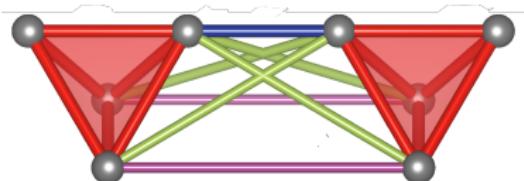


Chromium Breathing Pyrochlores

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

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- ▶ 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

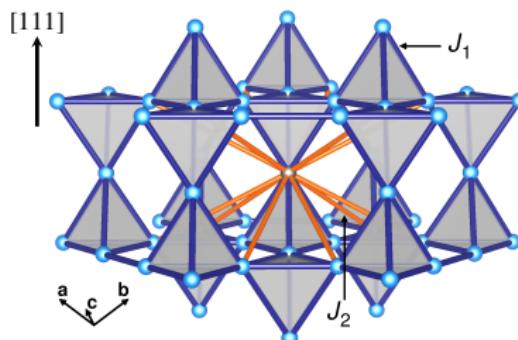
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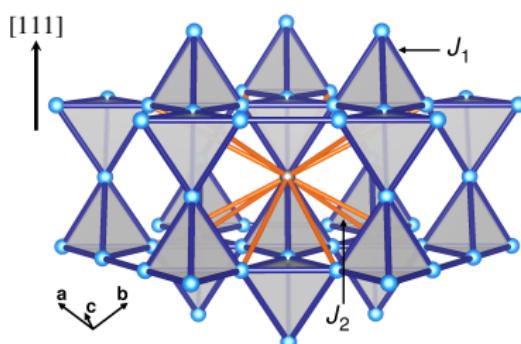
PYROCHLORE: CLASSICAL HEISENBERG MODEL

J_1 -only model



PYROCHLORE: CLASSICAL HEISENBERG MODEL

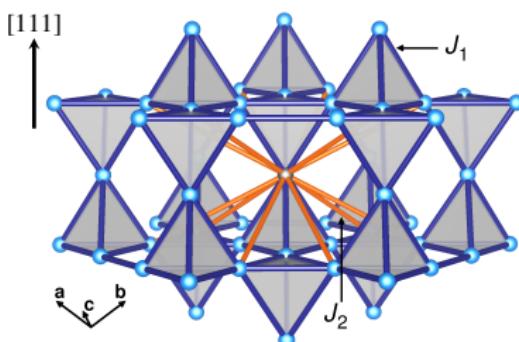
J_1 -only model



- ▶ extensive classical ground-state degeneracy

PYROCHLORE: CLASSICAL HEISENBERG MODEL

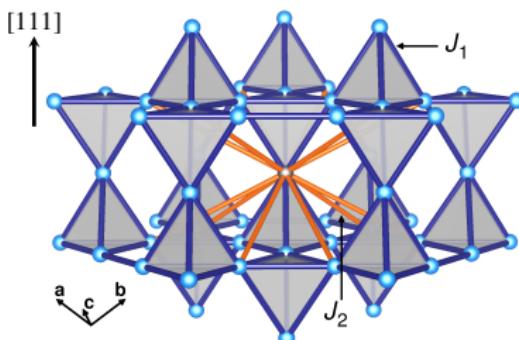
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- ▶ extensive classical ground-state degeneracy
- ▶ no magnetic long-range order down to $T = 0$

PYROCHLORE: CLASSICAL HEISENBERG MODEL

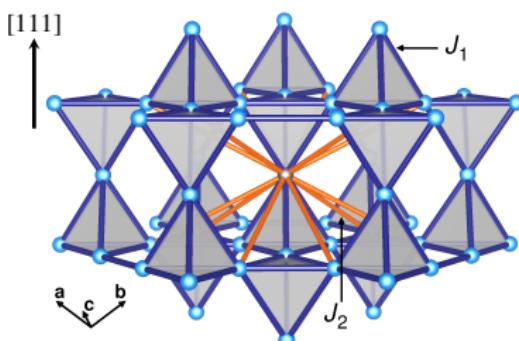
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- ▶ extensive classical ground-state degeneracy
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- ▶ cooperative paramagnet \Leftrightarrow “spin-ice”

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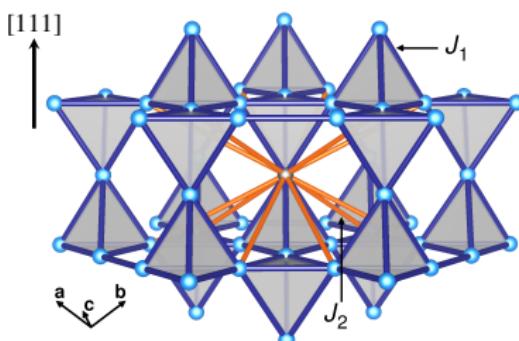
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- ▶ extensive classical ground-state degeneracy
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 (“ice rule”: $\sum_{i=1}^4 \vec{S}_i = 0$)

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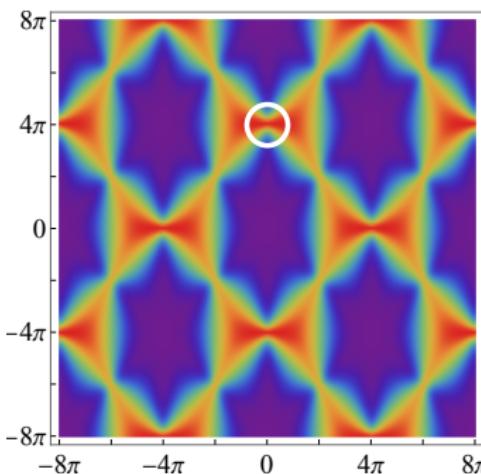
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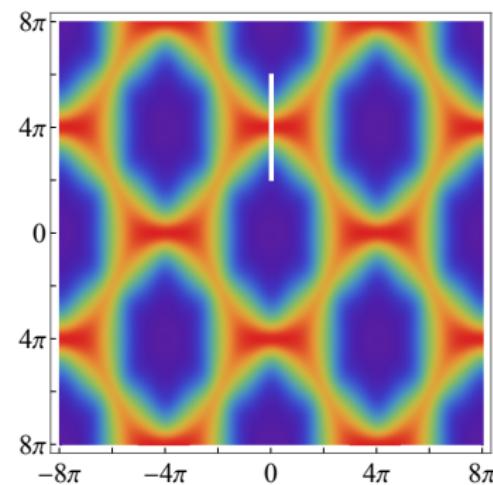
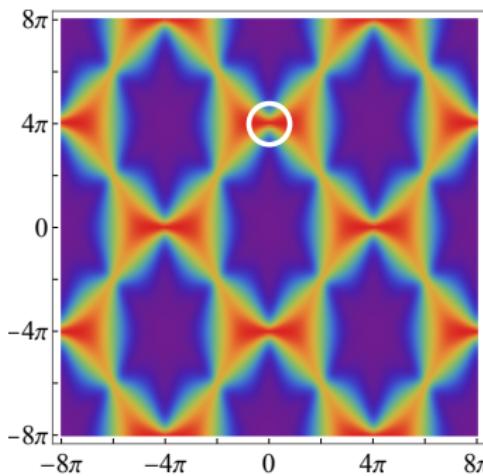
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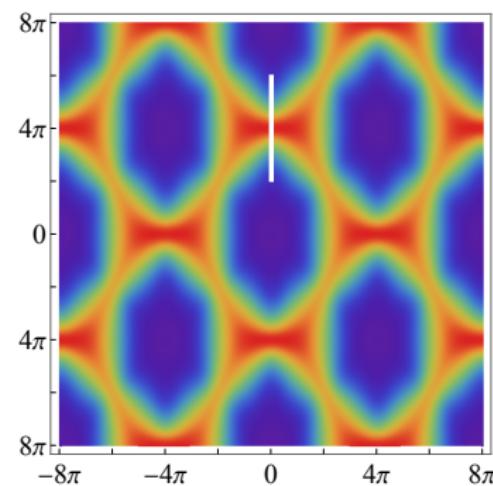
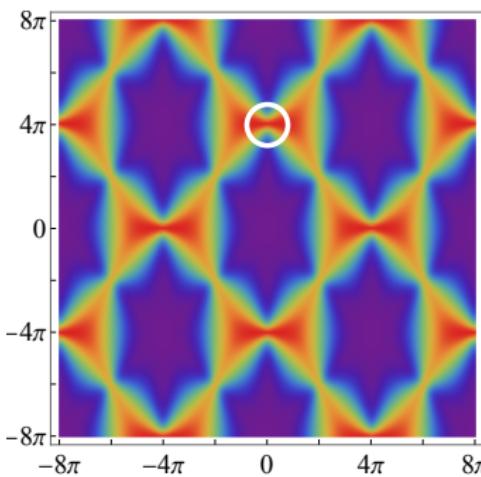
PYROCHLORE: QUANTUM HEISENBERG MODEL

