Experimental and theoretical investigation of the spin liquid candidate $PbCuTe_2O_6$

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UC Davis, July 13, 2018

Collaborators

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R. Thomale (Würzburg)

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arXiv:1712.07942

Outline

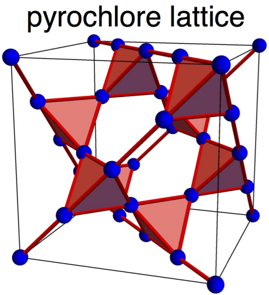
1. Known facts about $PbCuTe_2O_6$
2. Experimental neutron data
3. Theory results (DFT, pseudo-fermion functional renormalization group)
4. Conclusion

Known facts about $PbCuTe_2O_6$

Known facts about $PbCuTe_2O_6$

- Cu^{2+} ions carrying spin-1/2 magnetic moments
- μSR: no static magnetism down to 0.02K (PRL 116, 107203 (2016))
- No phase transition in heat capacity (PRB 90, 035141 (2014))
- Curie-Weiss-temperature: $\Theta_{\mathrm{CW}} = -22K$
  $\longrightarrow$ dominant antiferromagnetic interactions
- Lattice: (distorted) hyperkagome lattice
  $\longrightarrow$ hyper-hyperkagome lattice

Lattice structure of $PbCuTe_2O_6$



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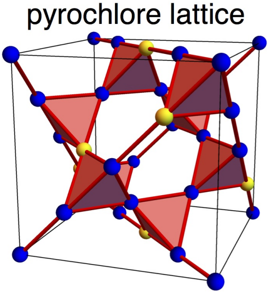

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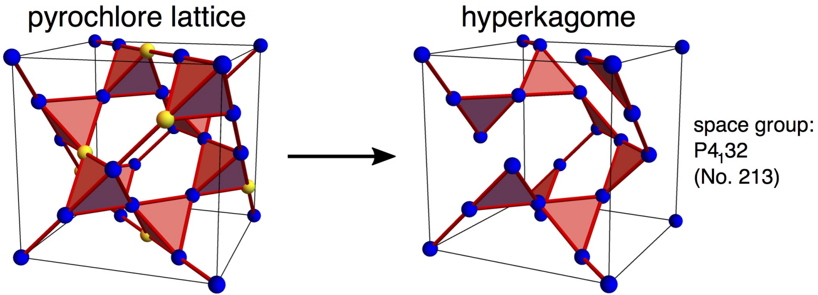

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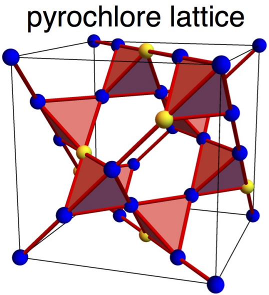
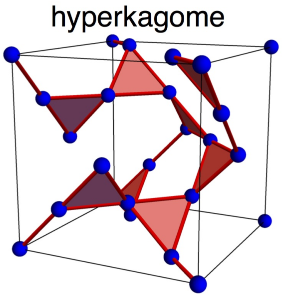
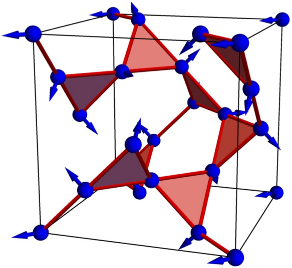




space group:
$P4_132$
(No. 213)



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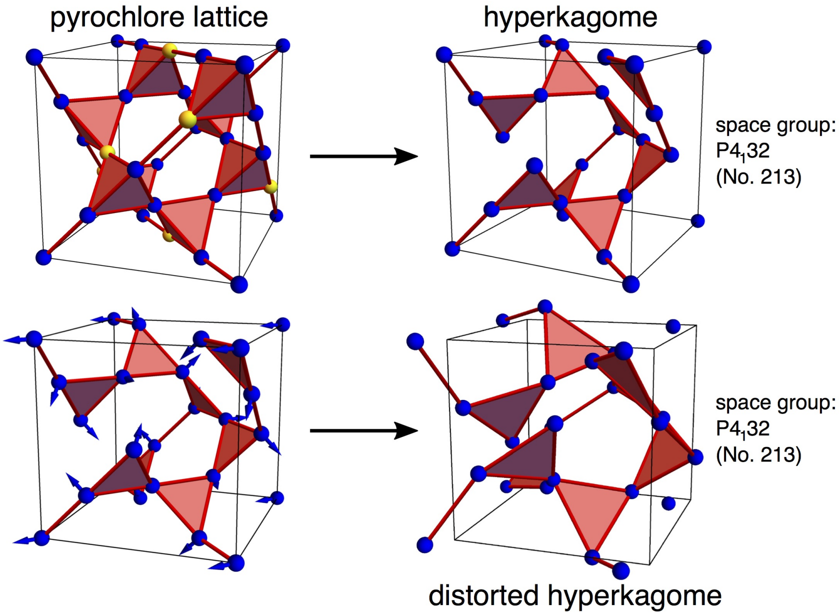

