Topological Magnon Dirac Points in a 3D Antiferromagnet

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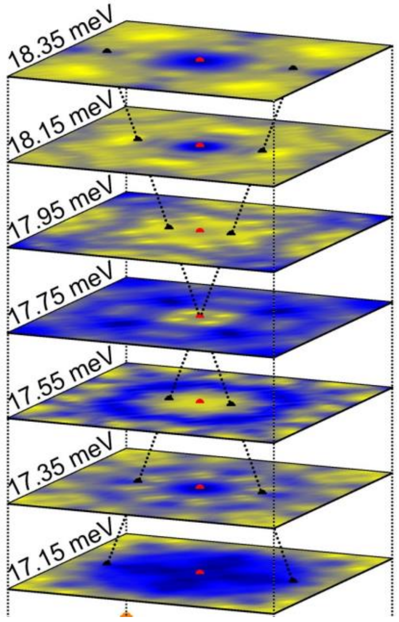

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K. Li


C. Li


C. Fang

theory


W. Yao


L. Wang

experiment

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Outline

- **Introduction**

  band topology + magnetism

- **Theoretical considerations**

  "Z_2 nodal lines", and the limiting case of Dirac points

  K. Li *et al.*, *Phys. Rev. Lett.* **119**, 247202 (2017)

- **Experiment and analysis**

  Spin-wave fitting + band-topology visualization

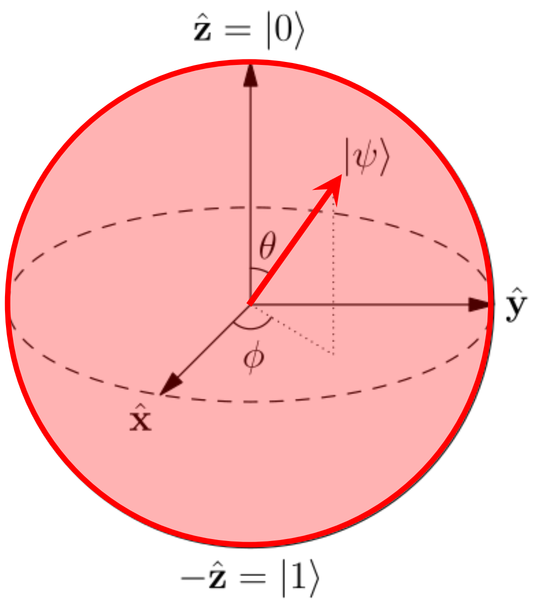
  W. Yao *et al.*, *Nat. Phys.* **14**, 1011 (2018),

- **Summary & outlook**

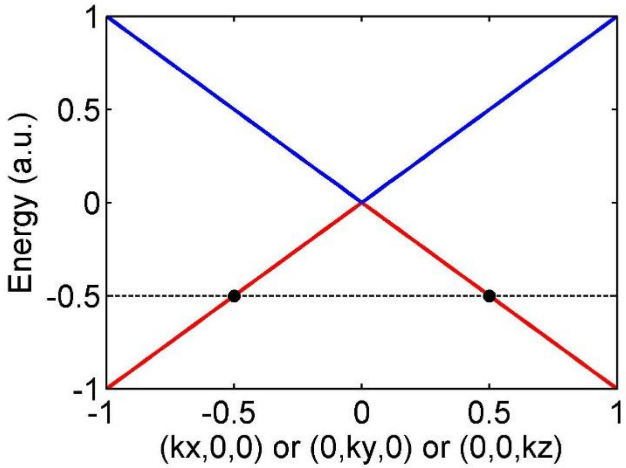
Topology on band structures

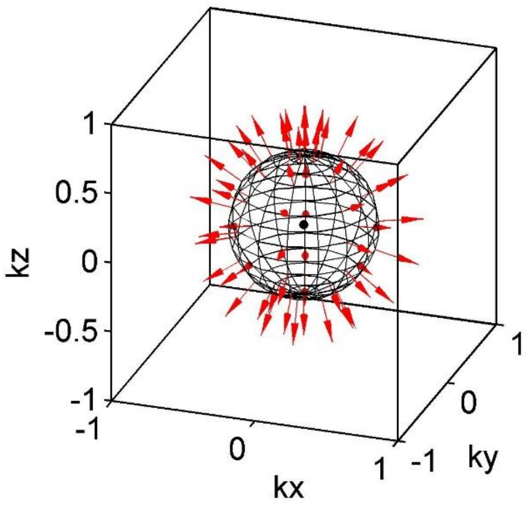
Two-band model near a Weyl point

$$H(\mathbf{k}) = \sum_{i=\{x,y,z\}} k_i \sigma_i + E_0 \sigma_0$$



Bloch sphere





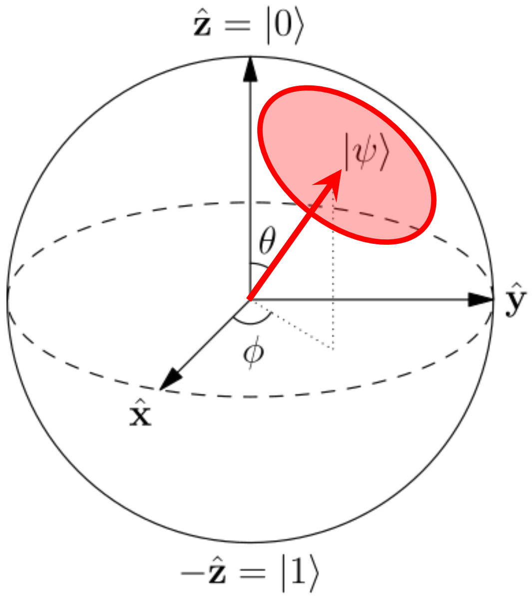
two bands in three dimensions

creation / annihilation only in pairs

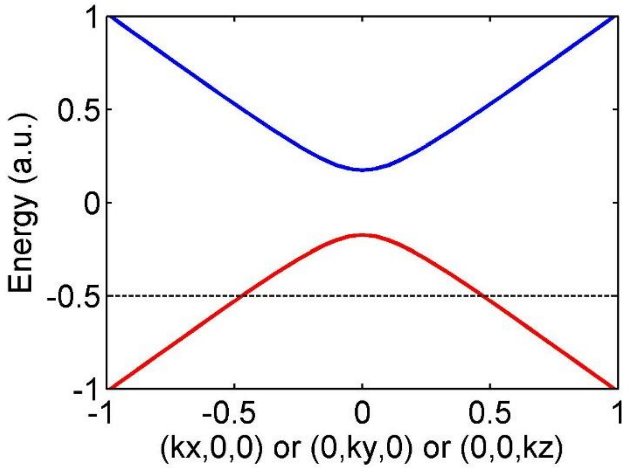
Topology on band structures

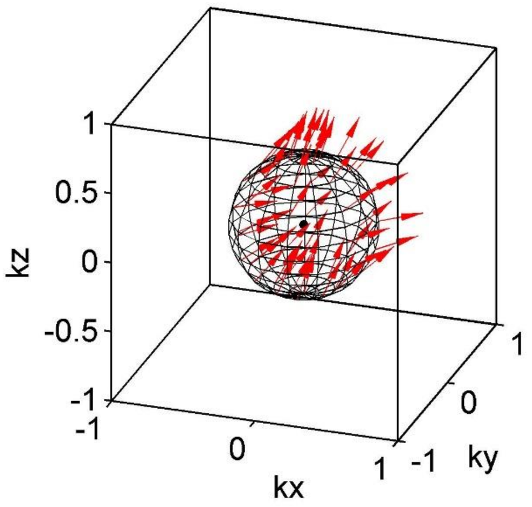
$$H(\mathbf{k}) = \sum_{i=\{x,y,z\}} \sigma_i \sqrt{m + k_i^2} + E_0\sigma_0$$

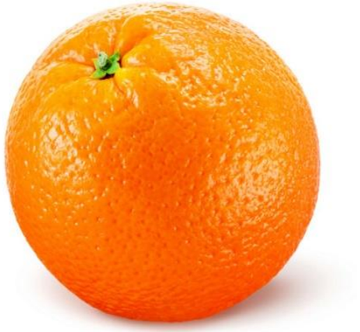
(cannot do this!)



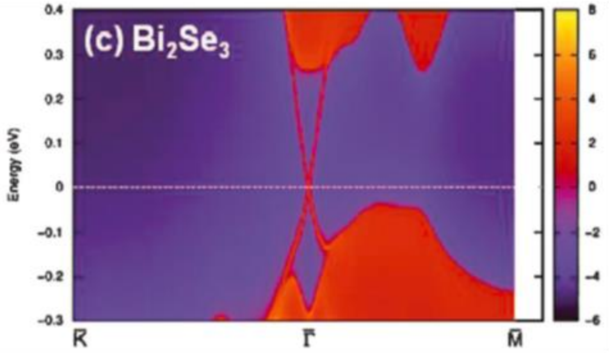
Bloch sphere





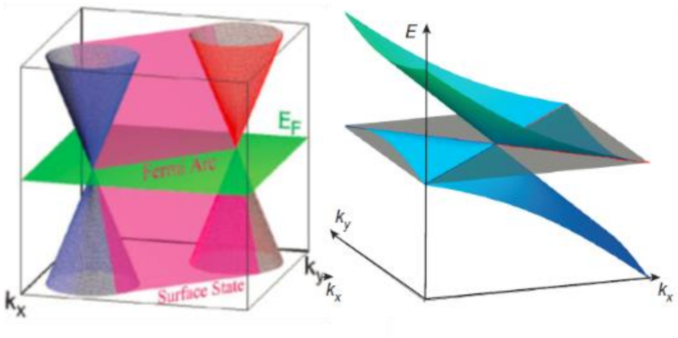


Topological insulators



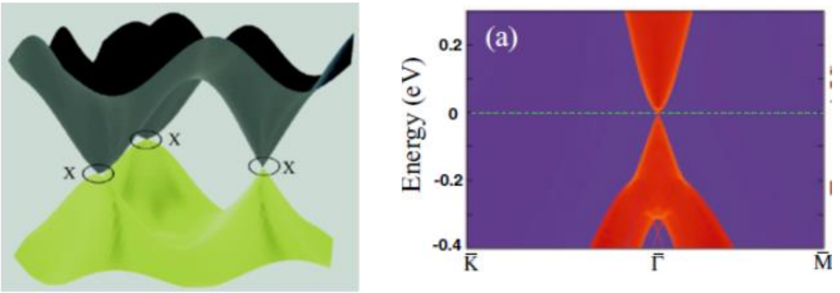
Hasan & Kane, RMP 2010
Qi & Zhang, RMP 2011

Weyl semimetals



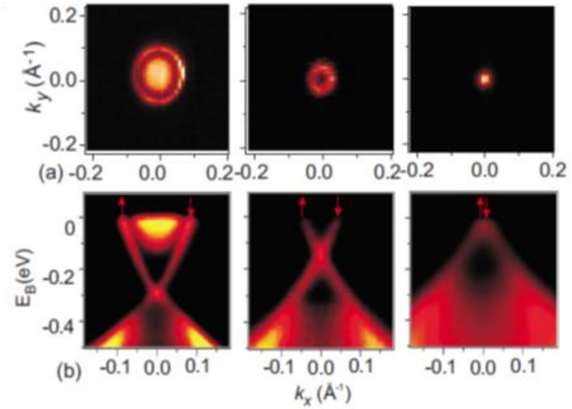
Wan et al., PRB 2011
Soluyanov et al., Nature 2015

Dirac semimetals

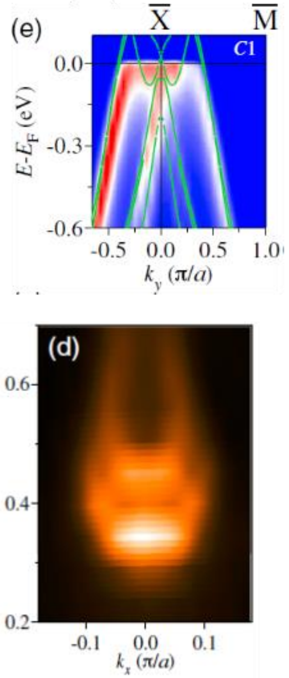


Young et al., PRL 2012
Wang et al., PRB 2012

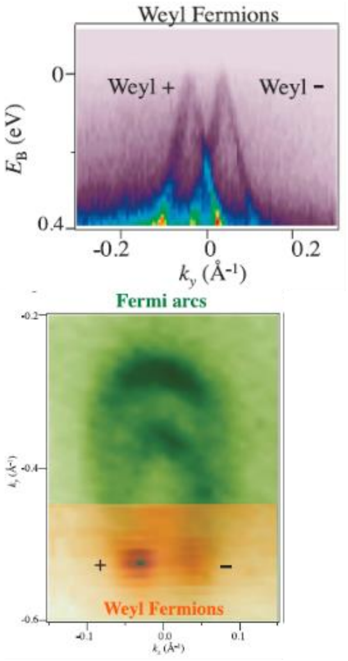
Hsieh et al., Nature 2009



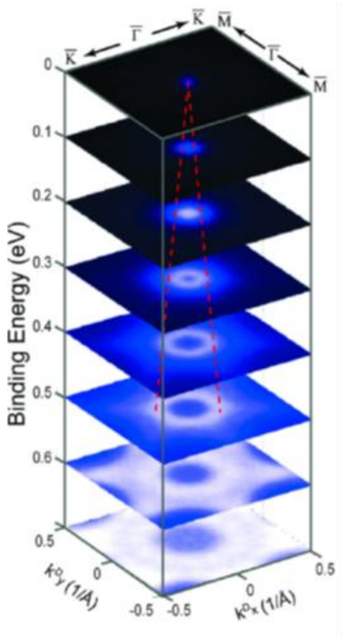
Lv et al., PRX 2015



Xu et al., Science 2015

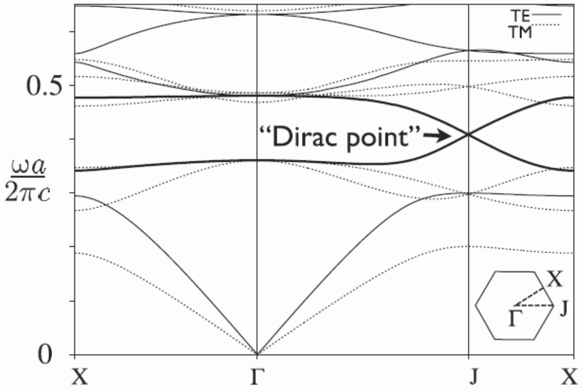


Liu et al., Science 2014



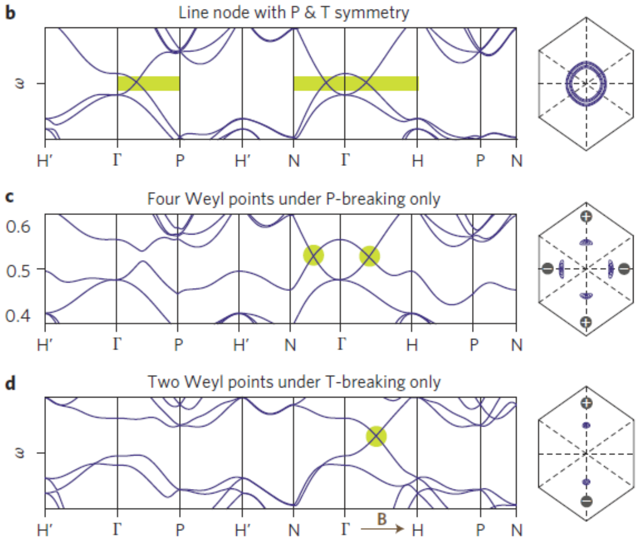
Idea of band topology not restricted to electrons (or Fermions)

Photonic analogue of quantum Hall



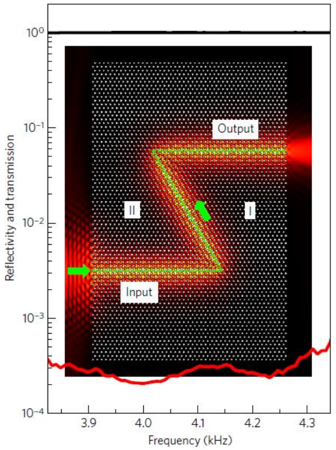
Haldane & Raghu, PRL 2008

Photonic analogue of semimetals



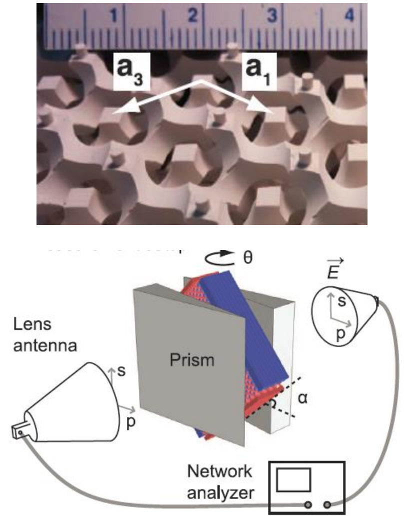
L. Lu et al., Nature Photonics 2013

Topological valley transport of sound

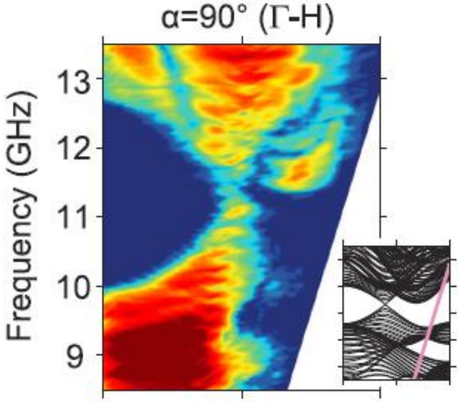


J. Lu et al., Nat. Phys. 2016

Classical waves in artificial structures



L. Lu et al., Science 2015



Why magnetic excitations?

