Randomness and frustration in a $S = 1/2$ square-lattice Heisenberg antiferromagnet

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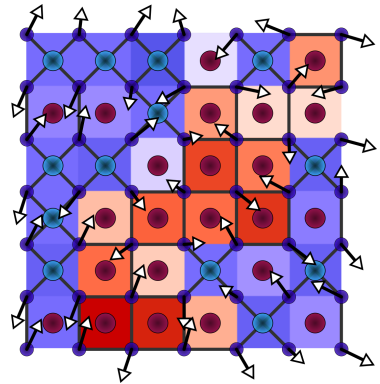

These are the people involved in this project

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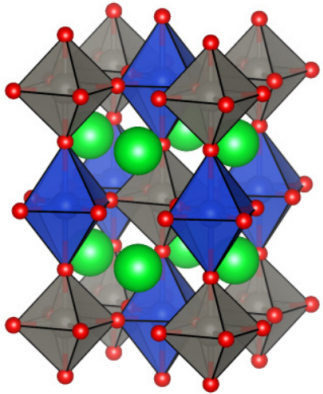
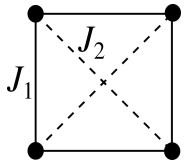
Aalto University

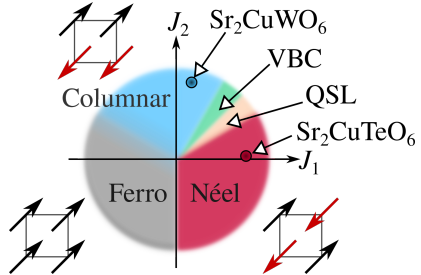
Further details can be found here: Fogh et al., *Phys. Rev. B* **105**, 184410 (2022)
Katukuri et al., *Phys. Rev. Lett.* **124**, 077202 (2020)

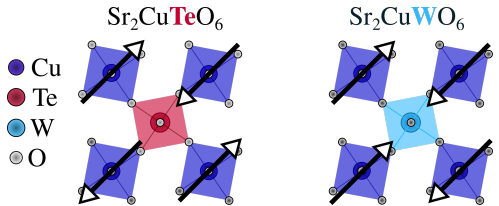
$Sr_2CuB''O_6$ (B'' = Te, W) looks like the perfect system to search for a *quantum spin liquid*



$S = 1/2$ Heisenberg spins on a square lattice







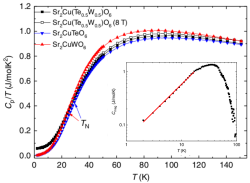
Mustonen et al., *Phys. Rev. B* **98**, 064411 (2018)

Walker et al., *Phys. Rev. B* **94**, 064411 (2016)

Babkevich et al., *Phys. Rev. Lett.* **117**, 237203 (2016)

Quantum spin liquid, valence bond glass, spin glass or something else?

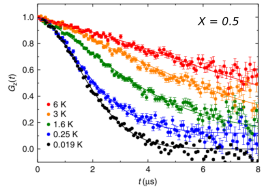
Specific heat is linear at low temperatures



→ quantum spin liquid

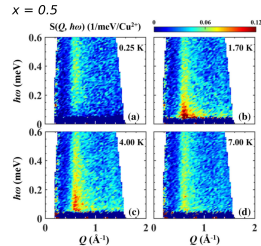
Mustonen et al., *Nature Comms.* **9**, 1085 (2018)

Muon spin relaxation measurements



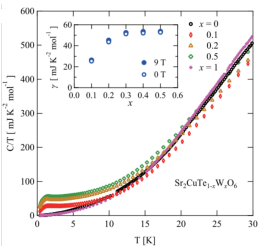
→ no order down to 19 mK

Inelastic neutron scattering measurements



→ spin liquid to partly frozen moments at 1.7 K

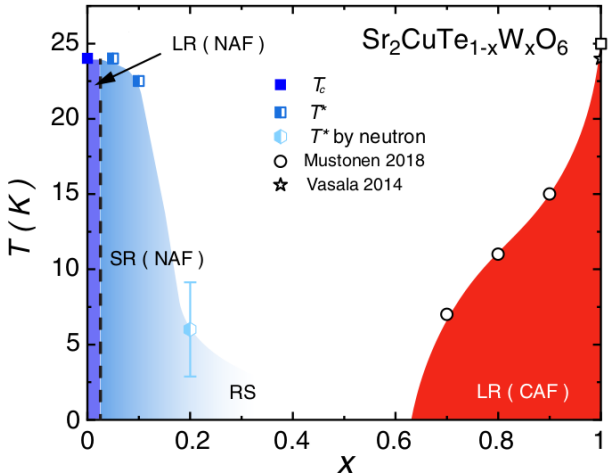
Hu et al., *Phys. Rev. Lett.* **127**, 017201 (2021)



