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

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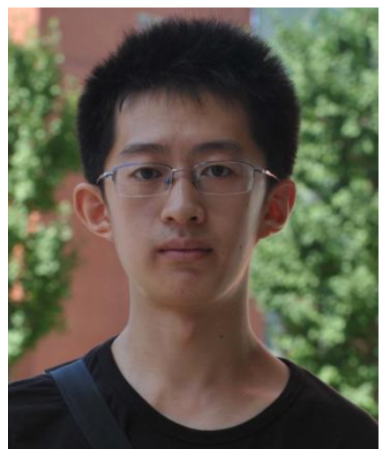
Collaborators

it is a student project !
it is a simple piece of work, there is
Not much creativity !



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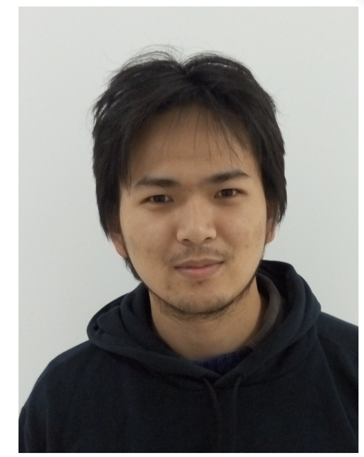


李耀东

with seniors: Prof. Yue Yu (虞跃)

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

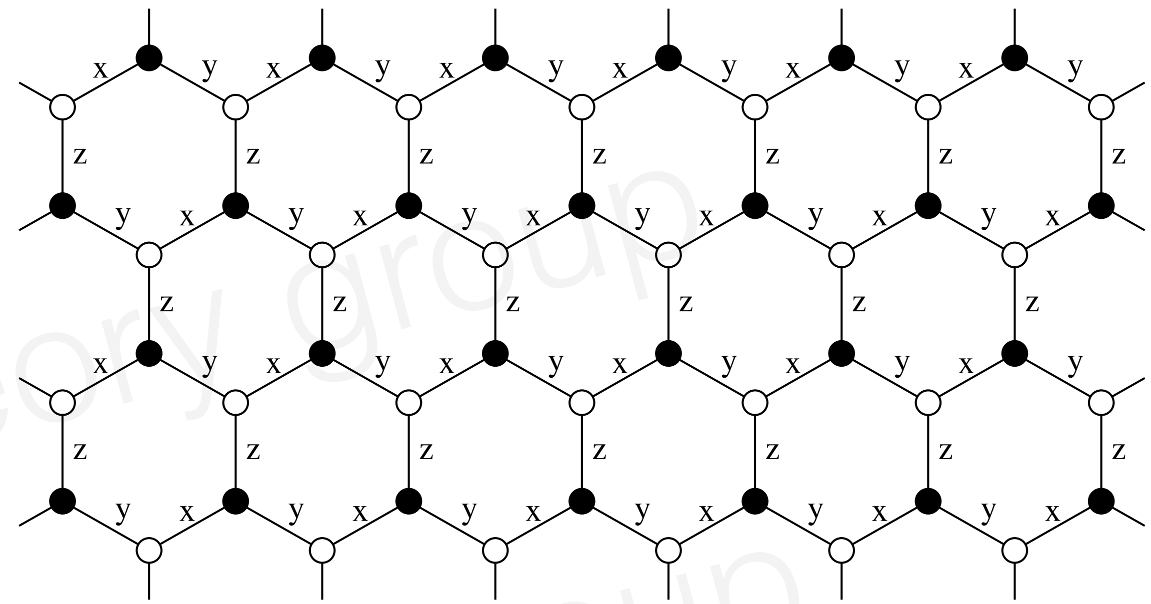
Outline

- A brief introduction to Kitaev materials
- Generalized Kitaev-Heisenberg model for rare-earth double perovskites
- Ground state selection and quantum excitation
- Conclusion

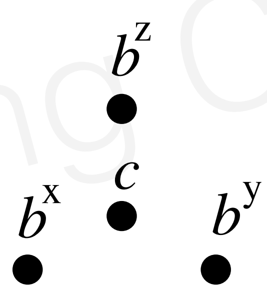
A Kitaev

Kitaev model

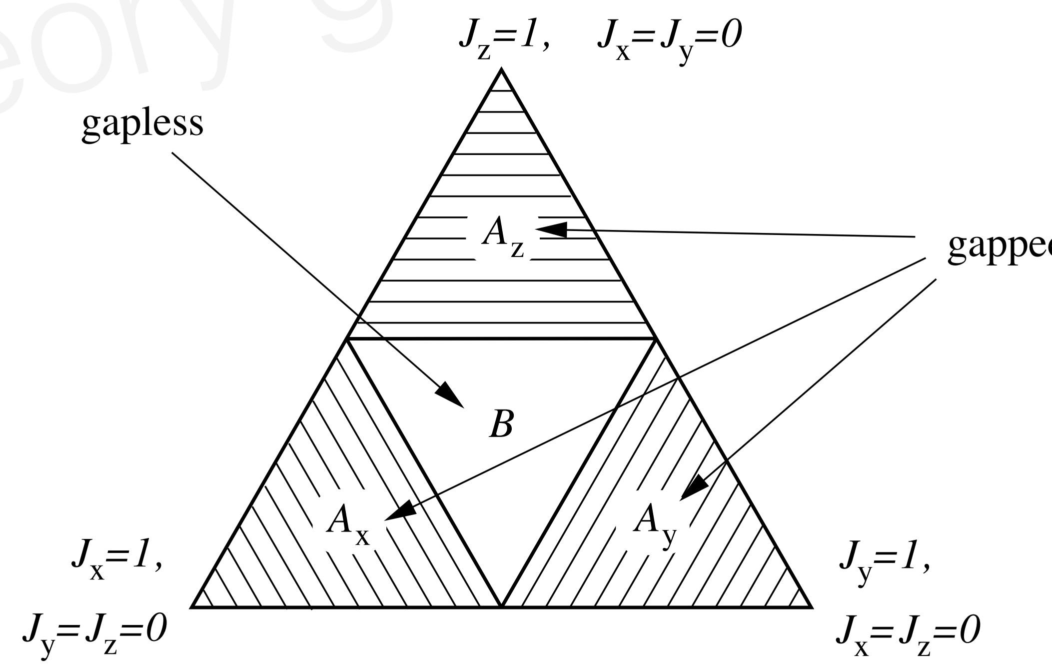
- A. Kitaev proposed and solved his model exactly with the majorana representation



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

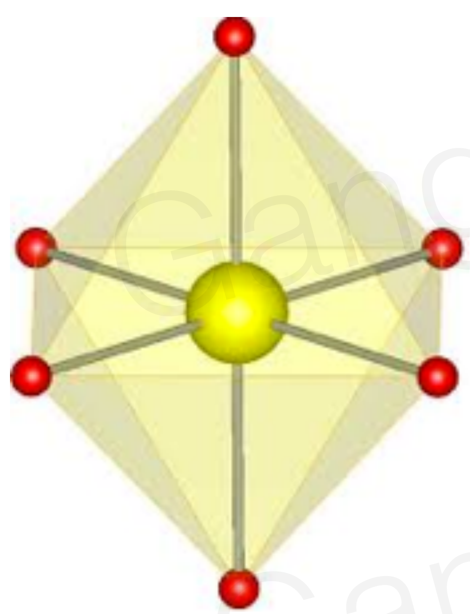


$$\widetilde{\sigma}^x = ib^x c, \quad \widetilde{\sigma}^y = ib^y c, \quad \widetilde{\sigma}^z = ib^z c.$$

