of Physics: Conference Series 200, no. 3 (January 1, 2010): 032041. https://doi.org/10.1088/1742-6596/200/3/032041.
2. Siemensmeyer, K., E. Wulf, H.-J. Mikeska, K. Flachbart, S. Gabáni, S. Mat'aš, P. Priputen, A. Efdokimova, and N. Shitsevalova. "Fractional Magnetization Plateaus and Magnetic Order in the Shastry-Sutherland Magnet TmB 4." *Physical Review Letters* 101, no. 17 (October 20, 2008). https://doi.org/10.1103/PhysRevLett.101.177201.
3. Dublenych, Yu. I. "Ground States of the Ising Model on the Shastry-Sutherland Lattice and the Origin of the Fractional Magnetization Plateaus in Rare-Earth-Metal Tetraborides." Physical Review Letters 109, no. 16 (October 16, 2012). https://doi.org/10.1103/PhysRevLett.109.167202.

Quantum evolution Markov chain without boundary conditions







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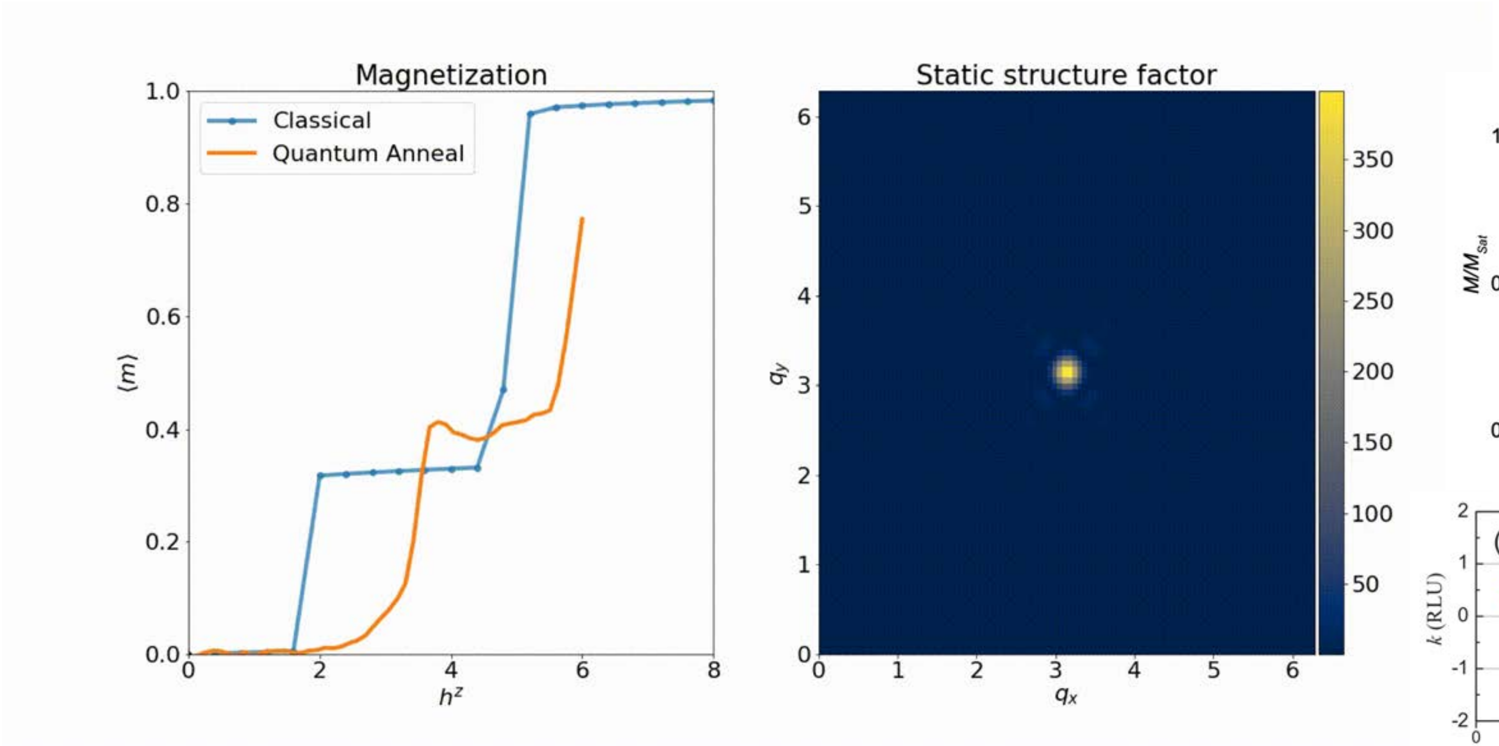
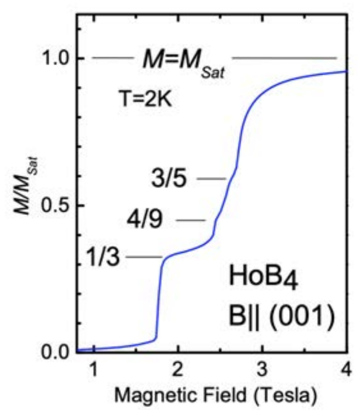
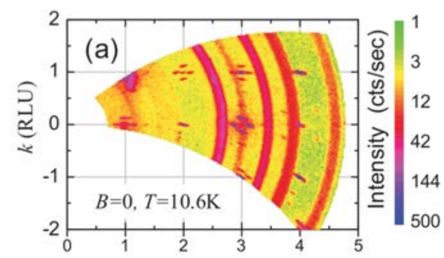
Forward Anneal - Tilt Embedding







