Recent developments in quantum magnetism

Gang Chen Fudan University, Shanghai China





There is no field theory, no exotic phenomenon, no fractionalization, no topological order, etc in this tutorial.



Part 1 Topological magnons: the case of Weyl magnon

- 1. What is Weyl semimetal?
- 2. Antiferromagnets and spin wave excitations
- 3. Weyl magnons: uniqueness and extension.

Part 2 Detecting hidden multipolar orders in quantum magnets

- 1. Hidden orders in condensed matter physics
- 2. Hidden orders with intertwined multipolar structure
 - in rare-earth magnets
- 3. An experimental example



Topological magnons: the case of Weyl magnon Part 1 Gang Gang Chen's theory group



Selected for a Viewpoint in *Physics*

PHYSICAL REVIEW B 83, 205101 (2011)

S

Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates

Xiangang Wan,¹ Ari M. Turner,² Ashvin Vishwanath,^{2,3} and Sergey Y. Savrasov^{1,4}

 ¹National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China
 ²Department of Physics, University of California, Berkeley, California 94720, USA
 ³Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
 ⁴Department of Physics, University of California, Davis, One Shields Avenue, Davis, California 95616, USA (Received 23 February 2011; published 2 May 2011)



Physics 4, 36 (2011)

Viewpoint

Weyl electrons kiss

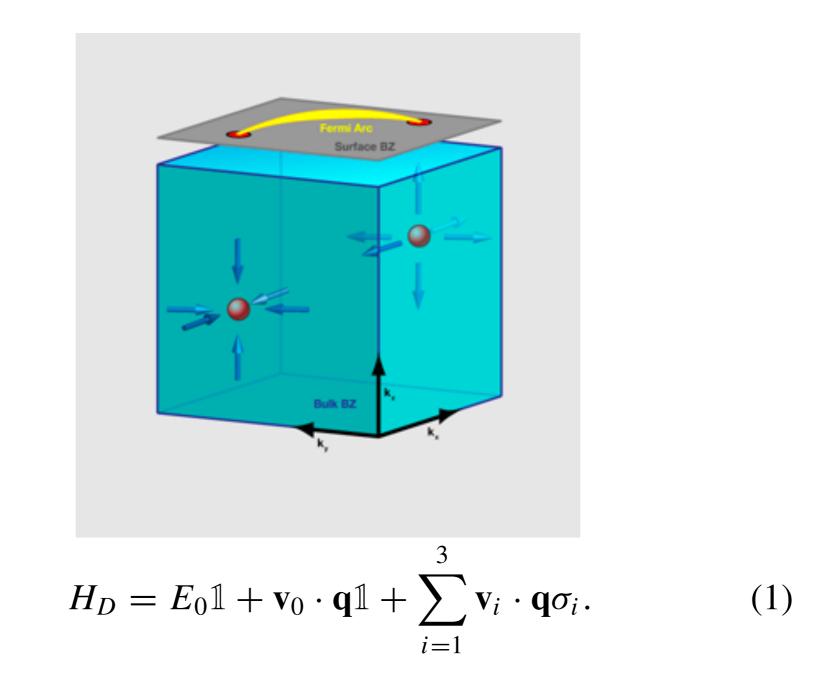
Leon Balents
Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA
Published May 2, 2011

Theorists predict the possibility of topological "Fermi arc" surface states in a system with broken time-reversal symmetry.

Subject Areas: Strongly Correlated Materials

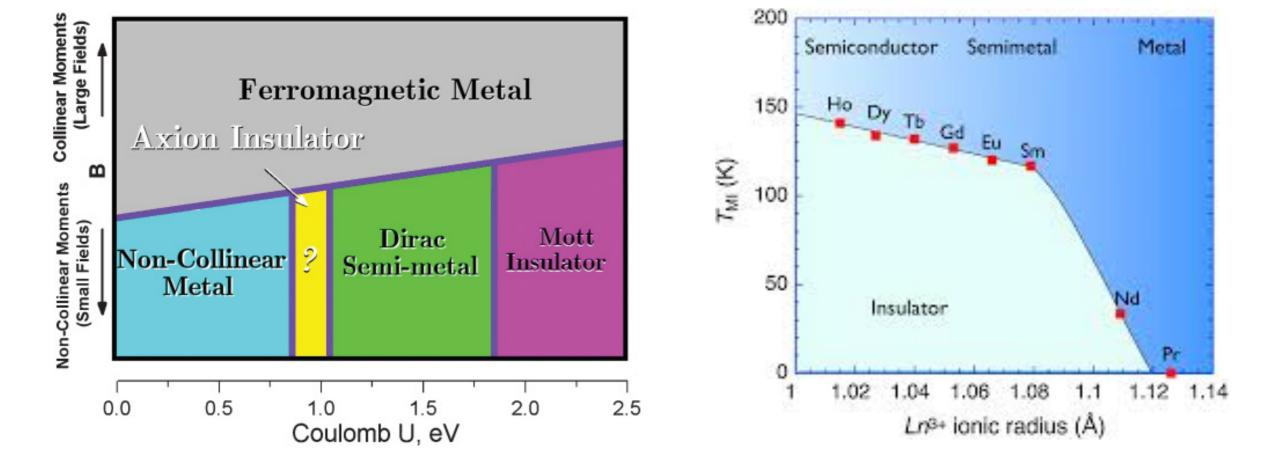


Weyl semimetal



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

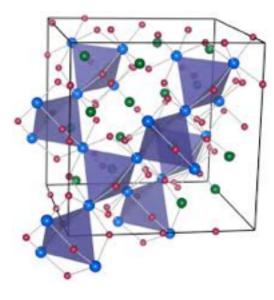


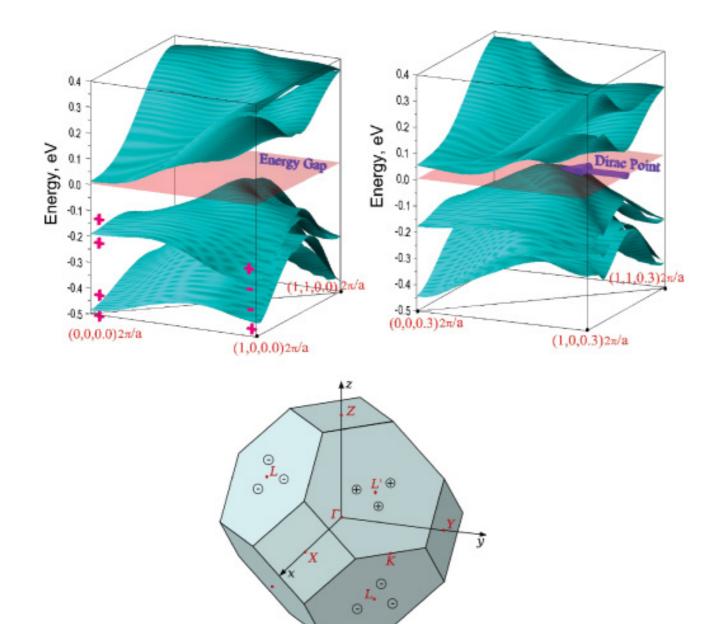


Weyl semimetal proposed in pyrochlore iridates

Xiangang Wan, Turner, Vishwanath, Savrasov, PhysRevB 2011, Magnetic Weyl semimetal from the Ir correlation driven all-in all-out order.







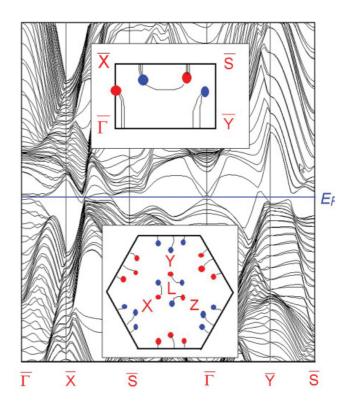


FIG. 4. (Color online) Semimetallic nature of the state at U = 1.5 eV according to the LSDA + U + SO method. (a) Calculated energy bands in the plane $K_z = 0$ with band parities shown; (b) energy bands in the plane $k_z = 0.6\pi/a$, where a Weyl point is predicted to exist. The lighter-shaded plane is at the Fermi level. (c) Locations of the Weyl points in the three-dimensional Brillouin zone (Ref. 29) (nine are shown, indicated by the circled + or - signs).