J_1 -only model



PYROCHLORE: QUANTUM HEISENBERG MODEL

J_1 -only model

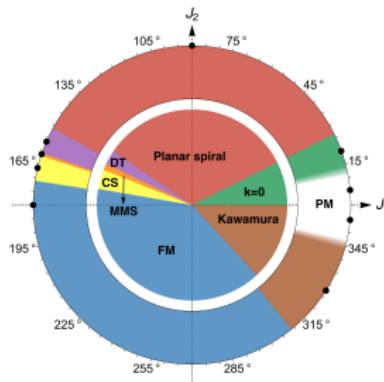


Coulomb spin-liquid

PYROCHLORE: QUANTUM PHASE DIAGRAM

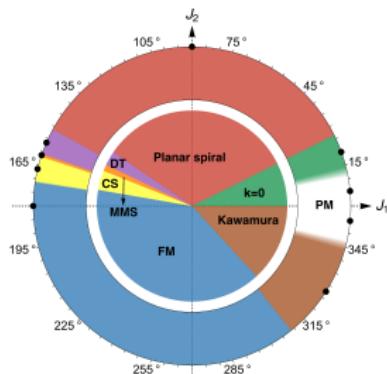
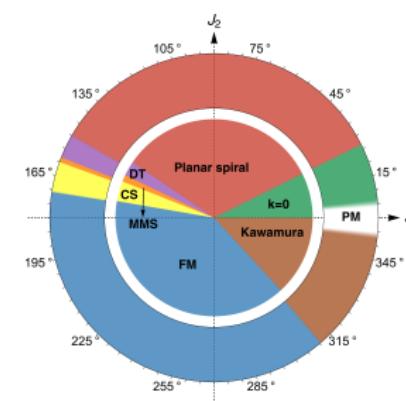
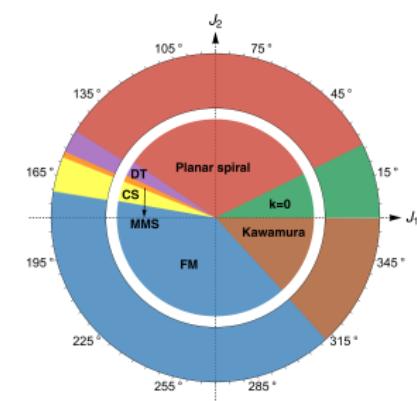
J_1 - J_2 model

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



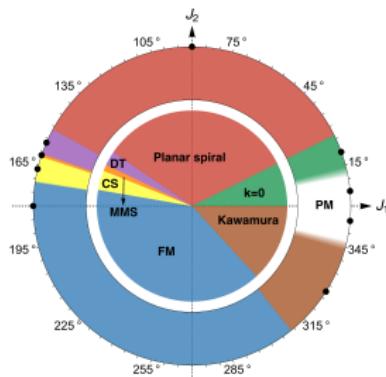
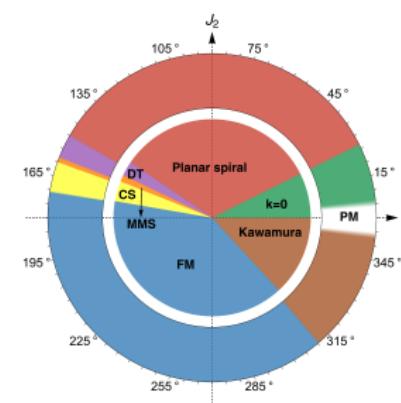
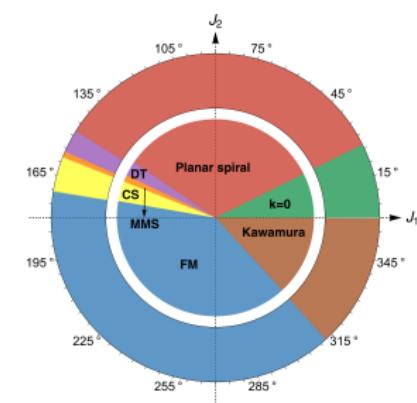
PYROCHLORE: QUANTUM PHASE DIAGRAM

J_1 - J_2 model

(a) $S = \frac{1}{2}$ (b) $S = 1$ (c) $S = \frac{3}{2}$ 

PYROCHLORE: QUANTUM PHASE DIAGRAM

J_1 - J_2 model

(a) $S = \frac{1}{2}$ (b) $S = 1$ (c) $S = \frac{3}{2}$ 

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

BREATHING PYROCHLORES

¹Phys. Rev. Lett. 110, 097203 (2013)

²Phys. Rev. B 91, 174435 (2015)

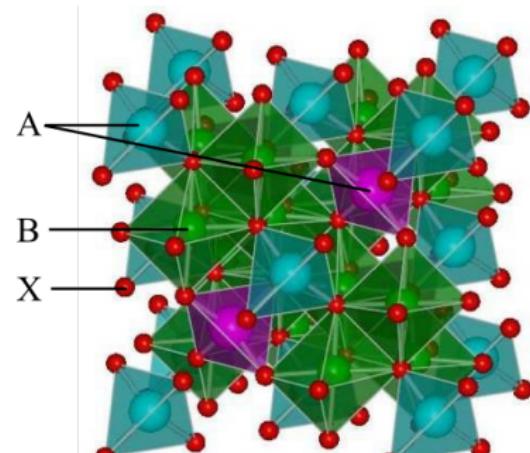
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BREATHING PYROCHLORES

- ▶ Pyrochlore (AB_2X_4)



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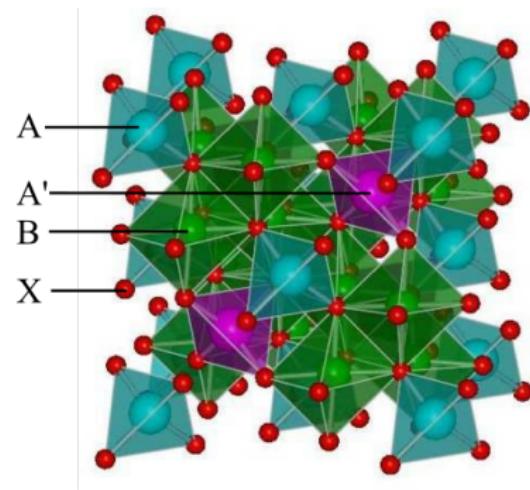
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BREATHING PYROCHLORES

- Pyrochlore (AB_2X_4) \Rightarrow Breathing Pyrochlore ($AA'B_4O_8$)