→ valence bond glass

Watanabe et al., *Phys. Rev. B* **98**, 054422 (2018)

Quantum spin liquid, valence bond glass, spin glass or something else?



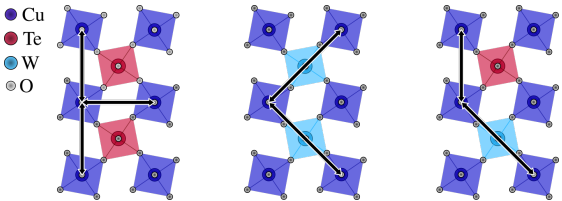
There is an interesting region for $0.1 < x < 0.6$

but

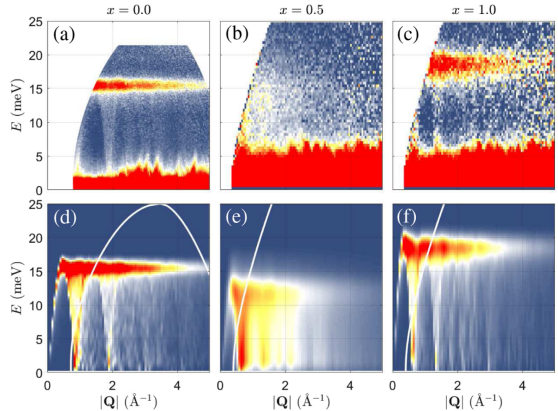
there is no consensus as to what it is

Hong et al., *Phys. Rev. Lett.* **126**, 037201 (2021)

There is evidence for a random-bond model in $Sr_2CuTe_{1-x}W_xO_6$

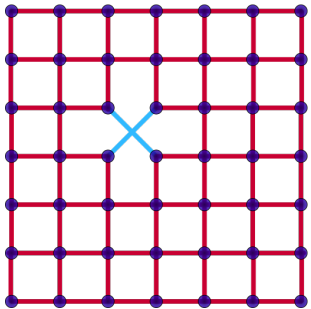


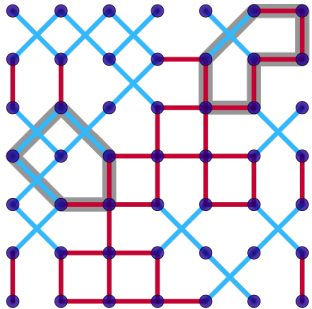
	Sr_2CuTeO_6		Sr_2CuWO_6	
	QC	INS	QC	INS
J_1	7.38	7.60(3)	0.68	1.02
J_2	0.05	0.60(3)	8.33	8.50
J_c	0.003	0.04	0.005	–

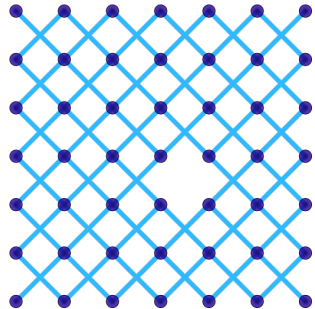


Katukuri et al., *Phys. Rev. Lett.* **124**, 077202 (2020)

What is the ground state for such a system of random bonds?



