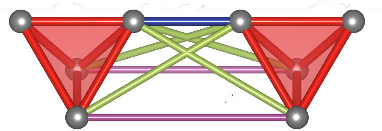
Chromium Breathing Pyrochlores

An exhibition of a variety of pyrochlore Hamiltonians

Pratyay Ghosh
Indian Institute of Technology Madras, Chennai, India



February 25, 2019

Collaborations

- Yasir Iqbal
- Tobias Müller
- Ronny Thomale
- Johannes Reuther
- Michel J. P. Gingras
- Harald O. Jeschke

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Acknowledgements

- Zenji Hiroi, Gøran Nilsen, Yoshihiko Okamoto, Owen Benton and Jason Gardner
- ICTS, Bengaluru, The 2nd Asia Pacific Workshop on Quantum Magnetism.
- SuperMUC

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INTRODUCTION

Spin systems, Frustration, Exotic quantum disorders, quantum-entangled spin liquid ground states, blah, blah, blah

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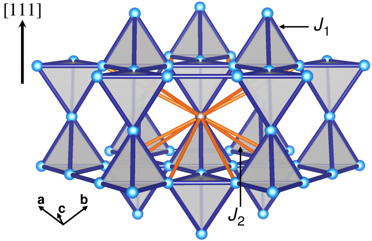
PYROCHLORE: CLASSICAL HEISENBERG MODEL

J_1-only model



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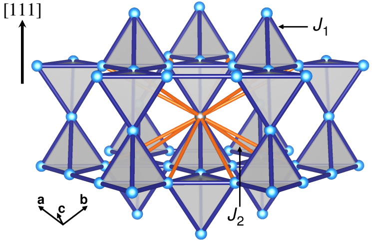

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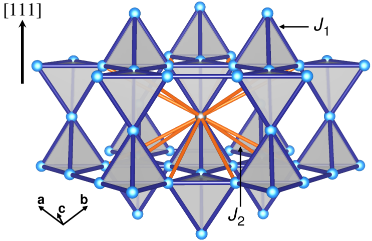

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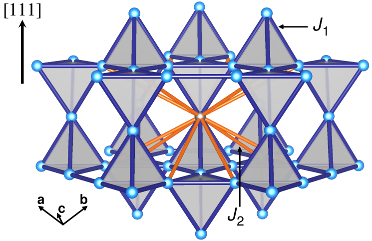

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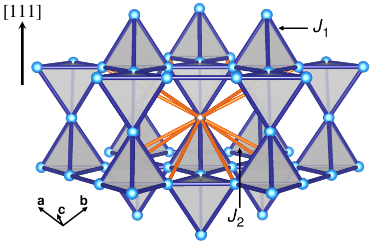

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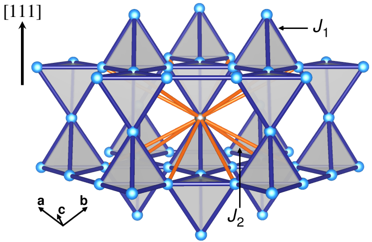

- extensive classical ground-state degeneracy
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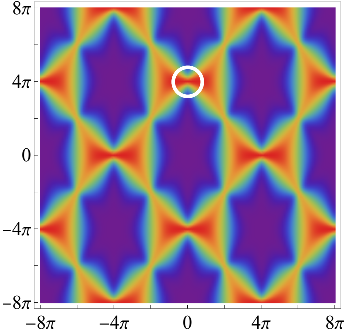

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PYROCHLORE: QUANTUM HEISENBERG MODEL

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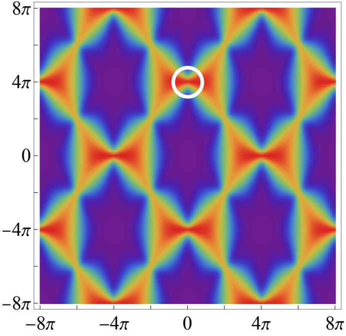

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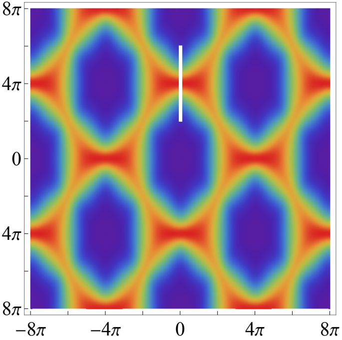

Phys. Rev. X 9, 011005 (2019)