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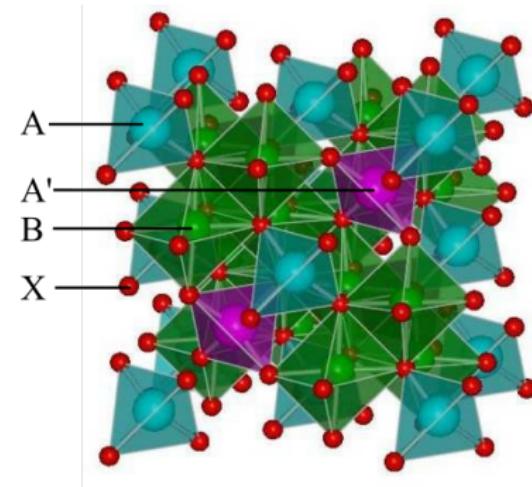
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BREATHING PYROCHLORES

- ▶ Pyrochlore (AB_2X_4) \Rightarrow Breathing Pyrochlore ($AA'B_4O_8$)
- ▶ **Size mismatch** between A and A'
 - ▶ $Fd\bar{3}m \rightarrow F\bar{4}3m$ (Symmetry reduction)



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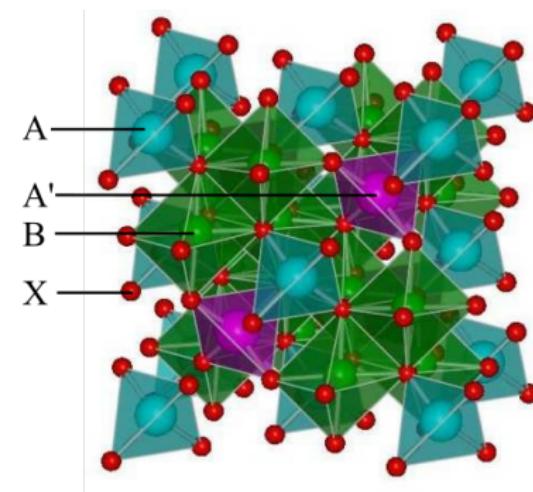
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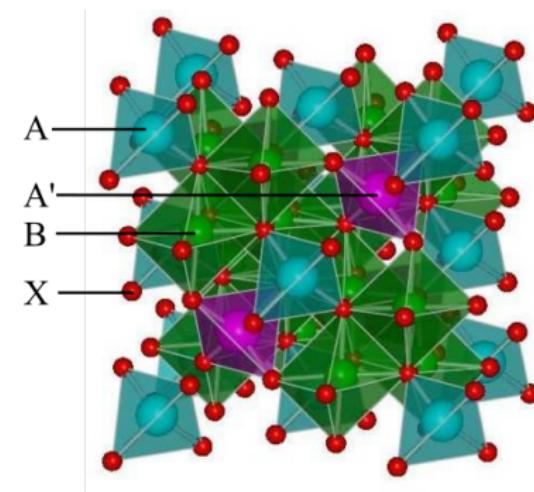
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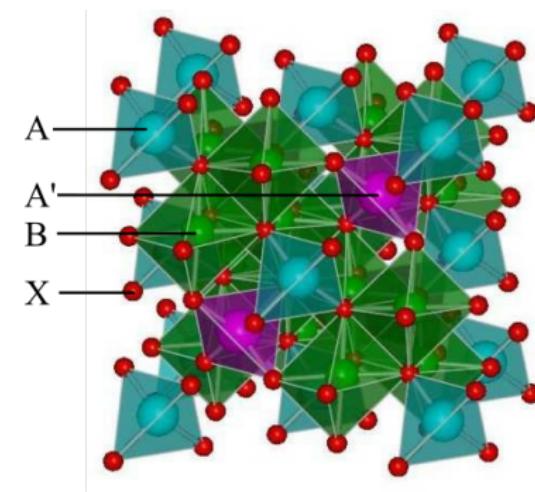
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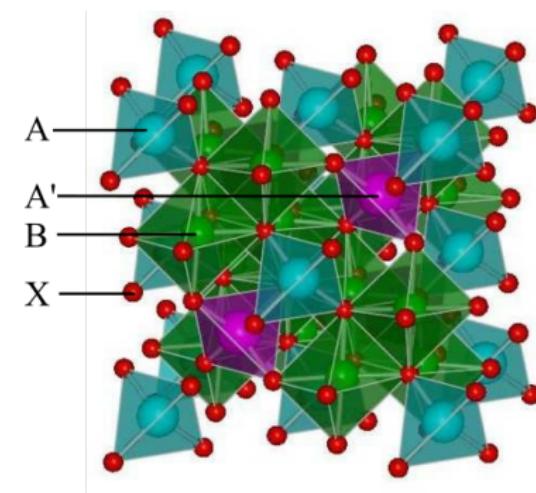
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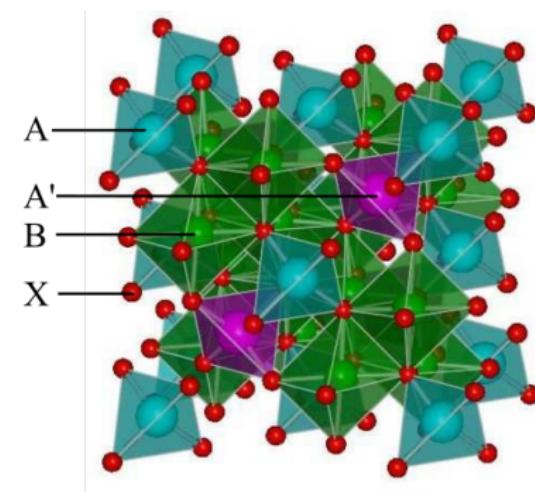
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- ▶ Energy mapping method ⇒ **model Hamiltonian**

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METHODOLOGY

- ▶ Energy mapping method ⇒ model Hamiltonian
- ▶ Iterative minimization method ⇒ classical ground state
- ▶ Pseudofermion functional renormalization group method
⇒ quantum ground state

PFFRG

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

PFFRG

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

Fermionic Hamiltonian:

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

PFFRG

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

Fermionic Hamiltonian:

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \rightarrow \frac{1}{4} \sum_{ij} J_{ij} \sum_{\mu} (f_i^{\dagger} \sigma^{\mu} f_i) (f_j^{\dagger} \sigma^{\mu} f_j)$$

PFFRG

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Diagrammatics in the fermion:

PFFRG

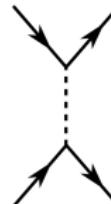
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Diagrammatics in the fermion:

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



interaction vertex: $\Gamma_0 = \sim J$



PFFRG

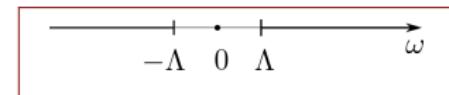
Functional Renormalization Group (FRG)

PFFRG

Functional Renormalization Group (FRG)

Infrared frequency cutoff

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

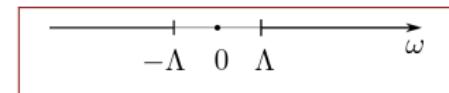


PFFRG

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Infrared frequency cutoff

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



Vertex functions become Λ -dependent

$$\Sigma = \text{Diagram with two external arrows pointing right} \rightarrow \Sigma^\Lambda$$

$$\Gamma = \text{Diagram with four external arrows forming a square loop} \rightarrow \Gamma^\Lambda$$

PFFRG

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

The diagram illustrates the flow equations for the self-energy and 2-particle vertex functions. The top row shows the flow equation for the self-energy, where the derivative $\frac{d}{d\Lambda}$ acts on a shaded loop diagram. The right side of the equation is the sum of two terms: a diagram with a vertical line and a curved line forming a loop, and a diagram with a curved line forming a loop. The middle row shows the flow equation for the 2-particle vertex function, where the derivative $\frac{d}{d\Lambda}$ acts on a shaded loop diagram. The right side of the equation is the sum of four terms, each enclosed in a brace and labeled 'vertex corrections'. The bottom row shows the 2-particle vertex function $\langle f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger \rangle$ and its components $\langle f_{i\alpha}^\dagger f_{j\alpha} \rangle$ and $\langle S_i^\mu \rangle = \frac{1}{2} \langle f_i^\dagger \sigma^\mu f_i \rangle$.

