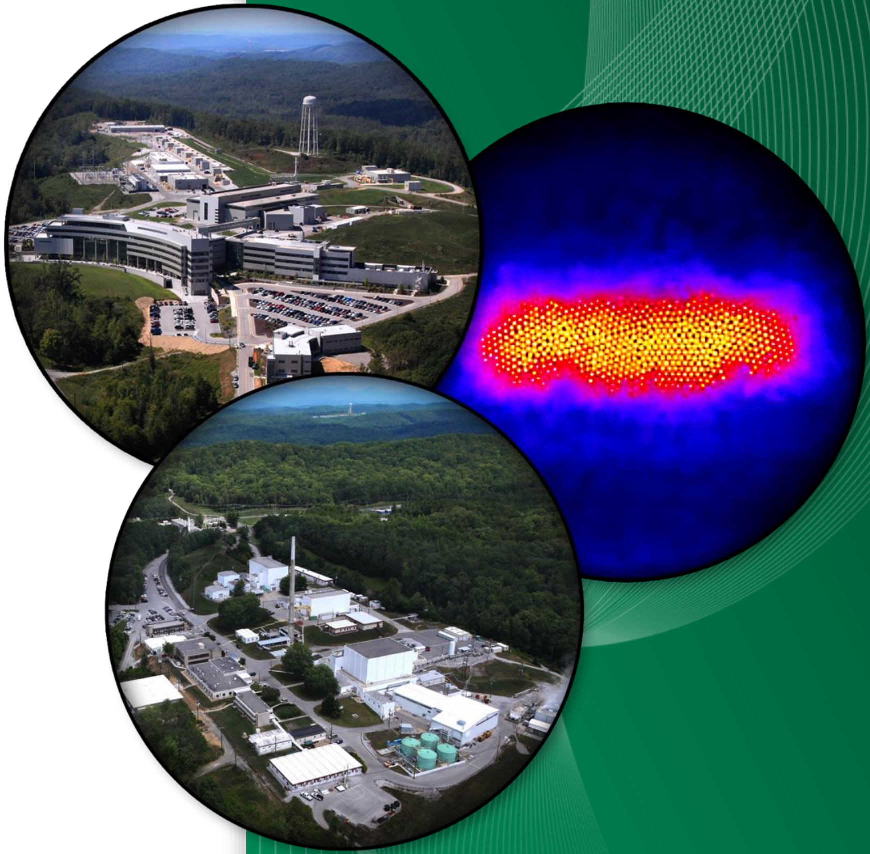
Possible Kitaev spin liquid physics and topological transitions in α-$RuCl_3$



Stephen Nagler
Oak Ridge National Laboratory

Outline

I. Kitaev's model

- Quick reminder of possible relevance to materials
- Basics of α-$RuCl_3$

II. Some inelastic neutron scattering

- Magnons and fractional excitations in INS
- Inelastic neutron scattering in α-$RuCl_3$

III. Recent results

- Higher fields and 3rd dimension
- Magnetocaloric effect and T- B phase diagram

Neutron Scattering Collaborators:

A. Banerjee, A. Aczel, C. Balz, C. Batista, S. Bhattacharjee, C. Bridges, H. Cao, B. Chakoumakos, G. Ehlers, O. Garlea, G. Granroth, Y. Kamiya, J. Knolle, D. Kovrizhin, P. Lampen-Kelley, L. Li, Y. Liu, Z. Lu, M. Lumsden, D. Mandrus, R. Moessner, M. Stone, D, Pajerowski, A. Samarakoon, D. A. Tennant, B. Winn, J.-Q. Yan, Y. Yiu, S. Zhang.