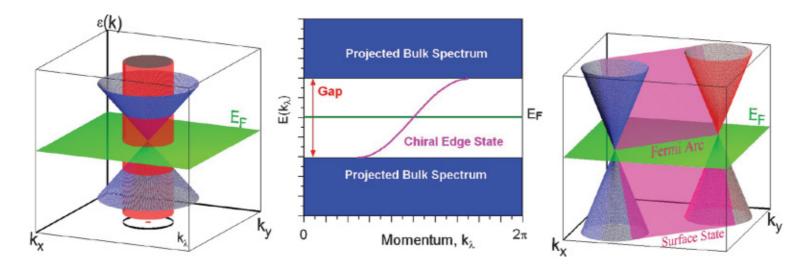


FIG. 5. (Color online) Illustration of surface states arising from bulk Weyl points. (a) The bulk states as a function of (k_x, k_y) (and arbitrary k_z) fill the inside of a cone. A cylinder whose base defines a one-dimensional circular Brillouin zone is also drawn. (b) The cylinder unrolled onto a plane gives the spectrum of the two-dimensional subsystem $H(\lambda, k_z)$ with a boundary. On top of the bulk spectrum, a chiral state appears due to the nonzero Chern number. (c) Meaning of the surface states back in the three-dimensional system. The chiral state appears as a surface connecting the original Dirac cone to a second one, and the intersection between this plane and the Fermi level gives a Fermi arc connecting the Weyl points.

The Weyl points behave like "magnetic" monopoles in momentum space whose charge is given by the chirality; they are actually a source of "Berry flux" rather than magnetic flux. The Berry connection, a vector potential in momentum space, is defined by $\mathcal{A}(\mathbf{k}) = \sum_{n=1}^{N} i \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle$, where N is the number of occupied bands. As usual, the Berry flux is defined as $\mathcal{F} = \nabla_{\mathbf{k}} \times \mathcal{A}$. To show that there are arcs connecting pairs of Weyl points, we argue that there is an arc on the surface Brillouin zone emanating from the projection (k_{0x}, k_{0y}) of each Weyl point.

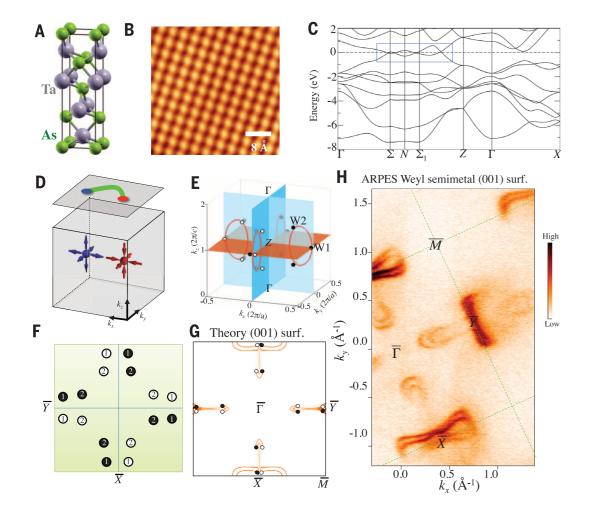


Weyl semimetal discovered in TaAs

TOPOLOGICAL MATTER

Discovery of a Weyl fermion semimetal and topological Fermi arcs

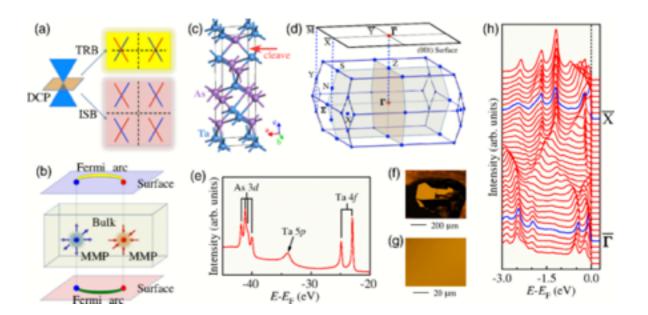
Su-Yang Xu,^{1,2*} Ilya Belopolski,^{1*} Nasser Alidoust,^{1,2*} Madhab Neupane,^{1,3*} Guang Bian,¹ Chenglong Zhang,⁴ Raman Sankar,⁵ Guoqing Chang,^{6,7} Zhujun Yuan,⁴ Chi-Cheng Lee,^{6,7} Shin-Ming Huang,^{6,7} Hao Zheng,¹ Jie Ma,⁸ Daniel S. Sanchez,¹ BaoKai Wang,^{6,7,9} Arun Bansil,⁹ Fangcheng Chou,⁵ Pavel P. Shibayev,^{1,10} Hsin Lin,^{6,7} Shuang Jia,^{4,11} M. Zahid Hasan^{1,2}†



PHYSICAL REVIEW X 5, 031013 (2015)

Experimental Discovery of Weyl Semimetal TaAs

B. Q. Lv,¹ H. M. Weng,^{1,2} B. B. Fu,¹ X. P. Wang,^{2,3,1} H. Miao,¹ J. Ma,¹ P. Richard,^{1,2} X. C. Huang,¹ L. X. Zhao,¹ G. F. Chen,^{1,2} Z. Fang,^{1,2} X. Dai,^{1,2} T. Qian,^{1,*} and H. Ding^{1,2,†}
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Extensions

- Type-II Weyl semimetal
- Hybrid Weyl semimetal
- Dirac fermion, type-II Dirac nodes
- nodal line semimetal
- hourglass fermion
- new fermion.....

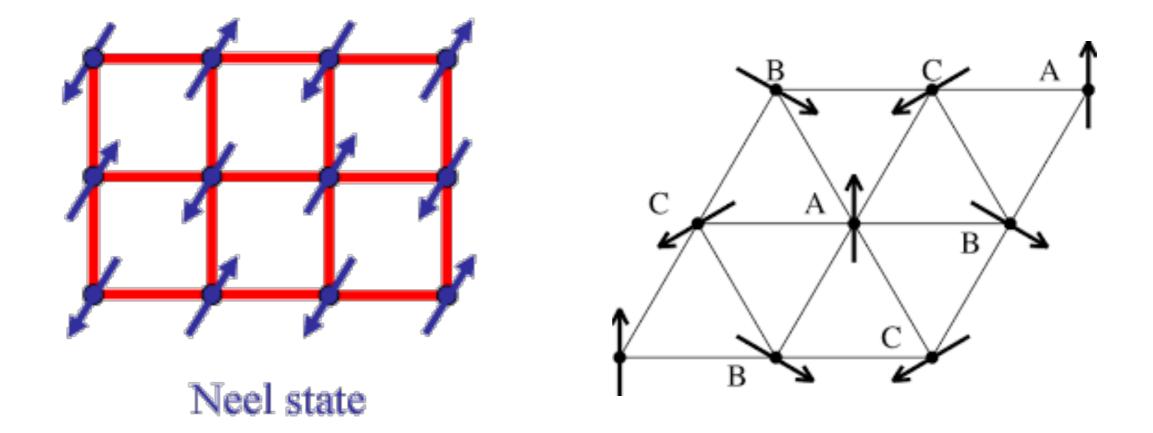


Part 1 Topological magnons: the case of Weyl magnon

2. Antiferromagnets and spin wave excitations



Ordered AFMs

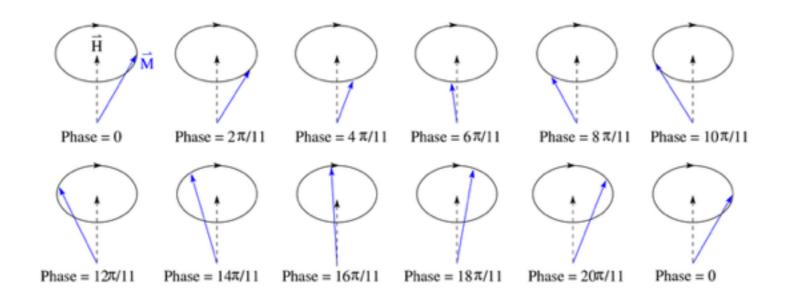


Ground state orders for AFMagnetic Heisenberg model.

Most known magnets are antiferromagnets.



