Kitaev materials beyond iridates: order by quantum disorder and Weyl magnons in rare-earth double perovskites

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Fei-Ye Li, Yao-Dong Li, Yue Yu, GC*, arXiv: 1607.05618
Outline

• A brief introduction to Kitaev materials
• Generalized Kitaev-Heisenberg model for rare-earth double perovskites
• Ground state selection and quantum excitation
• Conclusion
A. Kitaev proposed and solved his model exactly with the majorana representation

\[ H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z, \]

\( \tilde{\sigma}^x = ib^x c, \quad \tilde{\sigma}^y = ib^y c, \quad \tilde{\sigma}^z = ib^z c. \)
Iridates as Kitaev materials

2009 Jackeli and Khaliullin pointed out that Na$_2$IrO$_3$ may support a model with the Kitaev interaction in it.

IrO$_6$ octahedron

Red is iridium atom
A large families of Kitaev materials

hyperkagome: Na$_4$Ir$_3$O$_8$
H. Takagi, et al, PRL 2007,
GC and Balents PRB 2008.

A recent fashion
RuCl$_3$
Kitaev materials beyond iridates

- What gives the Kitaev interaction is the strong spin-orbit coupling, therefore, this does not restrict to iridates.

- The vast families of rare-earth magnets have never been discussed along the line of Kitaev interaction.

**Advantage:**

1. SOC of 4f electrons is much larger than 4d and 5d

2. 4f electron is more localized than 4d/5d electron, so most times the exchange is nearest neighbors, no perturbation from further neighbors

3. The rare earth elements do not suffer from the neutron absorption issue that prevails in iridates.
An example: rare-earth double perovskites
Rare-earth double perovskites

Lattice parameters for $\text{Ba}_2\text{LnSbO}_6$.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Space group</th>
<th>$a$ (Å)</th>
<th>$\alpha$ (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Ba}_2\text{LaSbO}_6$</td>
<td>$R3$</td>
<td>6.0866 (3)</td>
<td>60.30 (3)</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{PrSbO}_6$</td>
<td>$R3$</td>
<td>6.0527 (1)</td>
<td>60.16 (3)</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{NdSbO}_6$</td>
<td>$R3$</td>
<td>6.0383 (5)</td>
<td>60.10 (2)</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{SmSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.5069 (3)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{EuSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.4910 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{GdSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.4732 (2)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{TbSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.4505 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{DySbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.4297 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{HoSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.4146 (1)</td>
<td>90</td>
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<tr>
<td>$\text{Ba}_2\text{ErSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.3958 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{TmSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.3778 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{YbSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.3620 (1)</td>
<td>90</td>
</tr>
<tr>
<td>$\text{Ba}_2\text{LuSbO}_6$</td>
<td>$Fm\bar{3}m$</td>
<td>8.3484 (1)</td>
<td>90</td>
</tr>
</tbody>
</table>
Generalized Kitaev-Heisenberg model

\[ H = \sum_{\langle ij \rangle_{\gamma \pm}} \left[ J \mathbf{S}_i \cdot \mathbf{S}_j + K \mathbf{S}_i^\gamma \mathbf{S}_j^\gamma \pm F (\mathbf{S}_i^\alpha \mathbf{S}_j^\beta + \mathbf{S}_i^\beta \mathbf{S}_j^\alpha) \right] \]
Phase diagram

<table>
<thead>
<tr>
<th>Phase</th>
<th>Wavevector</th>
<th>Order Para.</th>
<th>Continuous deg</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>(2π, 0, 0)</td>
<td>along [100] axis</td>
<td>–</td>
</tr>
<tr>
<td>II</td>
<td>(2π, 0, 0)</td>
<td>in (100) plane</td>
<td>U(1)</td>
</tr>
<tr>
<td>III</td>
<td>(π, π, π)</td>
<td>along [111] axis</td>
<td>–</td>
</tr>
<tr>
<td>IV</td>
<td>(π, π)</td>
<td>in (111) plane</td>
<td>U(1)</td>
</tr>
<tr>
<td>V</td>
<td>(0, 0, 0)</td>
<td>any direction</td>
<td>O(3)</td>
</tr>
</tbody>
</table>