$$\frac{d}{d\Lambda} \text{ (shaded loop)} = - \text{ (vertical line, curved line loop)} + \text{ (curved line loop)}$$
$$\frac{d}{d\Lambda} \text{ (shaded loop)} = \underbrace{\text{ (shaded loop, double line loop)}}_{\text{vertex corrections}} + \underbrace{\text{ (shaded loop, triple line loop)}}_{\text{vertex corrections}} - \underbrace{\text{ (shaded loop, quadruple line loop)}}_{\text{vertex corrections}} + \underbrace{\text{ (shaded loop, five-line loop)}}_{\text{vertex corrections}}$$
$$\langle f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger \rangle \quad \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle \quad \langle S_i^\mu \rangle = \frac{1}{2} \langle f_i^\dagger \sigma^\mu f_i \rangle$$

PFFRG

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

The diagram shows two flow equations. The top equation is for the self-energy Σ , which starts with a bare self-energy Σ_0 (a grey circle with an arrow) and flows to a full self-energy Σ_f (a shaded box with an arrow), represented by the equation $\frac{d}{d\Lambda} \Sigma_0 = - \Sigma_f + \Sigma_f^*$. The bottom equation is for the 2-particle vertex function Γ , which starts with a bare vertex Γ_0 (a grey box with an arrow) and flows to a full vertex Γ_f (a shaded box with an arrow). This is shown as $\frac{d}{d\Lambda} \Gamma_0 = \Gamma_f + \text{vertex corrections}$, where the vertex corrections are represented by three diagrams: a double line with arrows, a double line with dashed arrows, and a loop of four circles with arrows.

$$\frac{d}{d\Lambda} \Sigma_0 = - \Sigma_f + \Sigma_f^*$$
$$\frac{d}{d\Lambda} \Gamma_0 = \Gamma_f + \text{vertex corrections}$$
$$\langle f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger \rangle \quad \langle f_{i\alpha}^\dagger f_{j\alpha} \rangle \quad \langle S_i^\mu \rangle = \frac{1}{2} \langle f_i^\dagger \sigma^\mu f_i \rangle$$

FRG flow starts with $\xrightarrow{\Lambda \rightarrow \infty}$ $\sim J$ and ends at $\Lambda = 0$.

PFFRG

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

$$\frac{d}{d\Lambda} \begin{array}{c} \text{circle with arrow} \\ \rightarrow \end{array} = - \begin{array}{c} \text{square with curved arrows} \\ \rightarrow \end{array} + \begin{array}{c} \text{square with curved arrows} \\ \leftarrow \end{array}$$
$$\frac{d}{d\Lambda} \begin{array}{c} \text{square with curved arrows} \\ \nearrow \searrow \end{array} = \underbrace{\begin{array}{c} \text{square with curved arrows} \\ \nearrow \searrow \end{array}}_{\langle f_i^\dagger f_j^\dagger \rangle} + \underbrace{\begin{array}{c} \text{square with curved arrows} \\ \nearrow \searrow \end{array}}_{\langle f_{i\alpha}^\dagger f_{j\alpha} \rangle} - \underbrace{\begin{array}{c} \text{square with curved arrows} \\ \nearrow \searrow \end{array}}_{\text{vertex corrections}} + \underbrace{\begin{array}{c} \text{square with curved arrows} \\ \nearrow \searrow \end{array}}_{\langle S_i^\mu \rangle = \frac{1}{2} \langle f_i^\dagger \sigma^\mu f_i \rangle}$$

FRG flow starts with $\xrightarrow{\Lambda \rightarrow \infty}$ $\sim J$ and ends at $\Lambda = 0$.

Magnetic response (static susceptibility):

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

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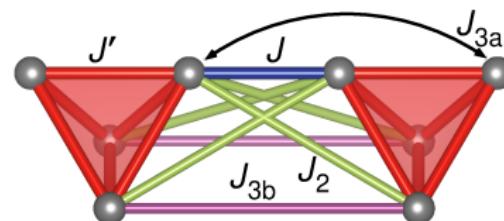
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Sulfides

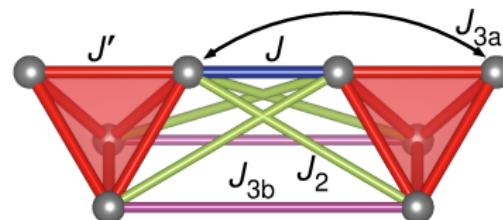
Selenide

CONCLUSIONS

MODEL HAMILTONIAN



MODEL HAMILTONIAN



Material	J (K)	J' (K)	J_2 (K)	J_{3a} (K)	J_{3b} (K)
$\text{LiInCr}_4\text{O}_8$	59.8(2)	22.0(2)	0.3(1)	1.9(1)	0.9(1)
$\text{CuInCr}_4\text{S}_8$	14.7(1)	-26.0(1)	1.1(1)	6.4(1)	4.5(1)
$\text{CuInCr}_4\text{Se}_8$	-25.4(2)	-31.0(1)	0.3(1)	4.8(1)	3.9(1)

OXIDES

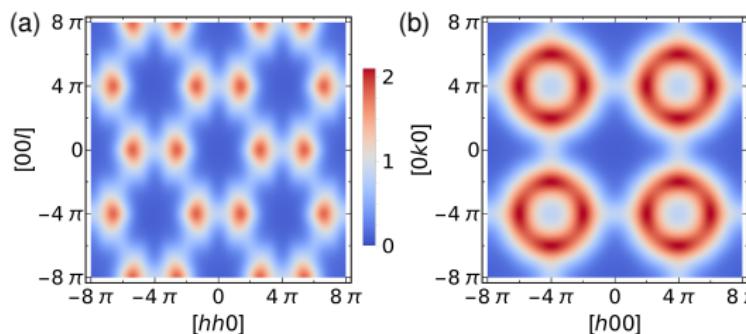
$\text{LiInCr}_4\text{O}_8$

⁶Phys. Rev. B, 81, 224413 (2010)

⁷Phys. Rev. B, 78, 144418 (2008)

OXIDES

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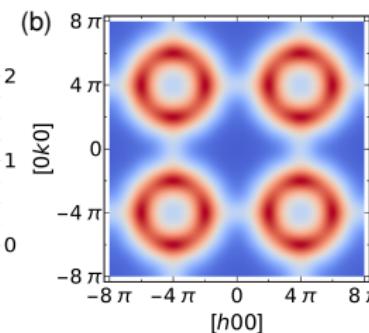
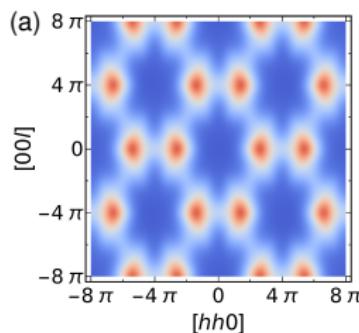


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OXIDES

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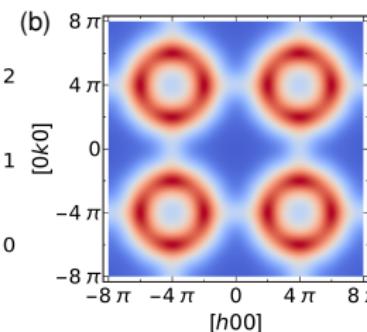
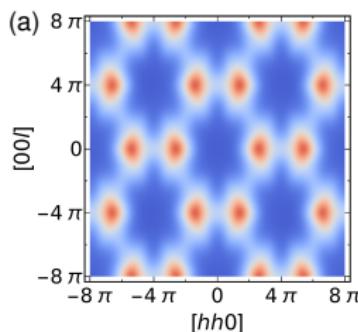