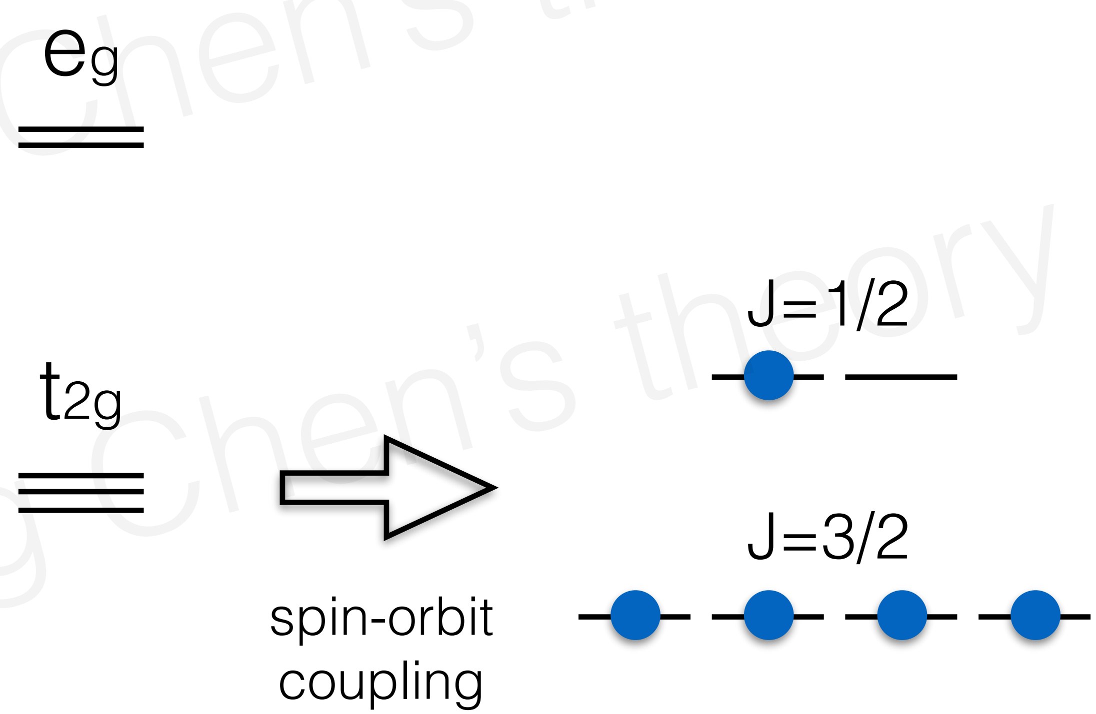


Iridates as Kitaev materials

2009 Jackeli and Khaliullin pointed out that Na_2IrO_3 may support a model with the Kitaev interaction in it.

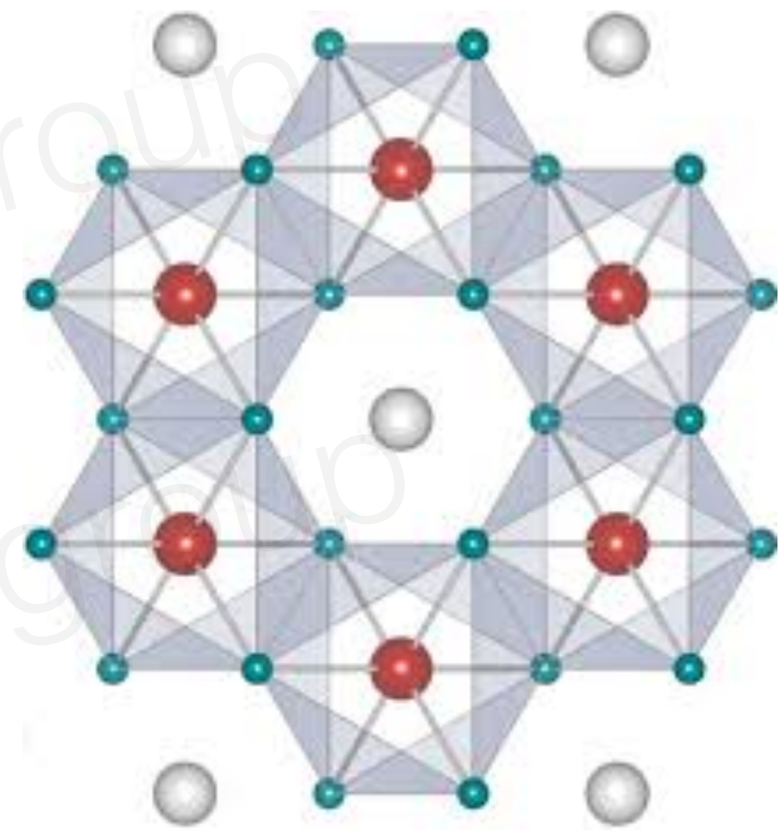


IrO_6 octahedron



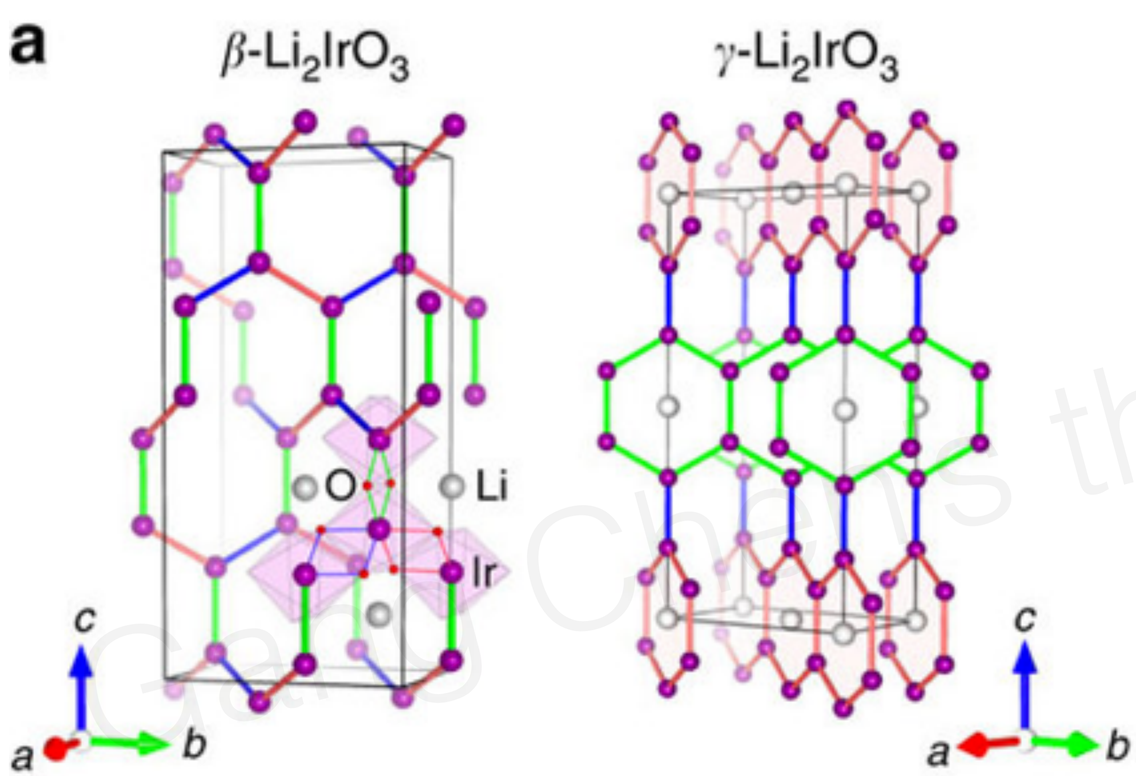
$Ir^{4+} : 5d^5$

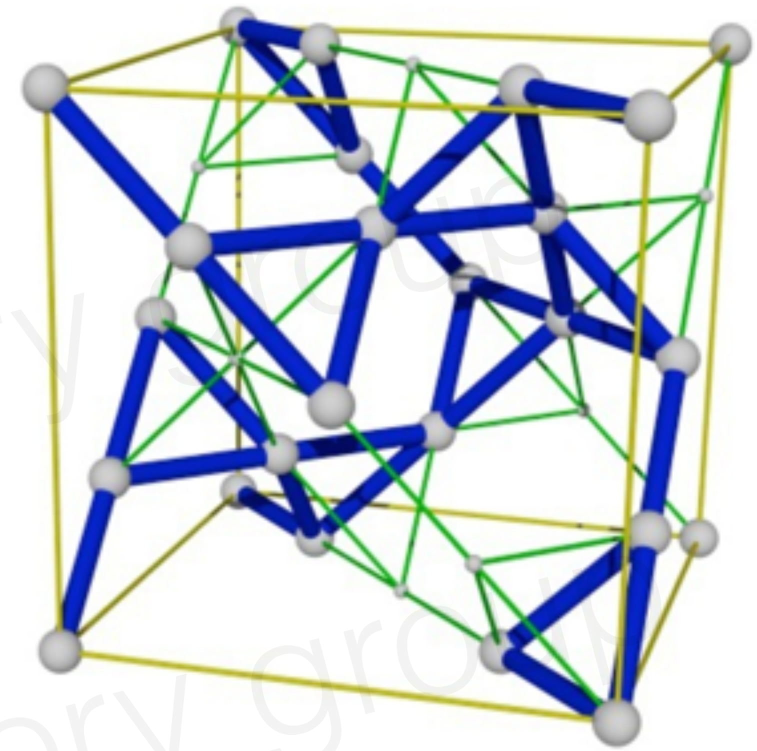
spin-orbit-entangled local moment



Na_2IrO_3
Red is iridium atom

A large families of Kitaev materials

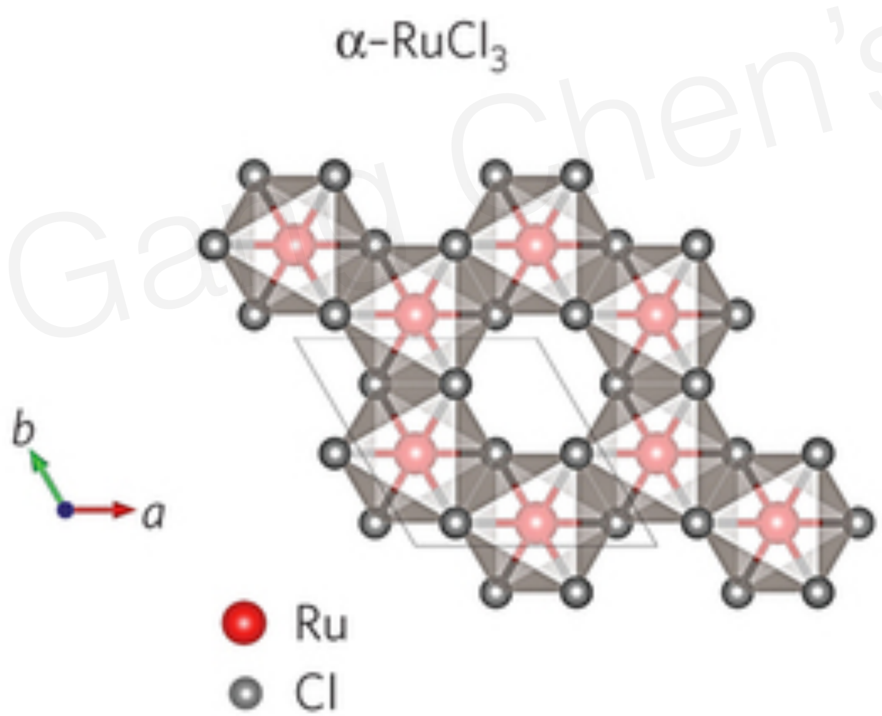




hyperkagome: $Na_4Ir_3O_8$

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.