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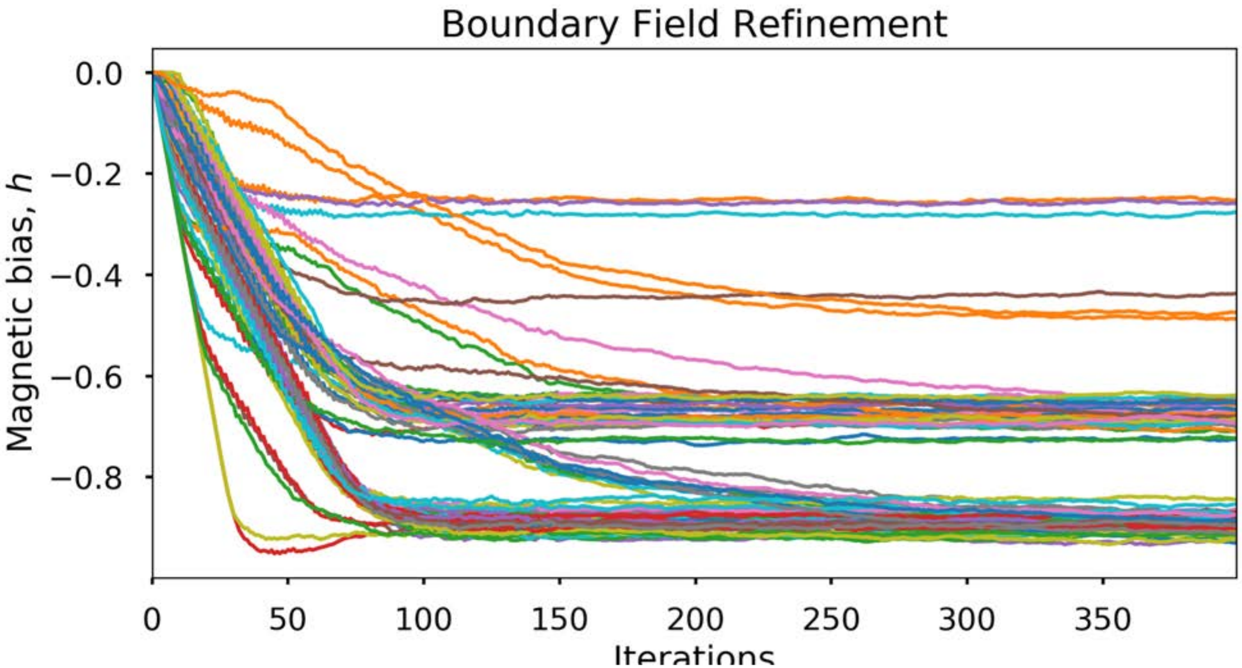
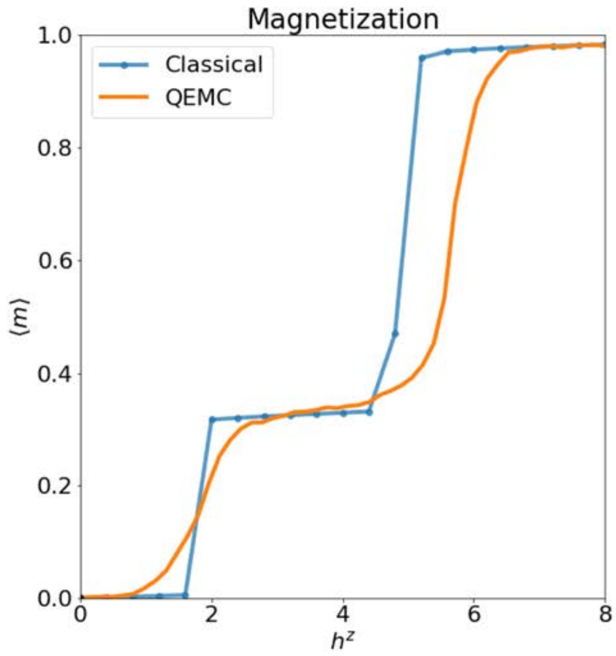
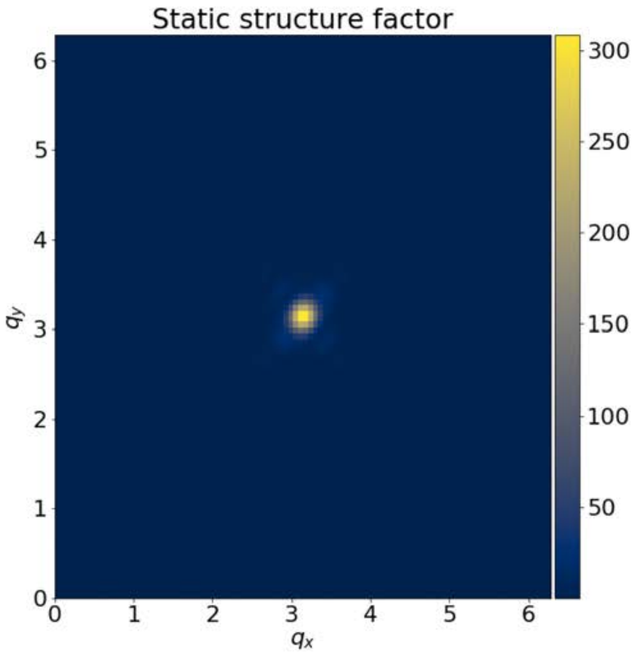
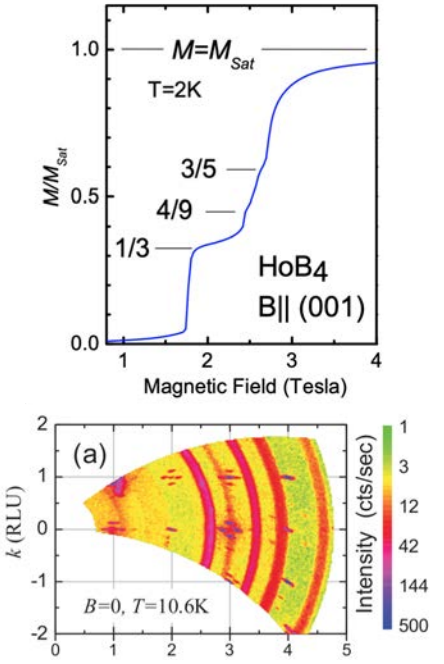
Boundary Refinement



Quantum evolution Markov chain: half-cell embedding







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