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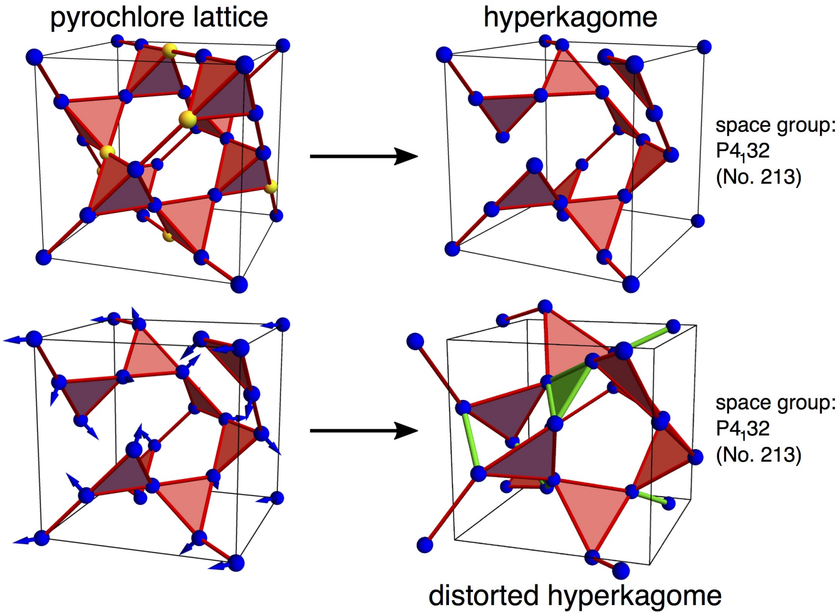

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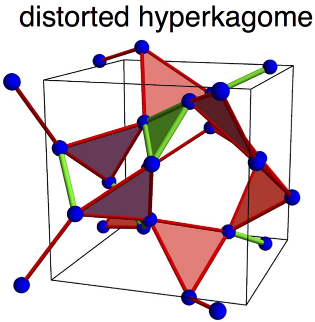
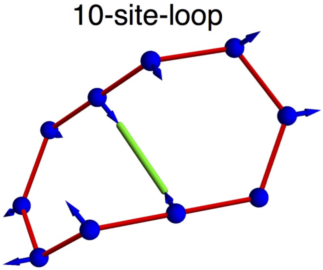
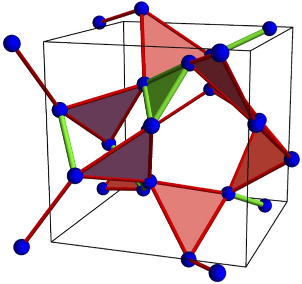