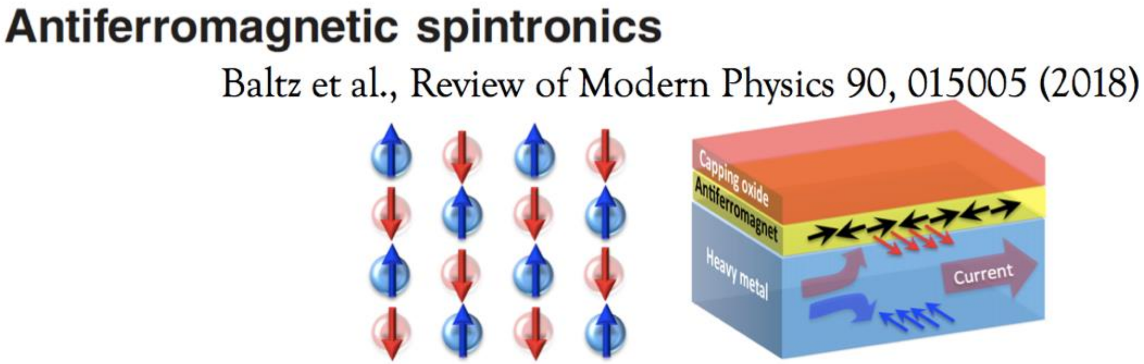
- **Band topology builds upon symmetry + dimensionality**

  1651 magnetic SGs vs. 230 crystallographic SGs

- **Magnetism is useful**

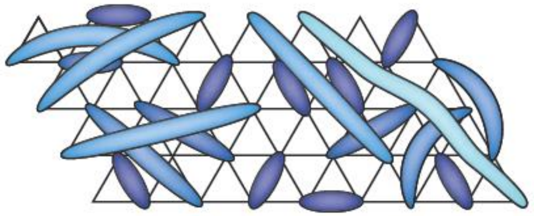
  spintronics, magnonics

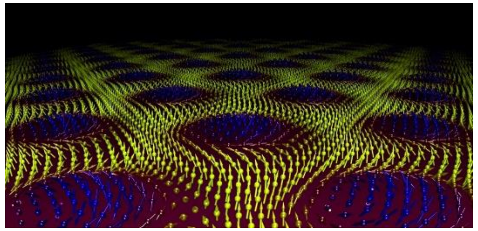
  surface, interfaces, heterostructures



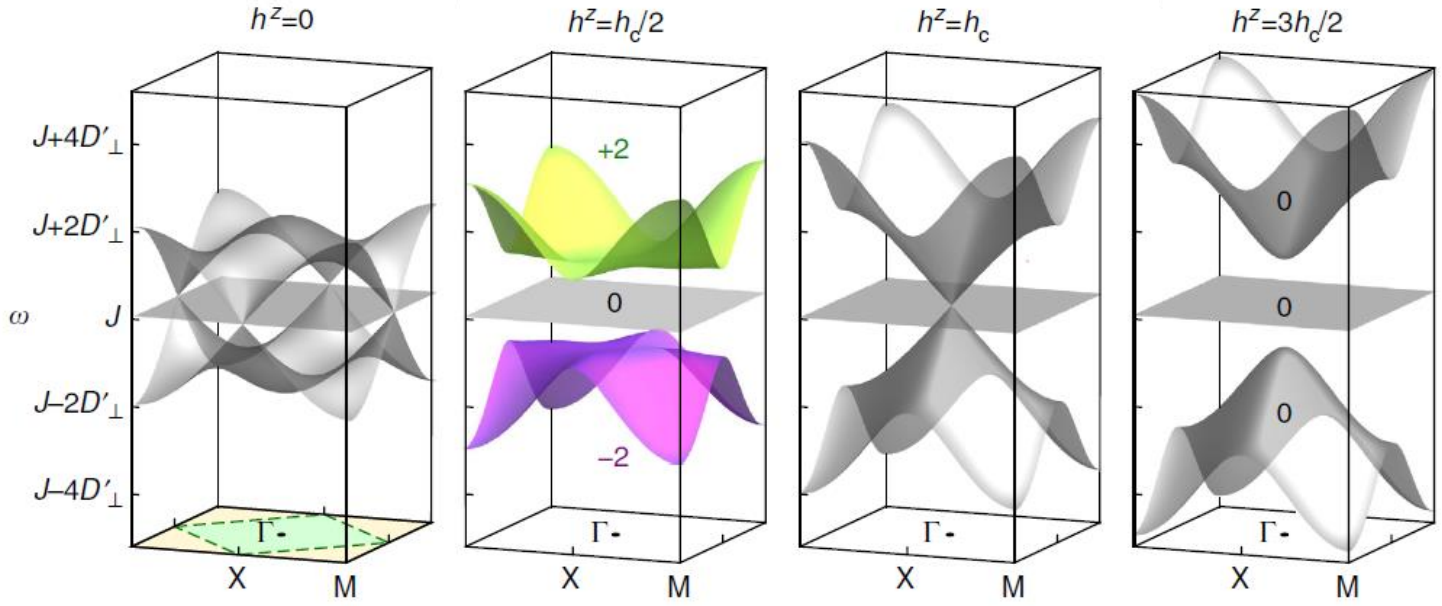
- **Topology in reciprocal space vs. real space**

  spin liquids, skyrmions …



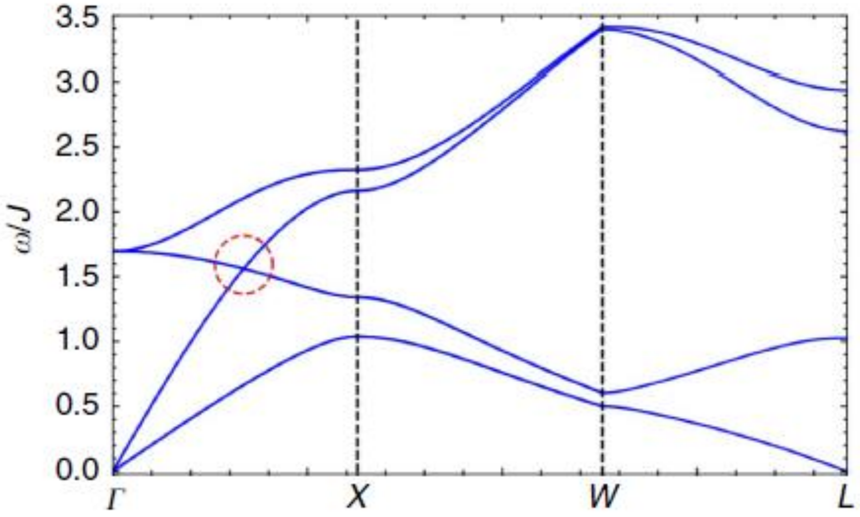


“magnon topological insulator”



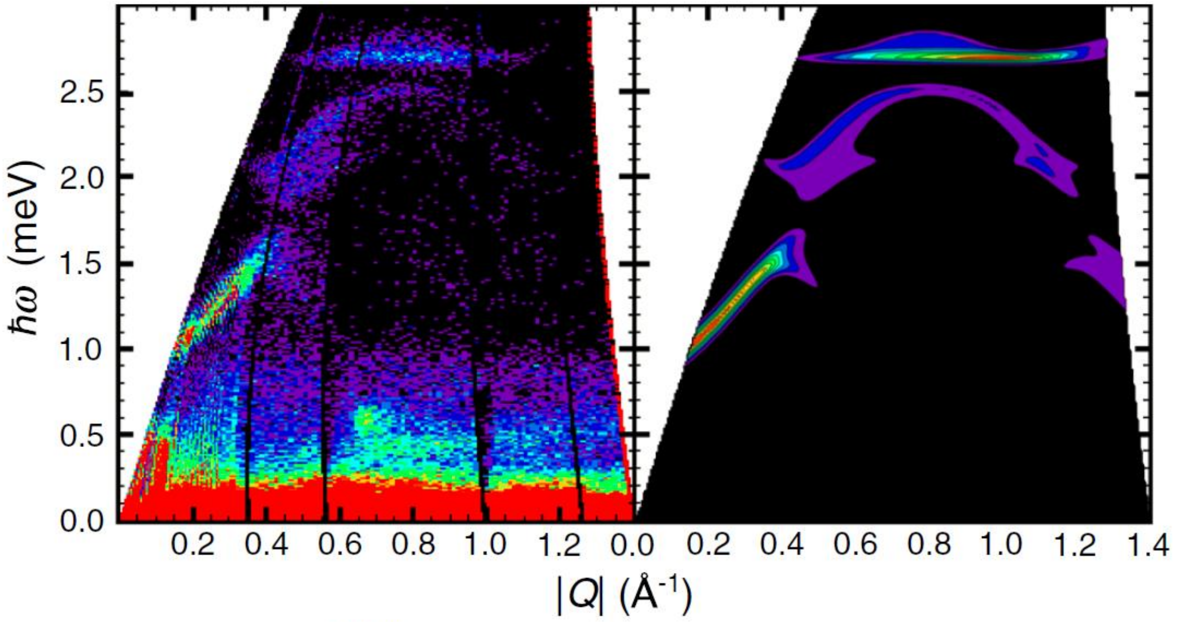
Romhanyi, Penc, Ganesh, Nat. Commun. 2015

“magnon topological semimetal”



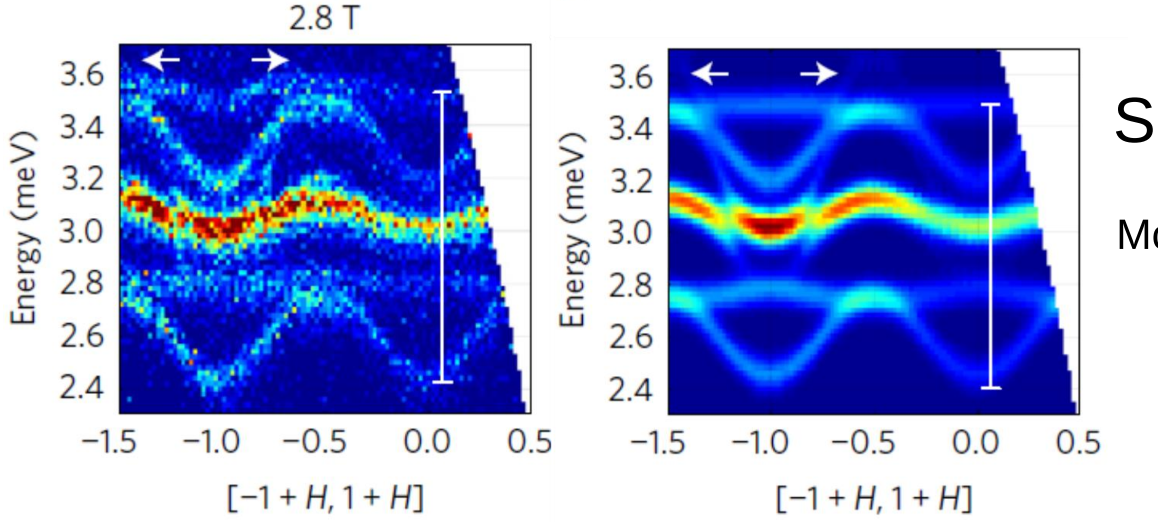
Gang Chen’s tutorial talk

Li et al., Nat. Commun. 2017



Cu(1,3-bdc) in 7 T

Chisnell et al., PRL 2015



$SrCu_2(BO_3)_2$ in 2.8 T

McClarty et al., Nat. Phys. 2017

- Bosonic “TI” not “semimetal”, need theory to detect topology
- Need magnetic fields

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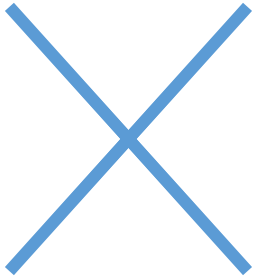
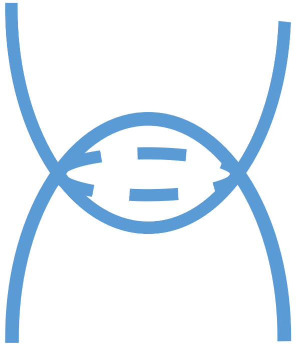
Nodal line with "Z_2-monopole" charge

C. Fang

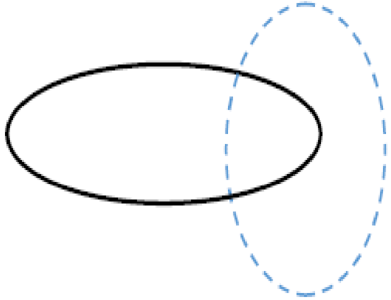
$$H(\mathbf{k}) = \sum_{i=\{x,y,z\}} k_i\sigma_i + E_0\sigma_0$$



Weyl point
2 bands, no *PT*



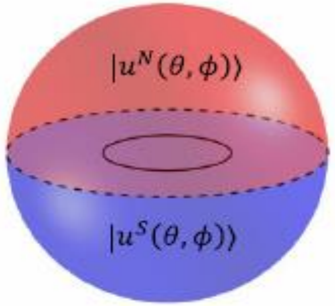
Nodal line
$(PT)^2 = +1$



Berry phase

$$\pi_1\left[\frac{O(M+N)}{O(M)\oplus O(N)}\right] = \mathbb{Z}_2$$

Burkov et al., PRB **84**, 235126 (2011)
Kim et al., PRL **115**, 036806 (2015)



Z_2-monopole charge

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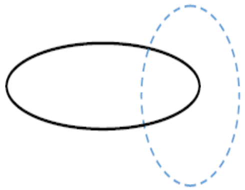
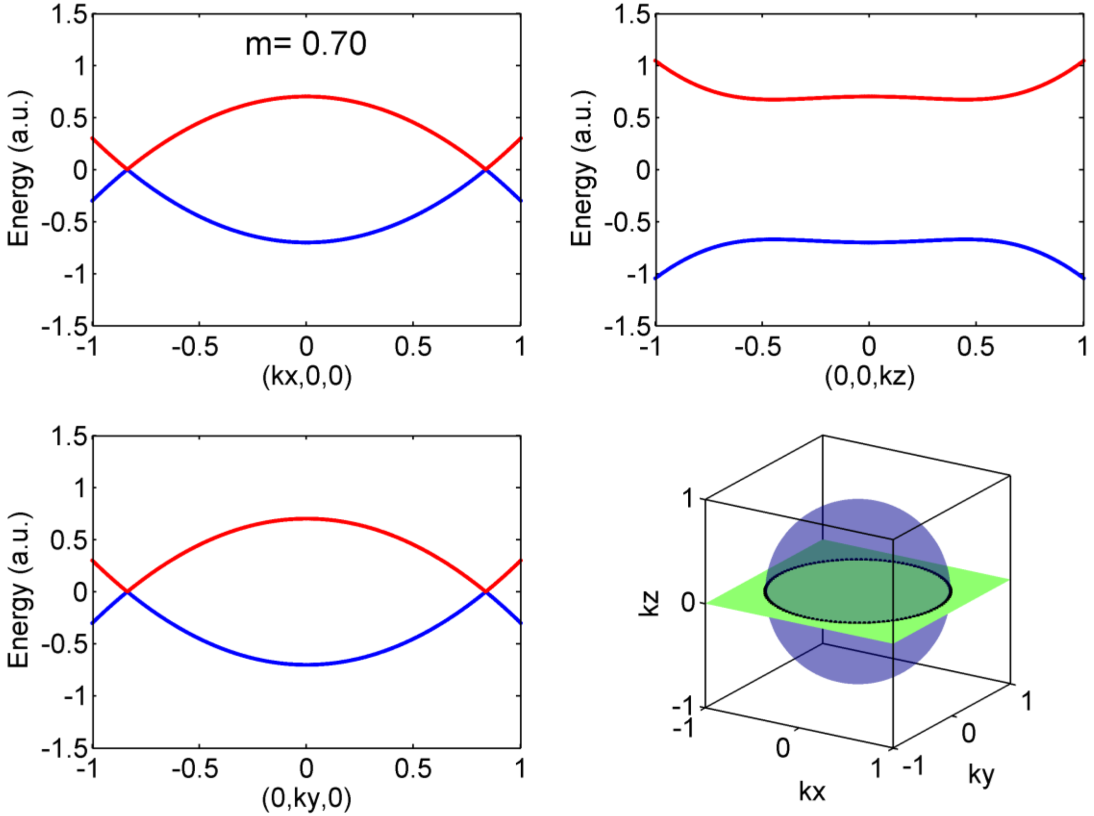
C. Fang, Y. Chen, H.-Y. Kee and L. Fu, Phys. Rev. B 92, 081201 (2015)