La 57	Ce 58	Pr 59	Nd 60	Pm 61	Sm 62	Eu 63	Gd 64	Tb 65	Dy 66	Ho 67	Er 68	Tm 69	Yb 70	Lu 71
Light Rare Earths							Heavy Rare Earths							

Advantage:

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

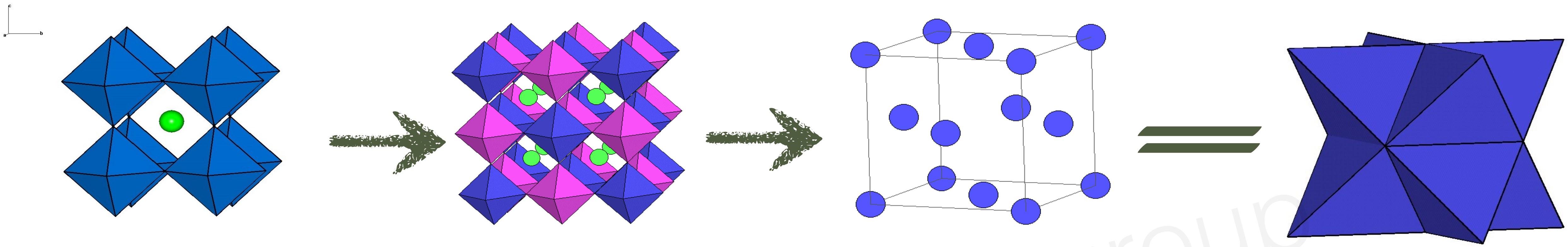
2. 4f electron is more localized than 4d/5d electron, so most times the exchange is nearest neighbors, no perturbation from further neighbors

3. The rare earth elements do not suffer from the neutron absorption issue that prevails in iridates.

Gang Chen's theory group

An example: rare-earth double perovskites

Rare-earth double perovskites



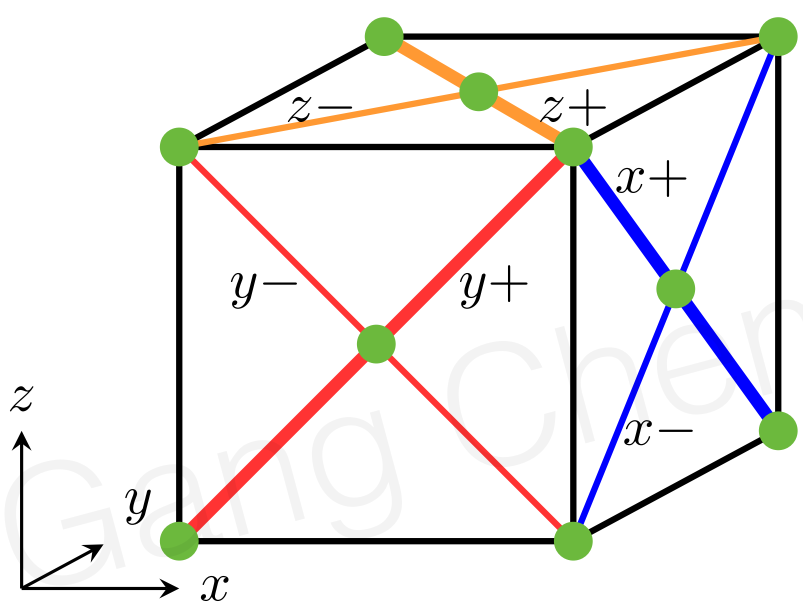
Lattice parameters for Ba_2LnSbO_6.

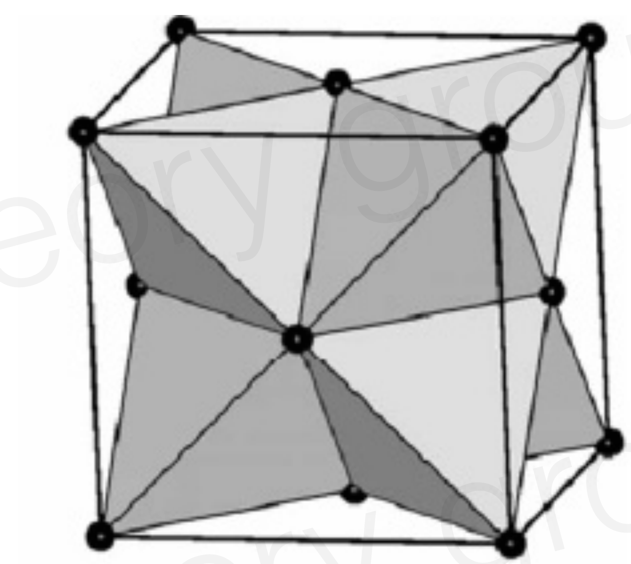
Compound	Space group	*a* (Å)	*α* (°)
Ba_2LaSbO_6	$R\bar{3}$	6.0866 (3)	60.30 (3)
Ba_2PrSbO_6	$R\bar{3}$	6.0527 (1)	60.16 (3)
Ba_2NdSbO_6	$R\bar{3}$	6.0383 (5)	60.10 (2)
Ba_2SmSbO_6	$Fm\bar{3}m$	8.5069 (3)	90
Ba_2EuSbO_6	$Fm\bar{3}m$	8.4910 (1)	90
Ba_2GdSbO_6	$Fm\bar{3}m$	8.4732 (2)	90
Ba_2TbSbO_6	$Fm\bar{3}m$	8.4505 (1)	90
Ba_2DySbO_6	$Fm\bar{3}m$	8.4297 (1)	90
Ba_2HoSbO_6	$Fm\bar{3}m$	8.4146 (1)	90
Ba_2ErSbO_6	$Fm\bar{3}m$	8.3958 (1)	90
Ba_2TmSbO_6	$Fm\bar{3}m$	8.3778 (1)	90
Ba_2YbSbO_6	$Fm\bar{3}m$	8.3620 (1)	90
Ba_2LuSbO_6	$Fm\bar{3}m$	8.3484 (1)	90

Shumpei Otsuka*, Yukio Hinatsu
Journal of Solid State Chemistry

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71
Light Rare Earths							Heavy Rare Earths							

Generalized Kitaev-Heisenberg model



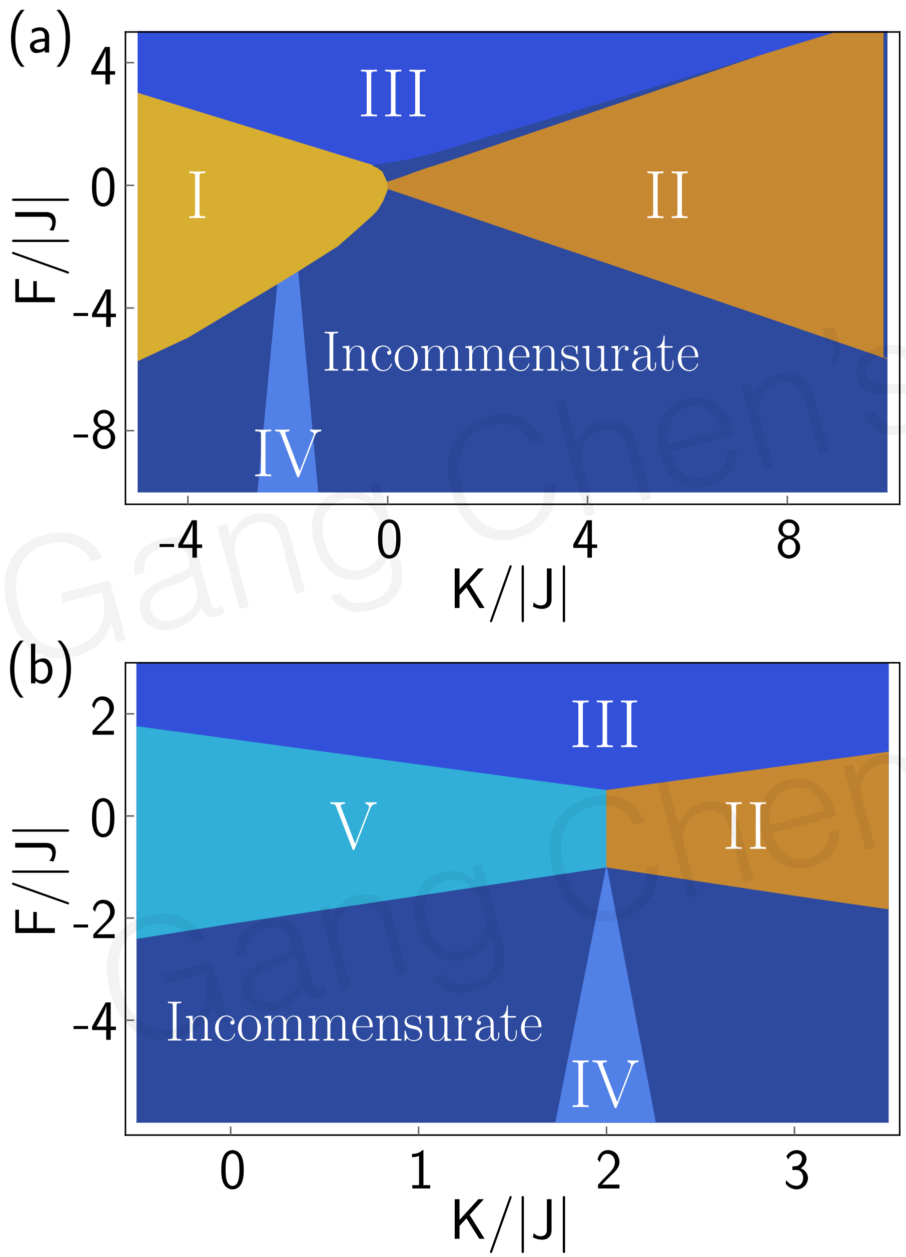


FCC lattice

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

Phase diagram

J>0



J<0

Phase	Wavevector	Order Para.	Continuous deg
I	$(2\pi, 0, 0)$	along [100] axis	–
II	$(2\pi, 0, 0)$	in (100) plane	$U(1)$
III	(π, π, π)	along [111] axis	–
IV	(π, π, π)	in (111) plane	$U(1)$
V	$(0, 0, 0)$	any direction	$O(3)$