Christian Balz

arXiv:1903.00056

Additional collaborators:
X. Hu, S. M. Yadav, Y. Takano

Outline

I. Kitaev's model
- Quick reminder of possible relevance to materials
- Basics of α-$RuCl_3$

Kitaev's model on honeycomb lattice – a special QSL

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Anyons in an exactly solved model and beyond

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California Institute of Technology, Pasadena, CA 91125, USA

Received 21 October 2005; accepted 25 October 2005

Kitaev's model on honeycomb lattice – a special QSL

$$H_{\text{Kitaev}} = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$

- Kitaev interaction: Bond-directional dependent Ising coupling
- Exactly solvable Hamiltonian

→ ***quantum spin liquid*** ground state

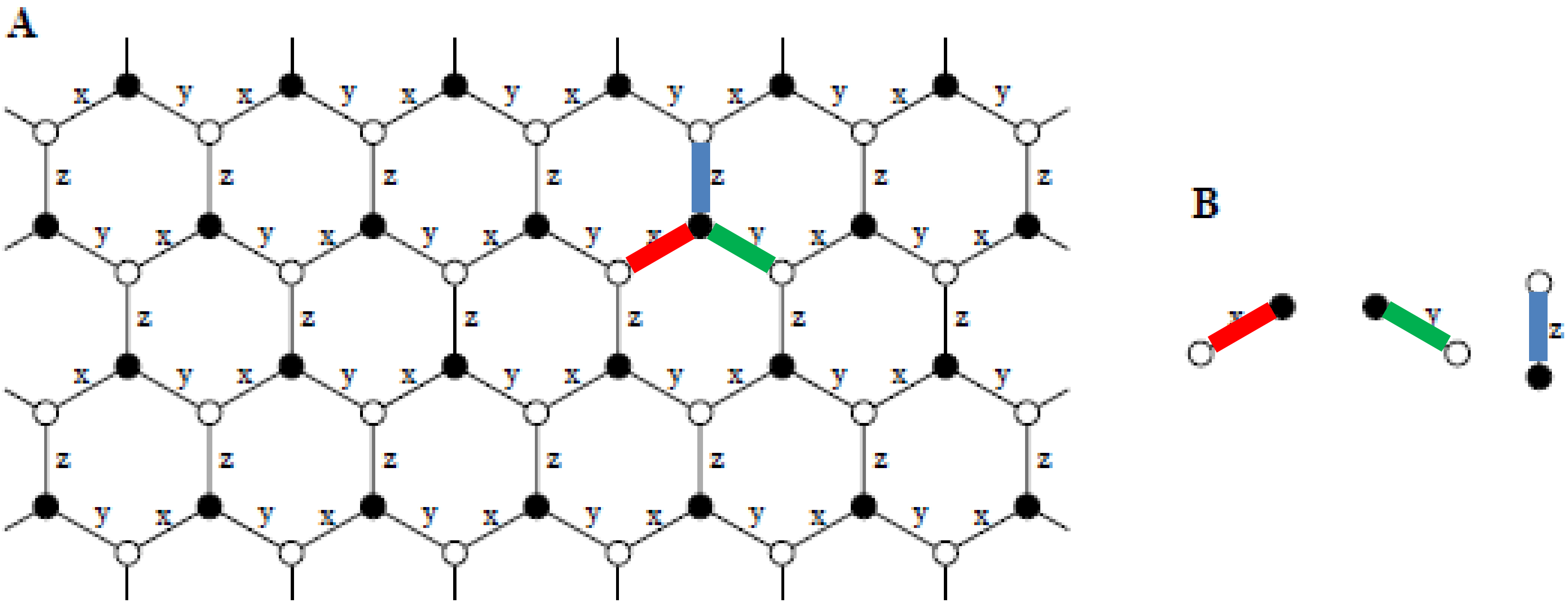