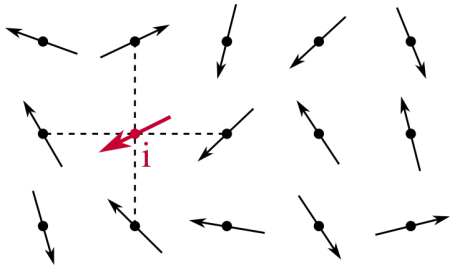


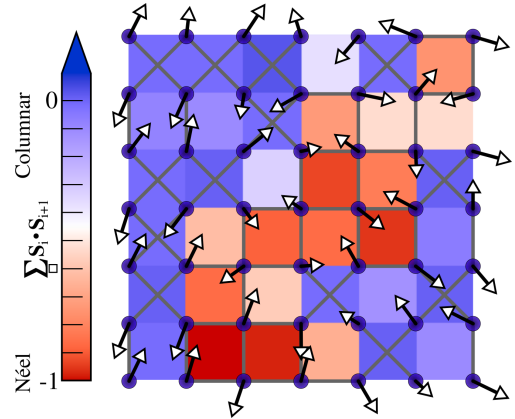


Inhomogeneous mean-field calculations are used to find the ground state

$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \mathbf{S}_i = \langle \mathbf{S}_i \rangle + \delta \mathbf{S}_i, \quad \langle \mathbf{S}_i \rangle = 1/2$

Calculations were performed in spinW
50×50 sites with W randomly placed
Periodic boundary conditions
10 different initial configurations for each value of x

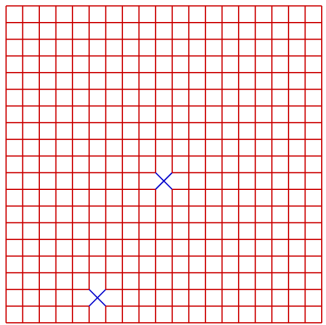


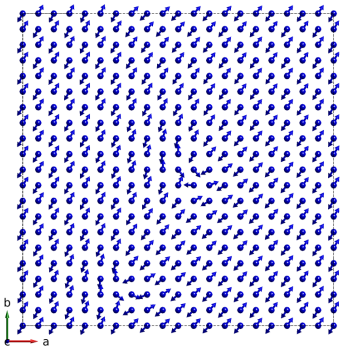


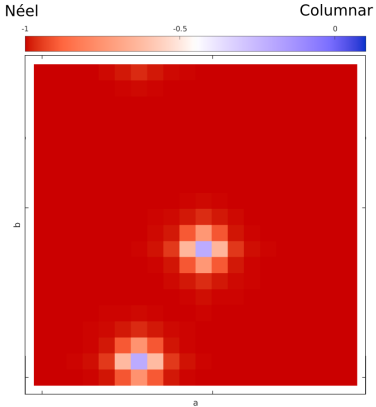
S. Toth and B. Lake, *J. Phys. Condens. Matter* **27**, 166002 (2015)