GS with accidental degeneracy

I: \( \mathbf{S}_i \equiv S \hat{m}_i = S \hat{x} e^{2\pi x_i} \),

II: \( \mathbf{S}_i \equiv S \hat{m}_i = S [\cos \theta \hat{y} + \sin \theta \hat{z}] e^{2\pi x_i} \),

III: \( \mathbf{S}_i \equiv S \hat{m}_i = \frac{S}{\sqrt{3}} (\hat{x} + \hat{y} + \hat{z}) e^{i\pi(x_i+y_i+z_i)} \).

IV: \( \mathbf{S}_i \equiv S \hat{m}_i = S (\cos \theta \hat{u}_1 + \sin \theta \hat{u}_2) e^{i\pi(x_i+y_i+z_i)} \),

V: \( \mathbf{S}_i \equiv S \hat{m}_i = S (\sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}) \),
This result indicates that one may find even simpler mod-
independent pseudospin interactions in Eq. 1. It is the
asymmetry in the symmetric pseudo-dipole interaction that de-
we have the well-known Kitaev exchange interaction as

TABLE I. The mean-field phases in Fig. 2. The incommen-
sation gives phase I. For the ferromagnetic Heisenberg in-
phase III but has a

\[ \Delta E = \sum_k \left[ \sum_{\mu} \frac{1}{2} (\omega_{\mu}(k) - A_{\mu\mu}(k)) + C(k) \right], \]

Quantum zero point energy

\[ H_{sw} = \sum_k \left[ \sum_{\mu,\nu} (A_{\mu\nu}(k)b_{k\mu}^\dagger b_{k\nu}^\dagger + B_{\mu\nu}(k)b_{-k,\mu}^\dagger b_{k,\nu}^\dagger) + B_{\mu\nu}^*(-k)b_{k\mu}^\dagger b_{-k,\nu}^\dagger + C(k) \right] + E_{cl}, \]

IV:  \[ \mathbf{S}_i \equiv S \hat{m}_i = S (\cos \theta \hat{u}_1 + \sin \theta \hat{u}_2)e^{i\pi(x_i+y_i+z_i)}, \]

V:  \[ \mathbf{S}_i \equiv S \hat{m}_i = S (\sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}), \]
Excitation: Pseudo-Goldstone mode and Weyl magnon

Pseudo-Goldstone mode:

Appear to be gapless at mean field level, but should be gapped when anharmonic spin-wave interactions is included.
In fact, as we show in Fig. X, there are in total four such zone for region I.

Although region I and III of the phase diagram have the tetrahedron with the strongest coupling and treat other phenomena known as “quantum order by disorder” [11–13].

To obtain the phase diagram in Fig. X, we have implemented the semiclassical approach and included the Holstein-Primakoff approximation. As we show in Fig. X, the spin wave spectrum along the high symmetry lines in the Brillouin zone is characterized by the chirality number that takes values from 0; 1 or 2. One may first consider the classical energy and is determined for every classical spin ground state.

Negative values of this parameter represent the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.

The resulting state is a non-collinear state and the spin wave modes depend on the angular variable $\vec{a}$ or $\vec{B}$ and is determined for every classical spin ground state. In these regimes, one may first consider the classical energy $\mathbf{B}$ and then work out the combination of the single-ion spin anisotropy is the 6$^\text{th}$-order $\vec{a}$ and is determined for every classical spin ground state.

The magnitude of $\mathbf{B}$ is the 6$^\text{th}$-order $\vec{a}$ and is determined for every classical spin ground state. The spin only couples to the field via a Zeeman coupling. This is quite different from the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.