PYROCHLORE: QUANTUM HEISENBERG MODEL

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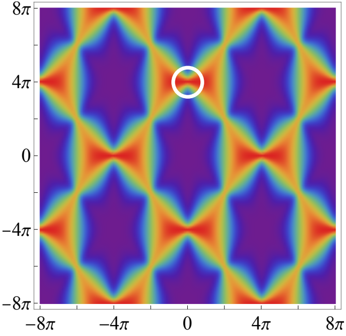

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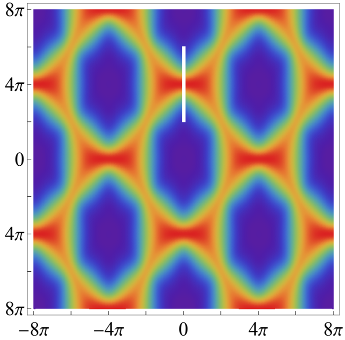


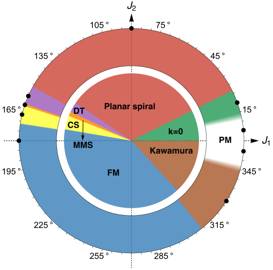
Coulomb spin-liquid

Phys. Rev. X 9, 011005 (2019)

PYROCHLORE: QUANTUM PHASE DIAGRAM

J_1-J_2 model

(a) $S = \frac{1}{2}$



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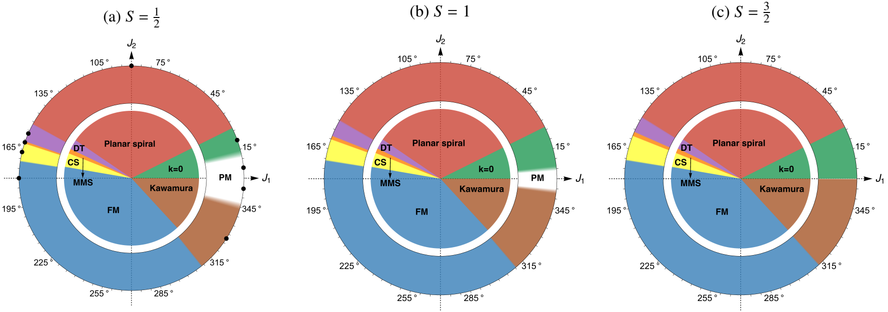
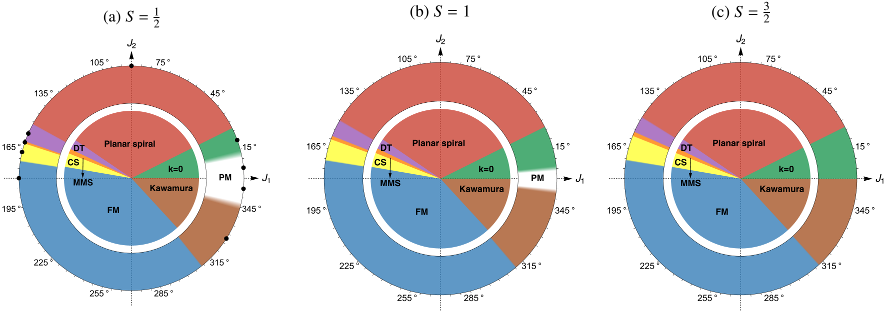


Phys. Rev. X 9, 011005 (2019)

Pyrochlore: Quantum Phase Diagram

J_1-J_2 model



We study the Cr^{3+} systems which are $S = 3/2$

Phys. Rev. X 9, 011005 (2019)

BREATHING PYROCHLORES

[1] Phys. Rev. Lett. 110, 097203 (2013)
[2] Phys. Rev. B 91, 174435 (2015)
[3] Phys. Rev. B 97, 134117 (2018)
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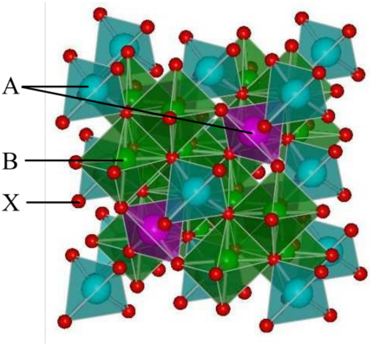
BREATHING PYROCHLORES

- Pyrochlore (AB_2X_4)



