Competing orders and topological excitations in spin-1 pyrochlore antiferromagnets

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Competing phases and topological excitations of spin-1 pyrochlore antiferromagnets

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PHYSICAL REVIEW B 98, 045109 (2018)

Everlasting success of spin-1/2 pyrochlores

Pauling entropy in spin ice

Classical spin ice

Ramirez, etc, Nature 1999,
Gingras, etc, Science, 2009
Castelnovo, Moessner, etc, Nature 2008
Everlasting success of spin-1/2 pyrochlores

Quantum spin ice,
Quantum spin liquid

Spinon deconfinement

Figs from Moessner & Schiffer, 2009

Gingras, Gaulin, Balents, Savary, SB Lee, GC, ...
Everlasting success of spin-1/2 pyrochlores

Order by quantum disorder

\textit{Er}_2\textit{Ti}_2\textit{O}_7 \textit{Hamiltonian}: The effective } S = 1/2 \textit{ description applies to } \textit{Er}_2\textit{Ti}_2\textit{O}_7 \textit{below about 74 K} [2, 11]. Nearest-neighbor exchange dominates, for which the Hamiltonian is constrained by symmetry to the form \cite{9}

\begin{align}
H &= \sum_{\langle ij \rangle} \left[ J_{zz} S_i^z S_j^z - J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) \right. \\
&\quad + J_{\pm\pm} \left[ \gamma_{ij} S_i^+ S_j^+ + \gamma_{ij} S_i^- S_j^- \right] \\
&\quad + J_{z\pm} \left[ S_i^z (\xi_{ij} S_j^+ + \xi_{ij}^* S_j^-) + i \leftrightarrow j \right].
\end{align}

(6)

\[ \epsilon_{\alpha}^w (\text{meV}) \]

FIG. 2. Zero-point fluctuation energy $\epsilon_{\alpha}^w$ in the classically degenerate manifold parametrized by $\alpha$. The peak-to-peak energy is $\lambda \approx 3.5 \times 10^{-4}$ meV.
The difference between spin-1/2 and spin-1

Due to Berry phase effect, spin-1/2 chain is gapless, spin-1 Heisenberg chain is gapped.

Building degree of freedom is $S=1$, but at there is $S=1/2$ edge state.
Spin-1 pyrochlores

<table>
<thead>
<tr>
<th>materials</th>
<th>magnetic ions</th>
<th>Θ_CW</th>
<th>magnetic transitions</th>
<th>magnetic structure</th>
</tr>
</thead>
<tbody>
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<td>Ru AFM order at 95K</td>
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</table>

Candidate spin-1 pyrochlore materials

References are listed in PRB 98, 045109

www.ptable.com
Model Hamiltonian

Local moment physics of the Ni$^{2+}$ ion in NaCaNi$_2$F$_7$  

\[ H = \sum_{\langle ij \rangle} \left[ J S_i \cdot S_j + D_{ij} \cdot (S_i \times S_j) \right] + \sum_i D_z (S_i \cdot \hat{z}_i)^2 \]

- Heisenberg (J$>$0)
- Dzyaloshinskii-Moriya
- Single ion anisotropy

\[ |D_{ij}|/J \sim O(\lambda/\Delta) \]
\[ |D_z|/\Delta \sim O(\lambda^2/\Delta^2) \]

\( \lambda \): SOC  \( \Delta \): CEF splitting
Phase diagram (overview)

Quant. Para. = quantum paramagnetic phase
Others are magnetic ordered phases
Quantum paramagnetic phase

Quant. Para. = quantum paramagnetic phase
Others are magnetic ordered phases
Quantum paramagnetic phase

$D_z \to +\infty \quad \text{(easy plane limit)}: \quad |\Psi\rangle = \prod_i |S_i^z = S_i \cdot \hat{z}_i = 0\rangle$

Flavor wave theory

start from the ground state in easy plane limit, one can introduce two flavors of bosons to represent the spin Hamiltonian

$$a_1^{\dagger} |S_i^z = 0\rangle = |S_i^z = 1\rangle$$

$$a_1^{\dagger} |S_i^z = 0\rangle = |S_i^z = -1\rangle$$

$$H_{fw} = \sum_k \Psi_k^{\dagger} M(k) \Psi_k$$

8 branches = 4 sublattices x 2 flavors

A. Joshi, et al. PRB 60, 6584 (1999)
Quantum paramagnetic phase

\[ D_z \to +\infty \text{ (easy plane limit): } |\Psi\rangle = \prod_i |S_i^z \equiv S_i \cdot \hat{z}_i = 0\rangle \]

Flavor wave theory

start from the ground state in easy plane limit, one can introduce two flavors of bosons to represent the spin Hamiltonian

\[ a^\dagger_1(i) |S_i^z = 0\rangle = |S_i^z = 1\rangle \]
\[ a^\dagger_1 |S_i^z = 0\rangle = |S_i^z = -1\rangle \]
\[ H_{fw} = \sum_\mathbf{k} \Psi_\mathbf{k}^\dagger M(\mathbf{k}) \Psi_\mathbf{k} \]