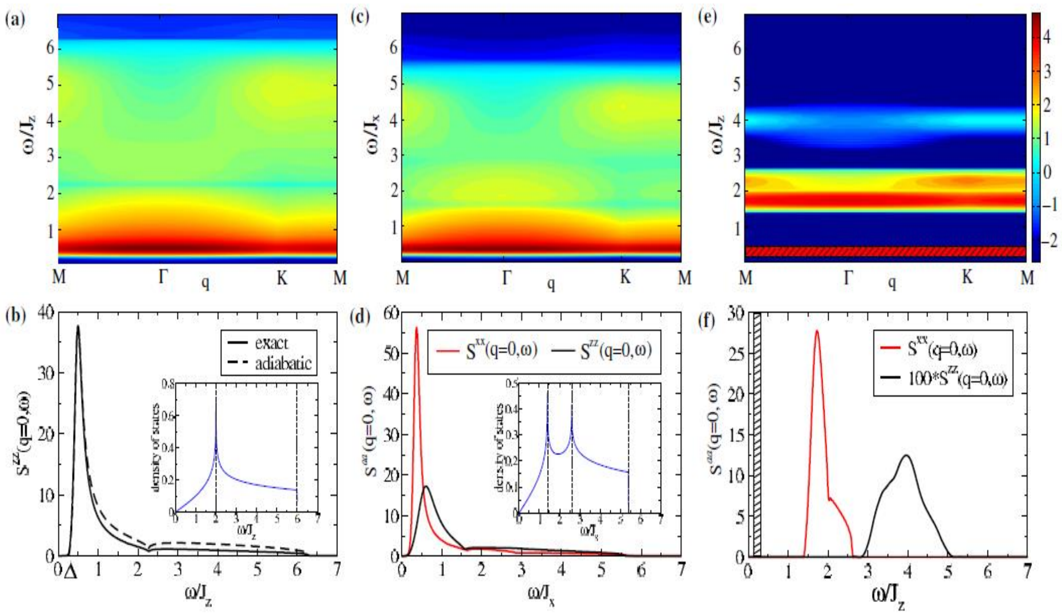
Fig. 3. Three types of links in the honeycomb lattice.

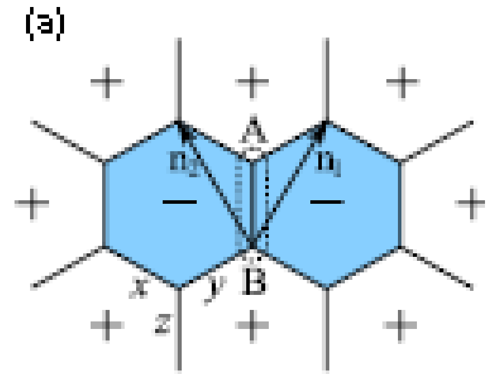
Dynamics of Kitaev QSL

PRL **112,** 207203 (2014)   Selected for a Viewpoint in *Physics*
PHYSICAL REVIEW LETTERS   week ending 23 MAY 2014

Dynamics of a Two-Dimensional Quantum Spin Liquid: Signatures of Emergent Majorana Fermions and Fluxes

J. Knolle,[1,*] D. L. Kovrizhin,[1,2] J. T. Chalker,[3] and R. Moessner[1]





Majorana: $a = a^\dagger \sim (f + f^\dagger)$

Kitaev interactions in materials

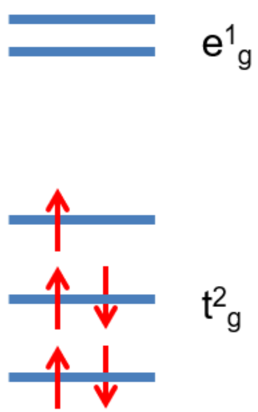
PRL 102, 017205 (2009) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

G. Jackeli[1,*] and G. Khaliullin[1]

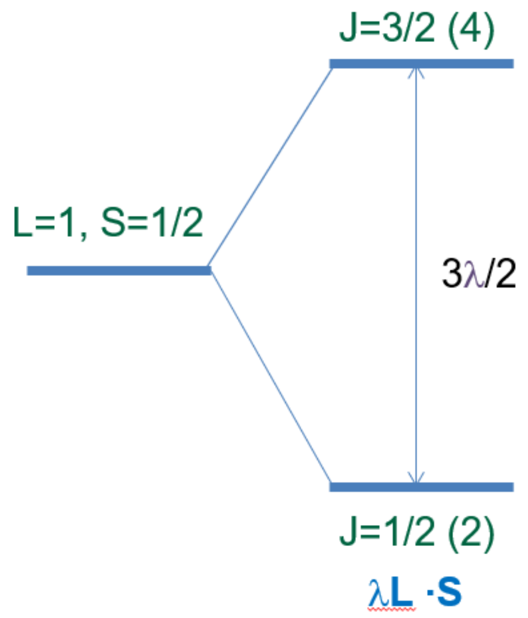
See also:
H. Takagi *et al.*,
Nature Reviews Physics 1, (2019)