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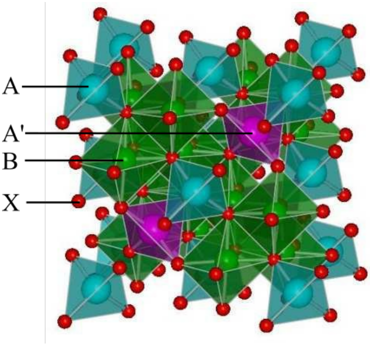

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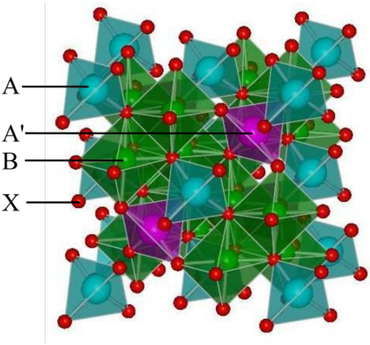

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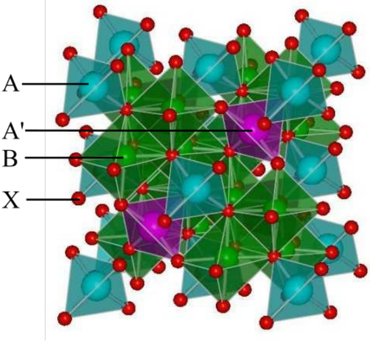

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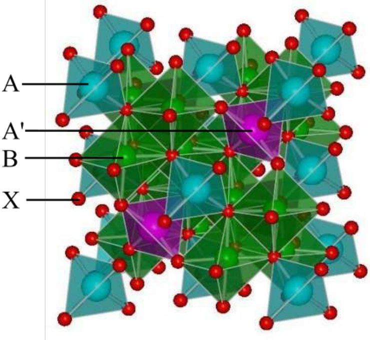

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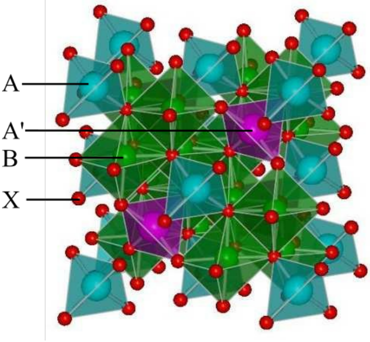

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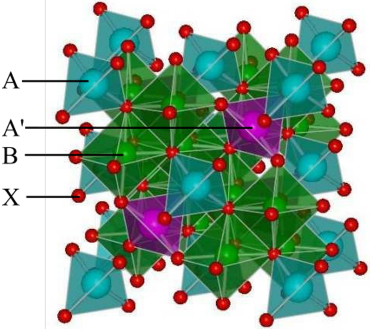

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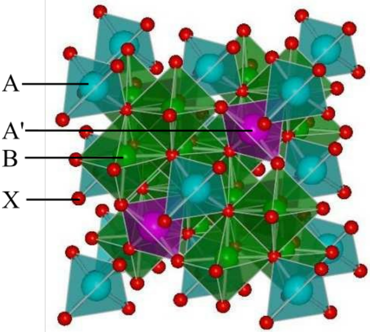

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Methodology

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- Pseudofermion functional renormalization group method ⇒ quantum ground state

PFFRG

Phys. Rev. B 83, 024402 (2011)
Phys. Rev. B 96, 045144 (2017)

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Fermionic Hamiltonian:

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

PFFRG

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Phys. Rev. B 96, 045144 (2017)

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Diagrammatics in the fermion:

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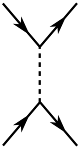
Diagrammatics in the fermion:

propagator: $G_0(i\omega) = \frac{1}{i\omega} =$ 

interaction vertex: $\Gamma_0 =$  $\sim J$

PFFRG

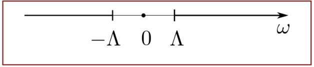
Functional Renormalization Group (FRG)

PFFRG

Functional Renormalization Group (FRG)

Infrared frequency cutoff

$$G_0(i\omega) = \frac{1}{i\omega} \rightarrow G_0^\Lambda(i\omega) = \frac{\Theta(|\omega|-\Lambda)}{i\omega}$$



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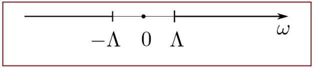
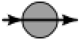