8 branches = 4 sublattices x 2 flavors

instability of the quantum paramagnet \(\leftrightarrow\) magnetic order

A. Joshi, et al. PRB 60, 6584 (1999)
Competing magnetic orders

Mean-field theory

\[ \langle H \rangle = \sum_{ij} J m_i \cdot m_j + D_{ij} \cdot (m_i \times m_j) + \sum_i D_z (m_i \cdot \hat{z}_i)^2 \]

All ordered states have \( Q=0 \)
Magnetic ordered phases

The ordered phases can be understood from degeneracy lifting:

\[ J \text{ term requires } \sum_{i \in I_{u/d}} S_i = 0 \text{ in one tetrahedron} \quad \text{(huge degeneracy)} \]

\[ -|D| \sum_i (S_i \cdot \hat{z}_i)^2 \]

“Z-type” order:
- local Z axis
- all-in all-out
- two-in two-out

“XY-type” order:
- local XY plane

Further selected by the sign of DM interaction

or

Quantum order by disorder

Weyl semimetal and extension

\[ H_D = E_0 \mathbb{1} + \mathbf{v}_0 \cdot \mathbf{q} + \sum_{i=1}^{3} \mathbf{v}_i \cdot \mathbf{q} \sigma_i. \]  

Energy is measured from the chemical potential, \( \mathbf{q} = \mathbf{k} - \mathbf{k}_0 \)

**Extension:** Type-II Weyl semimetal, Dirac semimetal, nodal line semimetal, hourglass fermion, new fermions
Topological magnons: Weyl magnon

F-Y Li, YD Li, Kim, Balents, Yu, GC, Nature communications 2016
Unique properties of topological Weyl magnon

Magnon Weyl nodes

Magnon surface arcs

Tune Weyl nodes with fields
Focus session: topological magnons

### Session Index

**Session V44: Topological Magnons**

<table>
<thead>
<tr>
<th>Date</th>
<th>Time</th>
<th>Title</th>
<th>Speaker</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thursday, March 7, 2019</td>
<td>2:30PM - 3:06PM</td>
<td><strong>V44.00001: Topological magnon bands in ultra-thin film pyrochlore iridates and iron jarosites</strong></td>
<td>Gregory Fiete</td>
</tr>
<tr>
<td>Thursday, March 7, 2019</td>
<td>3:06PM - 3:42PM</td>
<td><strong>V44.00002: Topological spin excitations in a three-dimensional antiferromagnet</strong></td>
<td>Yuan Li</td>
</tr>
<tr>
<td>Thursday, March 7, 2019</td>
<td>3:42PM - 4:18PM</td>
<td><strong>V44.00003: Topology of magnons: classification and application to honeycomb Kitaev magnets</strong></td>
<td>Yuan-Ming Lu</td>
</tr>
<tr>
<td>Thursday, March 7, 2019</td>
<td>4:18PM - 4:54PM</td>
<td><strong>V44.00004: Discovery of coexisting Dirac and triply degenerate magnons in a three-dimensional antiferromagnet</strong></td>
<td>Jinsheng Wen</td>
</tr>
<tr>
<td>Thursday, March 7, 2019</td>
<td>4:54PM - 5:30PM</td>
<td><strong>V44.00005: The surprising usefulness of magnons at intermediate and high energies: from frustration to topology</strong></td>
<td>Roderich Moessner</td>
</tr>
</tbody>
</table>

Room: BCEC 210C
Topological magnons for spin-1 pyrochlores

Triple degeneracy
Topological magnons for spin-1 pyrochlores

FIG. 7. Spin wave excitations of the ordered phases. The pa-

FIG. 8. The nodal lines and Weyl nodes of the spin wave exci-
tation. (a) For the same parameters as in Fig. 7(b), there is a nodal
Materials’ relevance

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on the systems with more known results. Ho$_2$Ru$_2$O$_7$ was studied using neutron scattering measurements in a nice paper [109] by C.R. Wiebe et al. The authors revealed the Ru moment order at ~95 K and the Ho moment order at ~1.4 K. The high temperature Ru magnetic order is consistent with the splayed FM with a splayed angle $\alpha \approx 41^\circ$. Under the internal exchange

The Heisenberg point requires more “quantum” treatment.

Heisenberg point $D = 0, D_z = 0$
- classical ground states are extensively degenerate
- strong quantum fluctuations and
- fundamental distinctions between spin-1/2 and spin-1
Relation to spin-3/2 pyrochlores:

- The same model actually applies to the spin-3/2 pyrochlore materials (e.g. Mn-based pyrochlores)

- Local spin anisotropy acts on it quite differently, \( D_Z (S_i \cdot \hat{z}_i)^2 \).

The quantum paramagnetic phase is absent since no Sz=0 state.

- The magnetic orders, if they occur, would be similar to the spin-1 pyrochlore system. The magnetic excitations would have similar properties, too.
Summary

1. We propose a minimal spin model for spin-1 pyrochlores

2. The competing phases and topological excitations are discussed.

3. Various materials’ realization and relevance are clarified.

Fei-Ye Li, GC, PRB 98, 045109 (2018)