GS with accidental degeneracy

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

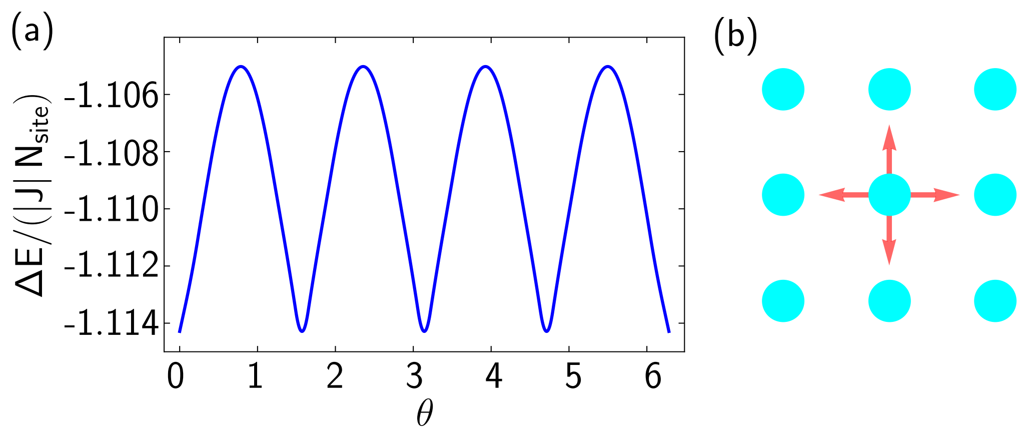
II: $\mathbf{S}_i \equiv S\,\hat{m}_i = S\,[\cos\theta\,\hat{y} + \sin\theta\,\hat{z}]\,e^{2\pi x_i}$,

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

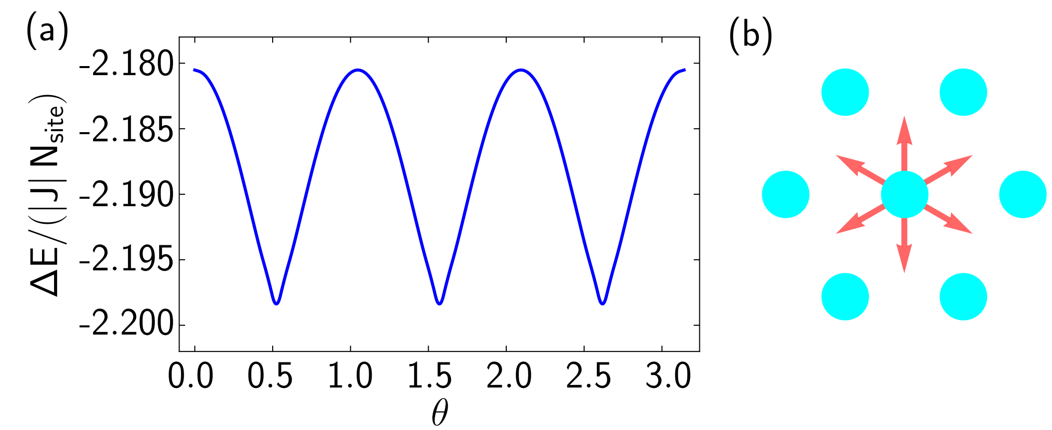
IV: $\mathbf{S}_i \equiv S\hat{m}_i = S(\cos\theta\,\hat{u}_1 + \sin\theta\,\hat{u}_2)e^{i\pi(x_i+y_i+z_i)}$,

V: $\mathbf{S}_i \equiv S\,\hat{m}_i = S\,(\sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z})$,

Ground state selection



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



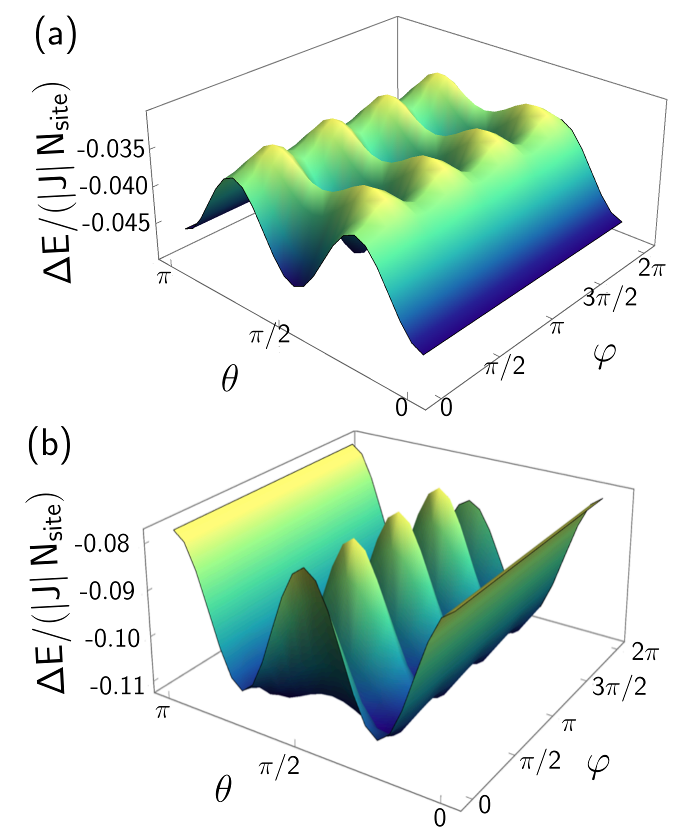
IV: $\mathbf{S}_i \equiv S\hat{m}_i = S(\cos\theta\,\hat{u}_1 + \sin\theta\,\hat{u}_2)e^{i\pi(x_i+y_i+z_i)},$

$$\mathbf{S}_i \cdot \hat{m}_i = S - b_i^\dagger b_i,$$

$$\mathbf{S}_i \cdot \hat{n}_i = \frac{(2S)^{\frac{1}{2}}}{2}(b_i + b_i^\dagger),$$

$$\mathbf{S}_i \cdot (\hat{m}_i \times \hat{n}_i) = \frac{(2S)^{\frac{1}{2}}}{2i}(b_i - b_i^\dagger),$$

$$H_{\rm sw} = \sum_{\mathbf{k}} \Big[\sum_{\mu,\nu} (A_{\mu\nu}(\mathbf{k}) b_{\mathbf{k}\mu}^\dagger b_{\mathbf{k}\nu} + B_{\mu\nu}(\mathbf{k}) b_{-\mathbf{k},\mu} b_{\mathbf{k}\nu} + B_{\mu\nu}^*(-\mathbf{k}) b_{\mathbf{k}\mu}^\dagger b_{-\mathbf{k},\nu}^\dagger) + C(\mathbf{k}) \Big] + E_{\rm cl},$$