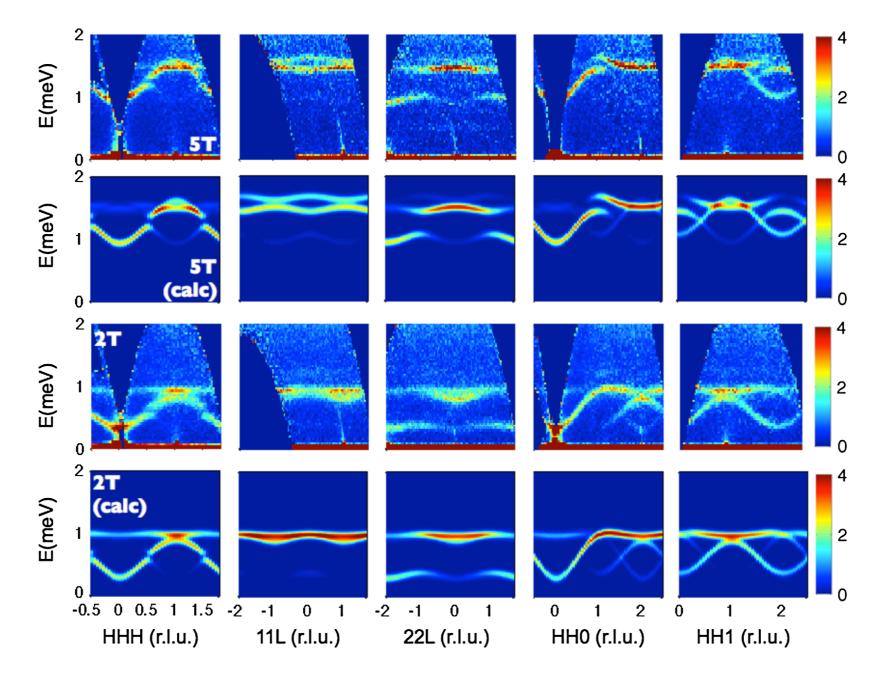
Propagating spin waves and Holstein-Primakoff spin wave



$$S_+=\hbar\sqrt{2s}\sqrt{1-rac{a^\dagger a}{2s}}\,a\ ,\qquad S_-=\hbar\sqrt{2s}a^\dagger\,\sqrt{1-rac{a^\dagger a}{2s}}\ ,\qquad S_z=\hbar(s-a^\dagger a)\ .$$



Spin wave excitations in ordered AFM: Pyrochlore Yb₂Ti₂O₇



Kate A. Ross,¹ Lucile Savary,² Bruce D. Gaulin,^{1,3,4} and Leon Balents^{5,*}



PHYSICAL REVIEW X 1, 021002 (2011)

Part 1 Topological magnons: the case of Weyl magnon

3. Weyl magnons: uniqueness and extension



Remark

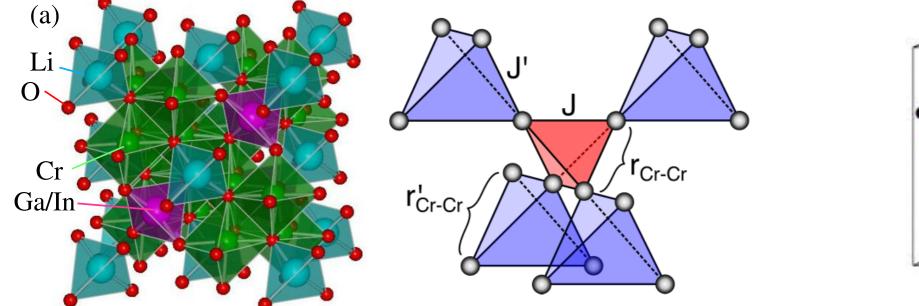
Weyl band touching is a topological property of the band structure, and is thus **independent** from the particle statistics.

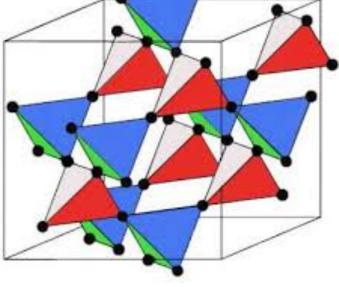
It can be fermion, e.g. electron, can also be boson, e.g. photon.



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.

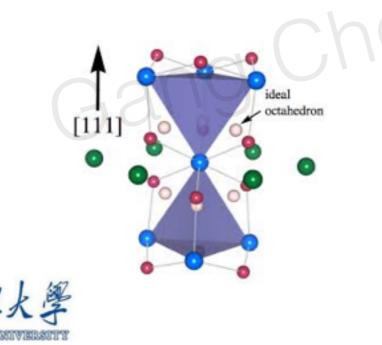


Minimal model and ground states

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

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

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



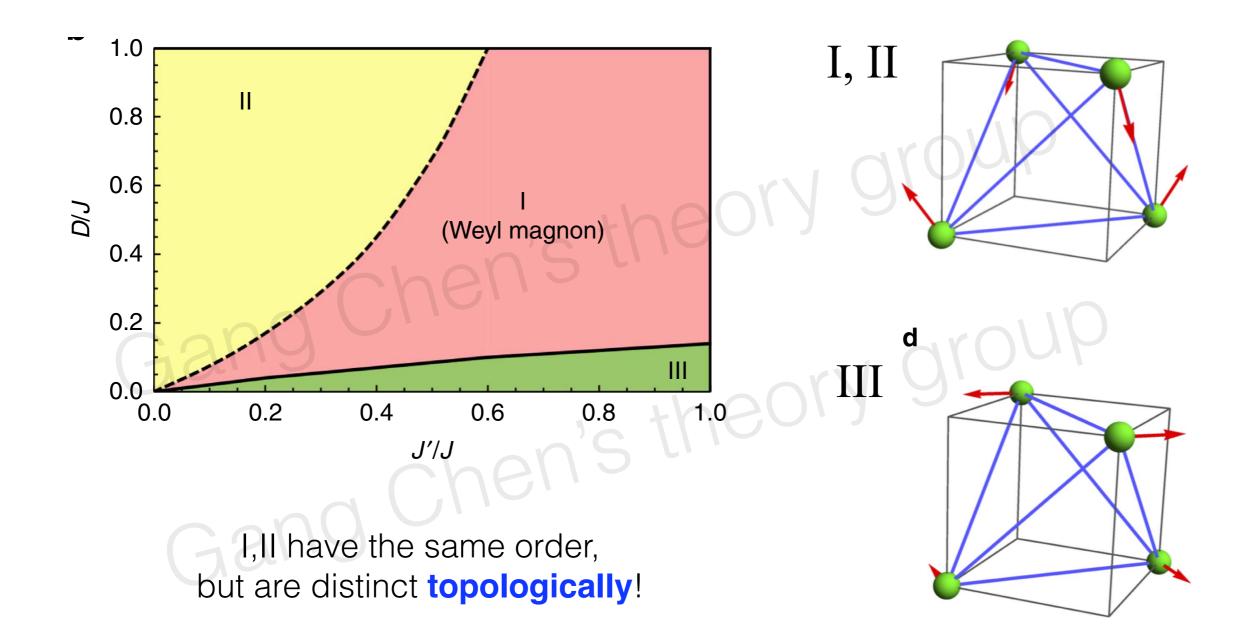
d'