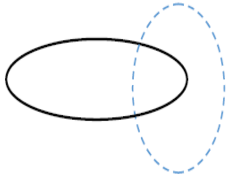
Type-I

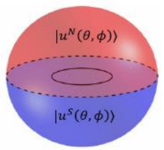
$$H(\mathbf{k}) = (m - k^2)\sigma_x + k_z\sigma_z$$



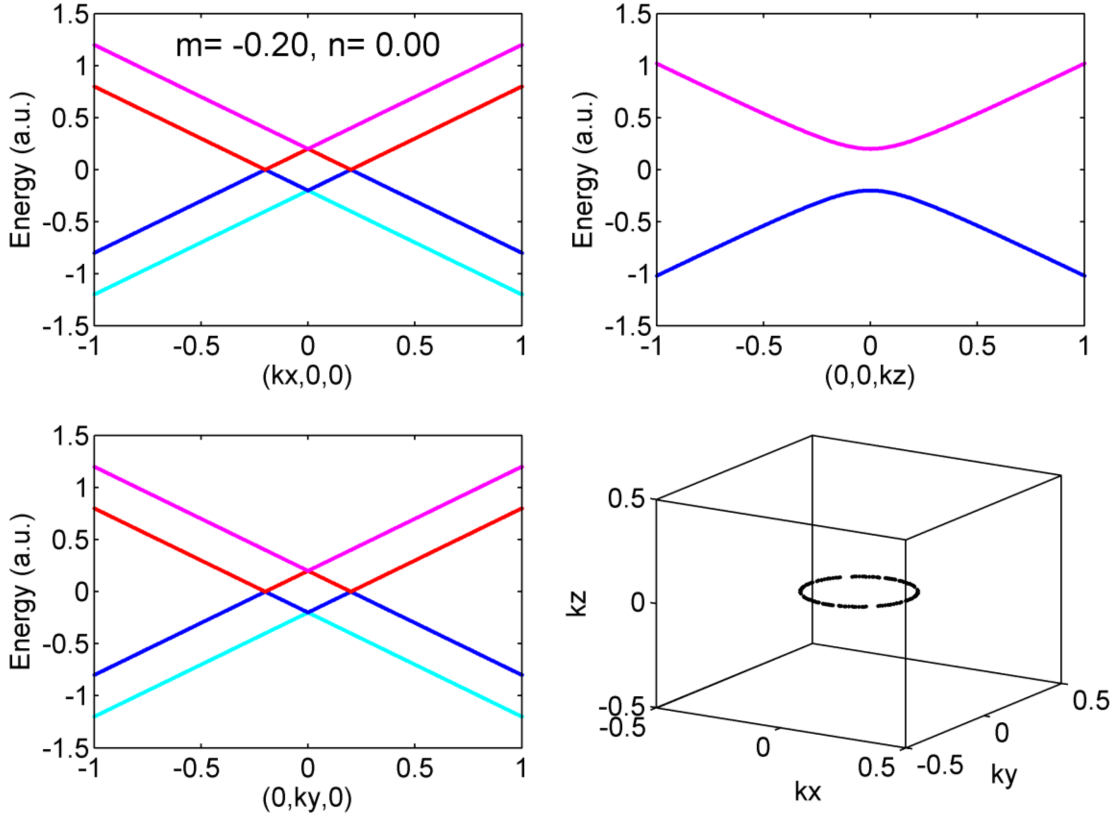
"shrink and gap"

Type-II





$$H(\mathbf{k}) = k_x\tau_0\sigma_x + k_y\tau_y\sigma_y + k_z\tau_0\sigma_z + m\tau_x\sigma_x + n\tau_z\sigma_z$$



cannot "shrink and gap"

Nodal line with "Z_2-monopole" charge

C. Fang

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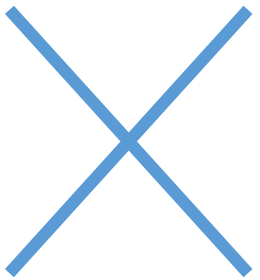

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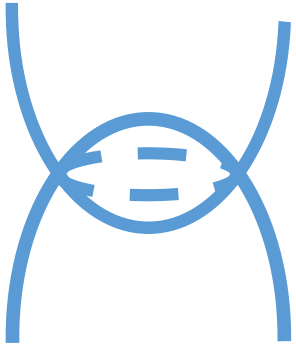
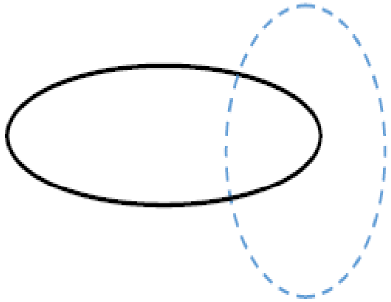


Nodal line
$(PT)^2 = +1$



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Z_2-monopole charge

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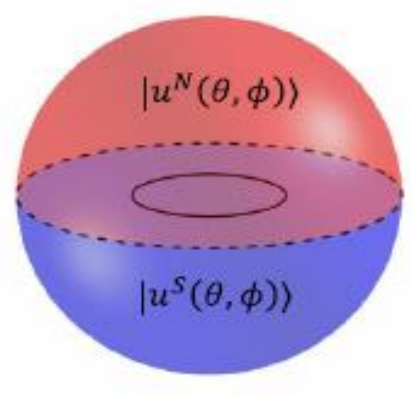
C. Fang, Y. Chen, H.-Y. Kee and L. Fu, Phys. Rev. B 92, 081201 (2015)

Idea: inheritage of (non-trivial) topology

Do it at home: keep cutting a Möbius band results in two twisted and entangled bands

… I'm like a hybrid between a nodal line and a Weyl point

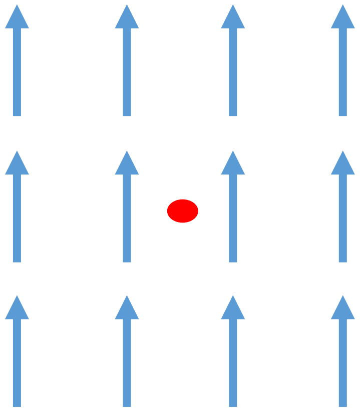
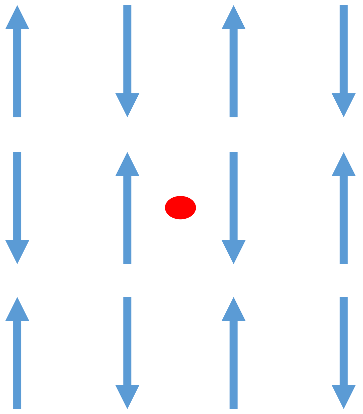
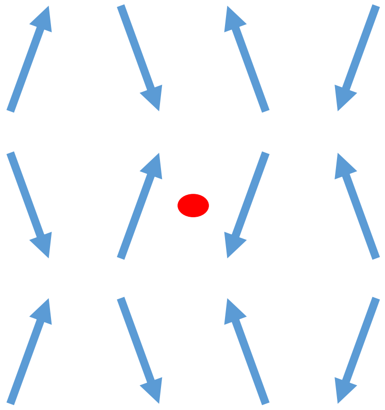


Step 1: Start with something like a Weyl point (a Dirac point in our case)

Step 2: Remove some of the required symmetry to form a type-II nodal line

Strategy: *PT* + *U*(1), then remove *U*(1)

$(PT)^2 = +1$ is always true for bosons

Not *PT*-symmetric	*PT* and *U*(1)	*PT* only
		
Ferromagnet	Collinear antiferromagnet	Non-collinear antiferromagnet
	Step 1	**Step 2**
	(focus of this talk)	

S^z conservation & linear spin-wave theory

Heisenberg spin interactions

$$\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+)$$

Holstein-Primakoff transformation

$$S^+ = (2S)^{\frac{1}{2}} \sqrt{1 - \frac{\hat{n}}{2S}}\, a$$

$$S^- = a^+ (2S)^{\frac{1}{2}} \sqrt{1 - \frac{\hat{n}}{2S}}$$

linear approximation

$$S^+ \approx (2S)^{\frac{1}{2}} a$$

$$S^- \approx (2S)^{\frac{1}{2}} a^+$$

$$S^z = S - a^+ a$$

For the spin-up sublattice:

$$S^+ \approx (2S)^{\frac{1}{2}} a; \quad S^- \approx (2S)^{\frac{1}{2}} a^+; \quad S^Z = S - a^+ a$$

For the spin-down sublattice:

$$S^+ \approx (2S)^{\frac{1}{2}} b^+; \quad S^- \approx (2S)^{\frac{1}{2}} b \quad S^z = -S + b^+ b$$

With the total S^z being a good quantum number, we must have:

LSWT Hamiltonian at a generic **k**-point

$$\begin{array}{c} \\ a^+ \\ b \\ a \\ b^+ \end{array} \begin{array}{c} \begin{array}{cccc} a & b^+ & a^+ & b \end{array} \\ \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix} \end{array}$$

S_z-conservation & LSWT approx.

PT-invariance

$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix} \rightarrow \begin{pmatrix} H_+ & 0 \\ 0 & H_+^* \end{pmatrix}$$

Can generally have Weyl Points (two at the same generic **k** point, with opposite monopole charges)

The block-diagonal form prevents them from annihilating each other.

→ A new way of getting (bosonic) Dirac points!

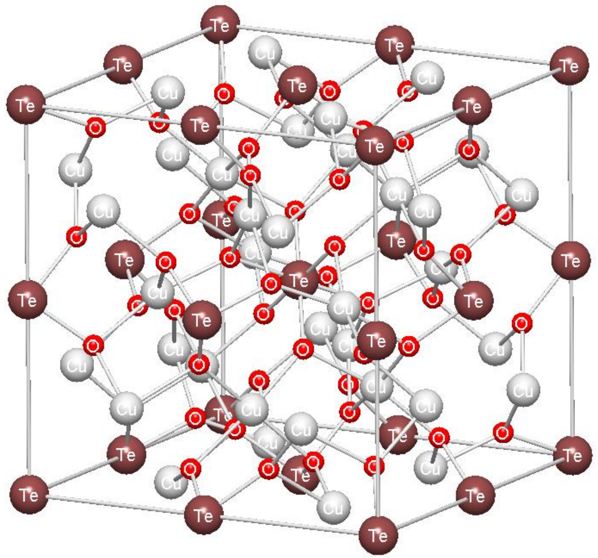
Magnon Dirac points

Need:

- *PT* + *U*(1) = centrosymmetric crystal structure + collinear AFM order
- Primitive cell with multiple spins

Properties:

- Anywhere in BZ, always in pairs
- Have surface arcs



Cu_3TeO_6: T_N = 61 K antiferromagnet, S.G. #206 *Ia-3*

two primitive cells (= 8 formula units) per cubic unit cell

12 Cu^{2+} spins in the magnetic primitive cell

Herak et al., J. Phys.: Condens. Matter 17, 7667 (2005)

Magnon Dirac points

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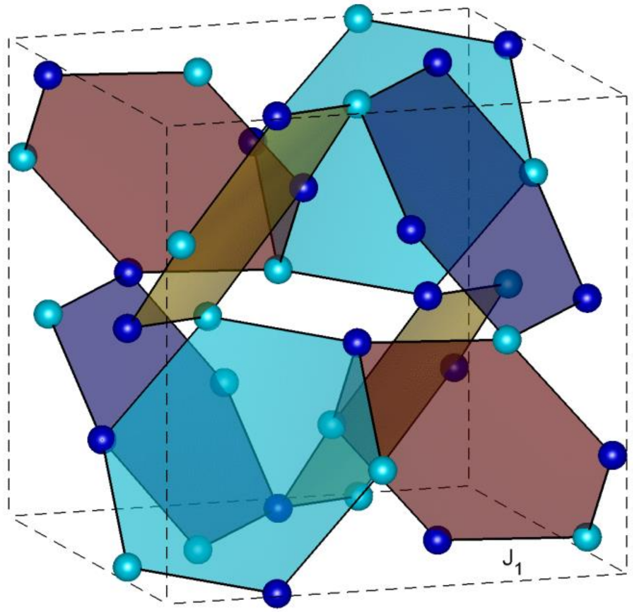
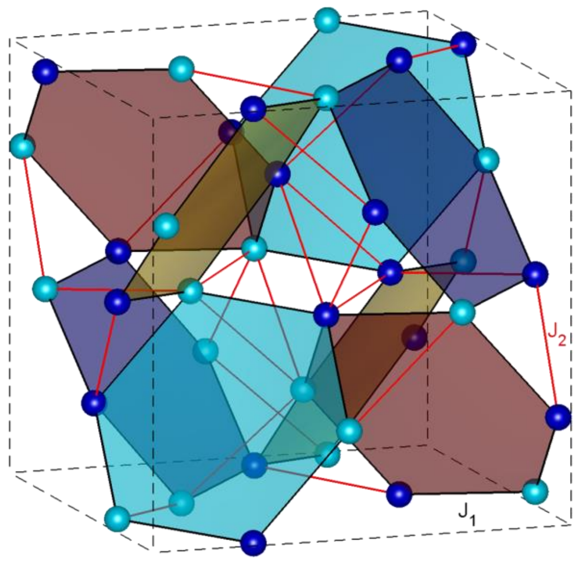


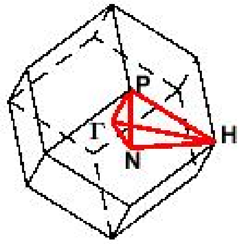
Colors of spheres: spins up and down on Cu^{2+}
(spins // a body diagonal of the cube)

Magnon Dirac points

Need:

- $PT + U(1)$ = centrosymmetric crystal structure + collinear AFM order
- Primitive cell with <u>multiple spins</u>





Properties:

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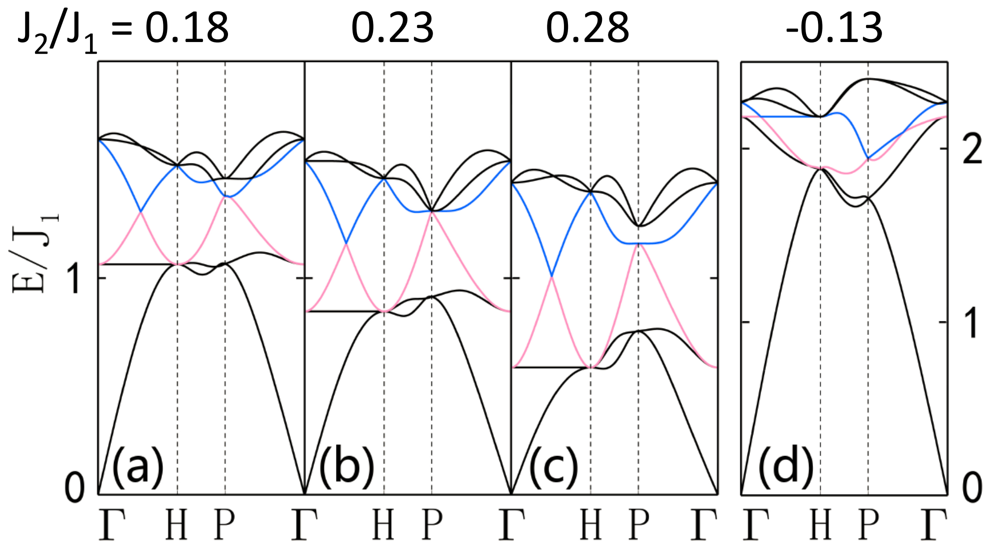
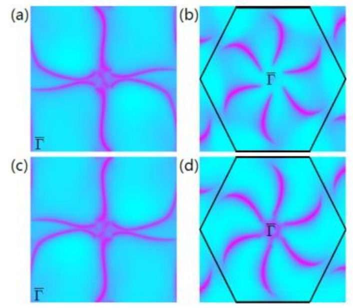
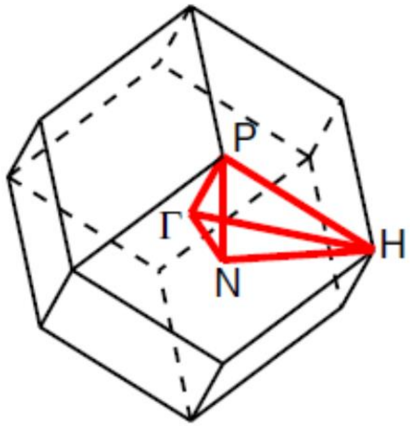
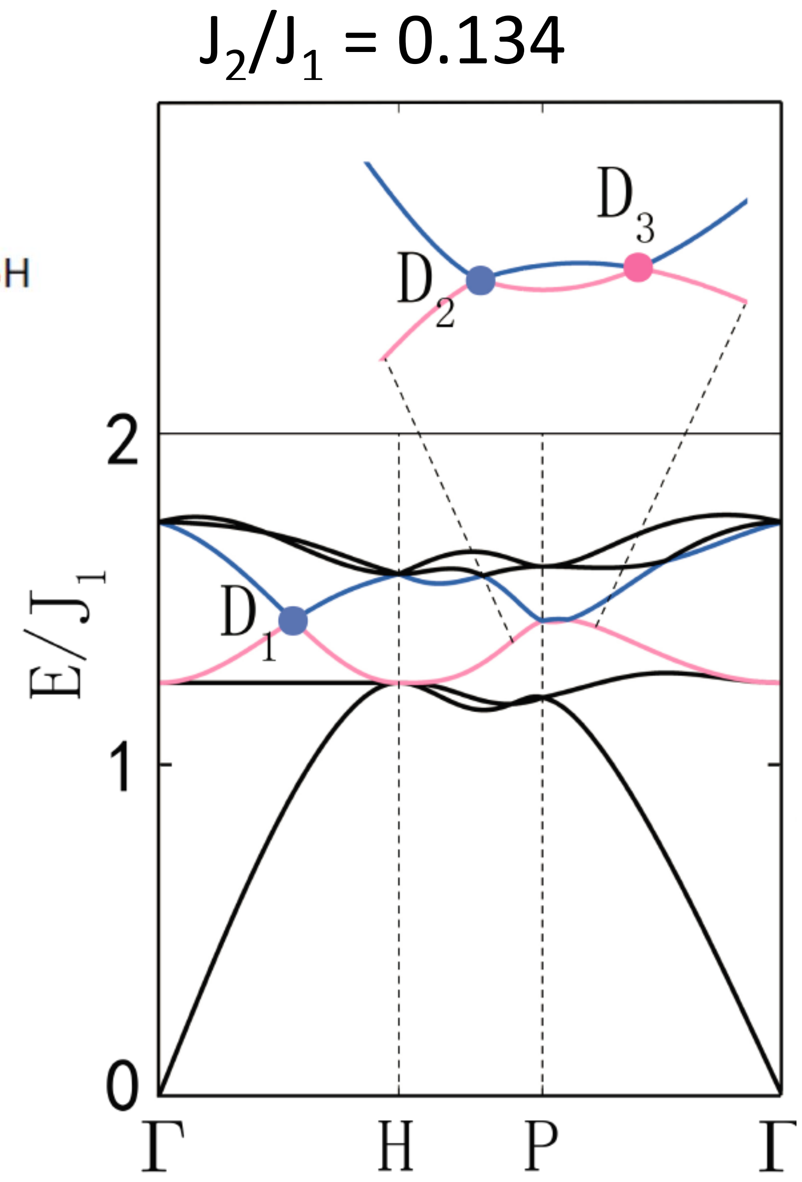








The P-point will always host Dirac points

The three screw rotations have anti-commutation relations forming a Clifford algebra:

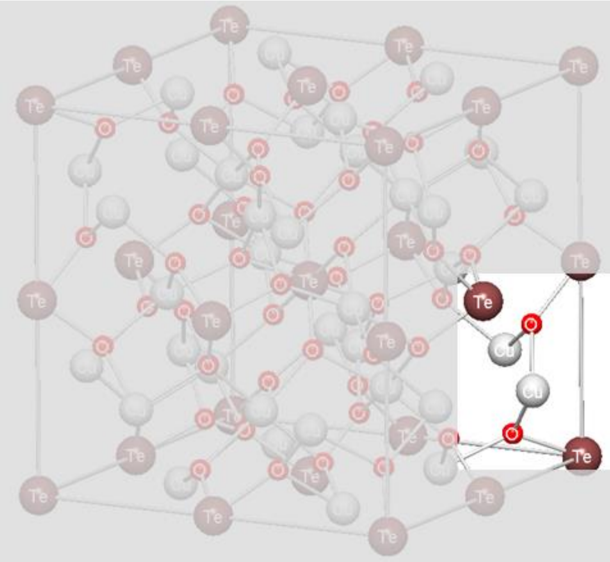
$$\{R_i, R_j\} = -2\delta_{ij}$$

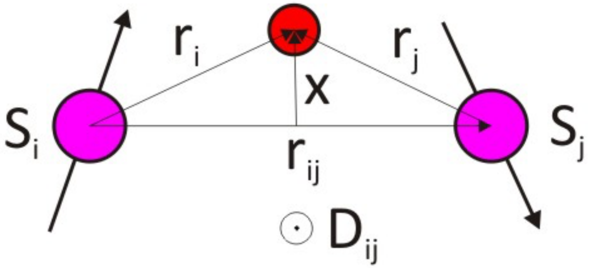
Since $[PT, C_{2i}] = 0$, the *PT*-symmetry enforces that the representations are real, and we have to use at least **4x4** Dirac matrices, *e.g.*:

$$R_x = i\sigma_y \otimes s_x,$$
$$R_y = is_y,$$
$$R_z = i\sigma_y \otimes s_z$$

(4D irrep)

Strategy: *PT* ~~+ *U*(1)~~

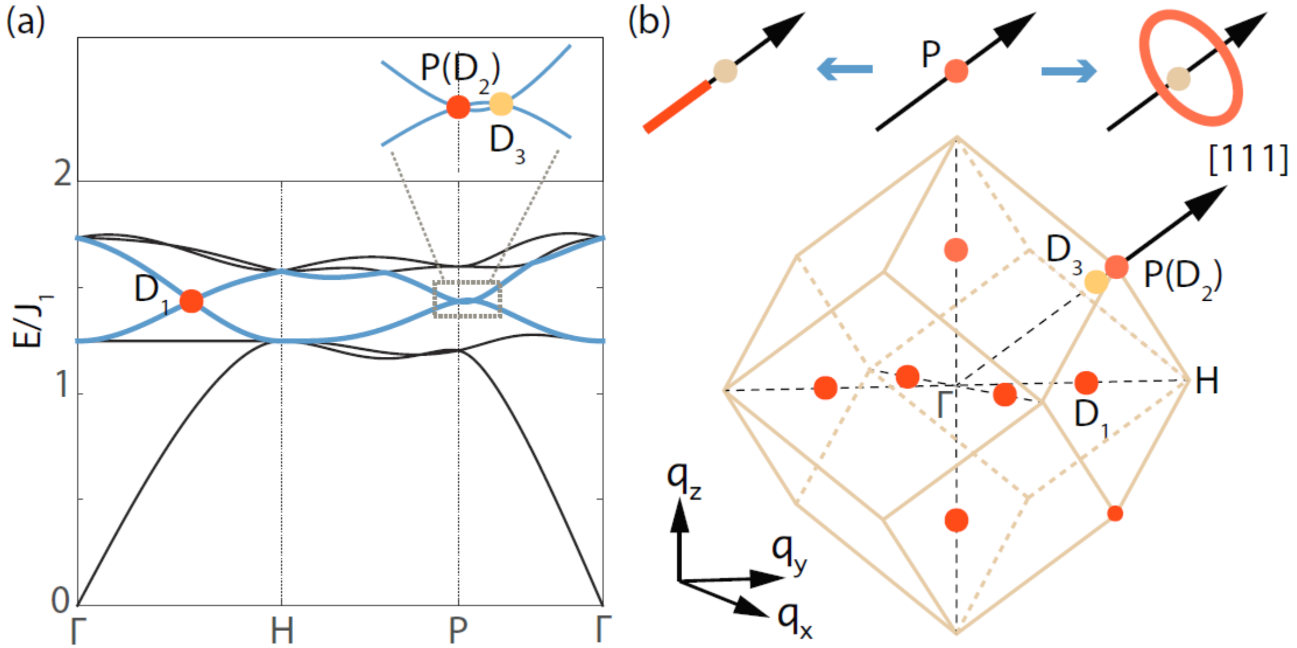




Dzyaloshinskii-Moriya interaction expected

~~S_z-conservation & LSWT approx.~~

~~$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}$$~~



Outline

- ❑ **Introduction**

  band topology + magnetism

- ❑ **Theoretical considerations**

  “Z_2 nodal lines”, and the limiting case of Dirac points

  K. Li *et al.*, *Phys. Rev. Lett.* **119**, 247202 (2017)

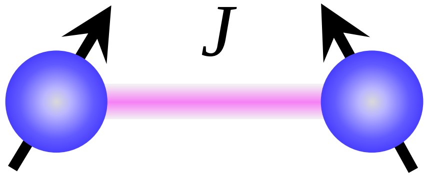
- ❑ **Experiment and analysis**

  Spin-wave fitting + band-topology visualization

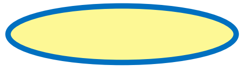
  W. Yao *et al.*, *Nat. Phys.* **14**, 1011 (2018).

- ❑ **Summary & outlook**

The “quantum” aspect of spin 1/2

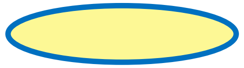


$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2$$

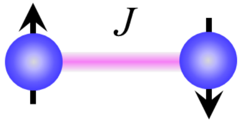
	Classical ground state	Quantum ground state
J < 0	FM	“↑↑” “↓↓” “↑↓ + ↓↑”
J > 0	AFM	“↑↓ - ↓↑” 

not even a quantum eigenstate!

Energy per link:

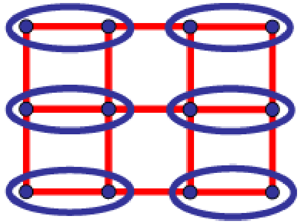


-3*J*/4



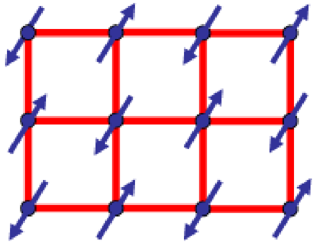
- *J*/4

Energy per site:



“VBS”

-3*J*/8



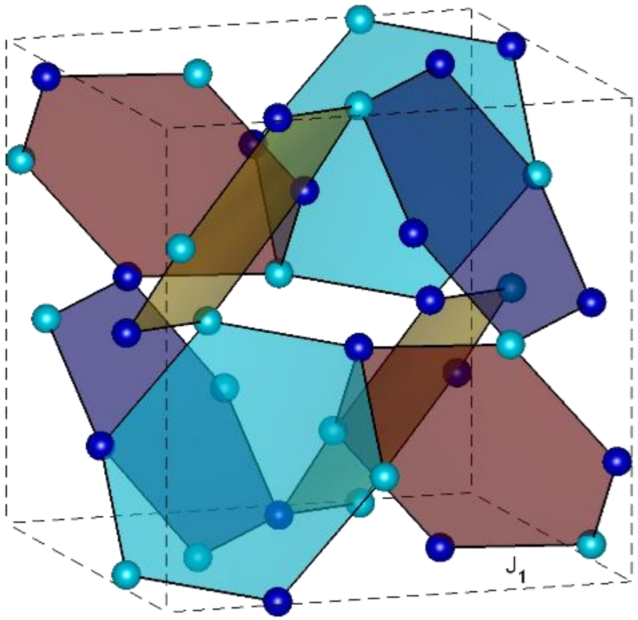
“Néel”

-*N***J*/8

Dimensionality (“cubic lattice”)	0	1	2	3
N	1	2	4	6

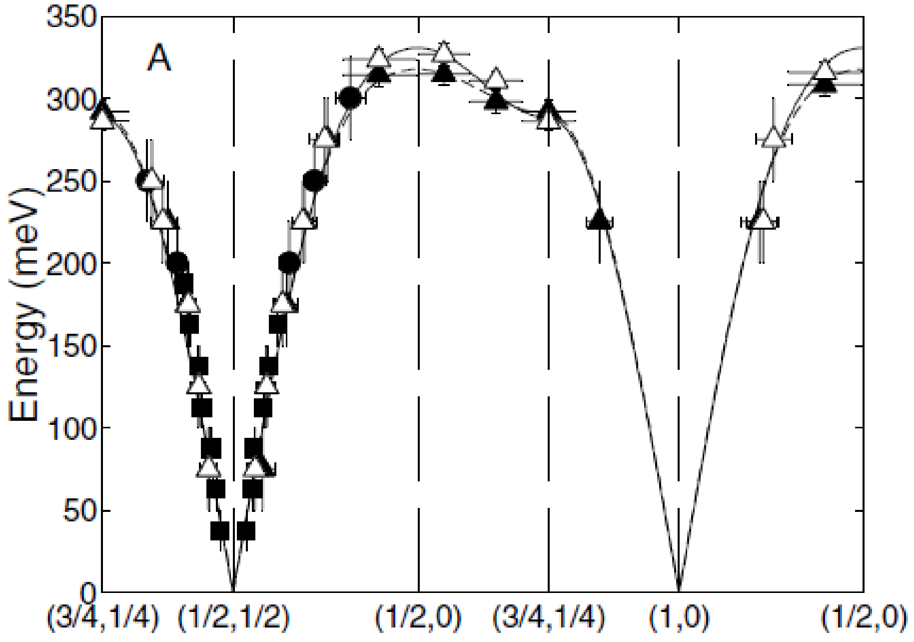
quantum ⟶ classical

Not a very optimistic situation for us…



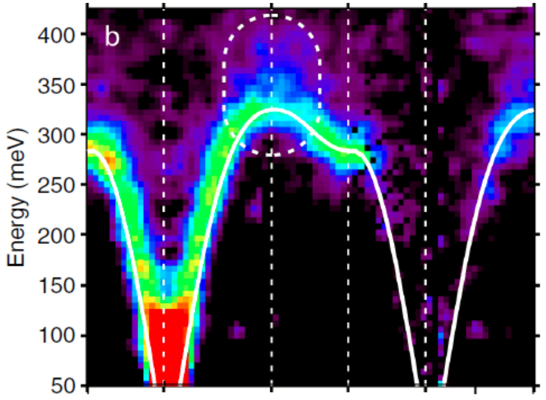
Although the lattice is 3D, *N* is only 4!

La_2CuO_4:
quasi-2D square lattice with $N = 4$

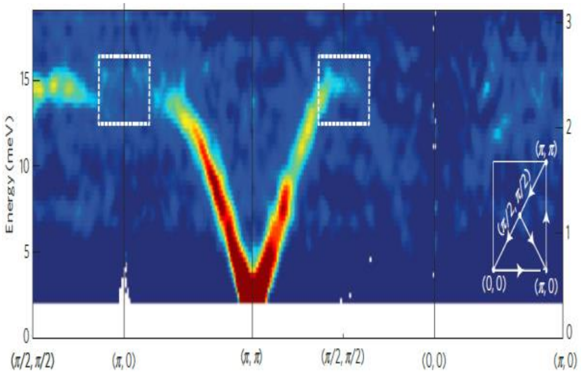


Coldea et al., PRL 2001

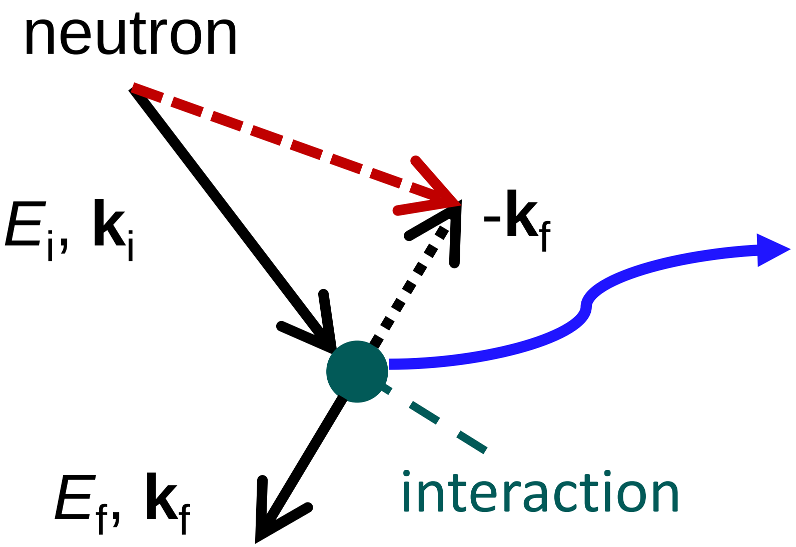
Headings et al., PRL 2010
La_2CuO_4, **2D square**