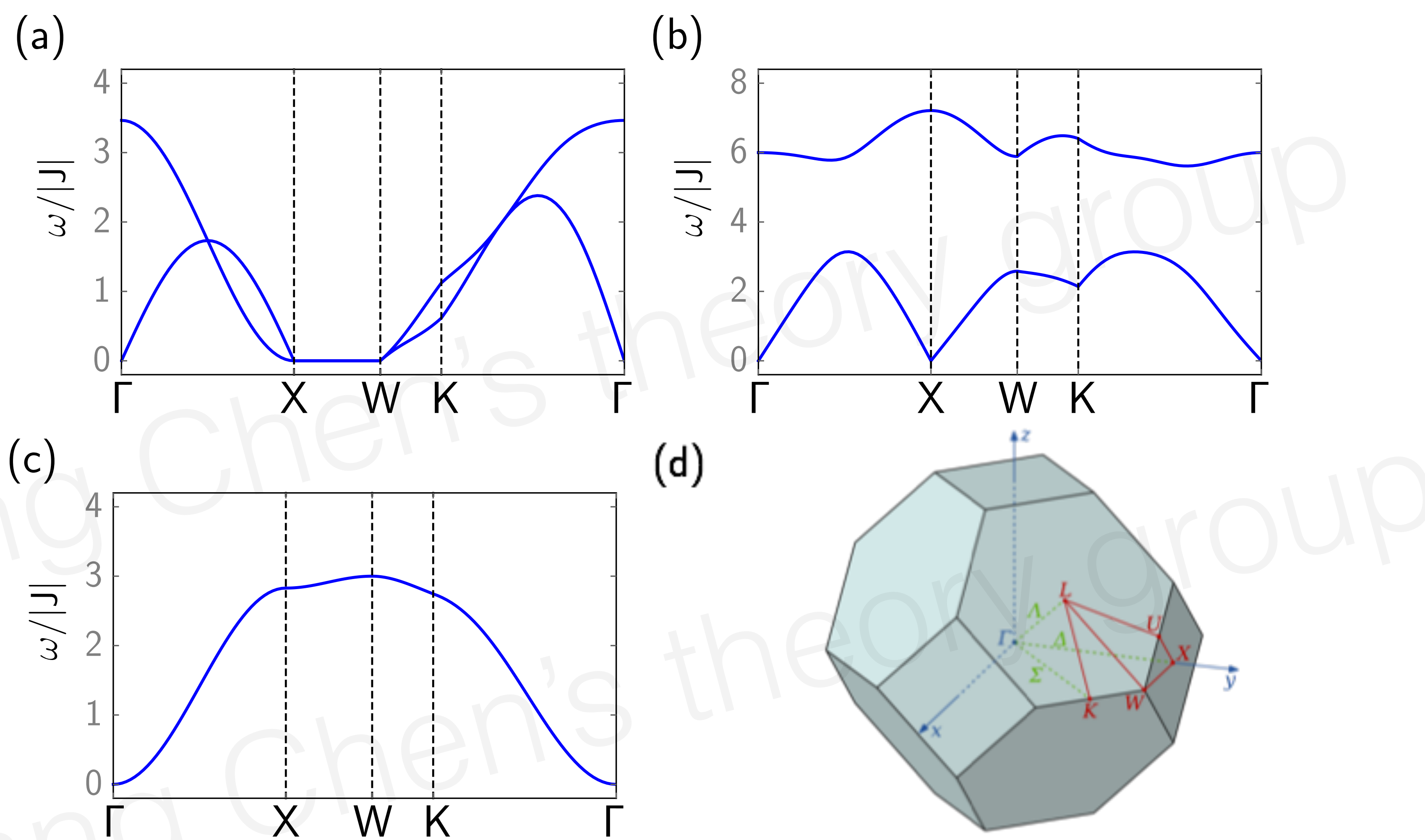


Quantum zero point energy

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

V: $\mathbf{S}_i \equiv S\,\hat{m}_i = S\,(\sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}),$

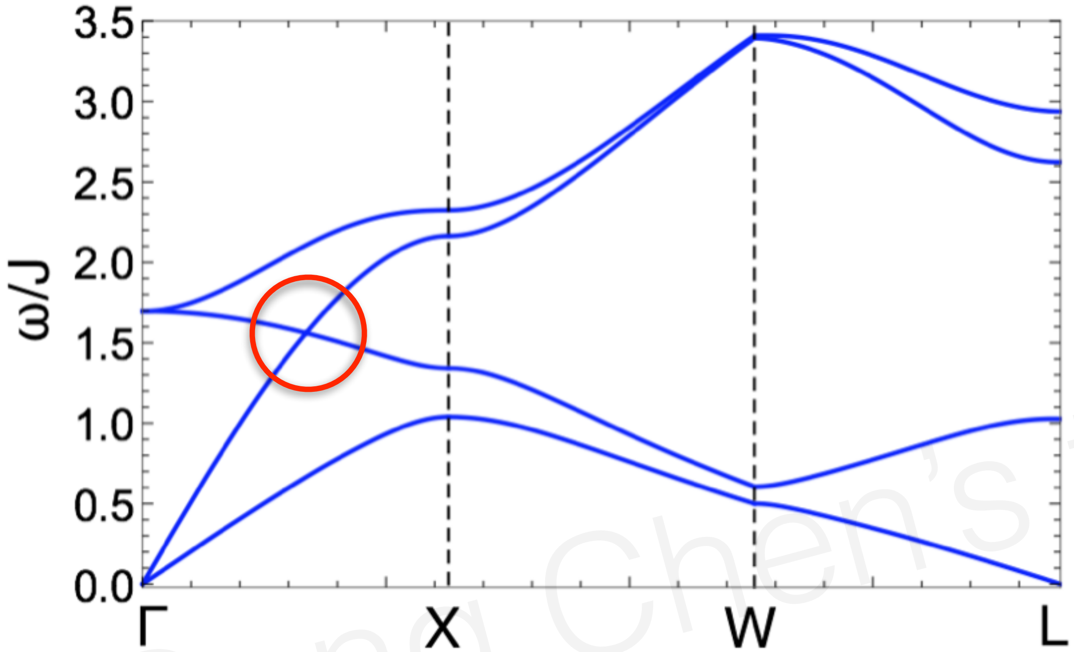
Excitation: Pseudo-Goldstone mode and Weyl magnon

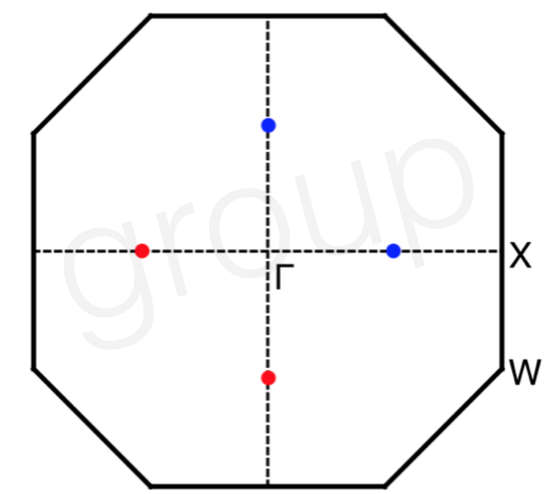


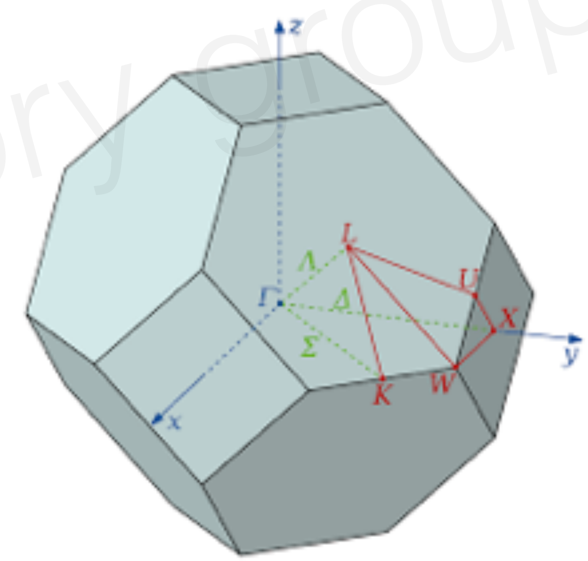
Pseudo-Goldstone mode:

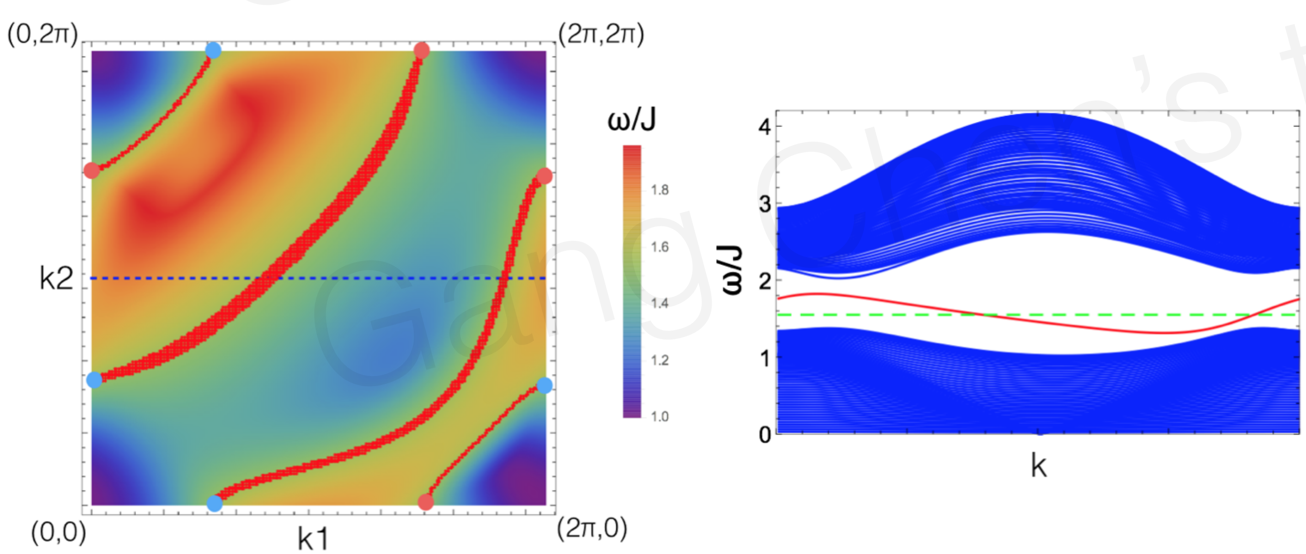
Appear to be gapless at mean field level, but should be gapped when anharmonic spin-wave interactions is included.