- $J'/J = 0.37$
- $J_2/J = 0.004$
- $J_{3a}/J = 0.03$
- $J_{3b}/J = 0.015$

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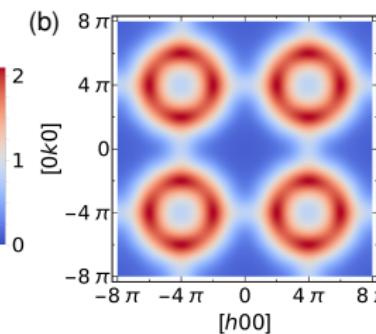
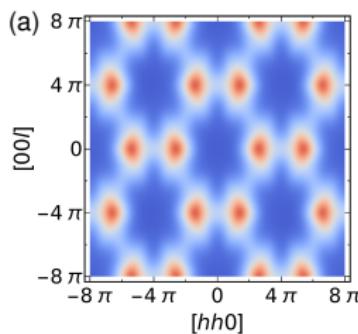
Ordering pitch vector

$$\mathbf{q} = \frac{2\pi}{a}(2, 1, 0) \Rightarrow$$

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OXIDES



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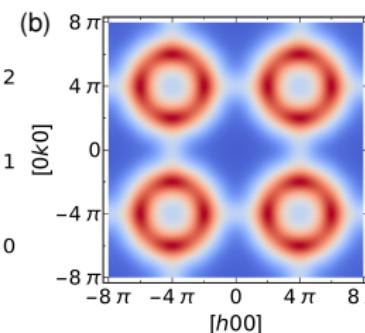
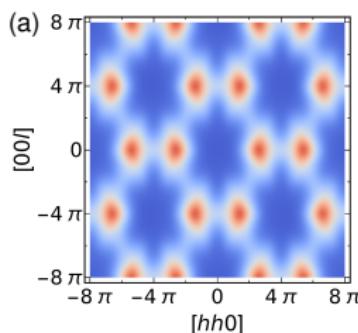
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- ▶ FM J_2 ⁶
- ▶ AFM J_3

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OXIDES



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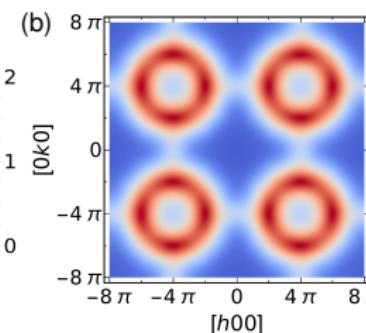
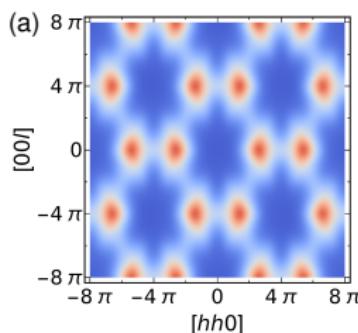
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For strong AFM NN interactions, J_2 in an ideal pyrochlore lattice is equivalent to a J_{3a} with opposite sign⁷.

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OXIDES



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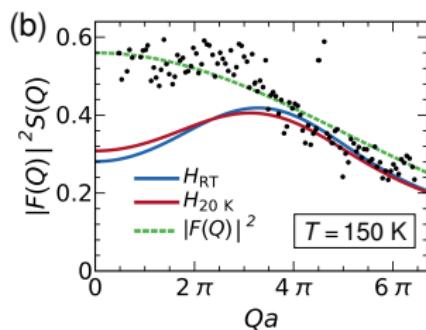
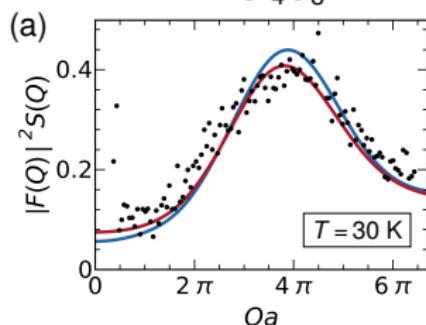
$$J_{3a}/J \rightarrow (J_{3a} - J_2)/J = 0.026$$

⁶Phys. Rev. B. 81, 224413 (2010)

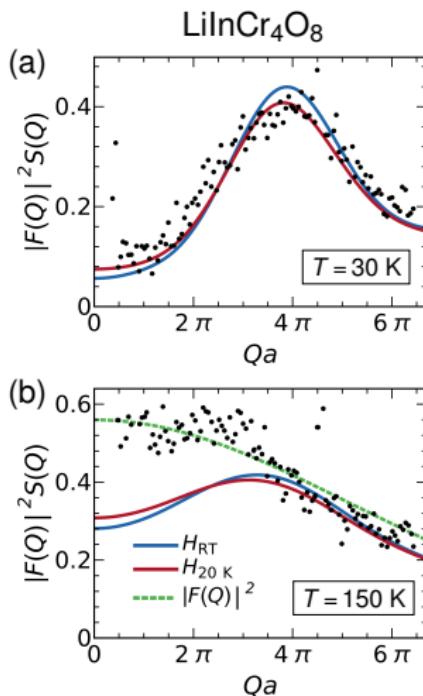
⁷Phys. Rev. B, 78, 144418 (2008)

OXIDES

LiInCr₄O₈



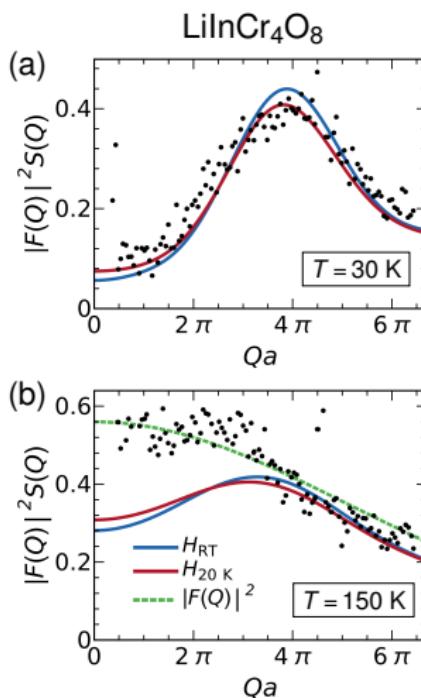
OXIDES



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

- ▶ Temperature dependent Hamiltonian

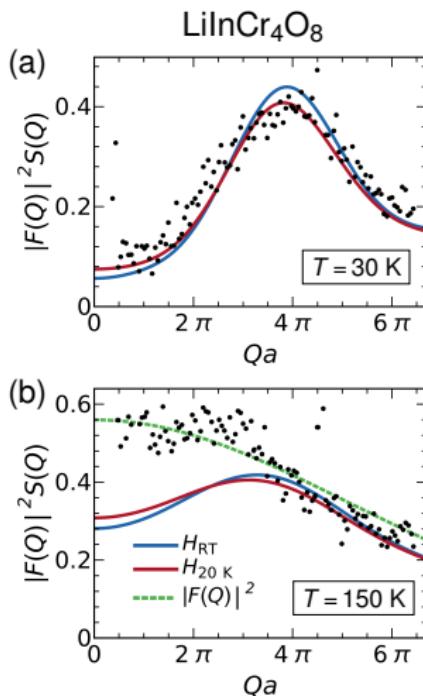
OXIDES



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

- ▶ Temperature dependent Hamiltonian
- ▶ absorption cross section in barns of In: 193.8
- ▶ absorption cross section in barns of Ga: 2.75

OXIDES



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

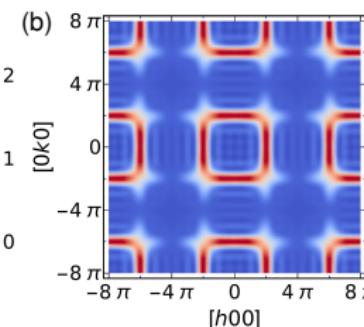
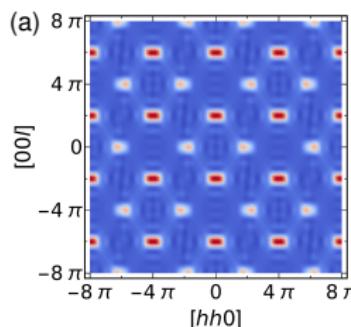
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SULFIDES