Dalla Piazza et al., Nat. Phys. 2015
$Cu(DCOO)_2 \cdot 4D_2O$, **2D square**



Inelastic neutron scattering

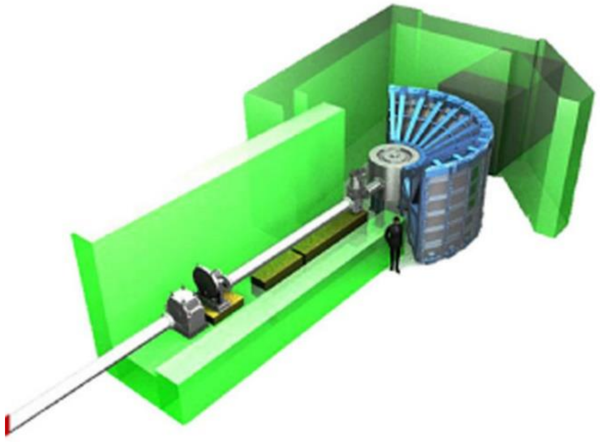


excitation:
energy $\omega = E_i - E_f$
momentum $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$

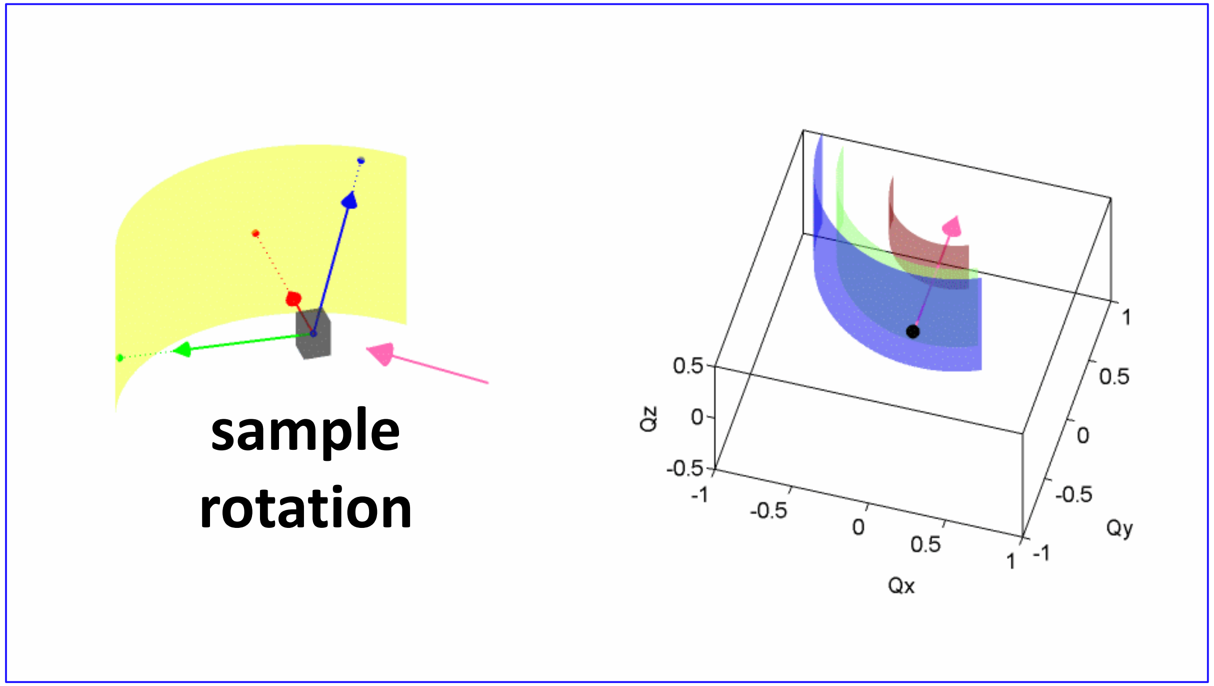
Measure scattering intensity, $S(\mathbf{Q},\omega)$

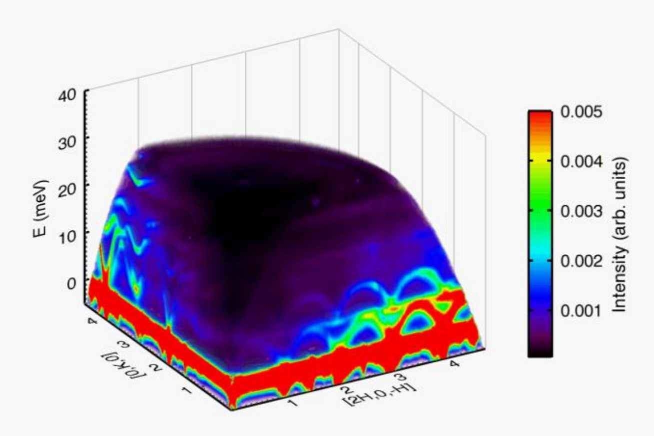
The time-of-flight (TOF) method

- Single-energy neutrons coming in pulses
- Large array of position-sensitive detectors (PSD)
- Final energy/momentum from TOF/PSD
- Event-by-event → histogram data → S(**Q**,ω)
- Data size ≳ 40 GB (gigabytes) per experiment



The 4SEASONS spectrometer @ J-PARC



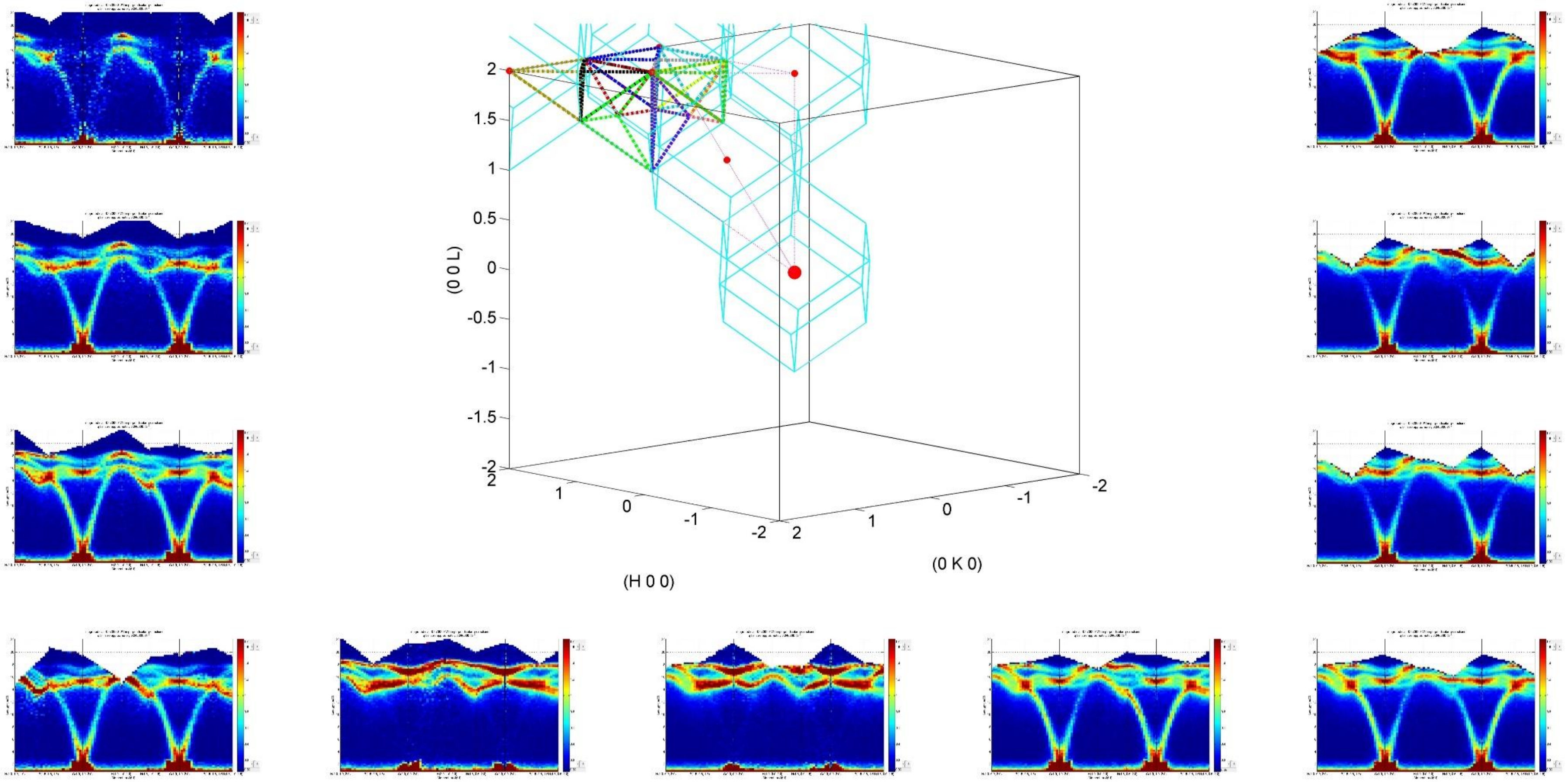


Phonons in $CuBr_2$
Wang et al., PRB **96**, 085111 (2017)

4D data set: ideal for mapping band dispersions

A BIG advantage from the cubic symmetry: “data folding”

S(**Q**,ω) available over many BZs

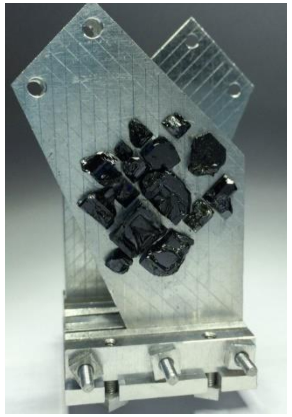


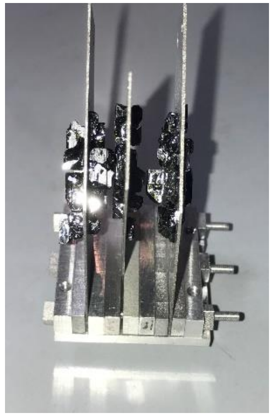
Single-crystal sample for INS experiment

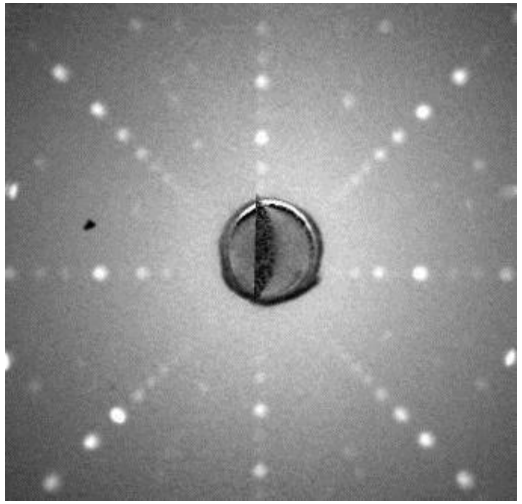
W. Yao

L. Wang

16.8 g single crystals
grown by a flux method

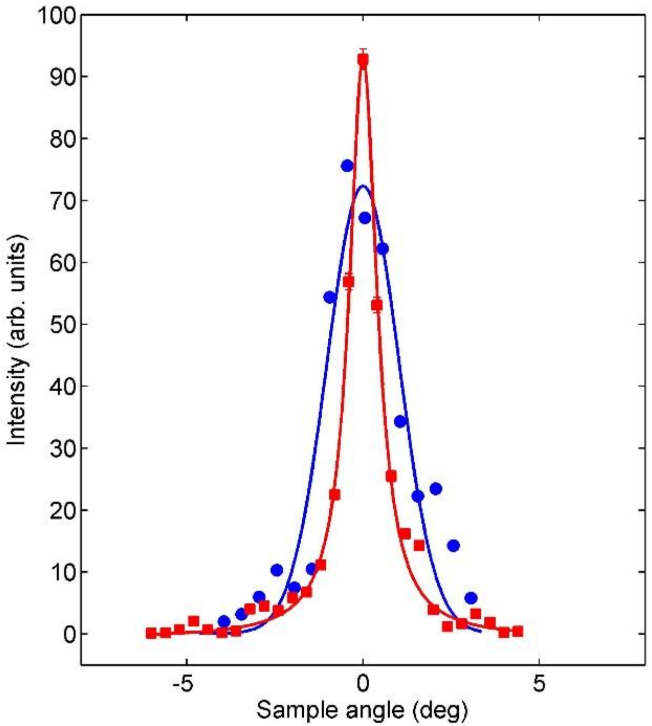




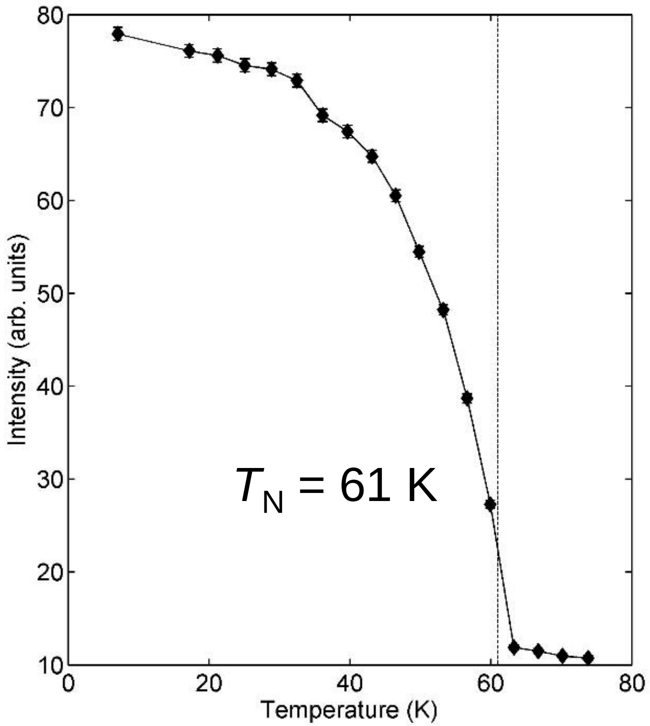


X-ray Laue

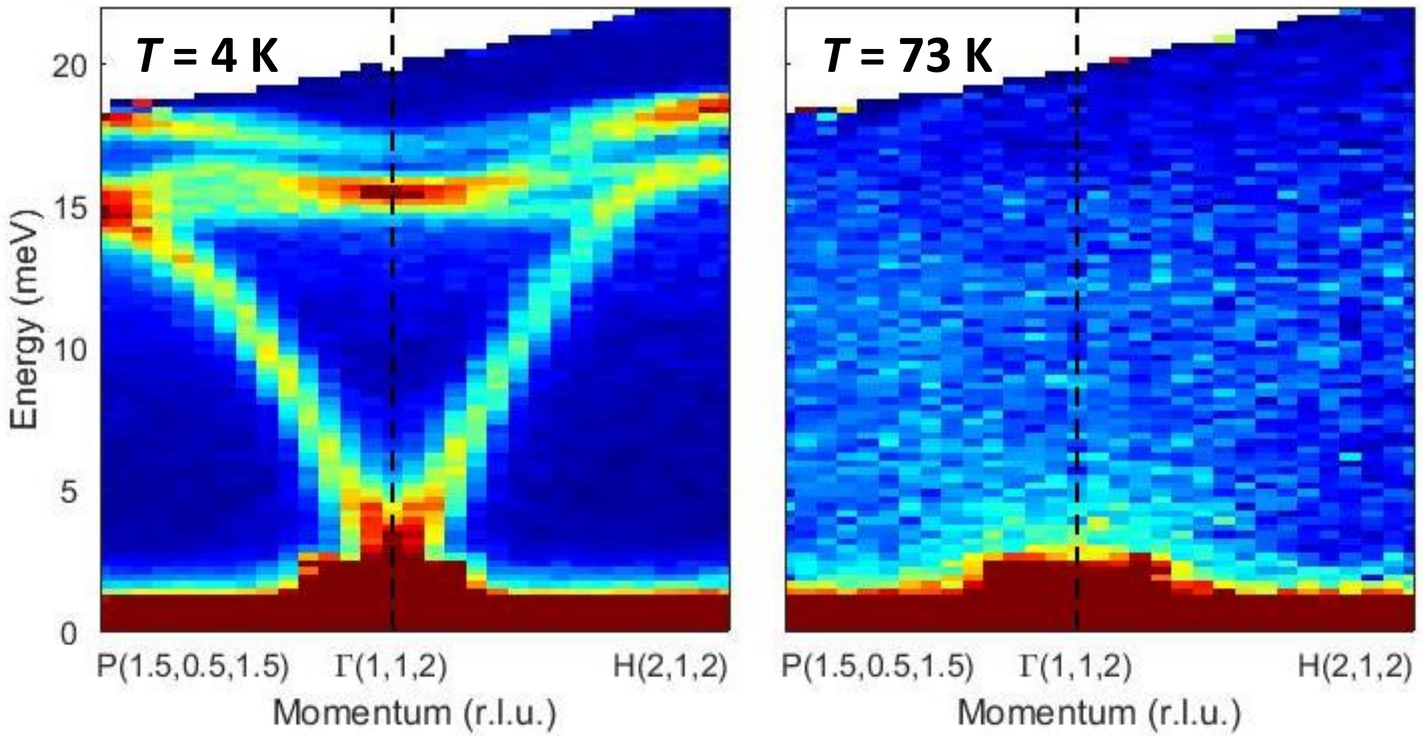
total mosaic spread:
about 2 degrees

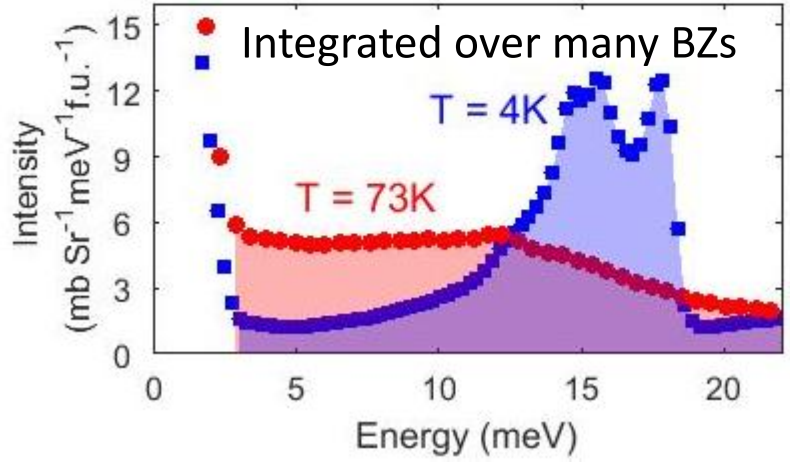


(1, 1, 0) magnetic
diffraction



“3D” AFM order and harmonic magnons



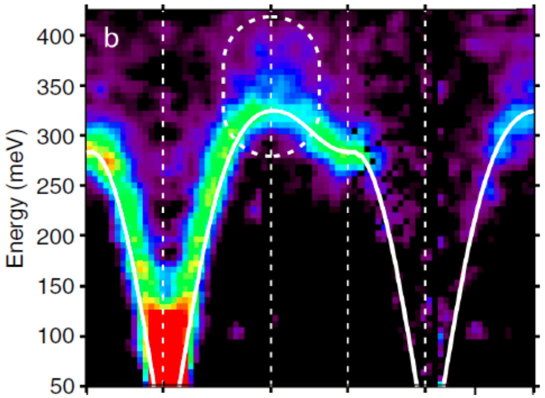


Very “3D” transition!