Dispersion along $(\Gamma X)$ does not change as we move from $(\Gamma X)$ to $(X W)$. As it is in Fig. X, the chiral semi-classical velocity of magnons. Likewise, due to the bulk-edge correspondence, the chiral surface magnon arc states also respond to $X$ and is determined for every classical spin ground state.

When we apply an external magnetic field to the system, the spin only couples to the field via a Zeeman coupling. This is quite different from the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.

To summarize, we have studied a realistic spin model that the combination of the single-ion spin anisotropy is the 6$^\text{th}$-order $\vec{a}$ and is determined for every classical spin ground state. The spin only couples to the field via a Zeeman coupling. This is quite different from the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.

# Weyl magnons

The resulting state is a non-collinear state and the spin wave modes depend on the angular variable $\vec{a}$ or $\vec{B}$ and is determined for every classical spin ground state. In these regimes, one may first consider the classical energy $\mathbf{B}$ and then work out the combination of the single-ion spin anisotropy is the 6$^\text{th}$-order $\vec{a}$ and is determined for every classical spin ground state. The spin only couples to the field via a Zeeman coupling. This is quite different from the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.

Our pump-probe approach to measure the optical absorption demonstrates that the combination of the single-ion spin anisotropy is the 6$^\text{th}$-order $\vec{a}$ and is determined for every classical spin ground state. The spin only couples to the field via a Zeeman coupling. This is quite different from the magnetic order in these two systems are not yet clear. This is the well-known phenomenon of quantum fluctuations. This is the well-known phenomenon of quantum fluctuations.
Weyl magnon in magnetic field

Unlike Weyl fermion in electron systems, there is no Lorenz coupling of the spins to the external magnetic field.

Via Zeeman coupling, the magnetic field modifies the magnetic order, and indirectly influences the band structure of the magnon.

The magnon Weyl points can be moved and annihilated by magnetic field, this provides a way to control Weyl magnons with magnetic fields.

FIG. 5. The evolution of Weyl nodes under the magnetic field. Applying a magnetic field along the global $z$ direction, $B = B[001]$, Weyl nodes are shifted but still in $k_z = 0$ plane. They are annihilated at $\Gamma$ when magnetic field is strong enough. Red and blue indicate the opposite chirality. (a) to (f): $B = 0, 0.1, 0.5, 0.9, 1.0, 1.1$. We have set $D = 0.2J, J' = 0.6J$ and $\theta = \pi/2$. 

[Diagram showing the evolution of Weyl nodes under magnetic field]
Summary

• We have pushed the Kitaev materials from iridates to rare-earth families.

• We predict the “order by quantum disorder” phenomenon in the rare-earth double perovskites.

• The pseudo-Goldstone mode and Weyl magnons are the excitations that we predict.

• We expect our work to inspire the experimental efforts on this series materials and alike. Some new states may be found.

arXiv: 1607.05618
“By Landau’s definition this is simply any parameter that is zero in the symmetric state and has a nonzero average uniquely specifying the state when the symmetry is broken.”
Weyl fermions

Hong Ding, Hasan, Ling Lu, Hongming Weng, Xi Dai, Zhong Fang, etc

Discovered in 2015 in various physical systems!
Weyl band touching is a topological property of the band structure, and is thus independent from the particle statistics.

It can be fermion, e.g. electron, can also be boson, e.g. photon.
Breathing Pyrochlore

Yoshihiko Okamoto, Gøran J. Nilsen, J. Paul Attfield, and Zenji Hiroi, PhysRevLett 2013,
As there is no orbital degeneracy for the $3d^3$ electron configuration of Cr$^{3+}$ ions, the orbital angular momentum is fully quenched and the Cr$^{3+}$ local moment is well described by the total spin $S = 3/2$ via the Hund’s rule. As

$$H = J \sum_{\langle ij \rangle \in u} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle \in d} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_i (\mathbf{S}_i \cdot \hat{n}_i)^2,$$