$\text{CuInCr}_4\text{S}_8$

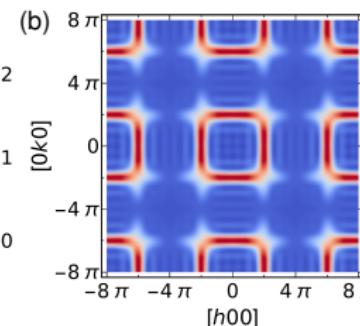
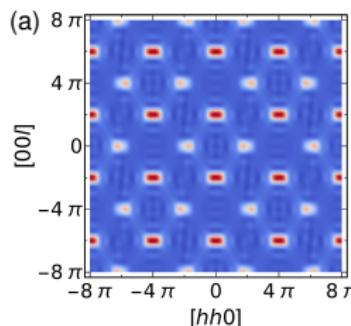
SULFIDES

$\text{CuInCr}_4\text{S}_8$



SULFIDES

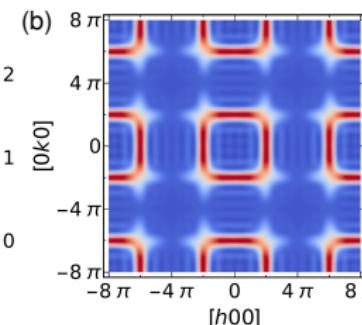
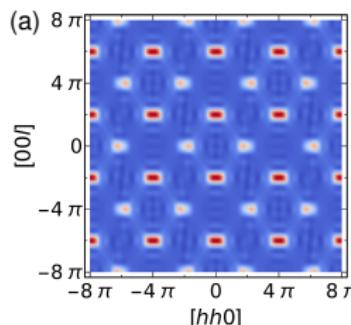
CuInCr₄S₈



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SULFIDES

CuInCr₄S₈

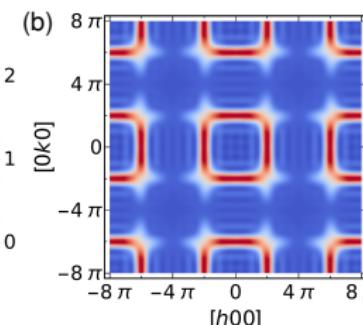
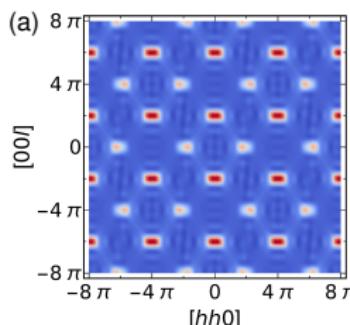


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SULFIDES

CuInCr₄S₈

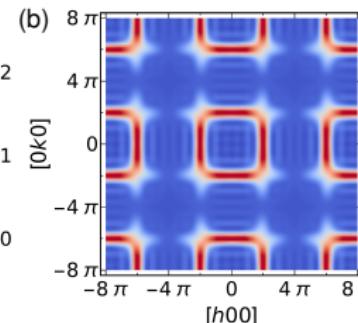
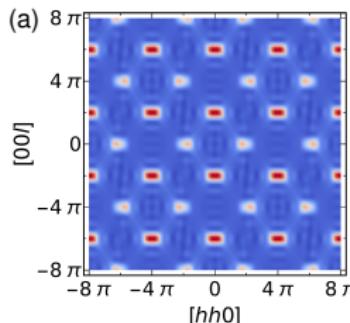


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- ▶ Pattern of almost degenerate line \Leftarrow AFM NN FCC \Rightarrow “spiral spin liquid”

SULFIDES

CuInCr₄S₈

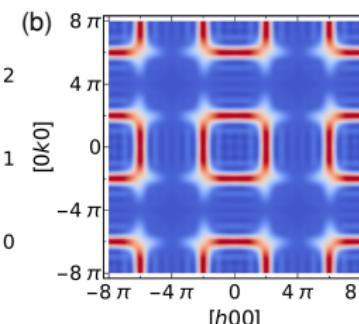
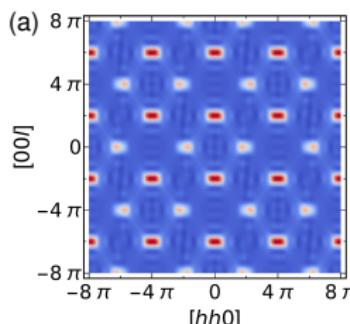


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SULFIDES

CuInCr₄S₈

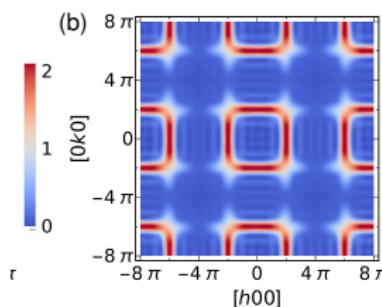


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 - ▶ $J_1^{fcc} = (J + 4J_2 + 2J_{3a} + 2J_{3b})/16$

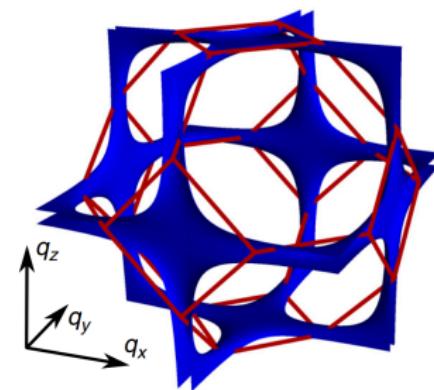
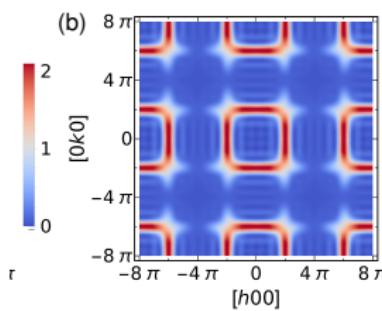
SULFIDES

CuInCr₄S₈



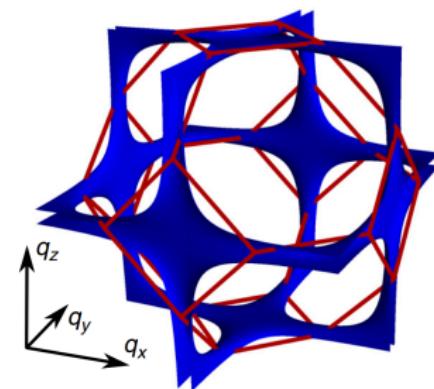
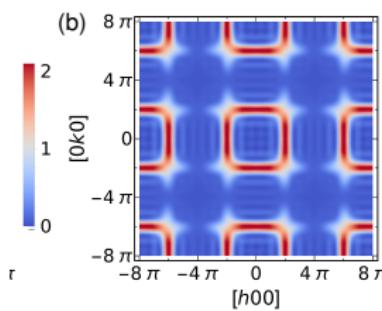
SULFIDES

$\text{CuInCr}_4\text{S}_8$



SULFIDES

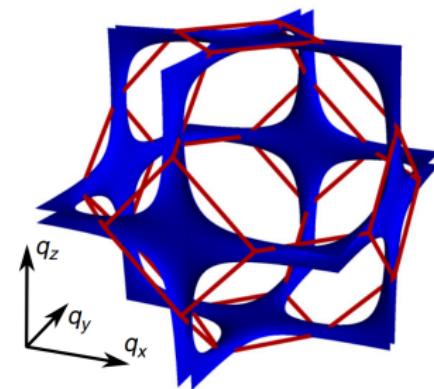
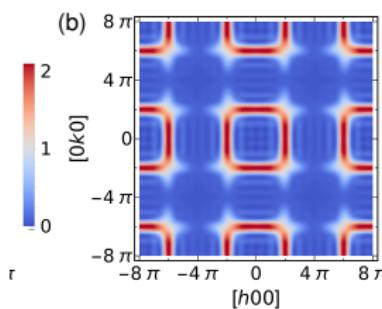
CuInCr₄S₈