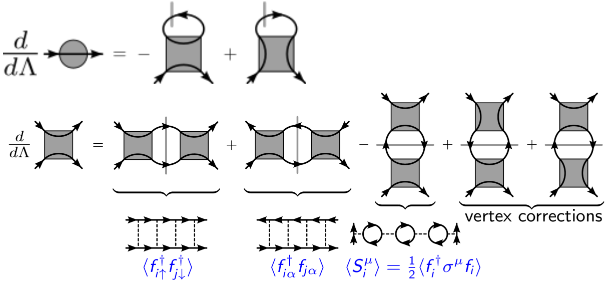
Vertex functions become Λ-dependent

$\Sigma =$  $\to \Sigma^\Lambda$

$\Gamma =$  $\to \Gamma^\Lambda$

PFFRG

Flow equations for self-energy and 2-particle vertex functions:



PFFRG

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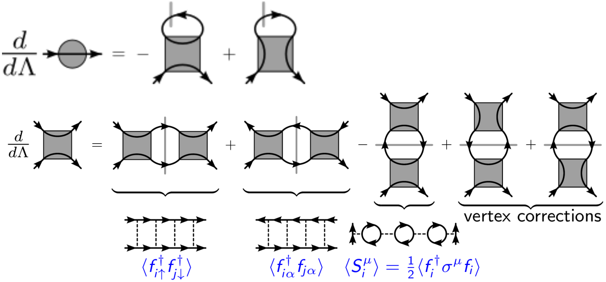
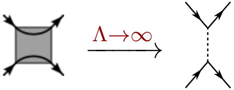


FRG flow starts with  $\sim J$ and ends at $\Lambda = 0$.

PFFRG

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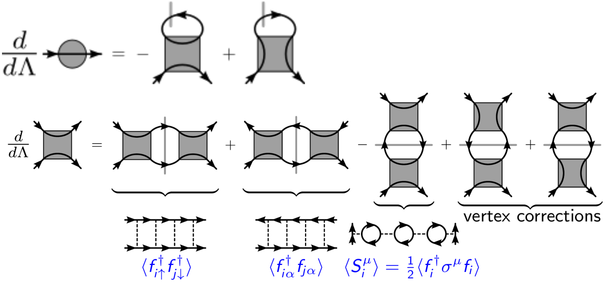
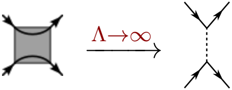
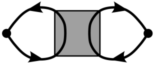


FRG flow starts with 

$\sim J$ and ends at $\Lambda = 0$.

Magnetic response (static susceptibility):

 $= \chi^\Lambda(\mathbf{k})$

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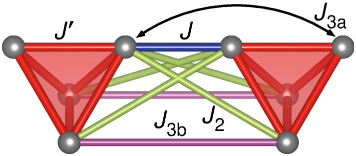
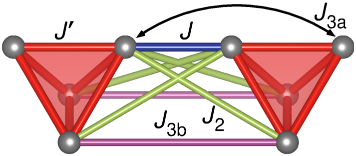
MODEL HAMILTONIAN



Model Hamiltonian



Material	J (K)	J' (K)	J_2 (K)	J_{3a} (K)	J_{3b} (K)
$LiInCr_4O_8$	59.8(2)	22.0(2)	0.3(1)	1.9(1)	0.9(1)
$CuInCr_4S_8$	14.7(1)	−26.0(1)	1.1(1)	6.4(1)	4.5(1)
$CuInCr_4Se_8$	−25.4(2)	−31.0(1)	0.3(1)	4.8(1)	3.9(1)

Oxides

$LiInCr_4O_8$

[6]Phys. Rev. B. 81, 224413 (2010)
[7]Phys. Rev. B, 78, 144418 (2008)

OXIDES

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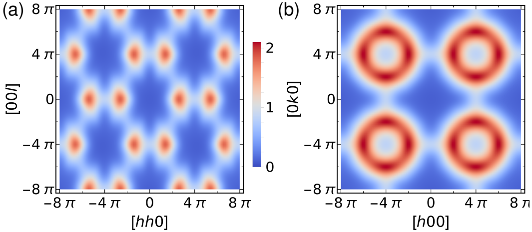

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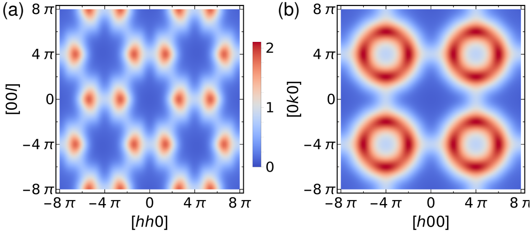