Cr

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

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

Phase diagram

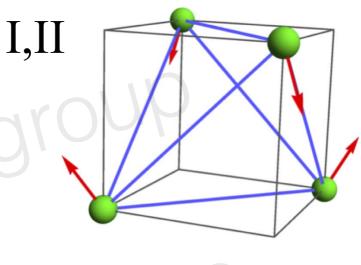


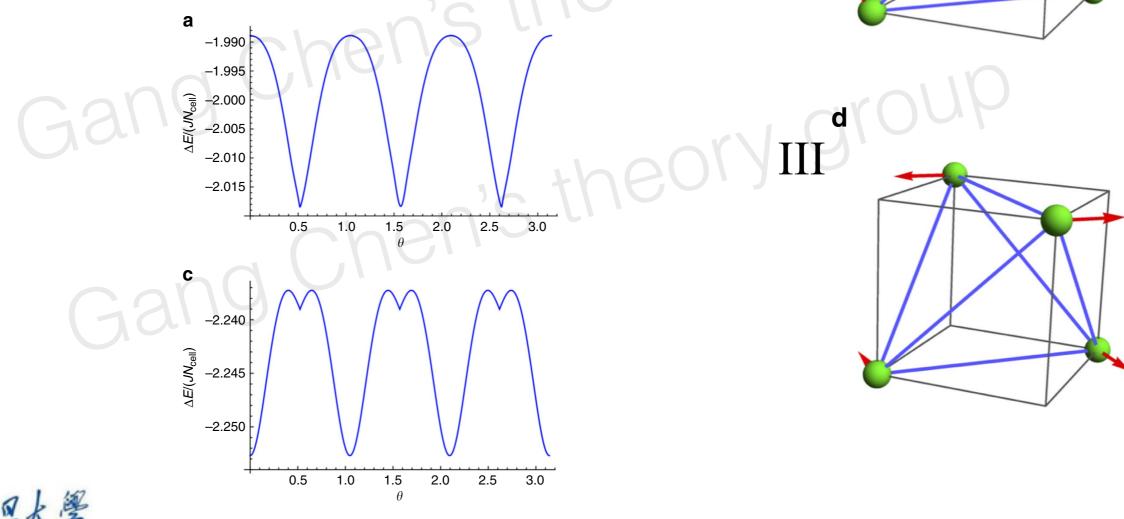


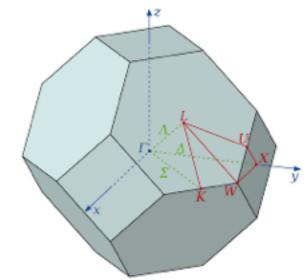
Quantum order by disorder

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

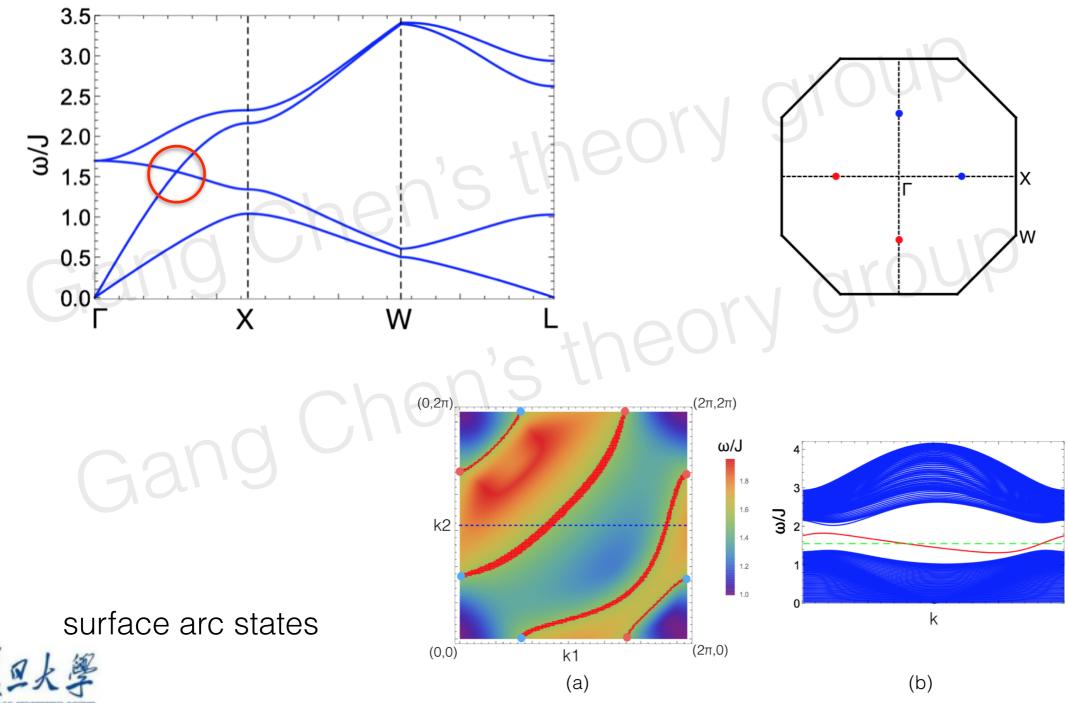
Holstein-Primarkoff bosons to express the spin operators as $\mathbf{S}_i \cdot \hat{m}_i = S - a_i^{\dagger} a_i$, $\mathbf{S}_i \cdot \hat{z}_i = (2S)^{1/2} (a_i + a_i^{\dagger})/2$, and $\mathbf{S}_i \cdot (\hat{m}_i \times \hat{z}_i) = (2S)^{1/2} (a_i - a_i^{\dagger})/(2i)$. Keeping terms in







Weyl magnons



Tune Weyl nodes with magnetic field

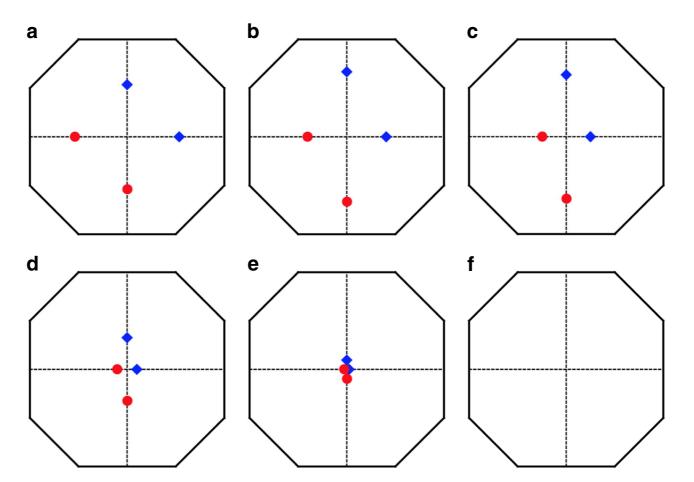


Figure 5 | The evolution of Weyl nodes under the magnetic field. Applying a magnetic field along the global *z* direction, $\mathbf{B}=B\hat{\mathbf{z}}$, Weyl nodes are shifted but still in $k_z = 0$ plane. They are annihilated at Γ when magnetic field is strong enough. Red and blue indicate the opposite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

different from Weyl electrons



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.

COMPARE TO Weyl fermion in the electron system



Extension

Dirac magnons (Yuan Li, Chen Fang, Jingsheng Wen) vs Dirac electron

nodal line magnon (??) vs nodal line semimetal

Magnon topological insulator (Schnyder, Katsura) vs electron topological insulator



Summary

Band topology of magnon can be another interesting thing to look at among these magnetically ordered systems.



Fei-Ye Li (Fudan)



Yaodong Li (Fudan->UCSB) and Yue Yu, Leon Balents, YongBaek Kim, Arun Paramekanti

Fei-Ye Li, Yao-dong Li, YB Kim, L Balents, Yue Yu, Gang Chen*, Nature Comms. 7, 12691 (2018) Fei-Ye Li, Yao-dong Li, Yue Yu, A Paramekanti, Gang Chen*, Phys. Rev. B, 95, 085132 (2017)



Part 2 Detecting hidden multipolar orders in quantum magnets

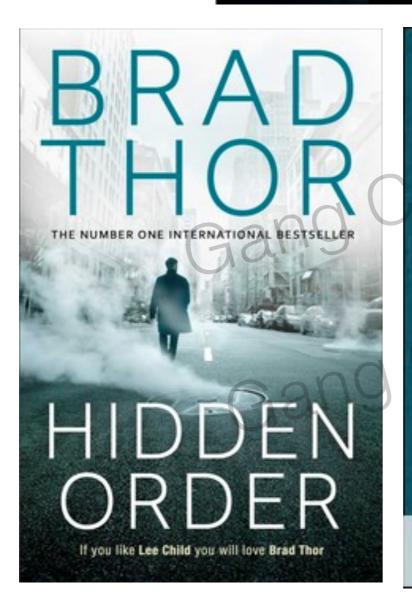
1. Hidden orders in condensed matter physics

we undertand the order/structure,

we know how thing work, function make prediction



R

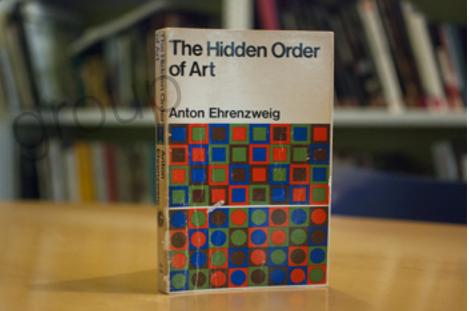


The Hidden Order of Corruption

An Institutional Approach

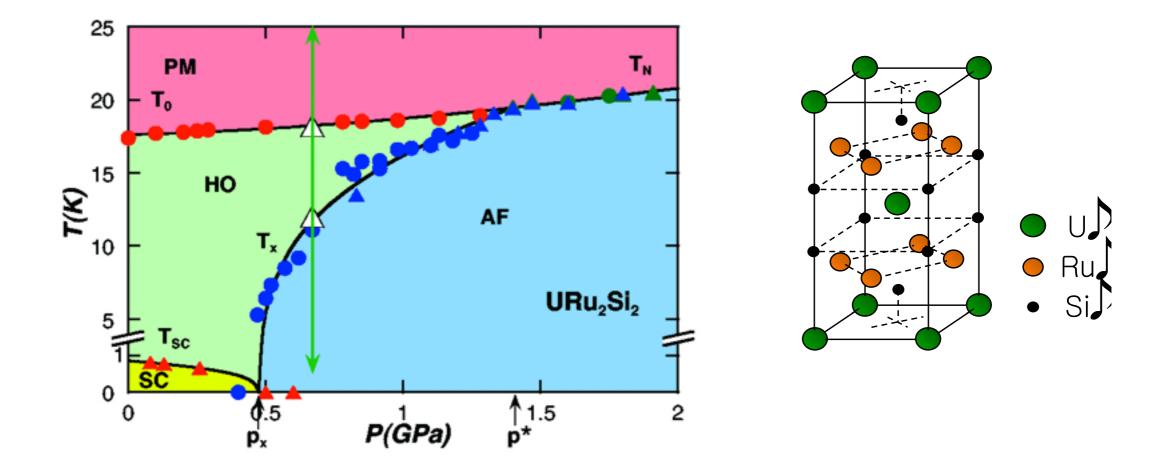
Kraina Ksiażek







Hidden order in condensed matter



- Hidden order: "dark matter" in CMT
- URu₂Si₂
 - Second order transition at ~17K, $\Delta \mathcal{S} \sim 0.42~Rln2$
 - Order parameters unknown after decades



Nature of hidden orders

 Magnetic multipolar order Quadrupolar order Octupolar order

2. Electric multipolar order

3. Orbital order

How to probe these hidden orders?