In contrast to …

Headings et al., PRL 2010

La_2CuO_4, 2D square



Dalla Piazza et al., Nat. Phys. 2015

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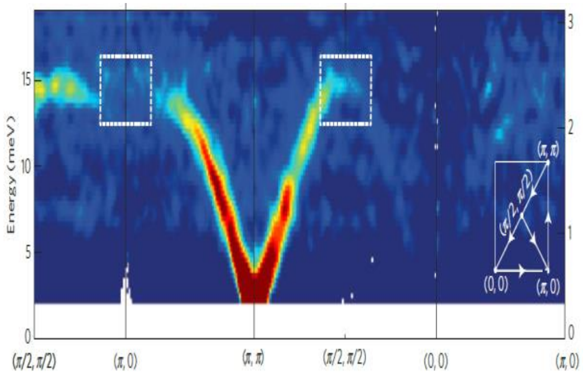
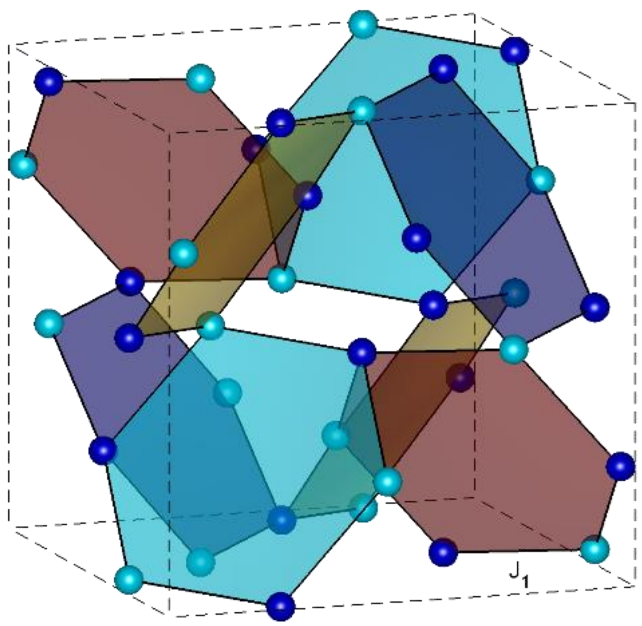
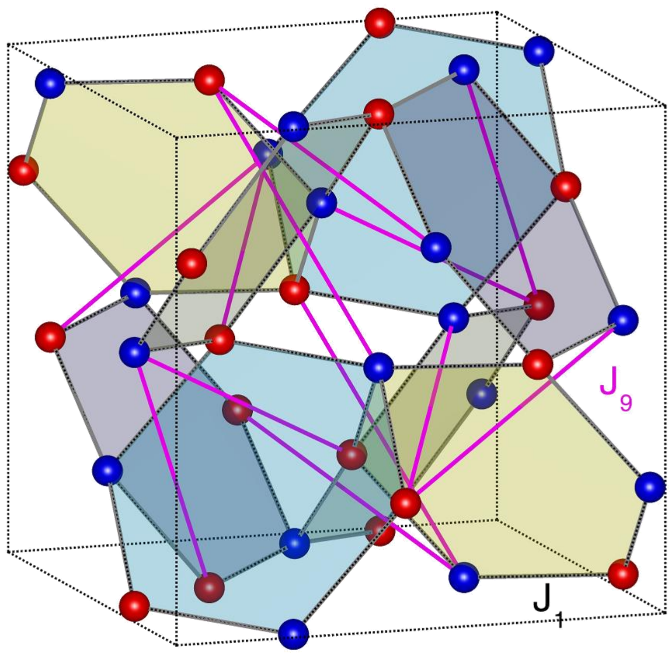
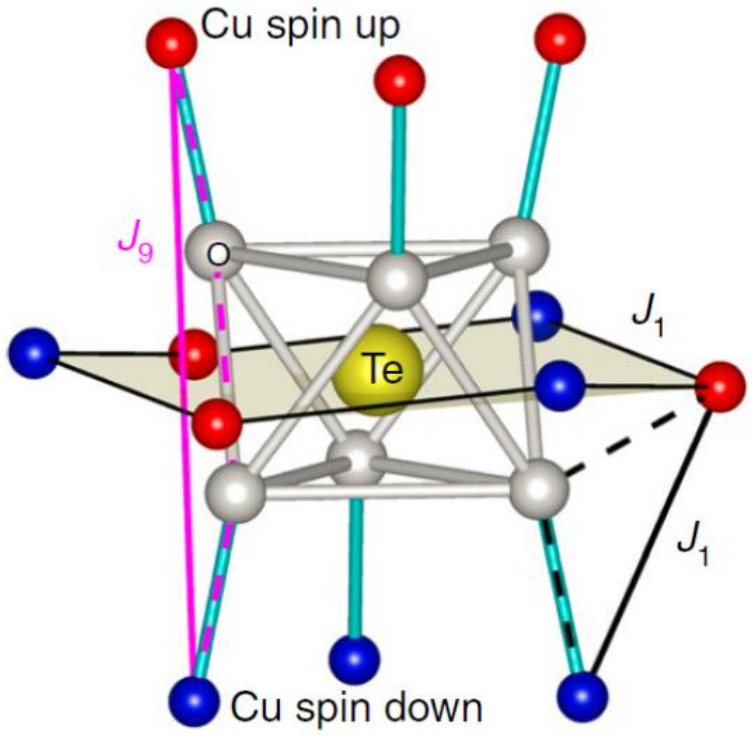




So we know it is harmonic, but how come?



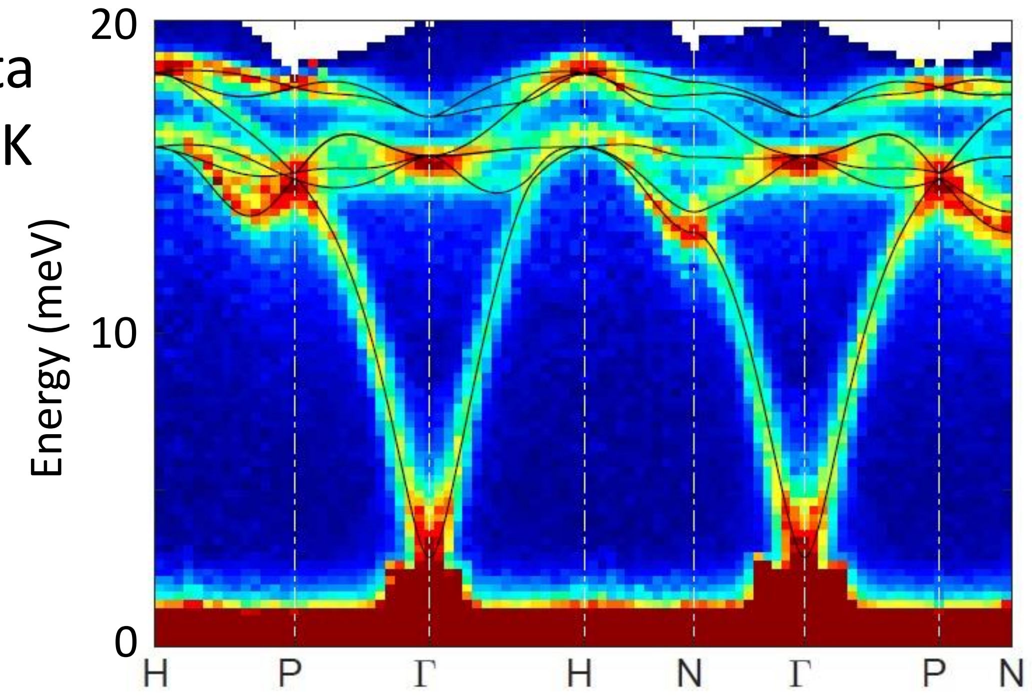
The true spin network (8 neighbors)

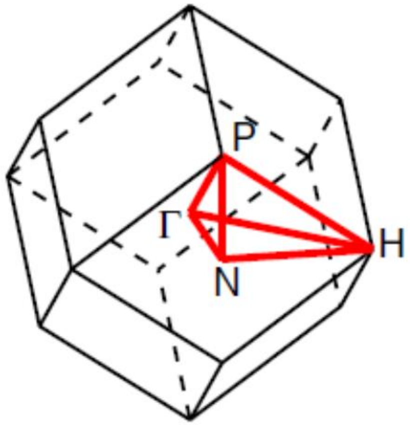


Bond angles matter!

Two-step linear spin-wave fitting

Raw data
at T = 4 K



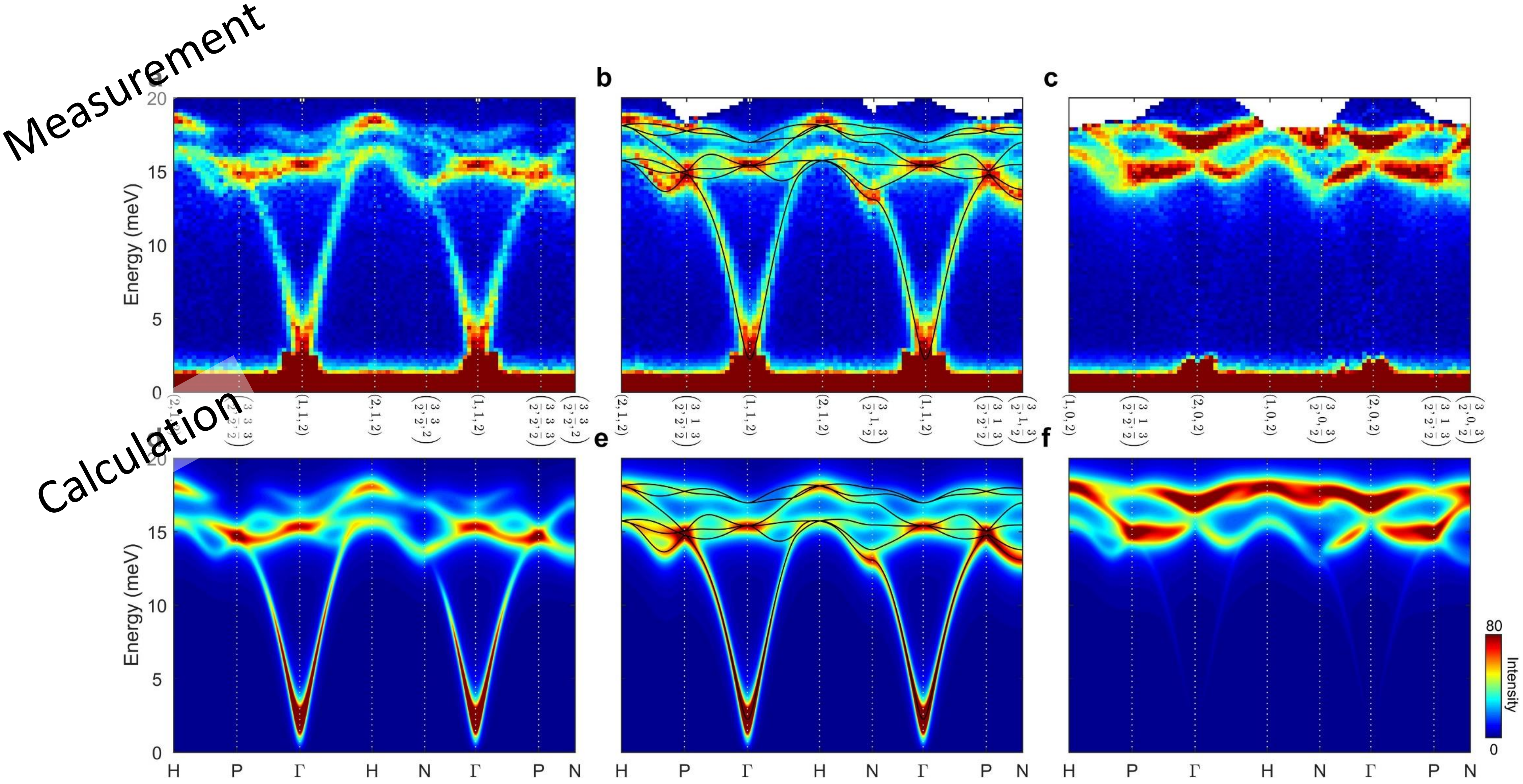


The first step:

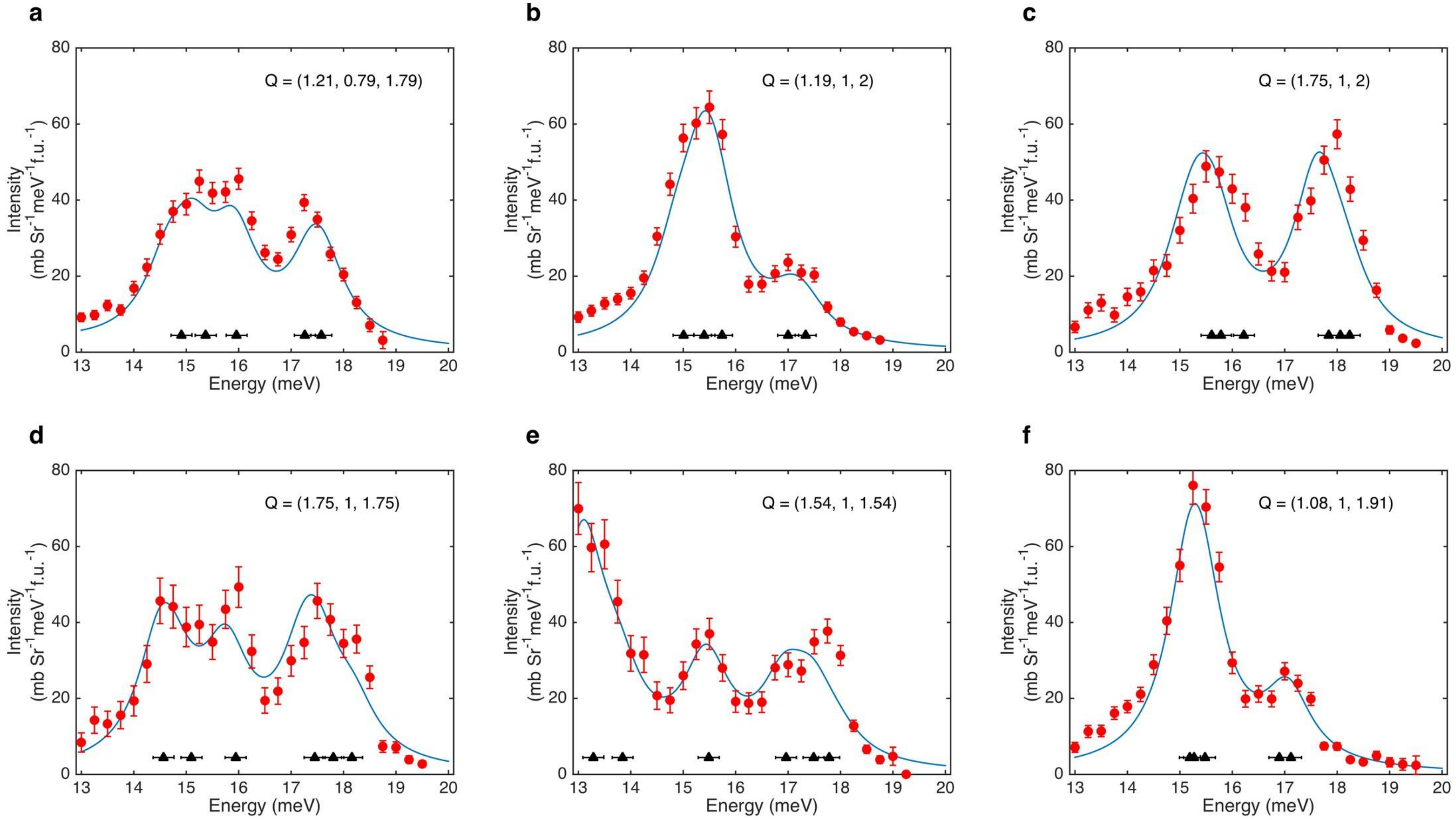
- Fit dispersions
- Consider interactions up to J_9

The second step:

- Fit S(**Q**,ω) with domain average
- Determine "dynamic moment size", and update *J* values



Extremely good agreement!