- $J'/J = 0.37$
- $J_2/J = 0.004$
- $J_{3a}/J = 0.03$
- $J_{3b}/J = 0.015$

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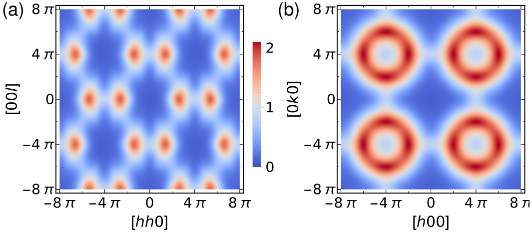

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Ordering pitch vector
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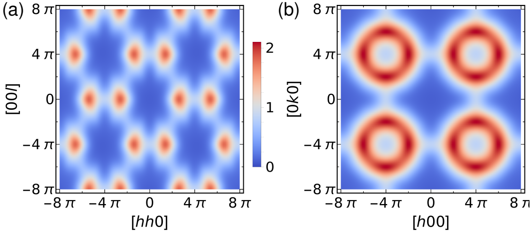
[7] Phys. Rev. B, 78, 144418 (2008)

OXIDES

$LiInCr_4O_8$



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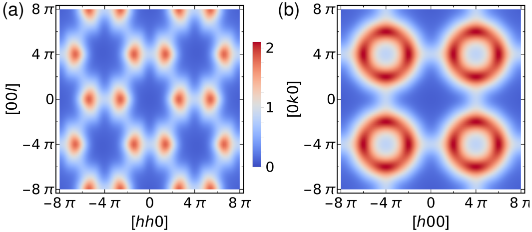

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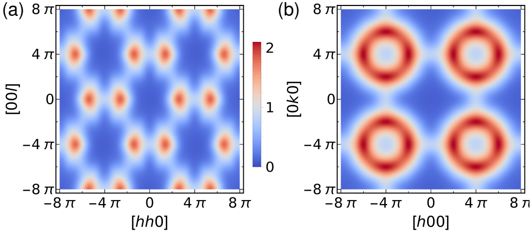

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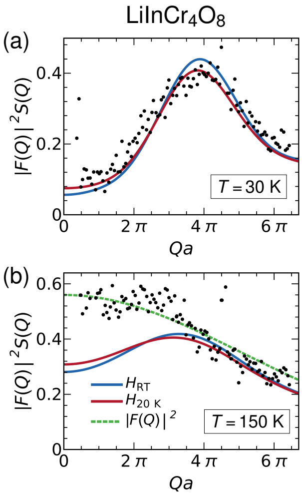
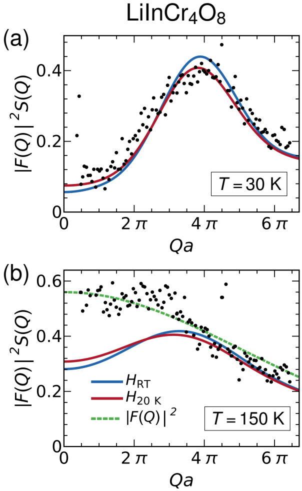
$J_{3a}/J \rightarrow (J_{3a} - J_2)/J = 0.026$

[6] Phys. Rev. B. 81, 224413 (2010)
[7] Phys. Rev. B, 78, 144418 (2008)

Oxides


LiInCr4O8
(a)
0.4
0.2
0
0
2 π
4 π
6 π
Qa
|F(Q)|²S(Q)
T = 30 K
(b)
0.6
0.4
0.2
0
0
2 π
4 π
6 π
Qa
|F(Q)|²S(Q)
H RT
H 20 K
|F(Q)|²
T = 150 K

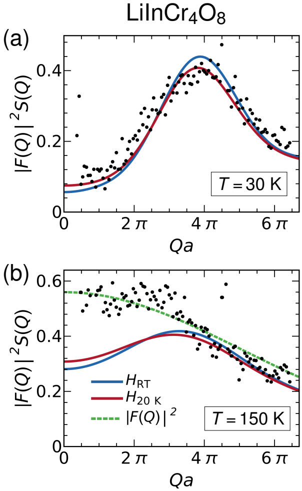
Oxides



Experimental data from J. Phys. Soc. Jpn. 84, 043707 (2015)

- Temperature dependent Hamiltonian

OXIDES



Experimental data from J. Phys. Soc. Jpn. 84, 043707 (2015)