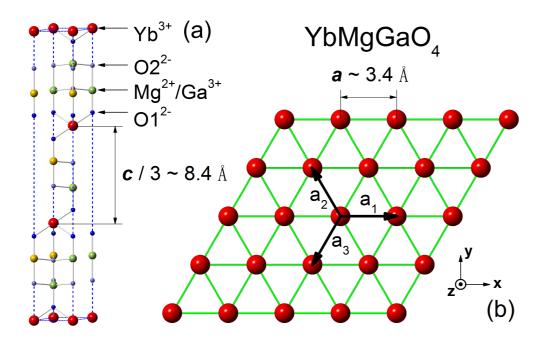
Part 2 Detecting hidden multipolar orders in quantum magnets

2. Hidden orders with intertwined multipolar structure in rare-earth magnets



A rare-earth triangular lattice quantum spin liquid: YbMgGaO4

collaboration with QM Zhang, Jun Zhao, Yuesheng Li, Yaodong Li





Qingming Zhang (Renmin)

- Hastings-Oshikawa-Lieb-Shultz-Mattis theorem.
- Recent extension to spin-orbit coupled insulators (Watanabe, Po, Vishwanath, Zaletel, PNAS 2015).
- This is likely the first strong spin-orbit coupled QSL with odd electron filling and effective spin-1/2.
- It is the first clear observation of T^{2/3} heat capacity. (needs comment.)
- Inelastic neutron scattering is consistent with spinon Fermi surface results.
- We think it is a spinon Fermi surface U(1) QSL.

Inelastic neutron scattering performed by Jun Zhao's group and M Mourigal's group



YMGO is not alone: lots of isostructural materials

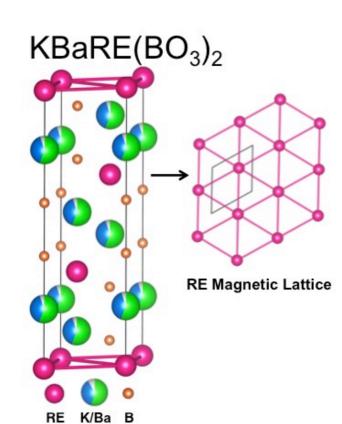
Compound	Magnetic ion	Space group	Local moment	$\Theta_{\mathrm{CW}}\left(\mathrm{K}\right)$	Magnetic transition	Frustration para. f	Refs.
YbMgGaO ₄	$Yb^{3+}(4f^{13})$	R3m	Kramers doublet	-4	PM down to 60 mK	<i>f</i> > 66	[4]
CeCd ₃ P ₃	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-60	PM down to 0.48 K	f > 200	[5]
CeZn ₃ P ₃	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-6.6	AFM order at 0.8 K	f = 8.2	[7]
CeZn ₃ As ₃	$Ce^{3+}(4f^1)$	$P6_3/mmc$	Kramers doublet	-62	Unknown	Unknown	[8]
PrZn ₃ As ₃	$Pr^{3+}(4f^2)$	$P6_3/mmc$	Non-Kramers doublet	-18	Unknown	Unknown	[8]
NdZn ₃ As ₃	$Nd^{3+}(4f^{3})$	$P6_3/mmc$	Kramers doublet	-11	Unknown	Unknown	[8]

YD Li, XQ Wang, GC*, PRB 94, 035107 (2016)

Magnetism in the KBaRE(BO₃)₂ (RE=Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) series: materials with a triangular rare earth lattice

M. B. Sanders, F. A. Cevallos, R. J. Cava Department of Chemistry, Princeton University, Princeton, New Jersey 08544

Many ternary chalcogenides NaRES2, NaRESe2, KRES2, KRES2, KRES2, KRES2, RbRES2, RbRES2, RbRES2, CsRES2, CsRES2, etc.)



C Liu, YD Li, GC*, PRB 98, 045119 (2018)



Model Hamiltonian for all cases

CHANGLE LIU, YAO-DONG LI, AND GANG CHEN

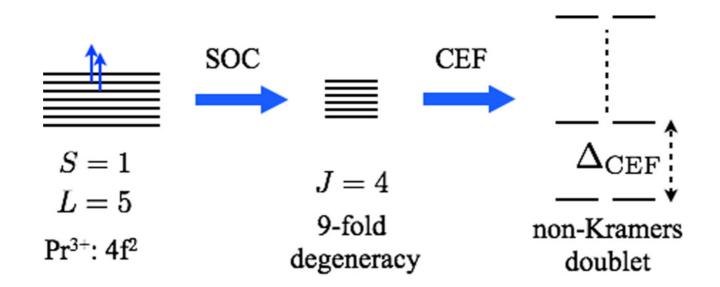
PHYSICAL REVI

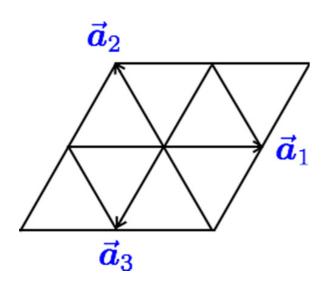
TABLE I. The relevant spin Hamiltonians for three different doublets on the triangular lattice. The models for th and the dipole-octupole doublet have been obtained in the previous works.

Local doublets	The nearest-neighbor spin Hamiltonians on the triangular lattice			
Usual Kramers doublet	$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) - \frac{iJ_{z\pm}}{2}$			
	$[(\gamma_{ij}^* S_i^+ - \gamma_{ij} S_i^-) S_j^z + S_i^z (\gamma_{ij}^* S_j^+ - \gamma_{ij} S_j^-)]$			
Dipole-octupole doublet	$H = \sum_{\langle ij \rangle} J_z S_i^z S_j^z + J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_{yz} (S_i^z S_j^y + S_i^y S_j^z)$			
Non-Kramers doublet	$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + J_{\pm} (S_i^{+} S_j^{-} + S_i^{-} S_j^{+}) + J_{\pm\pm} (\gamma_{ij} S_i^{+} S_j^{+} + \gamma_{ij}^* S_i^{-} S_j^{-})$			



Model for non-Kramers doublets





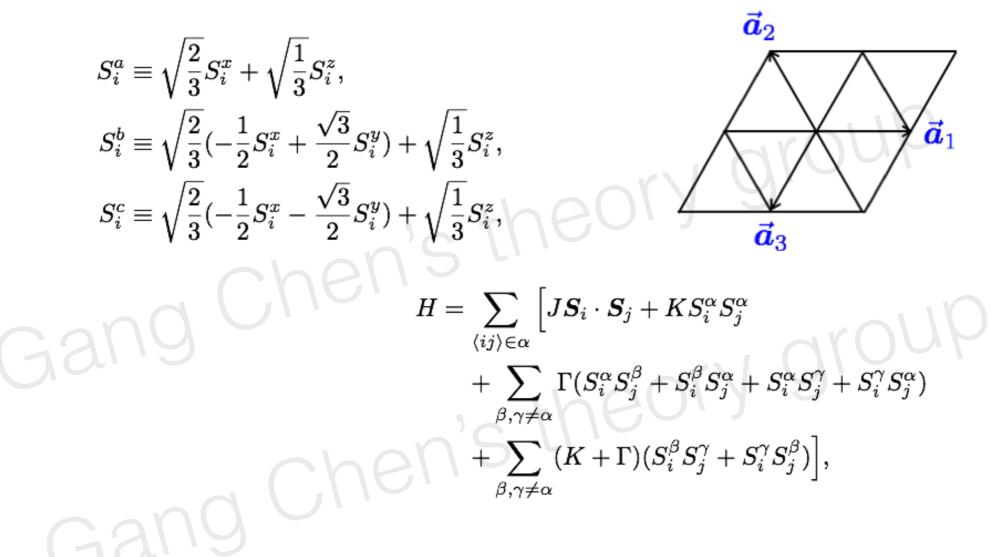
$$H = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z + J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-), \qquad (1)$$

in which, γ_{ij} is a bond-dependent phase factor, and takes 1, $e^{i2\pi/3}$ and $e^{-i2\pi/3}$ on the a_1, a_2 , and a_3 bond (see Fig. 2),

Time reversal symmetry forbids the coupling between transverse and Ising components.