The ground state consists of patches of Néel and columnar correlations

An example of a real space configuation for $x = 0.005$

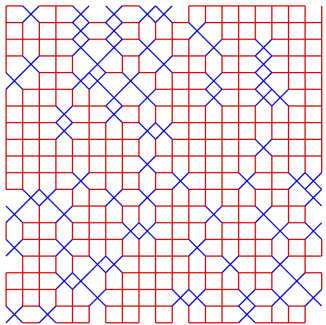


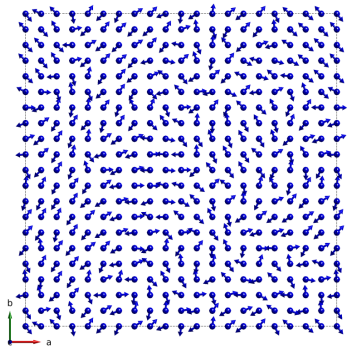


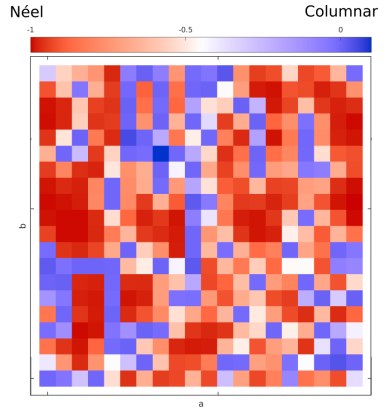


The ground state consists of patches of Néel and columnar correlations

An example of a real space configuation for $x = 0.2$

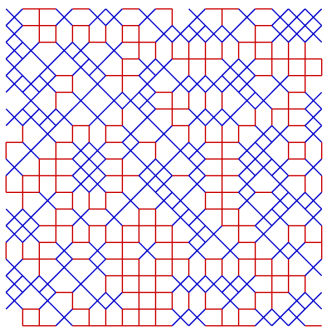


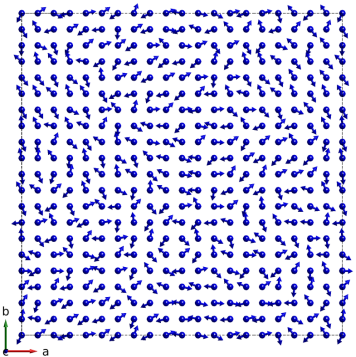


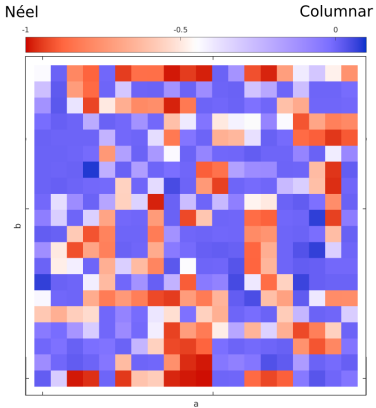


The ground state consists of patches of Néel and columnar correlations

An example of a real space configuation for $x = 0.4$

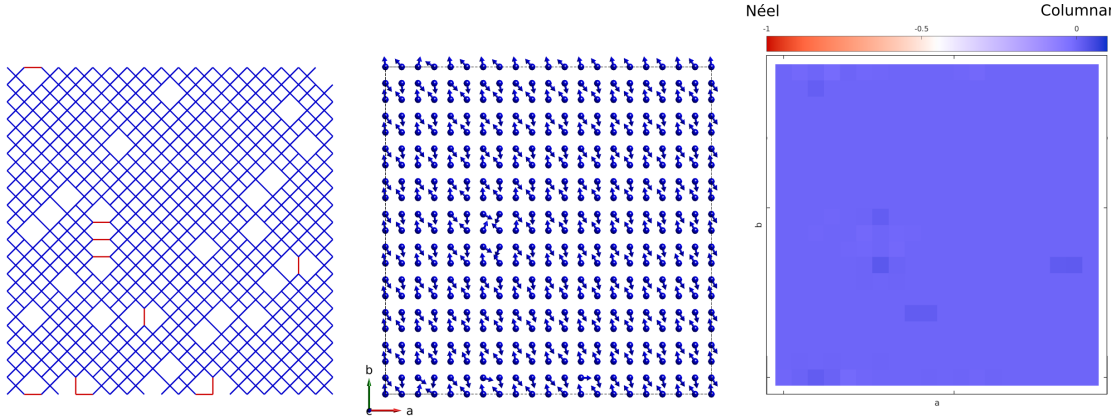






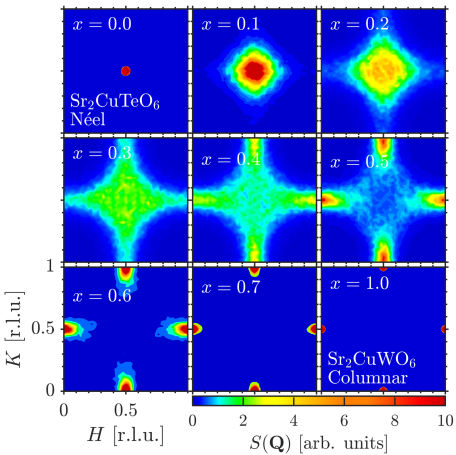
The ground state consists of patches of Néel and columnar correlations