Moment size responsible for the ‘coherent’ spectral weight:

~ 0.87 μ_B/Cu, compared to 0.3-0.4 μ_B/Cu in La_2CuO_4 [Bourges et al., PRL (1997)]

Interaction		Distance (nm)	Bond sequence and angles	Fit dispersion		Fit intensity
				Isotropic	Anisotropy = 0.46 meV	Anisotropy = 0.29 meV
				Strength (meV)		
J_1		0.318	A ∠106.2° B	**4.49**	**4.39**	**4.40**
J_2	J_{2A}	0.360	A ∠145.8° O1 ∠59.7° B	-0.22	-0.36	-0.41
	J_{2B}		A ∠102.1° O2 ∠101.2° A			
J_3		0.477	A ∠101.2° O2 ∠100.8° B (x2)	-1.49	-1.61	-1.63
J_4		0.481	A ∠147.5° O1 ∠102.6° B (x2)	1.33	1.30	1.31
J_5		0.481	N.A.	1.79	1.47	1,70
J_6		0.548	B ∠100.8° O2 ∠149.5° B	-0.21	-0.21	-0.21
J_7		0.573	A ∠102.1° O2 ∠149.5° B	-0.14	-0.20	-0.14
J_8		0.597	A ∠102.1° O2 ∠90.0° O1 ∠102.6° B (x2)	0.11	0.03	0.05
J_9		0.621	A ∠145.8° O1 ∠147.5° A	**4.51**	**4.51**	**4.26**

A: shorter Cu-O bond: 0.195 nm B: longer Cu-O bond: 0.203 nm

O1: shorter O-O bond: 0.262 nm O2: longer O-O bond: 0.281 nm

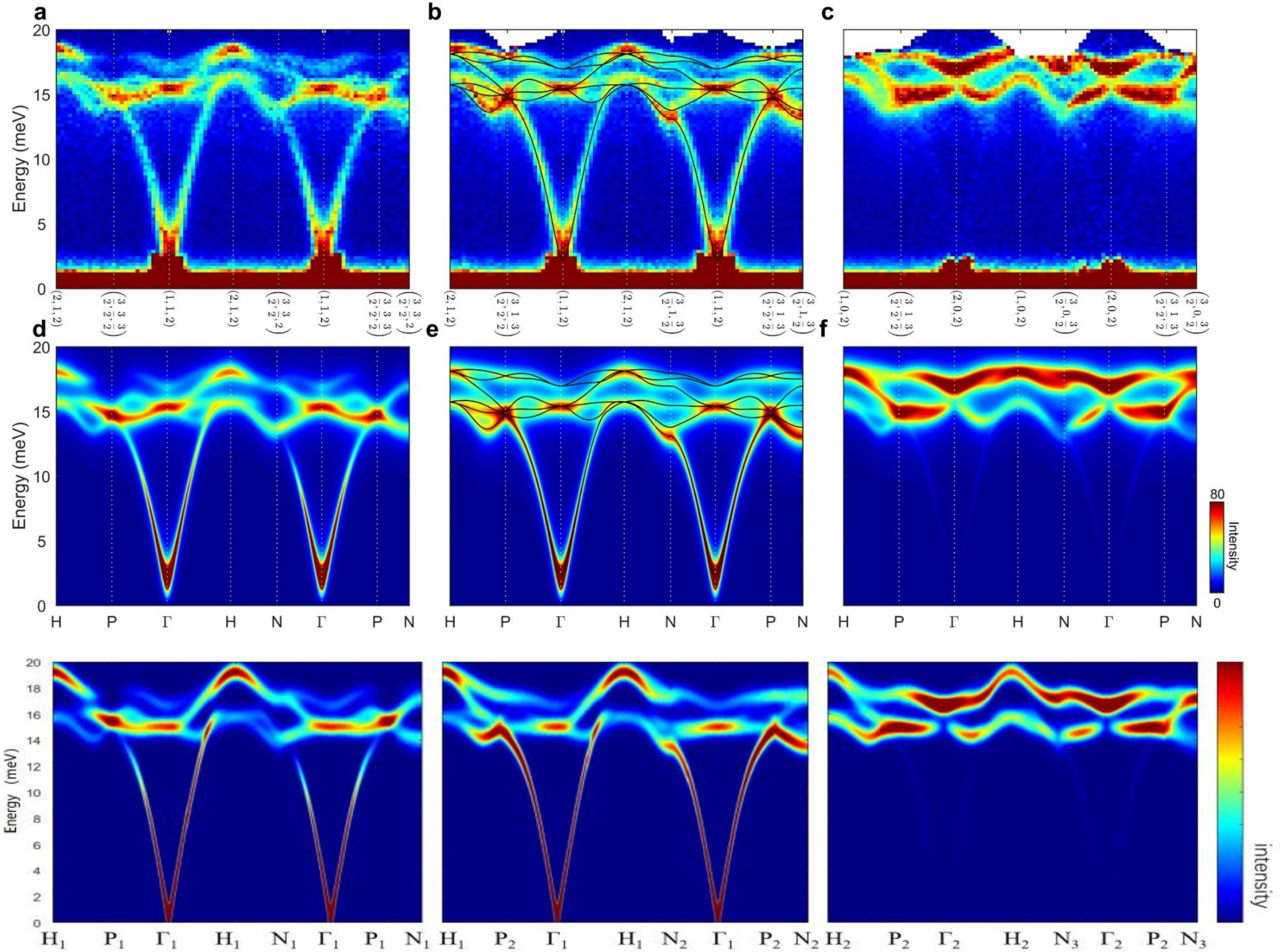
DFT calculation supports our finding

Related work by Nanjing University group:
Bao *et al.*, *Nat. Commun.* **9**, 2591 (2018)

Our work

	Distance(Å)	NN	Ref. [53]	Ref. [52]	Our results
J_1	3.18	4	9.07	4.49	7.05
J_2	3.60	4	0.89	-0.22	0.51
J_3	4.77	2	-1.81	-1.49	0.04
J_4	4.81	2	1.91	1.33	2.18
J_5	4.81	2	1.91	1.79	0.09
J_6	5.48	4	0.09	-0.21	0.01
J_7	5.73	4	1.83	-0.14	-0.01
J_8	5.97	4	–	0.11	0.04
J_9	6.21	4	–	4.51	3.77
J_{10}	6.34	2	–	–	0.56
J_{11}	6.34	2	–	–	-0.01
J_{12}	6.74	4	–	–	0.02

Wang et al.,
arXiv:1811.03603



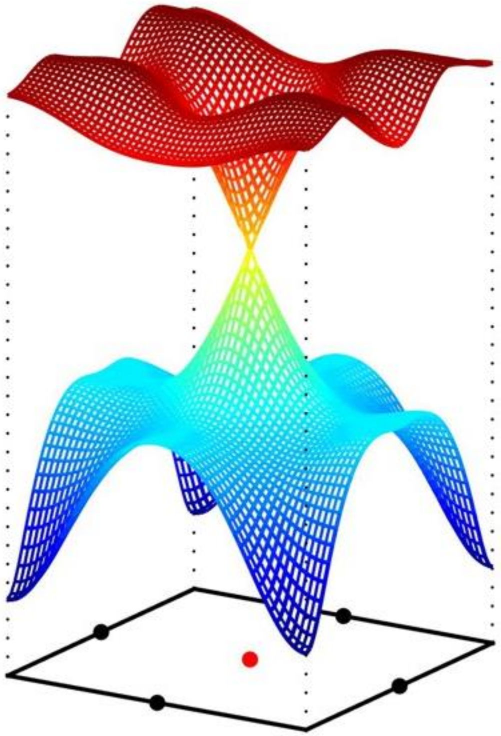
Experiment

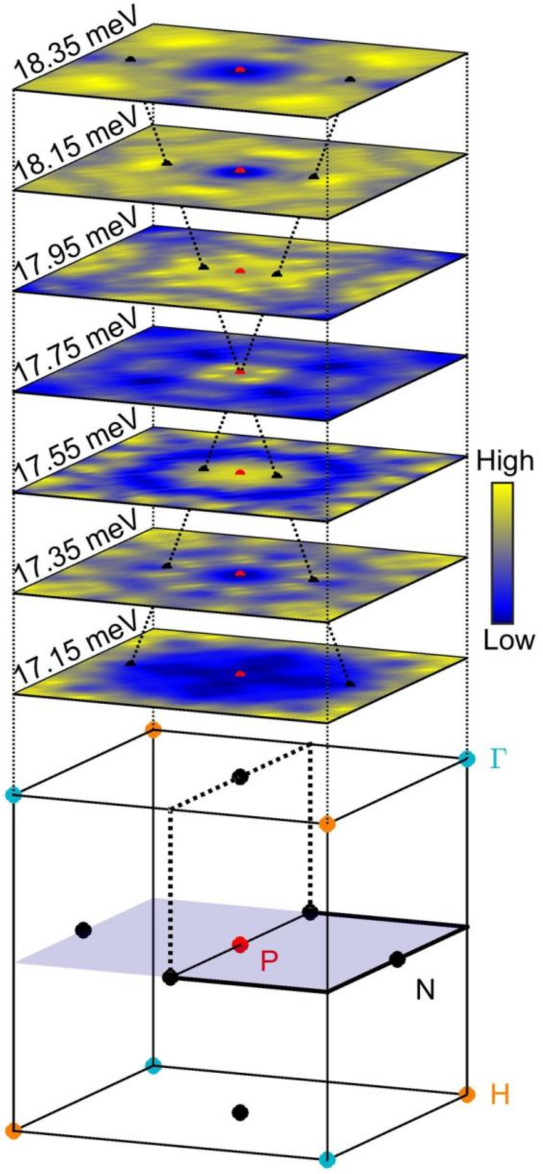
Our fitting

DFT + LSWT
arXiv:1811.03603

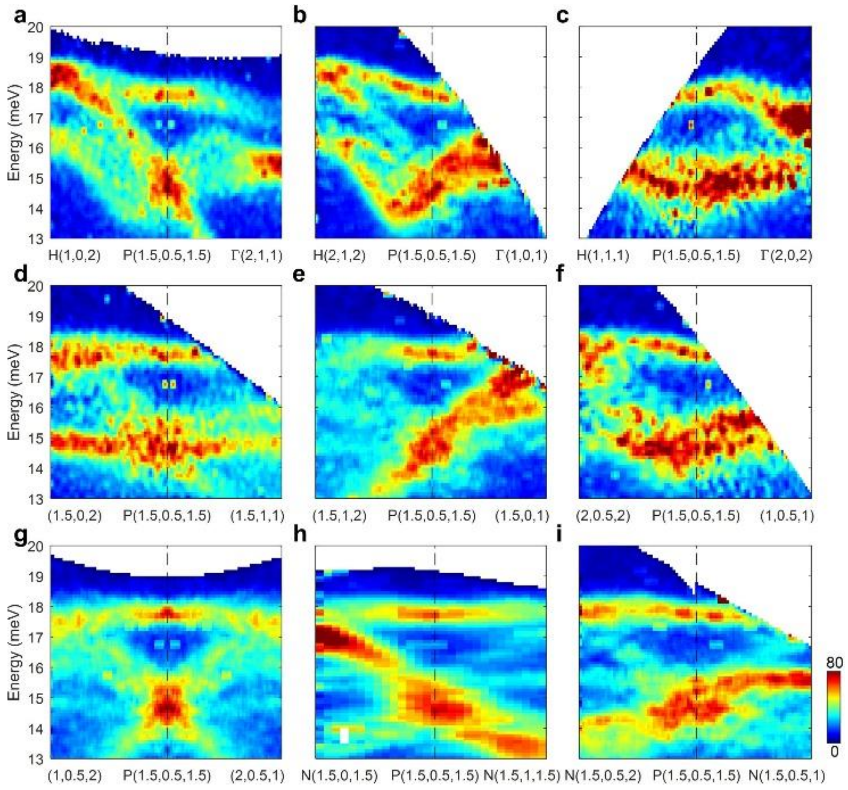
Visualization of the Dirac point (P-point at 17.8 meV)

Calculation





4D data "library"