Kitaev interaction

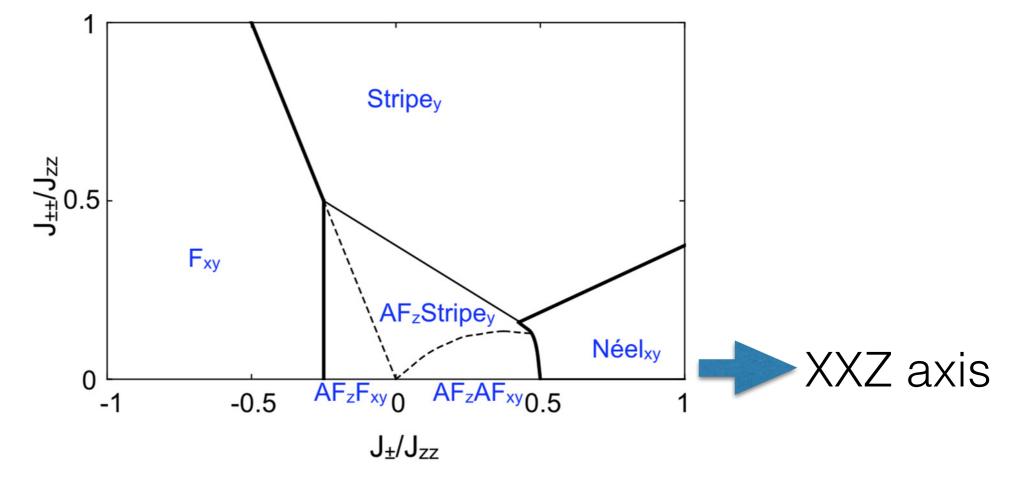


Kitaev material beyond iridates: the advantage of f electrons.

pointed out in Fei-Ye Li, YD Li, ..., GC, arXiv 2016, PRB 2017



Non-Kramers doublets: intertwined multipolar orders



We first notice that in the model, the spin rotation around the *z* direction by $\pi/4$ transforms $S^{\pm} \to \mp i S^{\pm}$ and the couplings in the model transform as

$$J_{zz} \to J_{zz}, \quad J_{\pm} \to J_{\pm}, \quad J_{\pm\pm} \to -J_{\pm\pm}.$$
 (2)

combined consequence of geometrical frustration and multipolar nature of the local moments



Non-Kramers doublets: intertwined multipolar orders

_		1 1		
-	States	Order types	Elastic neutron	
	F_{xy}	pure quadrupolar	no Bragg peak	
	120° Néel Stripe _v	pure quadrupolar pure quadrupolar	no Bragg peak no Bragg peak	
	AF_zF_{xy}	intertwined multipolar	Bragg peak at K	
	$AF_z AF_{xy}$	intertwined multipolar	Bragg peak at K	
	AF _z Stripe _y	intertwined multipolar	Bragg peak at K	
-	ohe	nsu		
	(a) F_{xy}	(b) Stripe_y	(c) Néel _{xy}	
			<u> </u>	
	y↑			
	$\diamond \longrightarrow x$		$ \longrightarrow x $	
	(d) AF_zF_x	(e) $AF_z AF_{xy}$	(f) $AF_zStripe_y$	
0 1 357				
四大學				

TABLE II. The list of ordered phases in the phase diagram of Fig. 3.



Quantum order by disorder

s. Assuming spins with sublattice index s has the direction pointing along the unit vector \mathbf{n}_s , one can always associate two unit vectors $\mathbf{u}_s \cdot \mathbf{n}_s = 0$ and $\mathbf{v}_s = \mathbf{n}_s \times \mathbf{u}_s$ so that \mathbf{n}_s , \mathbf{u}_s and \mathbf{v}_s are orthogonal with each other. Then we perform Holstein-Primakoff transformation for the spin operator $\mathbf{S}_{\mathbf{r}s}$,

$$\mathbf{n}_s \cdot \mathbf{S}_{\mathbf{r}s} = S - b_{\mathbf{r}s}^{\dagger} b_{\mathbf{r}s}, \qquad (4)$$

$$(\mathbf{u}_s + i\mathbf{v}_s) \cdot \mathbf{S}_{\mathbf{r}s} = (2S - b_{\mathbf{r}s}^{\dagger}b_{\mathbf{r}s})^{\frac{1}{2}}b_{\mathbf{r}s}, \qquad (5)$$

$$(\mathbf{u}_s - i\mathbf{v}_s) \cdot \mathbf{S}_{\mathbf{r}s} = b_{\mathbf{r}s}^{\dagger} (2S - b_{\mathbf{r}s}^{\dagger} b_{\mathbf{r}s})^{\frac{1}{2}}.$$
 (6)

After performing Fourier transformation

$$b_{\mathbf{r}s} = \sqrt{\frac{M}{N}} \sum_{\mathbf{k} \in \overline{\mathrm{BZ}}} b_{\mathbf{k}s} e^{i\mathbf{R}_{\mathbf{r}s} \cdot \mathbf{k}},\tag{7}$$

the spin Hamiltonian can be rewritten in terms of boson bilinears as

$$H_{\rm sw} = E_0 + \frac{1}{2} \sum_{\mathbf{k} \in \overline{\mathrm{BZ}}} \left[\Psi(\mathbf{k})^{\dagger} h(\mathbf{k}) \Psi(\mathbf{k}) - \frac{1}{2} \operatorname{tr} h(\mathbf{k}) \right], \quad (8)$$

where E_0 is the mean-field energy,

$$\Psi(\mathbf{k}) = [b_{\mathbf{k}1}, \dots, b_{\mathbf{k}M}, b_{-\mathbf{k}1}^{\dagger}, \dots, b_{-\mathbf{k}M}^{\dagger}]^{T}, \qquad (9)$$

and $h(\mathbf{k})$ is a $2M \times 2M$ Hermitian matrix, and $\overline{\text{BZ}}$ is the

magnetic Brillouin zone. H_{sw} can be diagonalized via a standard Bogoliubov transformation $\Psi(\mathbf{k}) = T_{\mathbf{k}} \Phi(\mathbf{k})$ where

$$\Phi(\mathbf{k}) = [\beta_{\mathbf{k}1}, \dots, \beta_{\mathbf{k}M}, \beta_{-\mathbf{k}1}^{\dagger}, \dots, \beta_{-\mathbf{k}M}^{\dagger}]^{T}, \qquad (10)$$

and $T_{\mathbf{k}} \in SU(M, M)$. Here SU(M, M) refers to indefinite special unitary group that is defined as [43]

$$SU(M,M) = \{g \in \mathbb{C}_{2M \times 2M} : g^{\dagger} \Sigma g = \Sigma, \det g = 1\}, \quad (11)$$

where Σ is the metric tensor and given as

$$\Sigma = \begin{pmatrix} I_{M \times M} & 0\\ 0 & -I_{M \times M} \end{pmatrix}.$$
 (12)

It is straightforward to prove that such transformation preserves the boson commutation rules. The diagonalized Hamiltonian reads

$$H_{\rm sw} = E_0 + \frac{1}{2} \sum_{\mathbf{k} \in \overline{\mathrm{BZ}}} \left[\Phi(\mathbf{k})^{\dagger} E(\mathbf{k}) \Phi(\mathbf{k}) - \frac{1}{2} \mathrm{tr} h(\mathbf{k}) \right]$$
$$= E_0 + E_r + \sum_{\mathbf{k} \in \overline{\mathrm{BZ}}} \omega_{\mathbf{k}s} \beta_{\mathbf{k}s}^{\dagger} \beta_{\mathbf{k}s}, \qquad (13)$$

where $E(\mathbf{k}) = \text{diag}[\omega_{\mathbf{k}1}, \dots, \omega_{\mathbf{k}M}, \omega_{-\mathbf{k}1}, \dots, \omega_{-\mathbf{k}M}]$ and

$$E_r = \frac{1}{4} \sum_{\mathbf{k} \in \overline{\mathrm{BZ}}} \operatorname{tr} \left[E(\mathbf{k}) - h(\mathbf{k}) \right]$$
(14)



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(b) (a)-0.7570-0.8254 Ξ -0.7575E -0.8255-0.7580-0.8256 $\pi/3$ $2\pi/3$ 0 $\pi/3$ $2\pi/3$ π 0 π θ θ

FIG. 5. Energy per spin taking into account quantum zeropoint energy vs the azimuth angle θ of spins for (a) the F_{xy} state and (b) the 120° Néel_{xy} state. Here we take the parameter $J_{\pm} = 0.4J_{zz}$, $J_{\pm\pm} = 0.4J_{zz}$ for the F_{xy} state and parameter $J_{\pm} = 0.9J_{zz}$, $J_{\pm\pm} = 0.2J_{zz}$ for the Néel_{xy} state. The zero-point energy is calculated within the linear spin-wave method.