An example of a real space configuation for $x = 0.9$

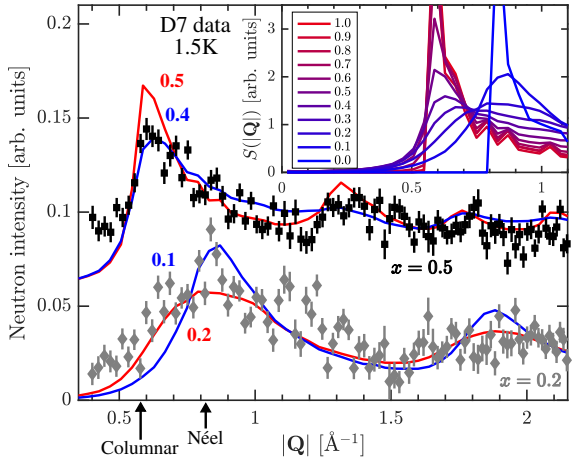


The ground state consists of patches of Néel and columnar correlations

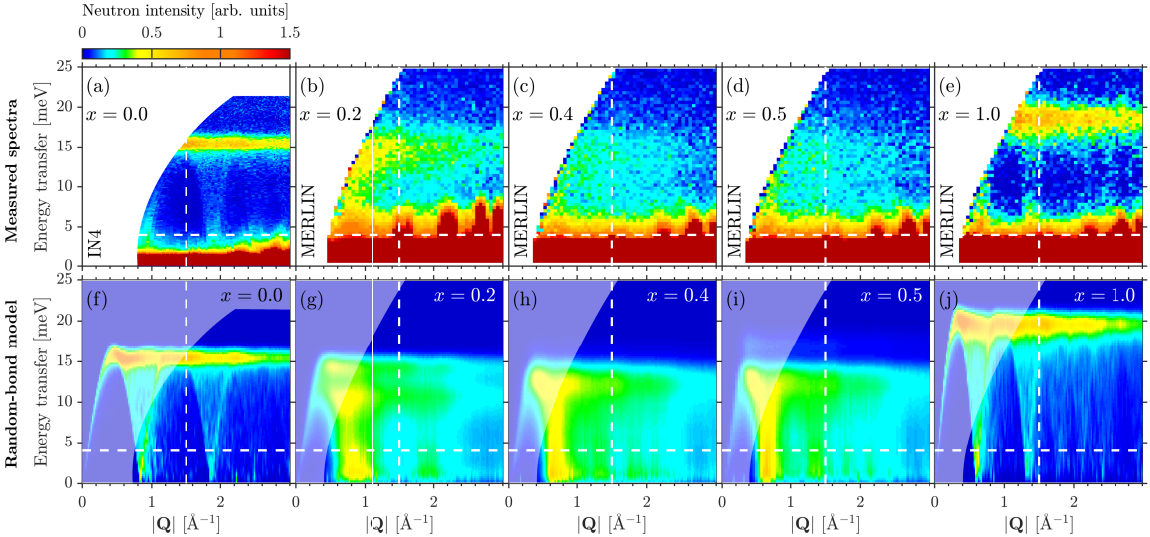
Predicted diffraction pattern



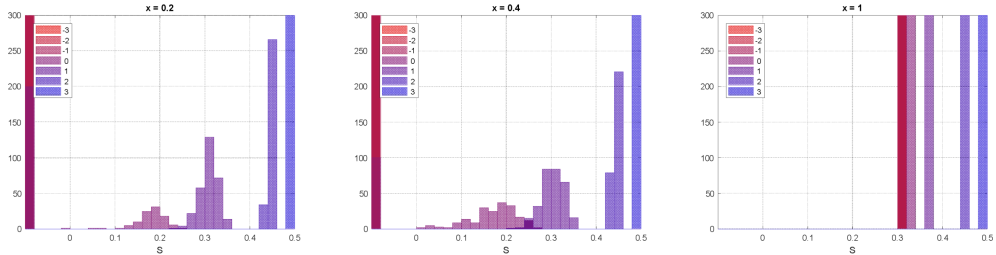
Diffuse neutron powder diffraction pattern



Linear spinwave calculations reproduce the features observed with inelastic neutron scattering



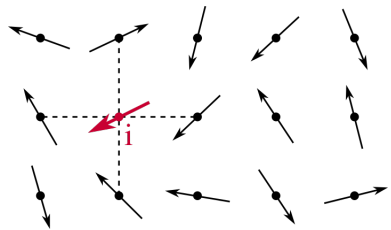
Is some part more *classical* and some part more *quantum mechanical*?



Reduced moment at some sites

Combination of frozen and fluctuating moments

Challenge and importance of theoretical understanding of inhomogenous systems



Conclusions

- $Sr_2CuTe_{1-x}W_xO_6$ is well-presented by a random-bond model
- The ground state in the mixed region has short-range correlations with patches of Néel and columnar correlations
- Randomness plays a larger role than frustration for governing the physics in the system