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

SULFIDES

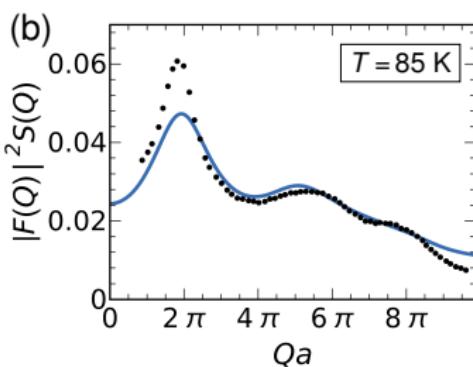
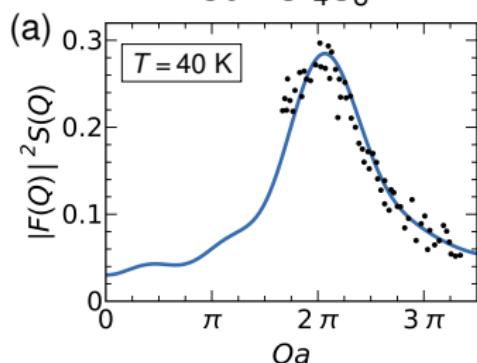
CuInCr₄S₈



- ▶ 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 $\mathbf{q} = \frac{2\pi}{a}(1, 0, 0)$

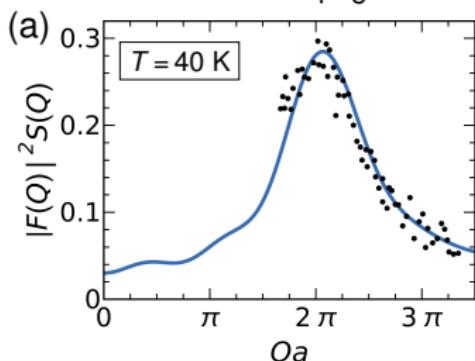
SULFIDES

CuInCr₄S₈

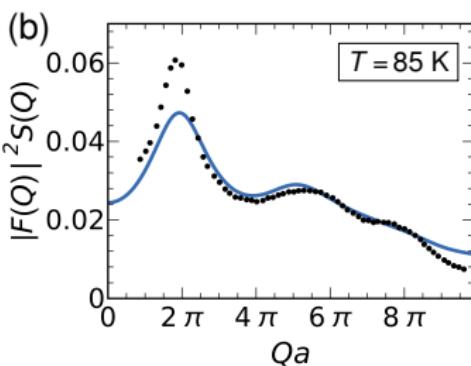


SULFIDES

CuInCr₄S₈

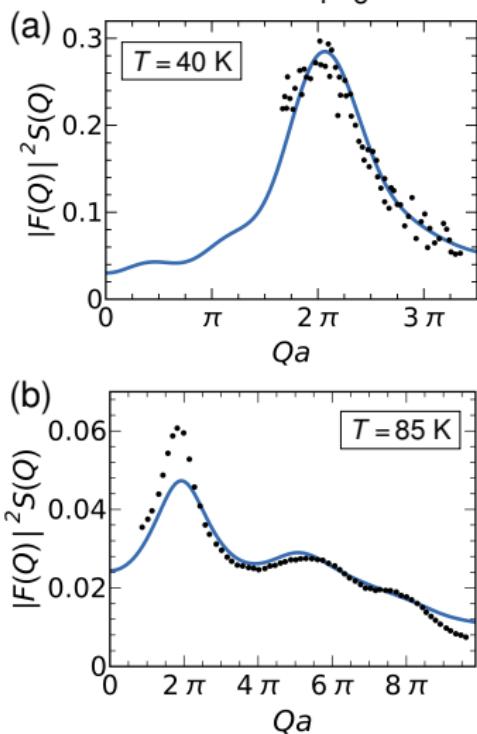


Experimental data from J. Phys. Colloques 32, C1-324 (1971) and Phys. Lett. 60A, 431 (1977).



SULFIDES

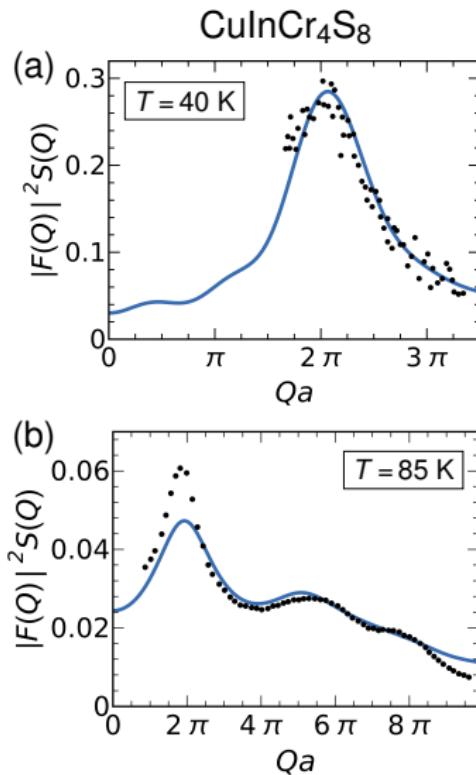
CuInCr₄S₈



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- ▶ absorption cross section in barns of Ga: 2.75(1.5)

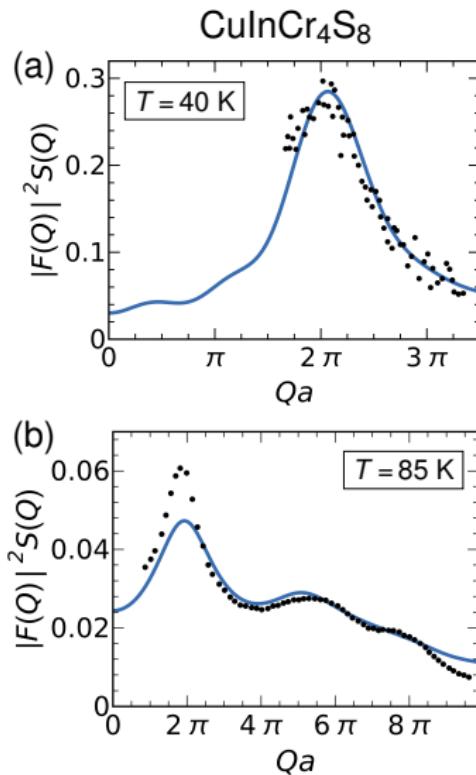
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SULFIDES



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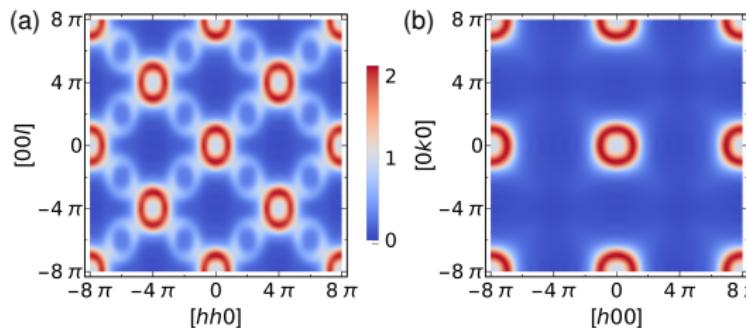
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- ▶ Experiments on $\text{LiGaCr}_4\text{S}_8$
- ▶ Experiments on $\text{LiInCr}_4\text{S}_8$ and $\text{CuInCr}_4\text{S}_8$