Quantum order by disorder

The idea of non-commutative observables

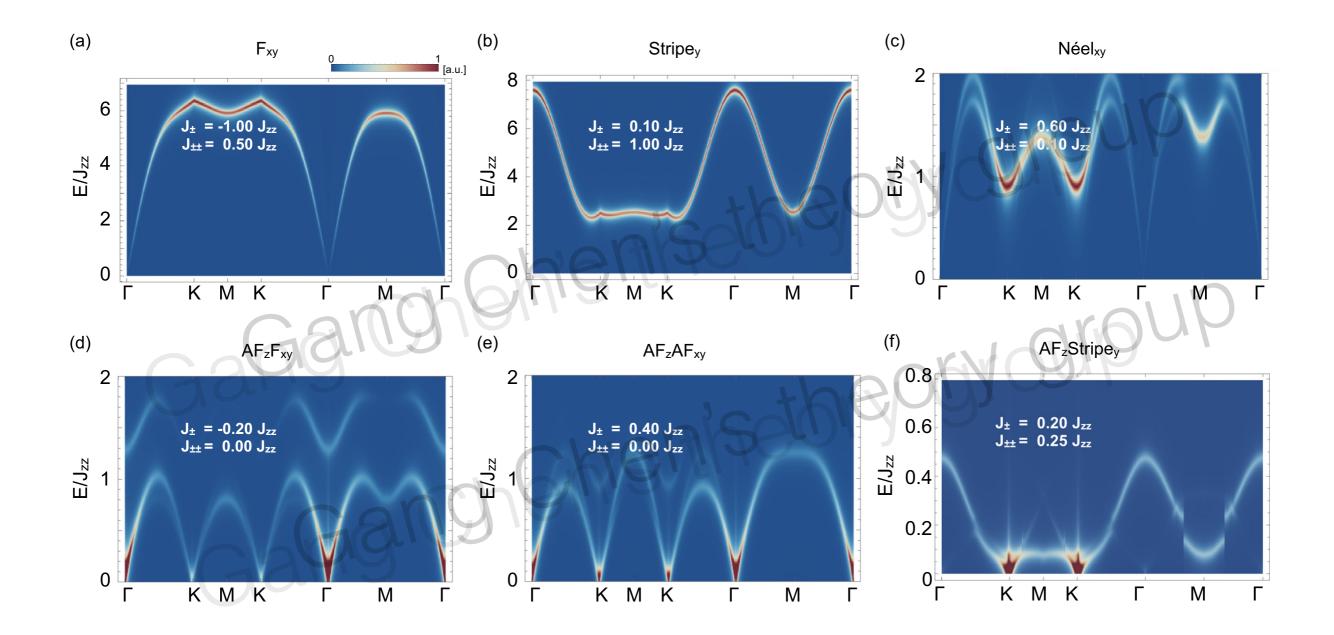
To detect intertwined multipolar orders, one can combine both elastic and inelastic neutron scattering measurements.

$$\mathcal{S}^{zz}(\mathbf{q},\omega>0) = \frac{1}{2\pi N} \sum_{ij} \int_{-\infty}^{+\infty} \mathrm{d}t \; e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)-i\omega t} \langle S_i^z(0)S_j^z(t) \rangle.$$

as if one is doing polarized neutron scattering measurements.



Detection of the intertwined multipolar orders: excitations





Selection rules

selection rule associated with the symmetry generated by

$$\hat{W} = T_{-\mathbf{a}_1 + \mathbf{a}_2} \otimes e^{i\pi \sum_j S_j^z},\tag{18}$$

where $T_{-\mathbf{a}_1+\mathbf{a}_2}$ denotes the lattice translation by $-\mathbf{a}_1 + \mathbf{a}_2$. The Hamiltonian stays invariant under \hat{W} , $[\hat{W}, H] = 0$.

From now on, we introduce the notation *s* and \bar{s} to denote the sublattice pair that is interchanged under the action of \hat{W} . In the labeling of Fig. 4, we find that $\bar{A} = B, \bar{C} = D, \bar{E} = F$.

For the elementary excitations, the effect of \hat{W} is such that

$$\text{Stripe}_{y}: \hat{W}b_{\mathbf{k},s}\hat{W}^{\dagger} = e^{i\phi(\mathbf{k})}b_{\mathbf{k},\bar{s}}, s = A, B, \qquad (19)$$

Stripe_yAF_z:
$$\hat{W}b_{\mathbf{k},s}\hat{W}^{\dagger} = e^{i\phi(\mathbf{k})}b_{\mathbf{k},\bar{s}}, s = A, \dots, F$$
, (20)

where $\phi(\mathbf{k}) = -k_x + k_y$.

The eigenmodes of \hat{W} take bonding/antibonding form,

$$\alpha_{\mathbf{k},s,\pm} = b_{\mathbf{k},s} \pm b_{\mathbf{k},\bar{s}},\tag{21}$$

whose eigenvalues are

$$\hat{W}\alpha_{\mathbf{k},s,\pm}\hat{W}^{\dagger} = \pm e^{i\phi(\mathbf{k})}\alpha_{\mathbf{k},s,\pm}.$$
(22)

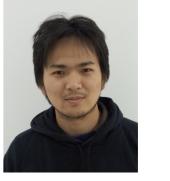
Since \hat{W} is a symmetry of the Hamiltonian, the energy eigenmodes are separate linear combinations of $\alpha_{\mathbf{k},s,\pm}$,

$$\beta_{\mathbf{k},t,\pm} = \sum_{s} c_{t,s} \alpha_{\mathbf{k},s,\pm} + d_{t,s} \alpha^{\dagger}_{-\mathbf{k},s,\pm}, \qquad (23)$$

and

$$\hat{W}\beta_{\mathbf{k},t,\pm}\hat{W}^{\dagger} = \pm e^{i\phi(\mathbf{k})}\beta_{\mathbf{k},t,\pm}.$$
(24)

The \pm branches do not mix, since they have distinct eigenvalues under \hat{W} .





Yaodong Li Fudan -> UCSB

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$$\sum_{n}^{MZZ}(\mathbf{q},\omega>0) = \sum_{n} \langle 0|\sum_{s=1}^{N} S_{s}^{Z}(-\mathbf{q},-\omega)|n\rangle \langle n|\sum_{s=1}^{N} S_{s}^{Z}(\mathbf{q},\omega)|0\rangle$$

$$\propto \sum_{n} \delta(\omega - (\epsilon_{n} - \epsilon_{0})) \langle 0|\sum_{s=1}^{M} (b_{\mathbf{q},s} + b_{-\mathbf{q},s}^{\dagger})|n\rangle \langle n|\sum_{s=1}^{M} (b_{-\mathbf{q},s} + b_{\mathbf{q},s}^{\dagger})|0\rangle$$

$$\propto \sum_{n} \delta(\omega - (\epsilon_{n} - \epsilon_{0})) \langle 0|\sum_{s=1}^{M} (\alpha_{\mathbf{q},s,+} + \alpha_{-\mathbf{q},s,+}^{\dagger})|n\rangle \langle n|\sum_{s=1}^{M} (\alpha_{-\mathbf{q},s,+} + \alpha_{\mathbf{q},s,+}^{\dagger})|0\rangle$$

It is thus obvious that the contribution is nonzero if and only if $|n\rangle$ is created by the $\beta_{k,t,+}$ operators. The $\beta_{k,t,-}$ states are not accessible. As a result, the $S^z - S^z$ correlation function only measures coherent excitations with even parity. The odd parity excitations, instead, are present in $S^x - S^x$ and $S^y - S^y$ correlation functions.