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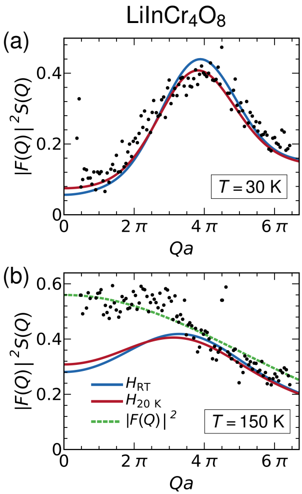
- absorption cross section in barns of Ga: 2.75

OXIDES



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$CuInCr_4S_8$

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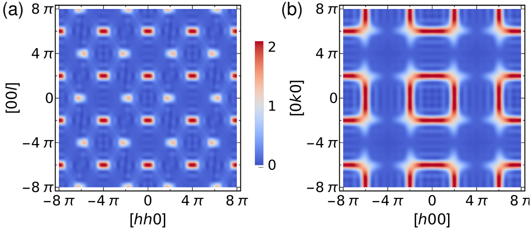

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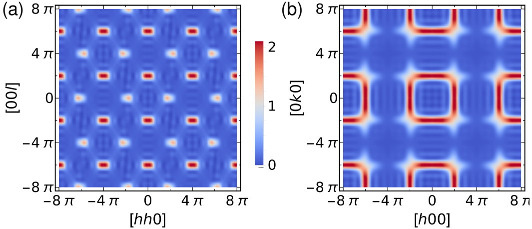

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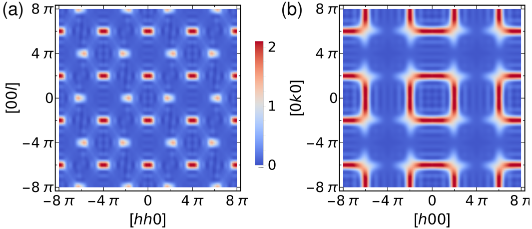

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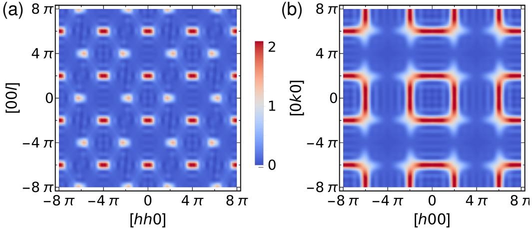

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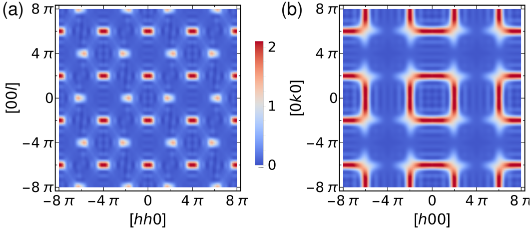

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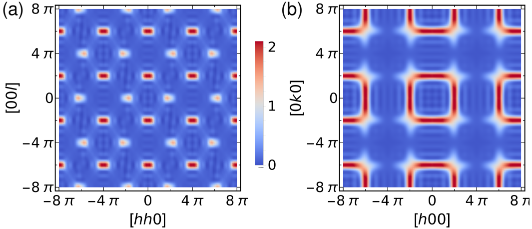

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  - $J_1^{fcc} = (J + 4J_2 + 2J_{3a} + 2J_{3b})/16$

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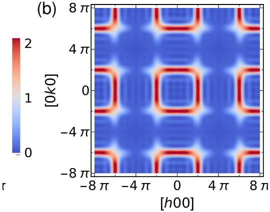

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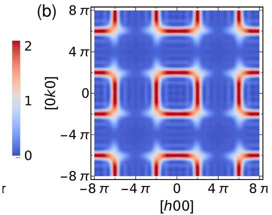

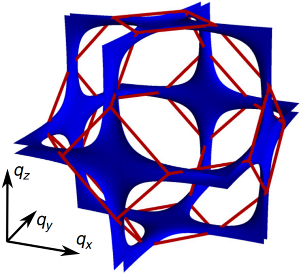

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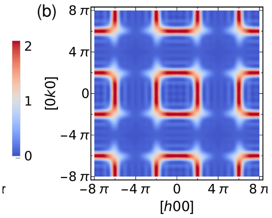

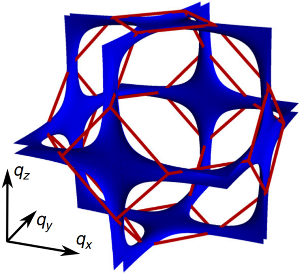

- Intersection of $\mathbf{q} = \frac{2\pi}{a}(1, \delta, 0)$ and $\mathbf{q} = \frac{2\pi}{a}(1, 0, \delta)$