Treating spins as classical vectors, simple algebra gives some rules for ground states

$$\sum_{\langle ij \rangle \in u} \mathbf{S}_i \cdot \mathbf{S}_j \sim \frac{1}{2} \left( \sum_{i \in u} \mathbf{S}_i \right)^2,$$

$$\sum_{\langle ij \rangle \in d} \mathbf{S}_i \cdot \mathbf{S}_j \sim \frac{1}{2} \left( \sum_{i \in d} \mathbf{S}_i \right)^2.$$
Quantum order by disorder

$$S^{\text{cl}}_{i} \equiv S\hat{m}_{i} = S(\cos \theta \hat{x}_{i} + \sin \theta \hat{y}_{i}),$$

Holstein-Primarkoff bosons to express the spin operators as $S_{i} \cdot \hat{m}_{i} = S - a_{i}^{\dagger}a_{i}$, $S_{i} \cdot \hat{z}_{i} = (2S)^{1/2}(a_{i} + a_{i}^{\dagger})/2$, and $S_{i} \cdot (\hat{m}_{i} \times \hat{z}_{i}) = (2S)^{1/2}(a_{i} - a_{i}^{\dagger})/(2i)$. Keeping terms in
In fact, as we show in Fig. X, there are in total four such action between the Holstein-Primarko small gap would eventually be created when the inter-

Although region I and III of the phase diagram have the phenomenon known as "quantum order by disorder" [11–13].

The spin wave Hamiltonian as

\[ B_\mu = \frac{1}{2} \left( \mathbf{P} \mathbf{\mu} \right), \]

is independent of

\[ \mathbf{a}_k, \mu \]

In these regimes, one may first consider the fluctuations in the parameter regimes when

\[ E_{\mu} = \frac{1}{2} \left( \mathbf{P} \mathbf{\mu} \right), \phi \]

is the classical ground state energy, and

\[ E_{cl} \]

is independent of

\[ \mathbf{a}_k, \mu \]

As we show in Fig. X, the spin wave spectrum along the high symmetry lines in the Brillouin directions of the local coordinate systems. Using the lin-

These linear band touchings occur towards the phase boundary with region III, the magnon Weyl nodes and surface states.

When we apply an external magnetic field to the systems where there exists an orbital coupling in addition to the Zeeman coupling. Because of this di-

The surface dependence of the magnon arc states, one can tune the Fermi energy to the Weyl nodes by varying the magnetic field merely shifts the positions of the magnon Weyl magnons.

Therefore, it is certainly of interest to confirm the magnetic order in these two systems are not yet clear.

The magnon Weyl nodes appear at finite energies, one necessarily needs to use the correspondence, the chiral surface magnon arc states also respond to the Zeeman coupling. Because of this di-

In these systems.

The blue indicate the opposite chirality. We have set

\[ FIG. 3. (Color Online.) (a) The spin wave spectrum along \Gamma X W L. \]

(3) When we apply an external magnetic field to the slab (cut in [110], (0 0 0), (0 0 0) and (2n 2n).

\[ FIG. 4. (Color Online.) Surface states of a slab (cut in [110] \]
How to probe in a REAL experiment?

1. Neutron scattering: detect the Weyl nodes as well as the consequence (the surface arc states that connect the Weyl nodes).

2. Thermal Hall effect: magnon Weyl nodes contribute the thermal currents that are tunable by external magnetic field.

3. Optically: as Weyl node must appear at finite energy, one needs to use pump-probe measurement.

可以对比 Weyl fermion in the electron system
Summary

We have studied a realistic spin model on the Cr-based breathing pyrochlore systems.

We show that the combination of the single-ion spin anisotropy and the superexchange interaction leads to conventional magnetic order.

We find the magnetic excitation in a large parameter regime develops magnon Weyl nodes in the magnon spectrum.