Weyl magnons









(a) (b)

surface arc states

Fei-Ye Li, Yao-Dong Li, YB Kim, L Balents, Yue Yu, **GC***, **Nat Comm**, in press.

Weyl magnon in magnetic field

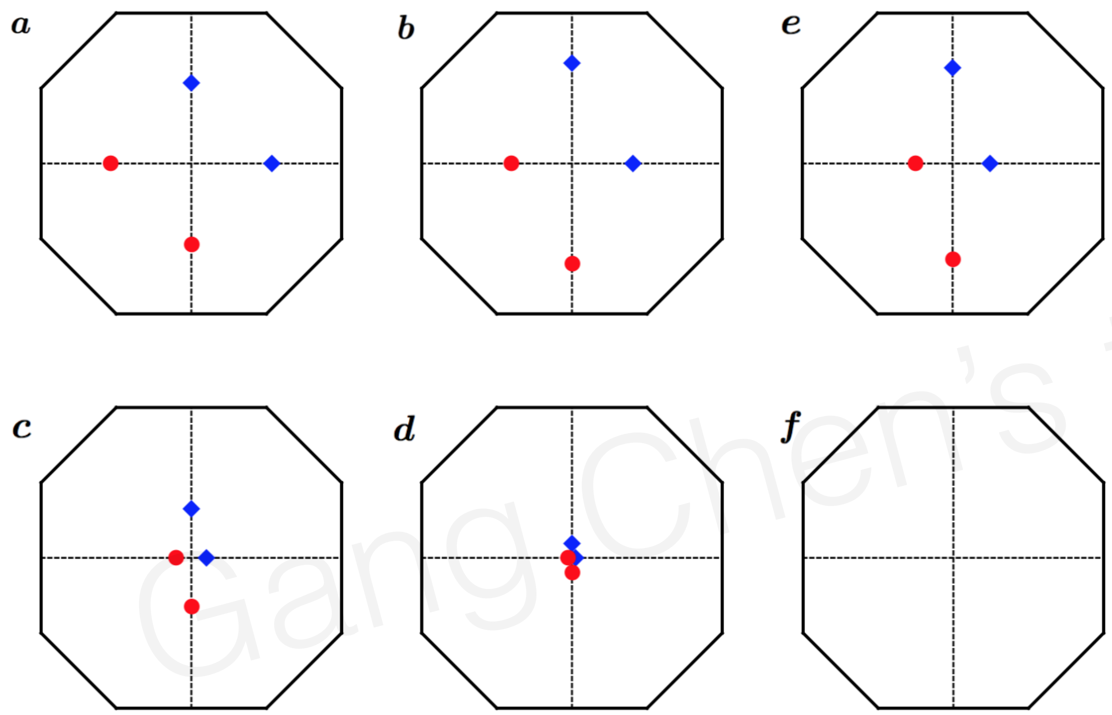


FIG. 5. **The evolution of Weyl nodes under the magnetic field**. Applying a magnetic field along the global z direction, $\mathbf{B} = B[001]$, Weyl nodes are shifted but still in $k_z = 0$ plane. They are annihilated at Γ when magnetic field is strong enough. Red and blue indicate the opposite chirality. (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 $\theta = \pi/2$.

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.

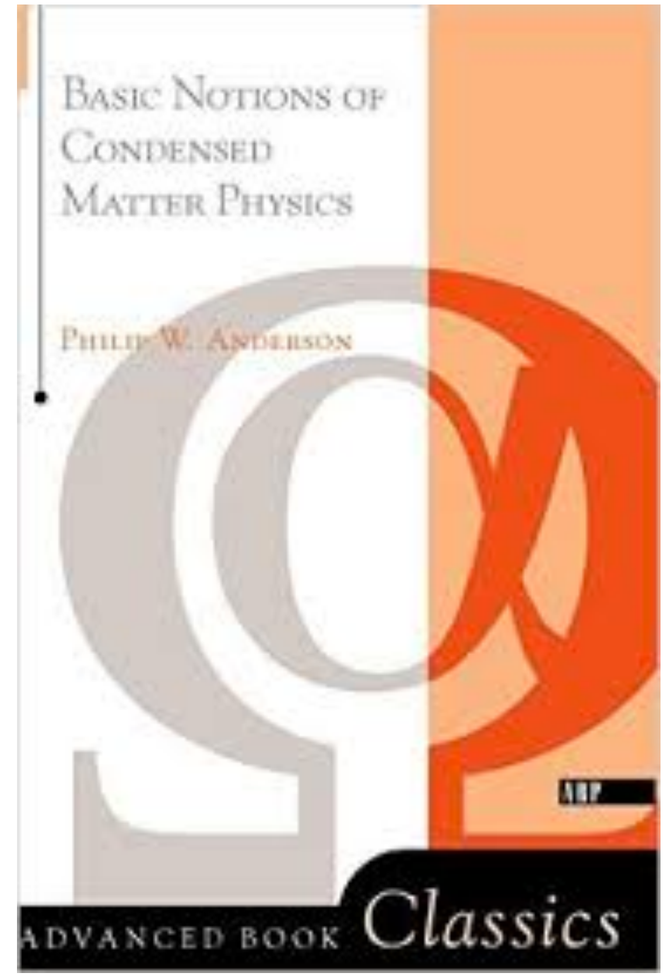
The magnon Weyl points can be moved and annihilated by magnetic field, this provides a way to control Weyl magnons with magnetic fields.

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

P W Anderson

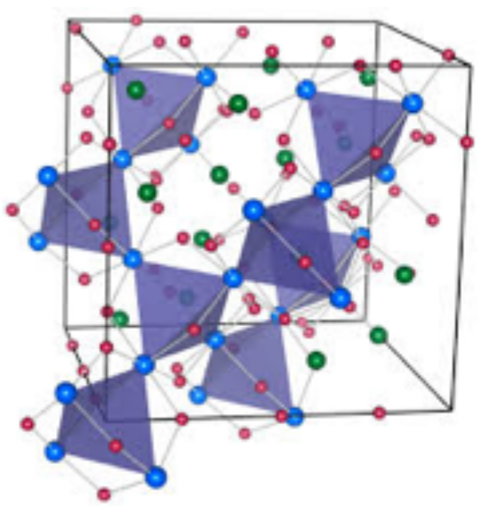


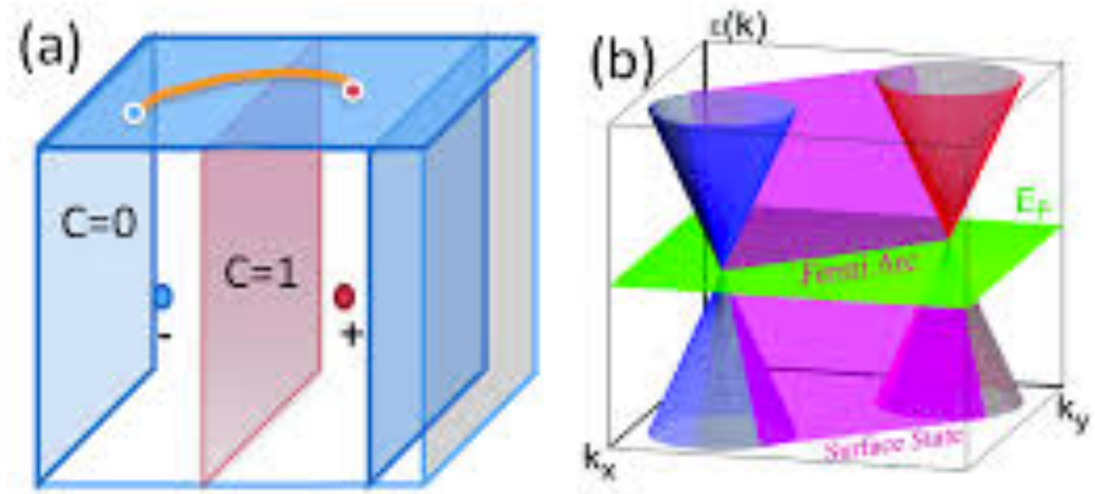
1984

“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.”

explain the history

Weyl fermions





Xiangang Wan, Vishwanath, etc 2011, Burkov, Balents 2011

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

Discovered in 2015 in various physical systems !