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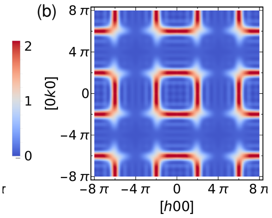
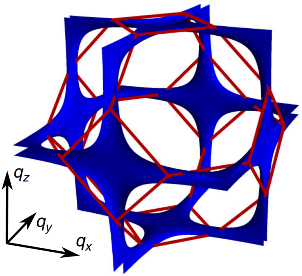
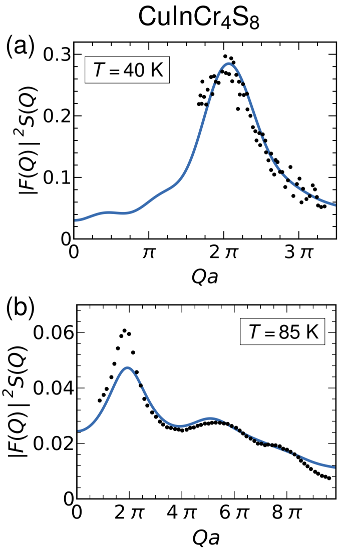


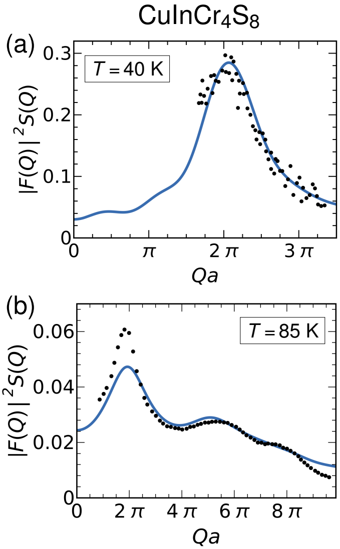


- Intersection of $\mathbf{q} = \frac{2\pi}{a}(1, \delta, 0)$ and $\mathbf{q} = \frac{2\pi}{a}(1, 0, \delta)$
- "Order by disorder" selects $\mathbf{q} = \frac{2\pi}{a}(1, 0, 0)$

SULFIDES

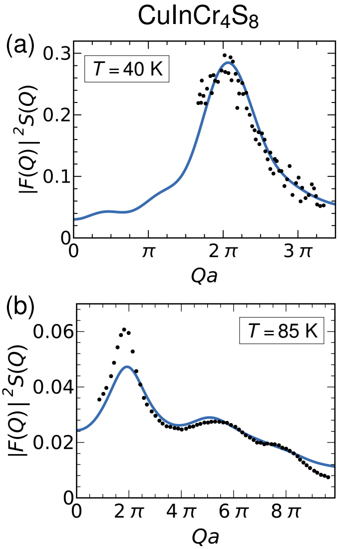

CuInCr4S8
(a)
T = 40 K
|F(Q)|2S(Q)
0.3
0.2
0.1
0
0
π
2 π
3 π
Qa
(b)
T = 85 K
|F(Q)|2S(Q)
0.06
0.04
0.02
0
0
2 π
4 π
6 π
8 π
Qa

Sulfides



Experimental data from J. Phys. Colloques 32, C1-324 (1971) and Phys. Lett. 60A, 431 (1977).

SULFIDES



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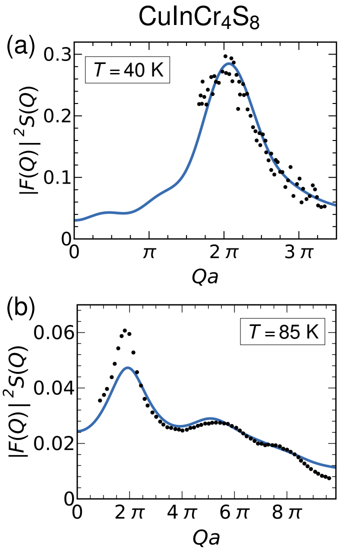
Sulfides