SELENIDE

$\text{CuInCr}_4\text{Se}_8$

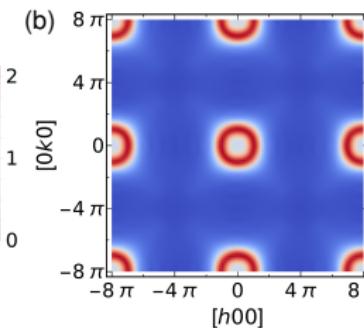
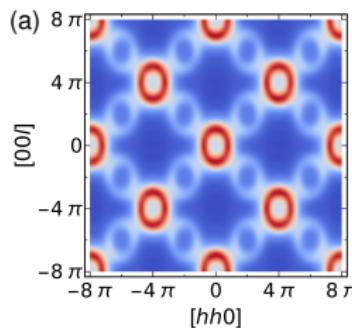
SELENIDE

CuInCr₄Se₈



SELENIDE

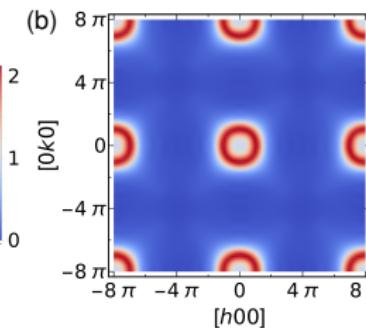
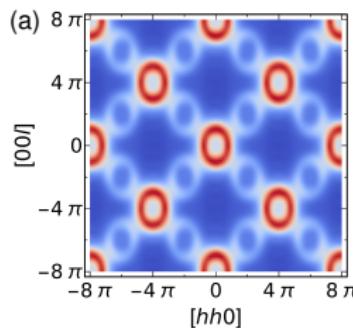
CuInCr₄Se₈



- $|J'|/|J| = 1.18$
- $J_2/|J| = 0.016$
- $J_{3a}/|J| = 0.2$
- $J_{3b}/|J| = 0.16$

SELENIDE

CuInCr₄Se₈

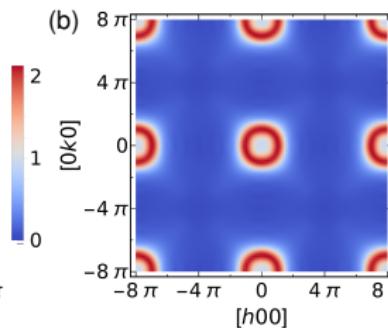
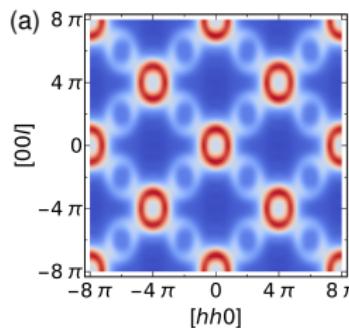


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- ▶ FM J and J'

SELENIDE

CuInCr₄Se₈

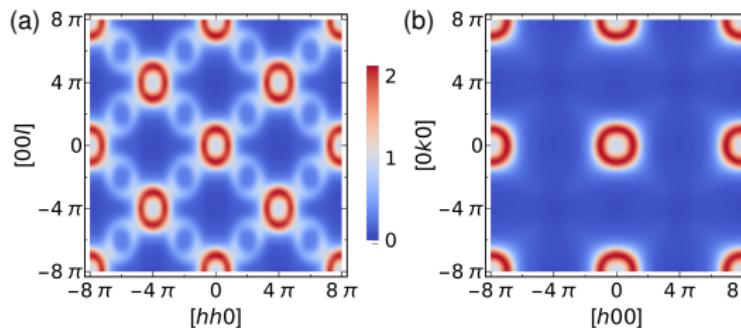


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- ▶ FM J and J'
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SELENIDE

CuInCr₄Se₈

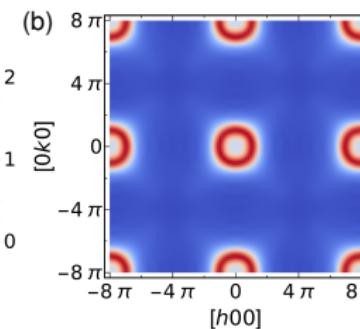
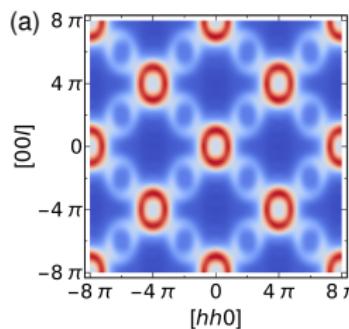


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- ▶ Observed for the pyrochlore material ZnCr₂Se₄⁸

SELENIDE

CuInCr₄Se₈

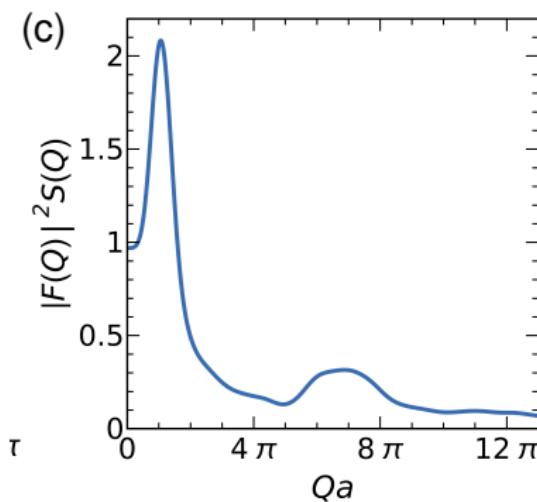


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- ▶ Ordering pitch vector: $\mathbf{q} = (0.521278, 0, 0)$
- ▶ Observed for the pyrochlore material ZnCr₂Se₄⁸
- ▶ “spiral spin liquid”?

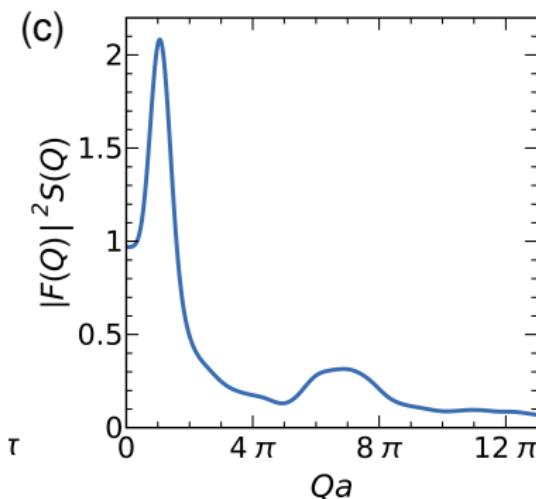
SELENIDE

CuInCr₄Se₈



SELENIDE

$\text{CuInCr}_4\text{Se}_8$



“Inarticulated” matching with
the unpolarized neutron
scattering data

*MAGNETIC ORDERING IN
THE NORMAL SPINEL*

$\text{Cu}_{0.5}\text{In}_{0.5}\text{Cr}_2\text{Se}_4$

R. Plumier and M. Sougi

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

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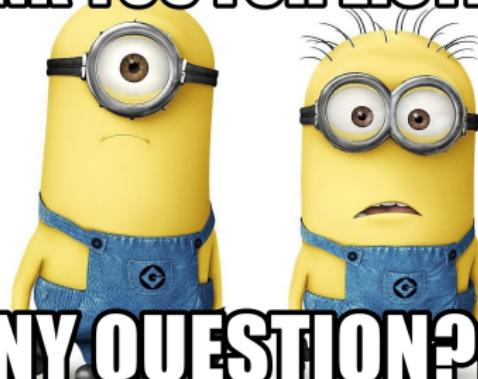
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- ▶ The temperature dependence of these systems?

THANK YOU FOR LISTENING



ANY QUESTION???

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