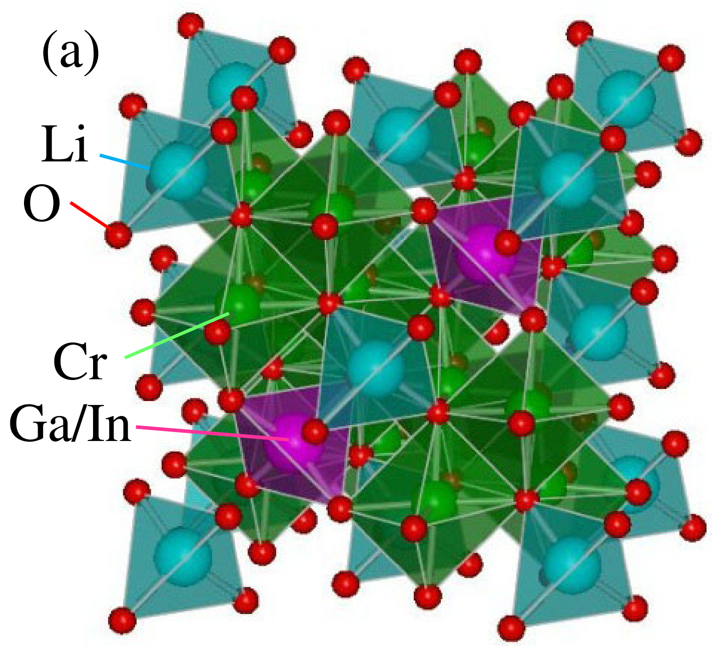
Remark

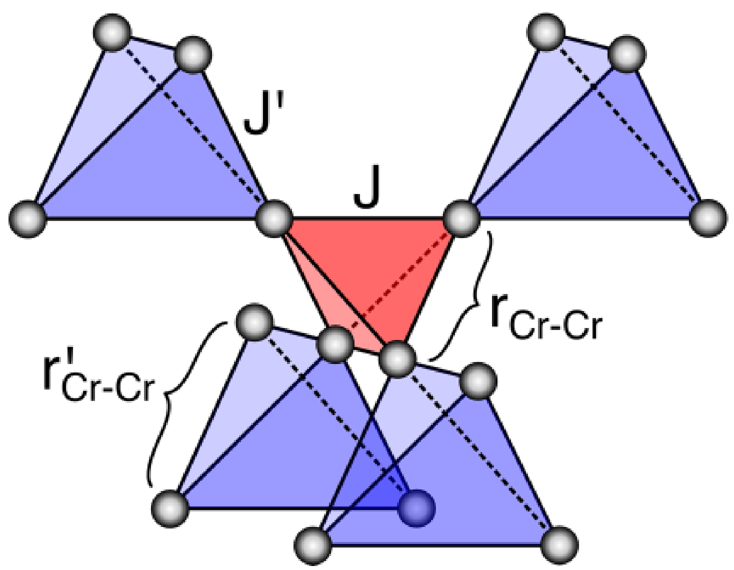
Weyl band touching is a topological property of the band structure, and is thus **independent** from the particle statistics.

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

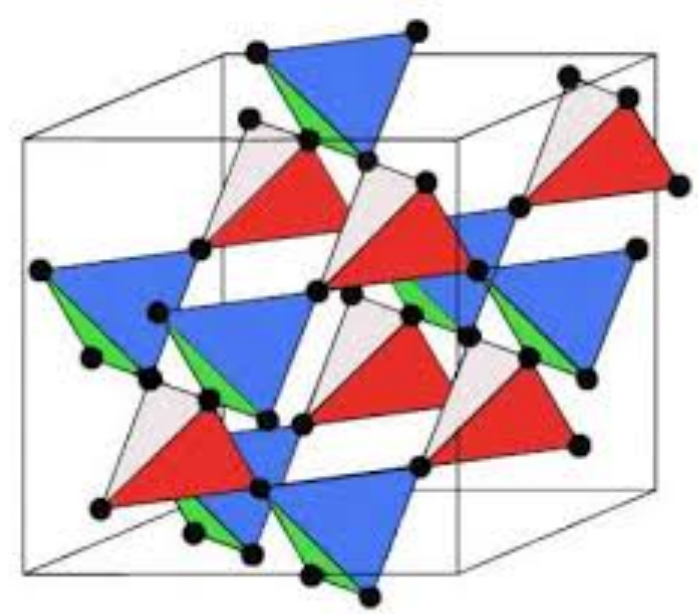
类似于 breathing

Breathing Pyrochlore





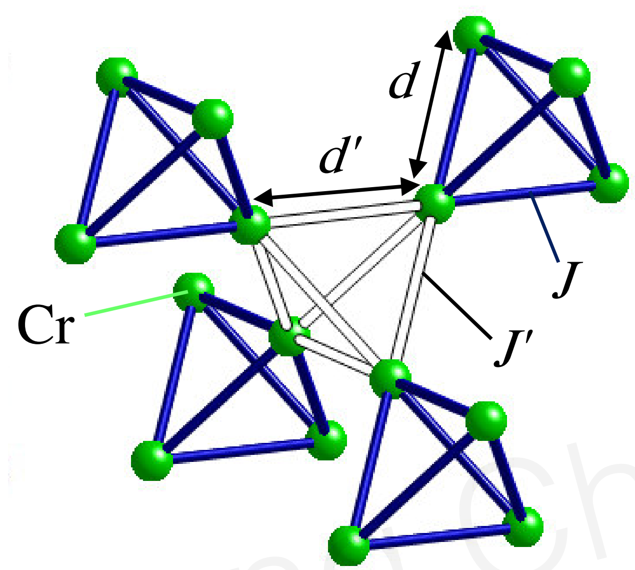
Breathing Pyrochlore



Regular Pyrochlore

K. Kimura, S. Nakatsuji, and T. Kimura, **PhysRevB** 2014,
Yoshihiko Okamoto, Gøran J. Nilsen, J. Paul Attfield, and Zenji Hiroi, **PhysRevLett** 2013,
Yu Tanaka, Makoto Yoshida, Masashi Takigawa, Yoshi- hiko Okamoto, and Zenji Hiroi, **PhysRevLett** 2014.

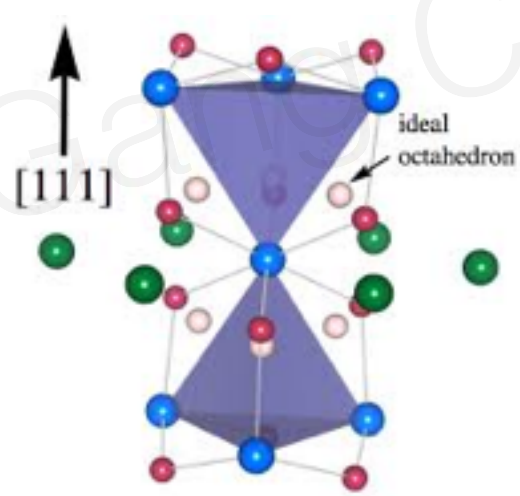
Minimal model and ground states



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

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

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



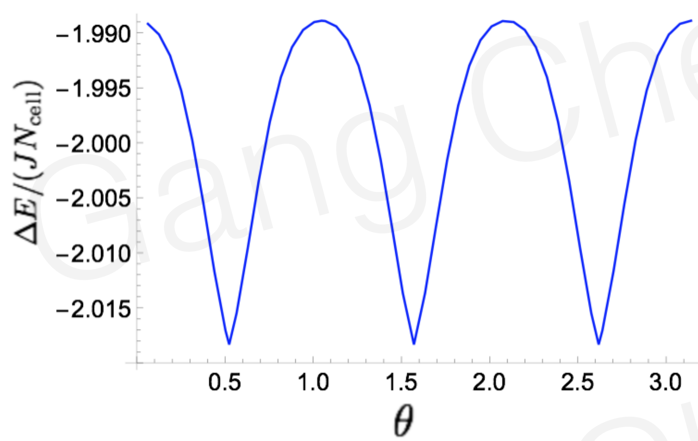
$$\sum_{\langle ij \rangle \in \mathrm{u}} \mathbf{S}_i \cdot \mathbf{S}_j \sim \frac{1}{2} \Big(\sum_{i \in \mathrm{u}} \mathbf{S}_i \Big)^2$$

$$\sum_{\langle ij \rangle \in \mathrm{d}} \mathbf{S}_i \cdot \mathbf{S}_j \sim \frac{1}{2} \Big(\sum_{i \in \mathrm{d}} \mathbf{S}_i \Big)^2$$

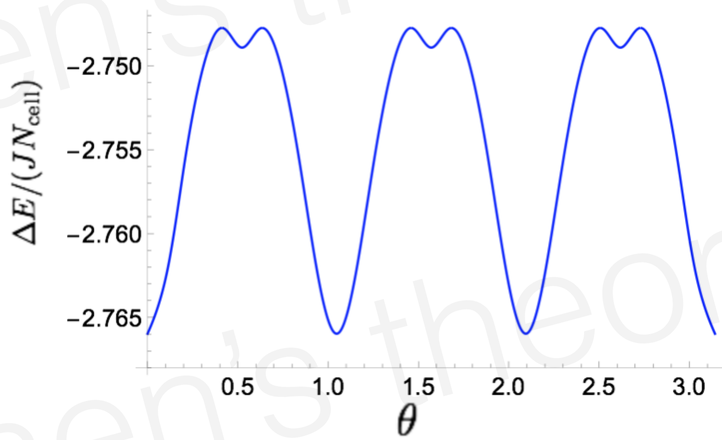
Quantum order by disorder

$$\mathbf{S}_i^{\rm cl} \equiv S\hat{m}_i = S(\cos\theta\,\hat{x}_i + \sin\theta\,\hat{y}_i),$$

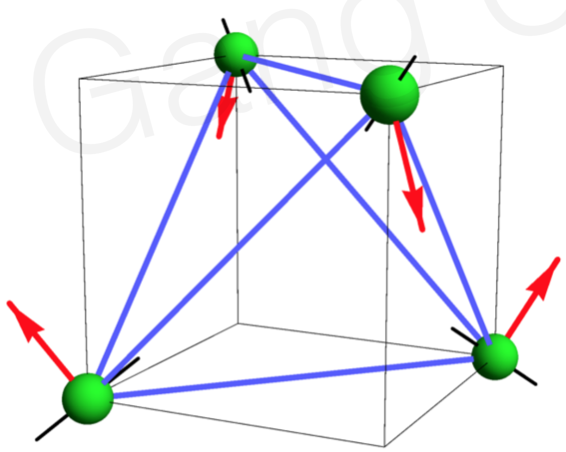
Holstein-Primarkoff bosons to express the spin operators as $\mathbf{S}_i \cdot \hat{m}_i = S - a_i^\dagger a_i$, $\mathbf{S}_i \cdot \hat{z}_i = (2S)^{1/2}(a_i + a_i^\dagger)/2$, and $\mathbf{S}_i \cdot (\hat{m}_i \times \hat{z}_i) = (2S)^{1/2}(a_i - a_i^\dagger)/(2i)$. Keeping terms in