Intertwined multipolar order in TmMgGaO4



Changle Liu (Fudan)



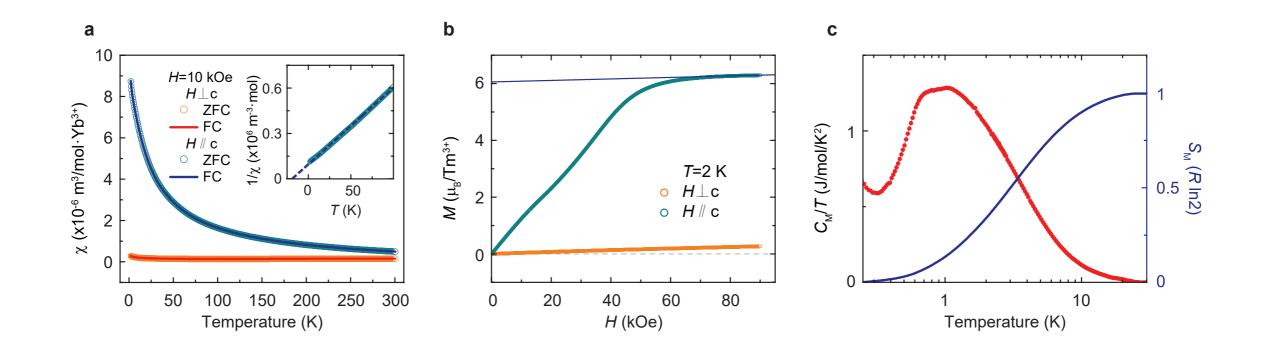
Yao Shen (Fudan)

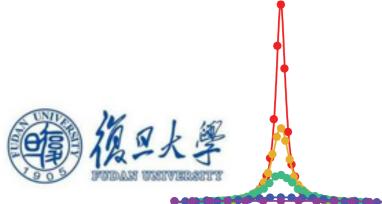


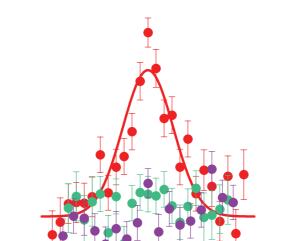
Jun Zhao (Fudan)

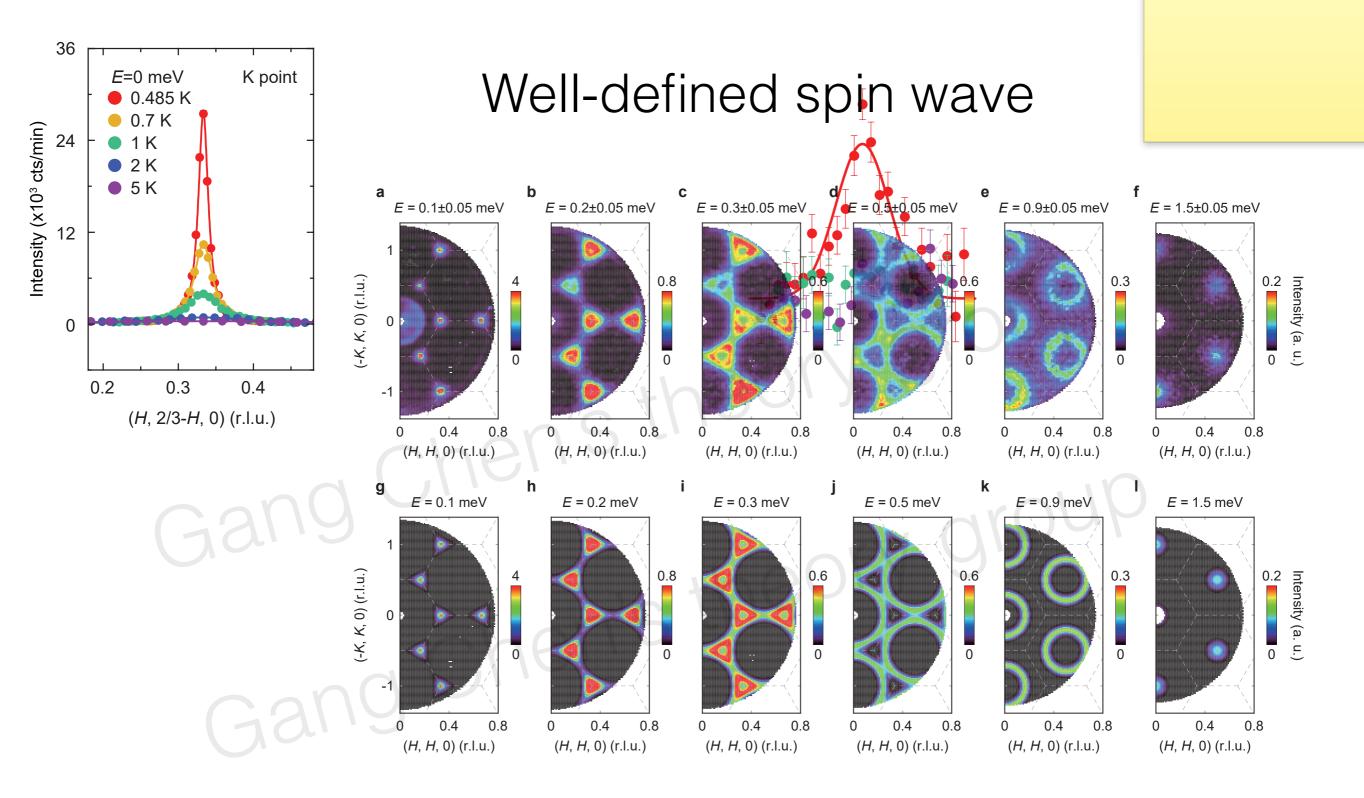


approximately thought as non-Kramers doublets





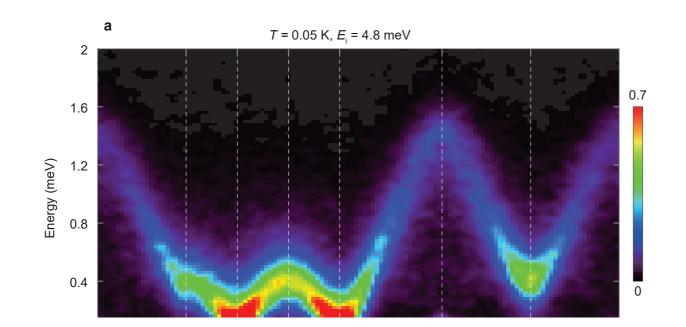


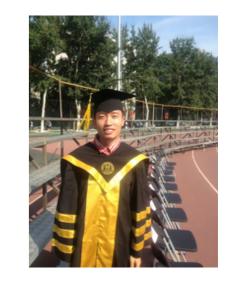


The presence of well-defined spin wave indicates the presence of the hidden order !

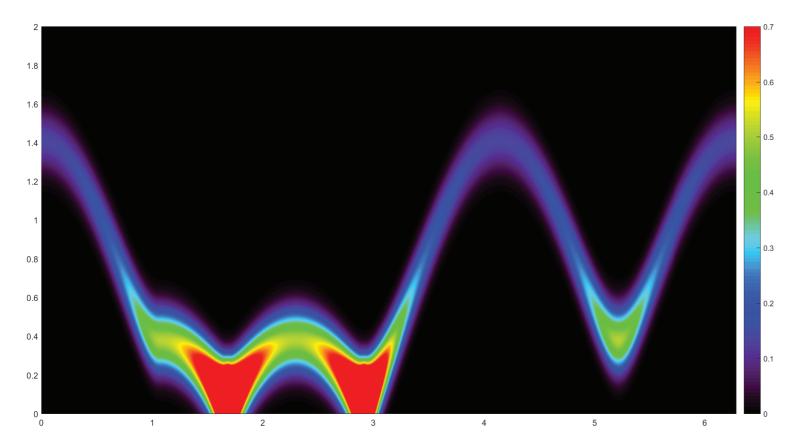


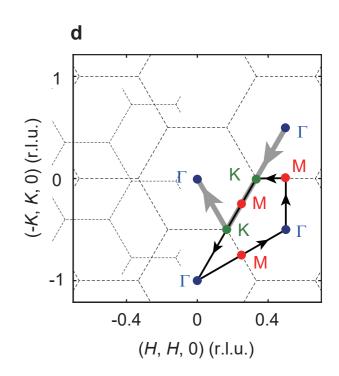
Comparison with theory





Changle Liu







Summary

- 1. The interplay between geometrical frustration and multipolar local moments leads to rich phases and excitations.
- 2. The manifestation of the hidden multipolar orders is rather nontrivial, both in the static and dynamic measurements.
- 3. The non-commutative observables/operators can be used to reveal the dynamics of hidden orders. This is general and can be adapted to many other hidden order systems.
- 4. Finally, the non-trivial Berry phase effect has not yet been discussed. This thought has been hinted in Kivelson's recent work (PNAS 2018).