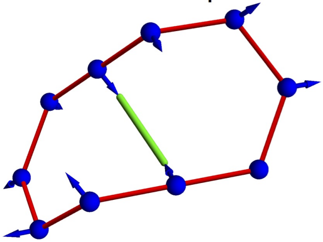


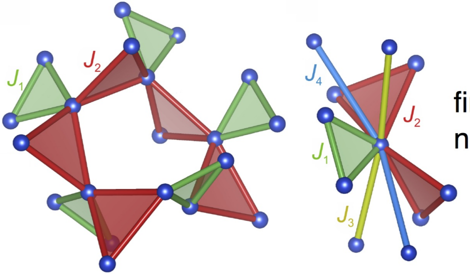
Lattice structure of $PbCuTe_2O_6$

distorted hyperkagome



10-site-loop

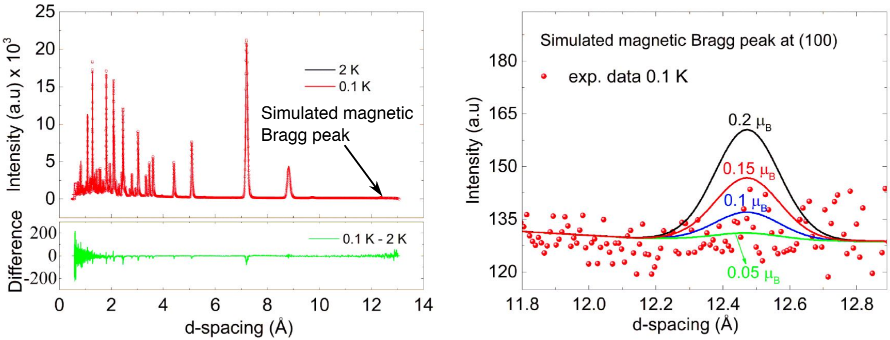




first to fourth neighbor bonds

Experimental neutron data

Powder neutron diffraction

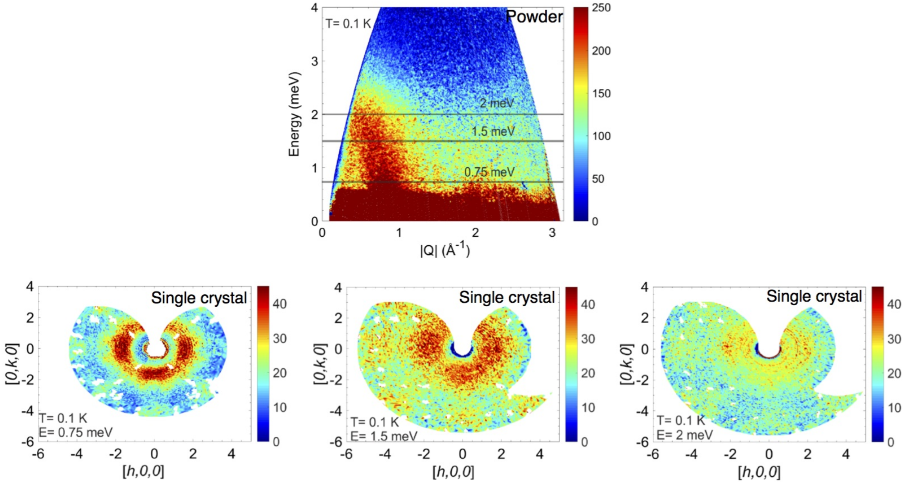


Diffraction peaks entirely described by crystal structure of $PbCuTe_2O_6$

$\longrightarrow$ no magnetic Bragg peak

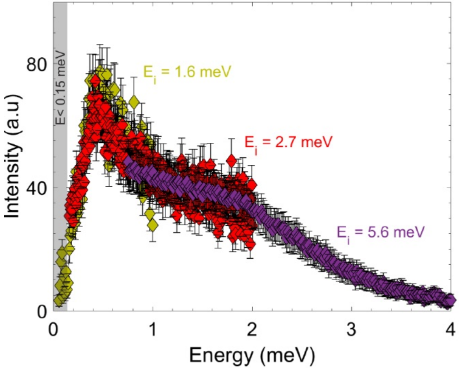
Upper bound: $0.05\mu_B$ per Cu^{2+} from iso-structural compound $SrCuTe_2O_6$.

Inelastic neutron scattering



Diffuse/broad rings of scattering suggestive of multi-spinon excitations in a quantum spin liquid.

Gapped/gapless ground state?



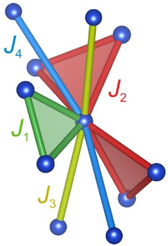
Low energy behavior: Decreasing intensity with decreasing energy.

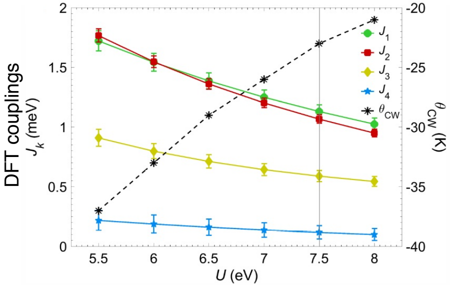
If a gap exists, it is smaller than 0.15meV.