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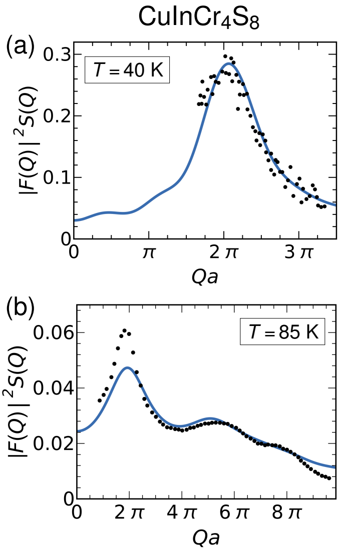

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SELENIDE

$CuInCr_4Se_8$

[9] Phys. Rev. B. 81, 224413 (2010)

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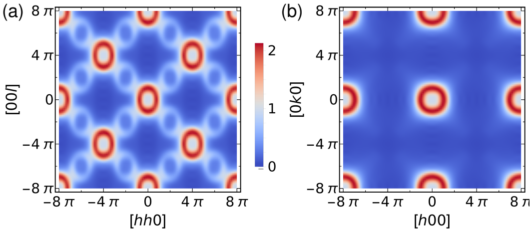

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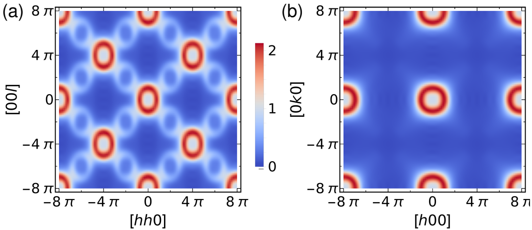

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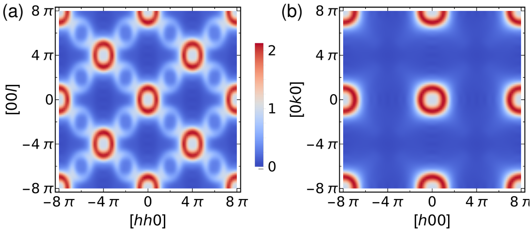

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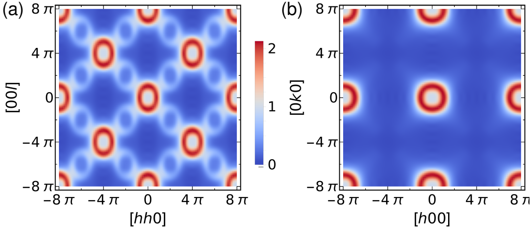

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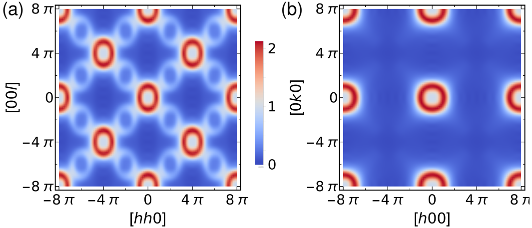

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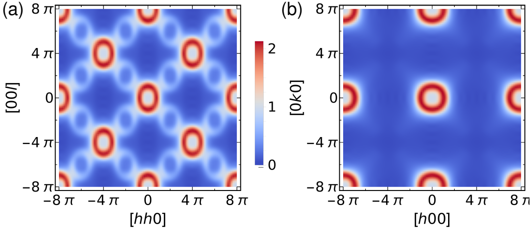

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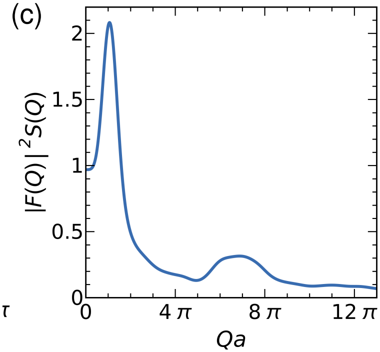

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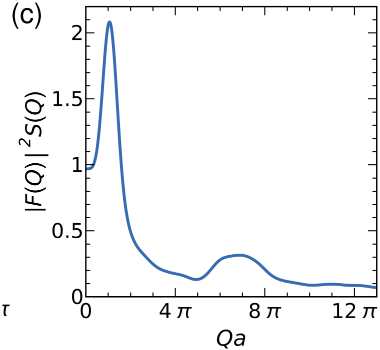

"Inarticulated" matching with the unpolarized neutron scattering data

MAGNETIC ORDERING IN THE NORMAL SPINEL $Cu_{0.5}In_{0.5}Cr_2Se_4$

R. Plumier and M. Sougi

Solid State Communications, Vol. 69, No. 4, pp.341-345, 1989.

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- The temperature dependence of these systems?


THANK YOU FOR LISTENING
ANY QUESTION???
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