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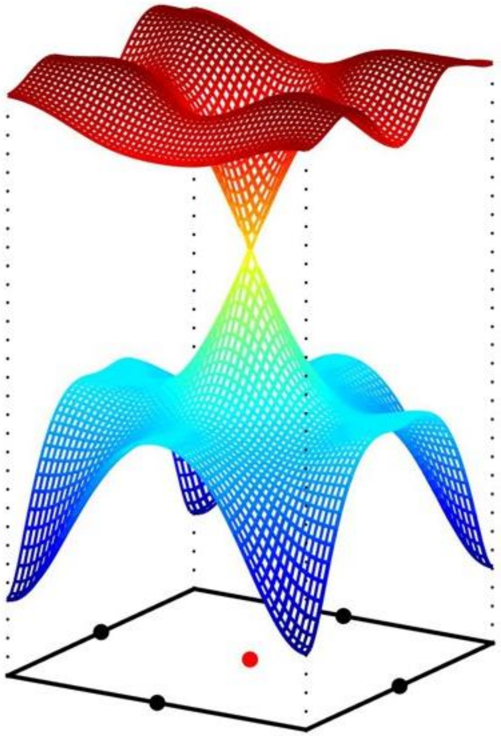
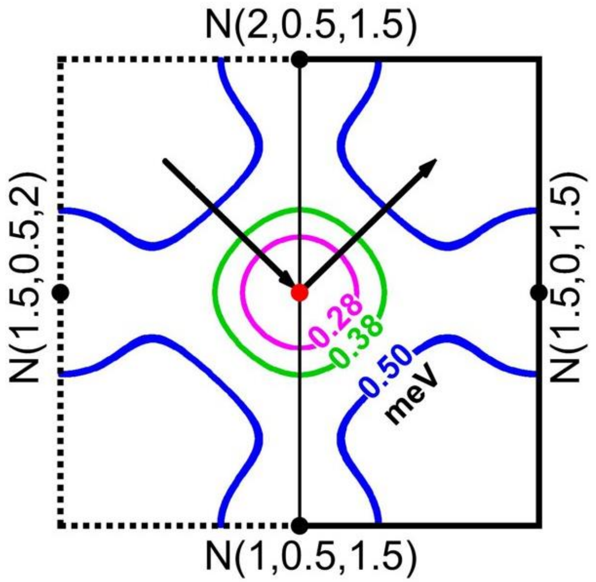
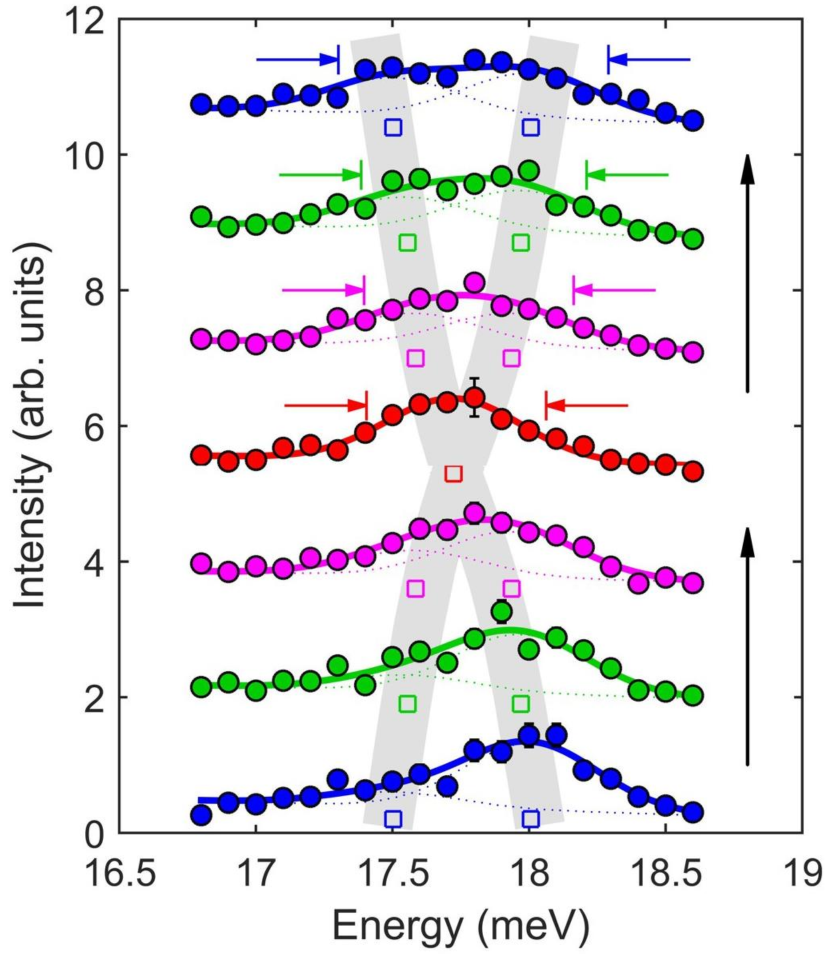
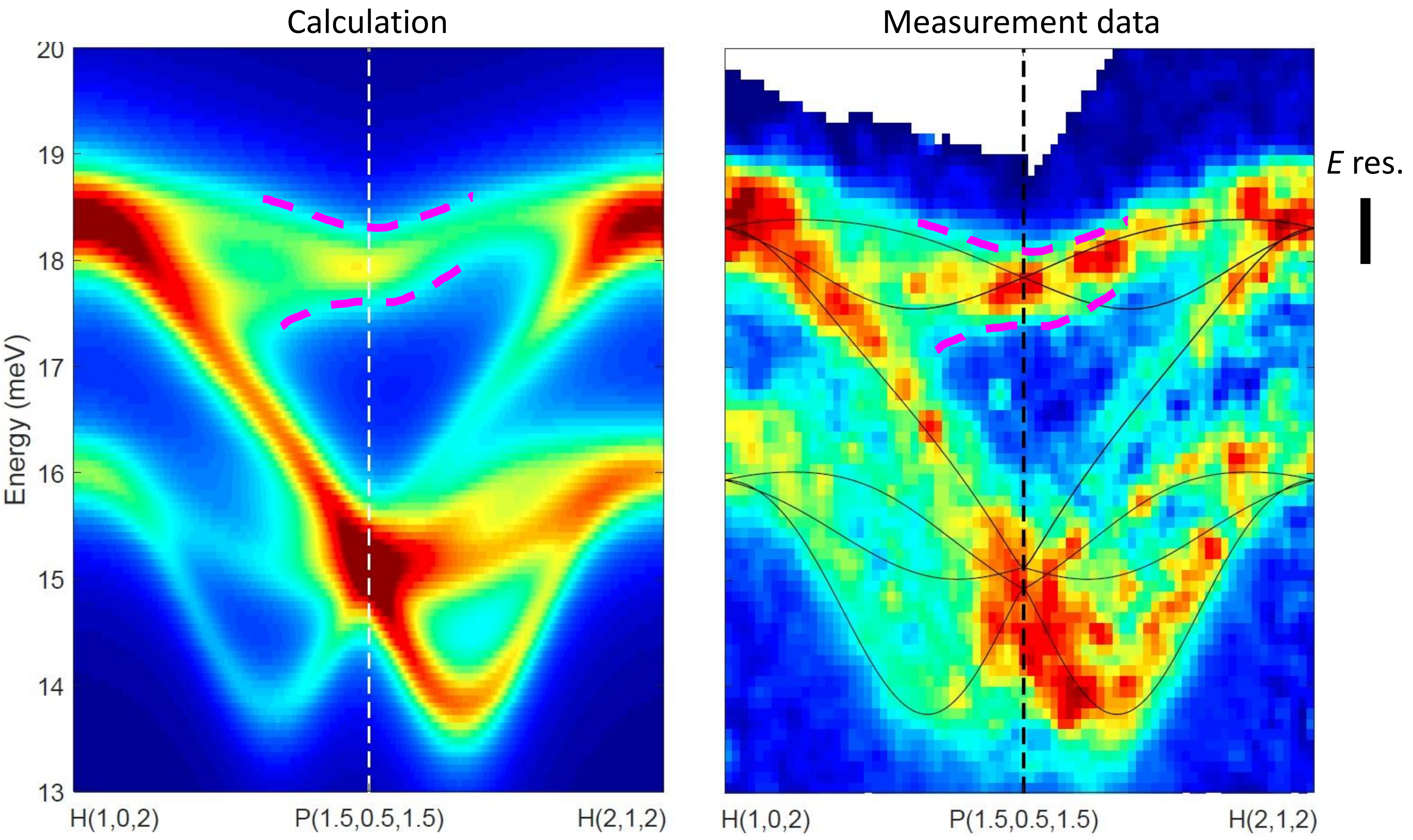






Check the wave functions



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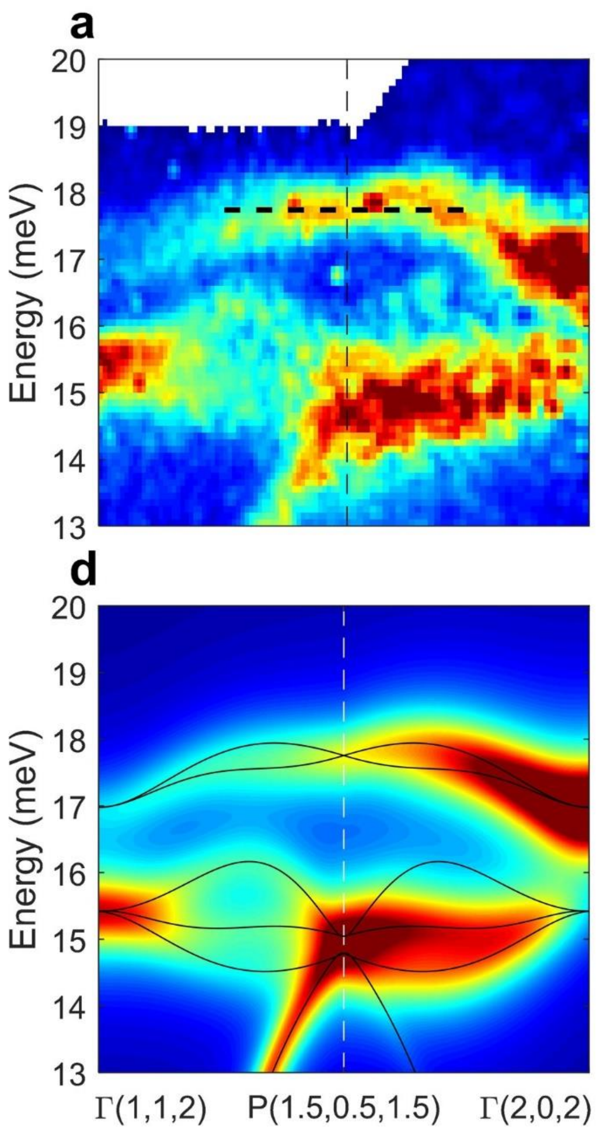

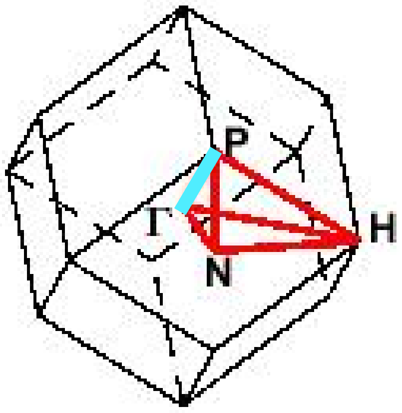

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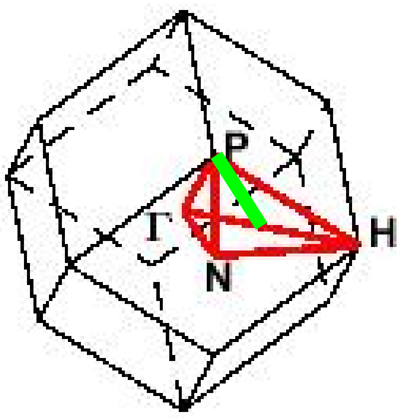
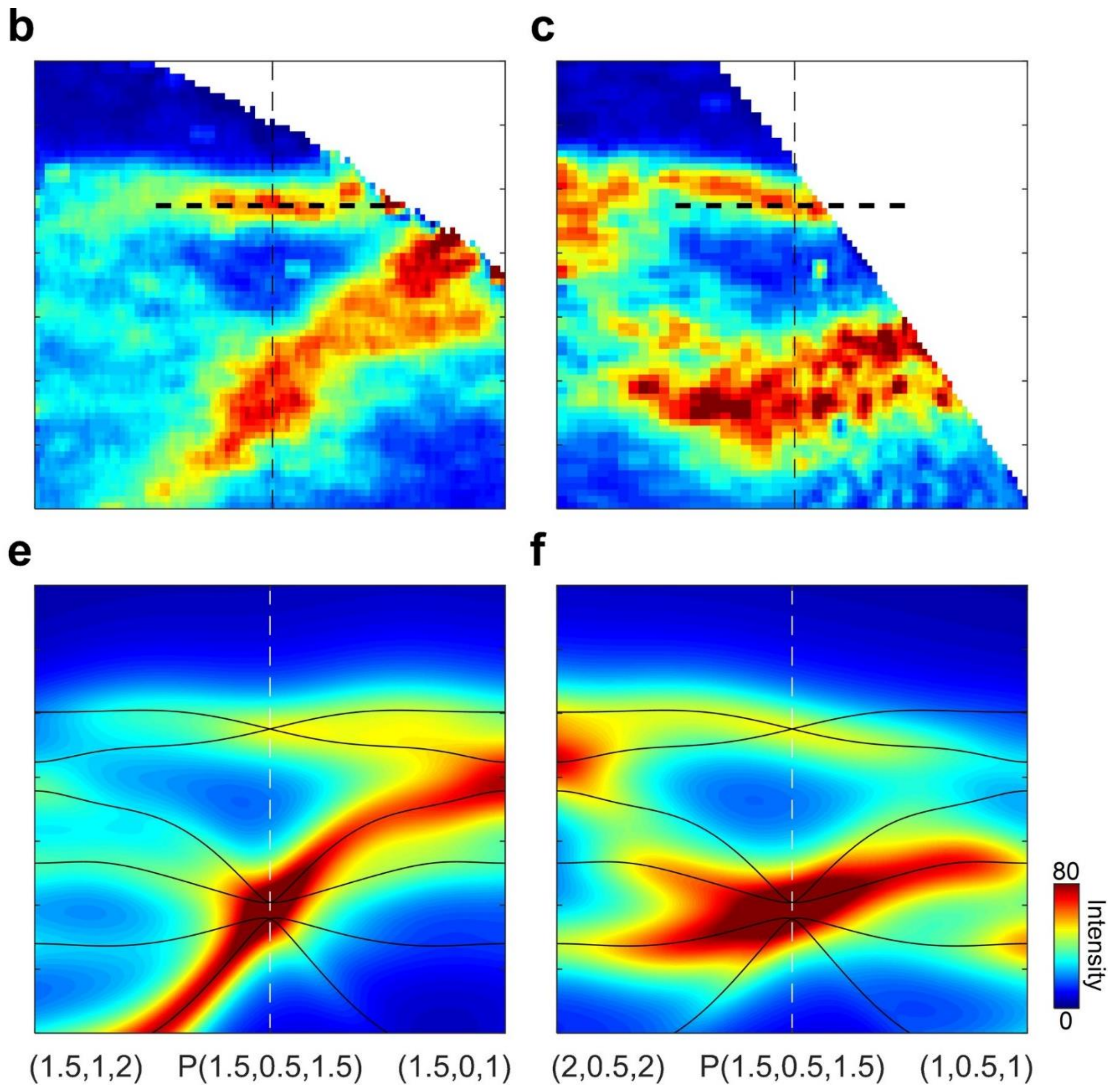
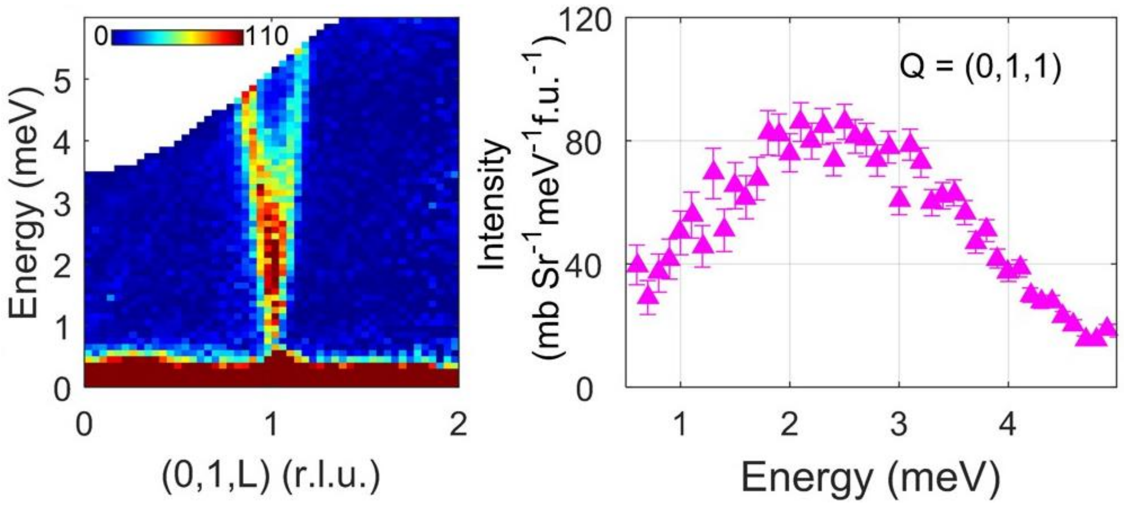


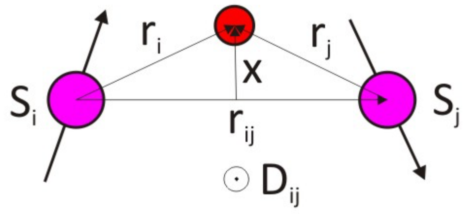


About the U(1) symmetry

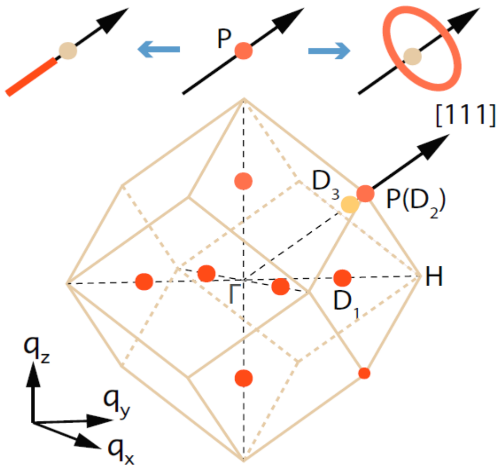


Anisotropy gap of about 2 meV

cannot be caused by U(1)-preserving global single-ion anisotropy



- Must be exchange anisotropy, most likely DMI, which favors non-collinear order.
- All observed DPs are actually tiny nodal lines!



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  band topology + magnetism

- **Theoretical considerations**

  "Z_2 nodal lines", and the limiting case of Dirac points

  K. Li *et al.*, *Phys. Rev. Lett.* **119**, 247202 (2017)

- **Experiment and analysis**

  Spin-wave fitting + band-topology visualization

  W. Yao *et al.*, *Nat. Phys.* **14**, 1011 (2018).

- **Summary & outlook**

Summary

- A new type of nodal lines with a Z_2-monopole charge has been theoretically predicted for magnons in a large class of PT-antiferromagnets
- With additional U(1) symmetry: a new type of Dirac points

K. Li *et al.*, *PRL* **119**, 247202 (2017)

- The Dirac points are experimentally confirmed in Cu_3TeO_6
- Long-range super-superexchange (J_9) is important

W. Yao *et al.*, *Nat. Phys.* **14**, 1011 (2018)

Outlook

- Magnon band topology may be found in lots of materials
- Beware of long-range interactions!
- Nodal-ring diameter ∝ $[\mathrm{DMI}]^2$, need large U(1)-breaking interactions
- Topological thermal Hall effects (spintronics / magnonics)
- Magnon surface states (RIXS / EELS / INS)
- Neutron scattering is a very powerful tool to detect 3D band topology

topological phonon band crossing in CoSi (Work in progress)