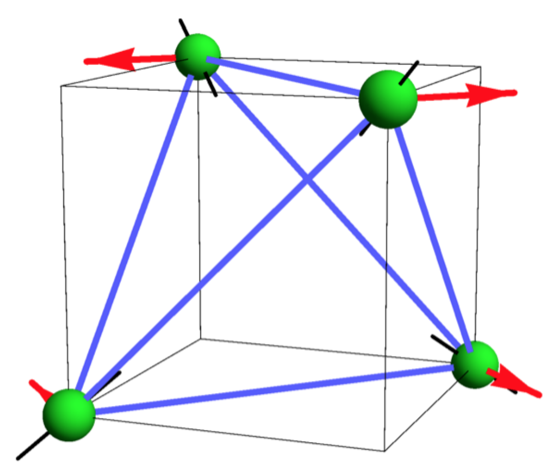
(a)



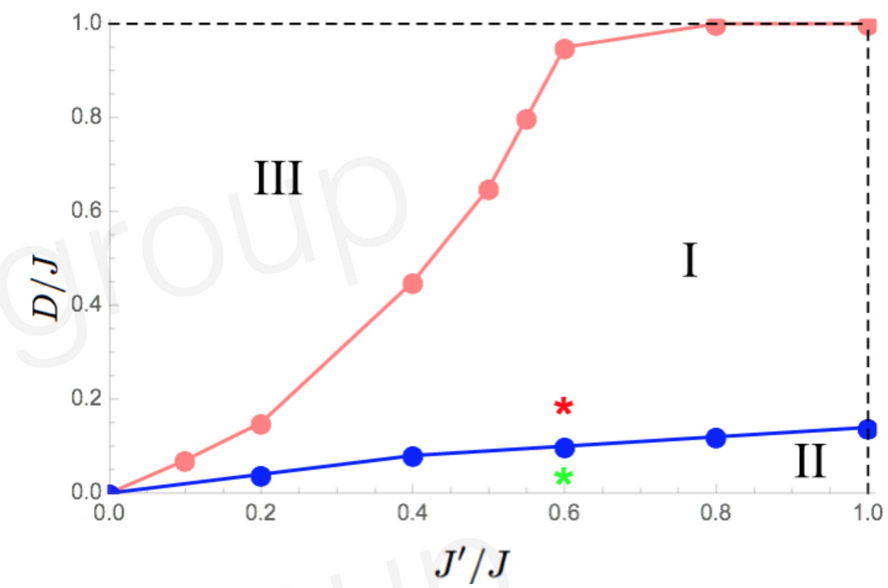
(b)



(c)



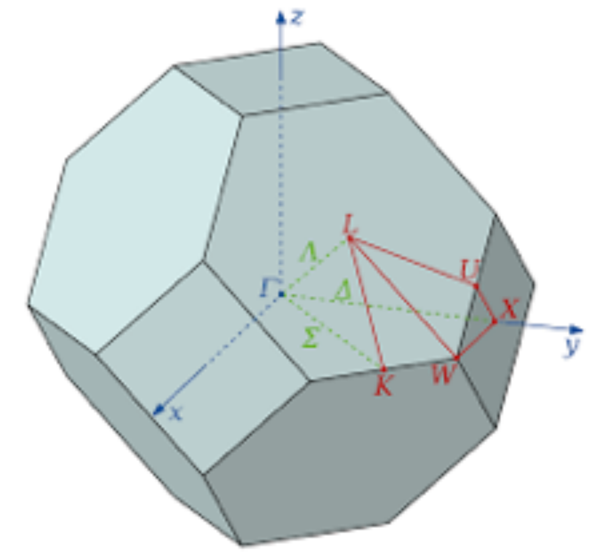
(d)

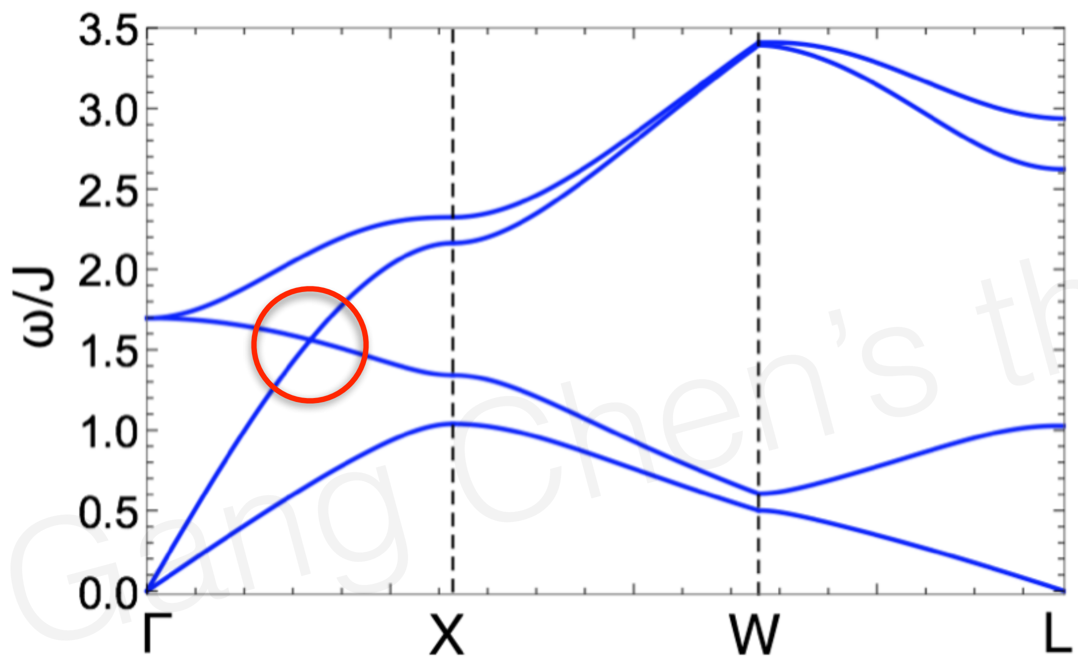


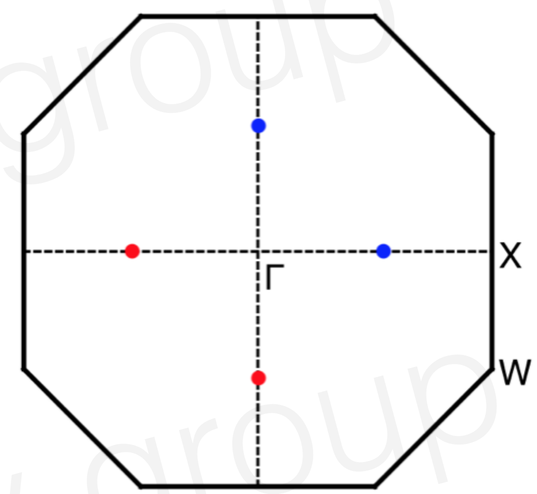
I,III have the same order,
but are distinct **topologically**!

CL Henley 1987

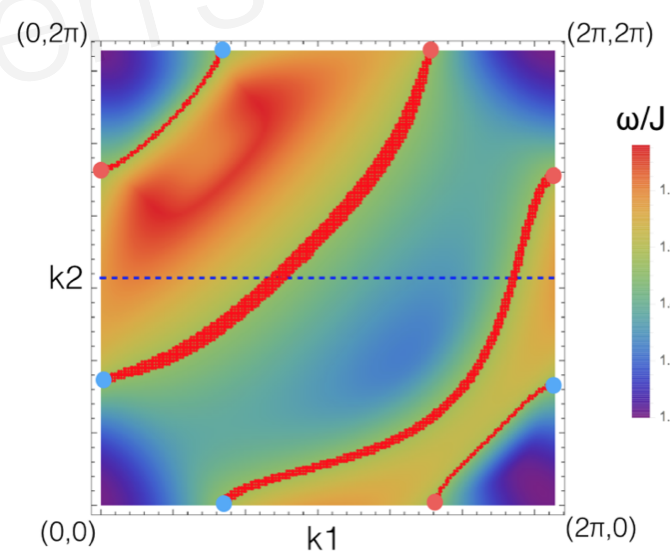
Weyl magnons



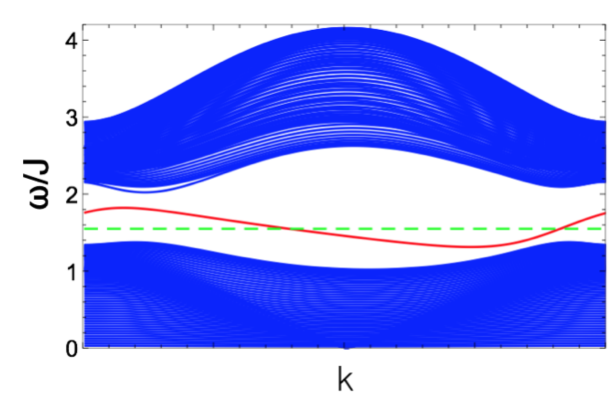




surface arc states



(a)



(b)

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.