Theory results (DFT, pseudo-fermion functional renormalization group)

Magnetic Hamiltonian from DFT

$$H = J_1 \sum_{\langle i,j \rangle_1} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle i,j \rangle_2} \vec{S}_i \vec{S}_j + J_3 \sum_{\langle i,j \rangle_3} \vec{S}_i \vec{S}_j + J_4 \sum_{\langle i,j \rangle_4} \vec{S}_i \vec{S}_j$$





DFT and fit to Curie-Weiss temperature:

$$J_1/J_2 = 1.06,\ J_3/J_2 = 0.55,\ J_4/J_2 = 0.11$$

$J_1 \approx J_2 \implies$ **hyper-hyperkagome lattice**

Comparison to previous second order perturbation theory (PRB 90, 035141):

$$J_1/J_2 = 0.54,\ J_3/J_2 = 0.77,\ J_4/J_2 = 0$$

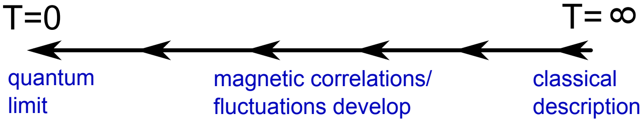
Pseudo-fermion functional renormalization group (PFFRG)

Express spin operators S_i^μ in terms of fermions ($f_{i\uparrow}$, $f_{i\downarrow}$ for each site i):

$$S_i^\mu = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^\mu f_{i\beta}$$

$\longrightarrow$ allows to use Feynman diagram techniques

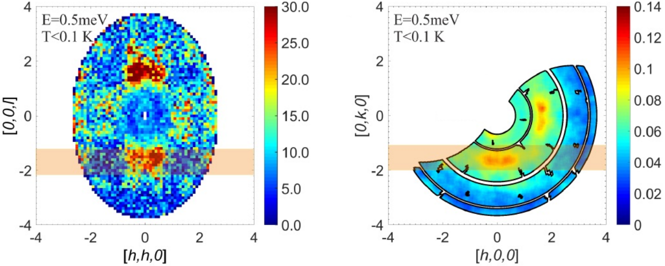
Renormalization group method: Calculate evolution of the magnetic susceptibility as a function of temperature $\frac{d}{dT}\chi(\mathbf{Q})$
($\sim$ simulate slow cooling process)



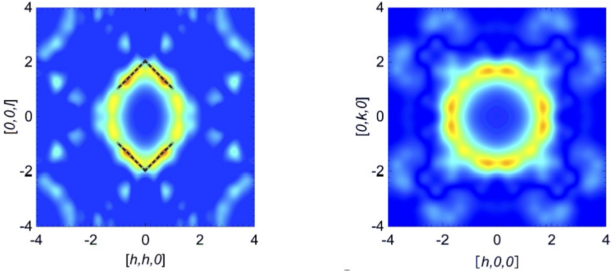
Magnetic order and non-magnetic phases can be investigated on equal footing.

Theory versus experiment

Neutron data:



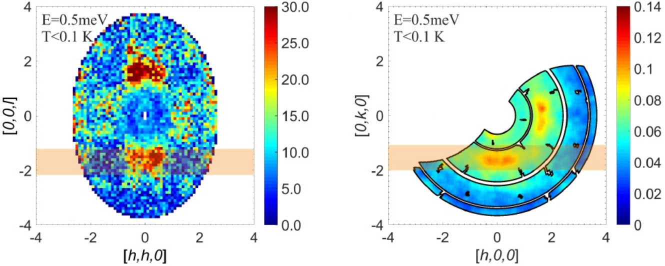
PFFRG results:



diffuse spinon-like scattering reproduced:
ring-like features, double peaks

Theory versus experiment

Neutron data:



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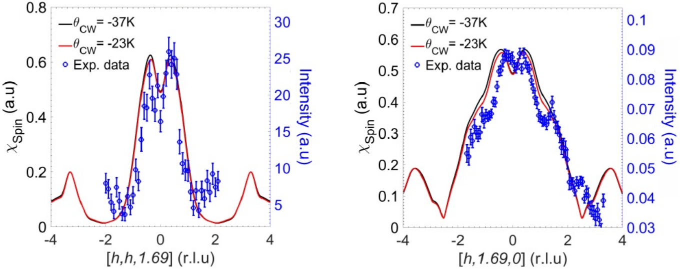
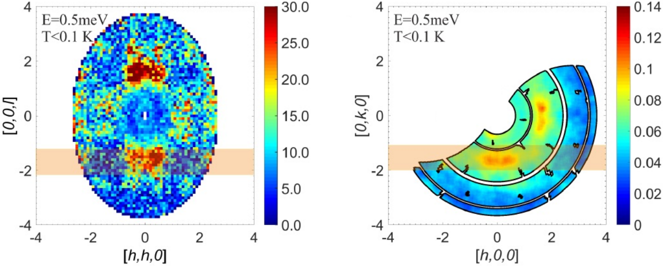


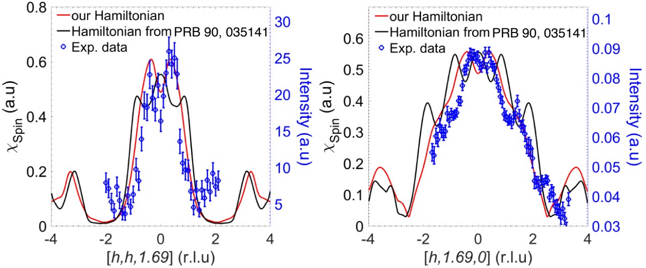
quantitative agreement of results!

Theory versus experiment

Neutron data:



PFFRG results for previous model:



$J_1/J_2=0.54$

$J_3/J_2=0.77$

$J_4=0$

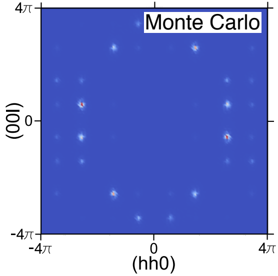
peak structures disagree

Discussion of experimental/theoretical results

Origin of the proposed spin liquid? Classical degeneracy?

Susceptibility from classical Monte Carlo for full J_1-J_2-J_3-J_4 model:

Magnetic order, no extensive classical degeneracy!



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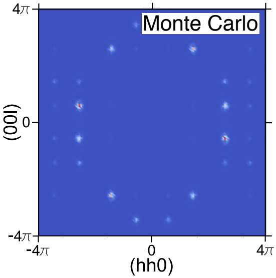
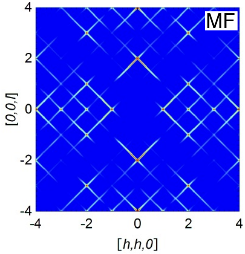
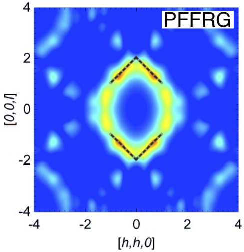


J_1-J_2-only model: streaks of intensity in classical mean-field susceptibility:





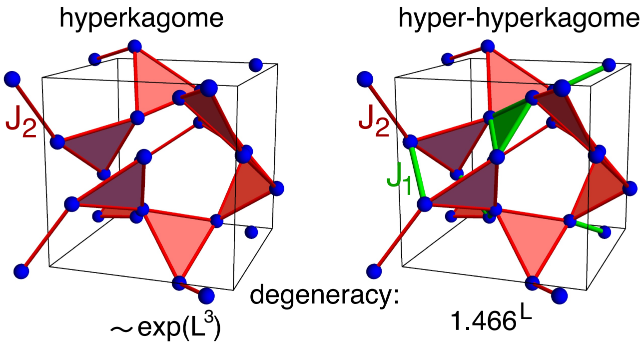
Classical degeneracy.

Qualitative agreement with full PFFRG result.

Classical degeneracy

Origin of classical degeneracy of J_1-J_2-only model:

"Ice rule" for each corner-sharing triangle: $\vec{S}_1 + \vec{S}_2 + \vec{S}_3 = 0$



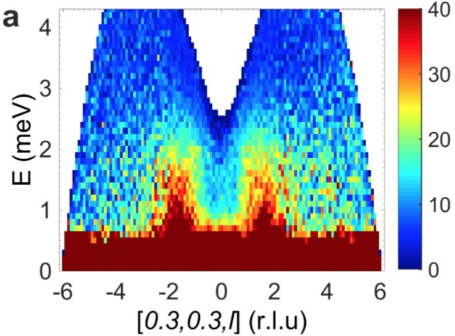
Subextensive degeneracy in the classical hyper-hyperkagome model (J_1-J_2-only model)

Conclusion

Conclusion

- $PbCuTe_2O_6$ exhibits characteristic features of a quantum spin liquid: Absence of static magnetism, diffuse dispersionless spinon-like excitations.
- Complex hyper-hyperkagome lattice Hamiltonian with J_1, J_2, J_3, J_4 interactions yields excellent agreement with PFFRG simulations.
- Minimal J_1-J_2-only model exhibits corner-sharing triangles and a subextensive classical degeneracy, possibly explaining the origin of strong frustration.

Thank you for your attention!


a
E (meV)
0
1
2
3
4
-6
-4
-2
0
2
4
6
[0.3,0.3,l] (r.l.u)
0
10
20
30
40