d^5 in low spin octahedral configuration

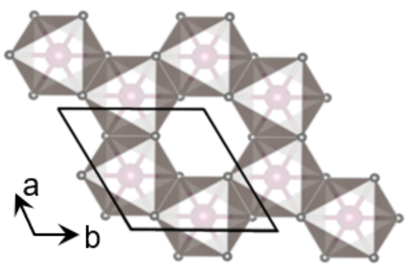


strong field limit
S=1/2, L_{eff} =1
e.g. $(5d^5)$ Ir^{4+}
$(4d^5)$ Ru^{3+}

strong spin-orbit coupling



edge-sharing octahedra



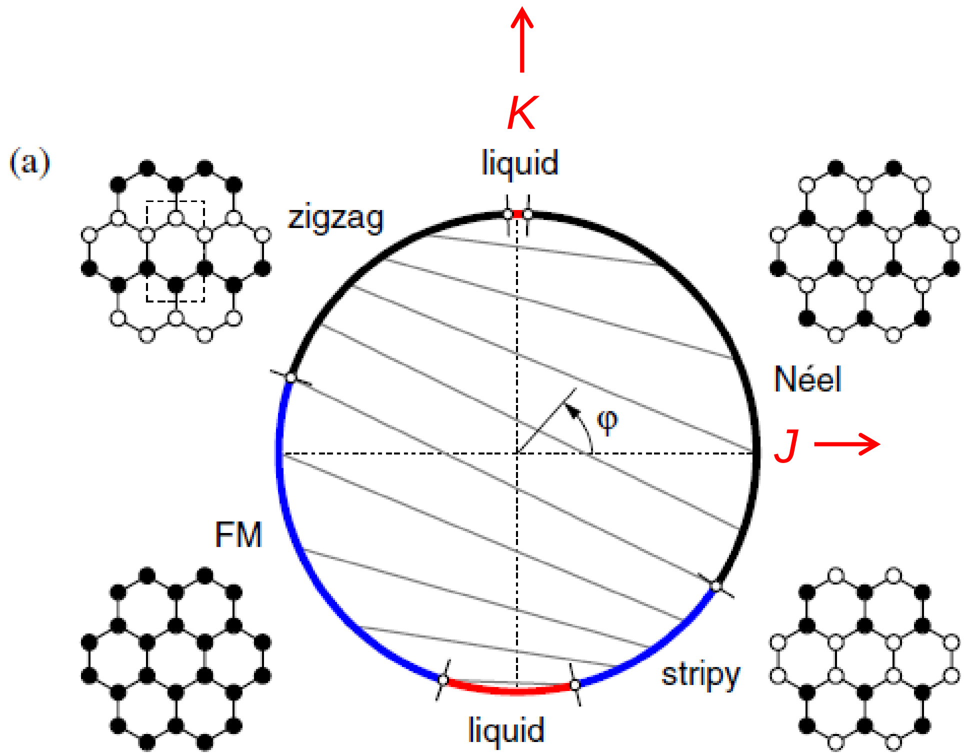
Heisenberg – Kitaev Phase Diagram

PRL **110,** 097204 (2013) PHYSICAL REVIEW LETTERS week ending 1 MARCH 2013

Zigzag Magnetic Order in the Iridium Oxide Na_2IrO_3

Jiří Chaloupka,[1,2] George Jackeli,[1,*] and Giniyat Khaliullin[1]

$$\mathcal{H}_{ij}^{(\gamma)} = 2KS_i^\gamma S_j^\gamma + J\mathbf{S}_i \cdot \mathbf{S}_j.$$



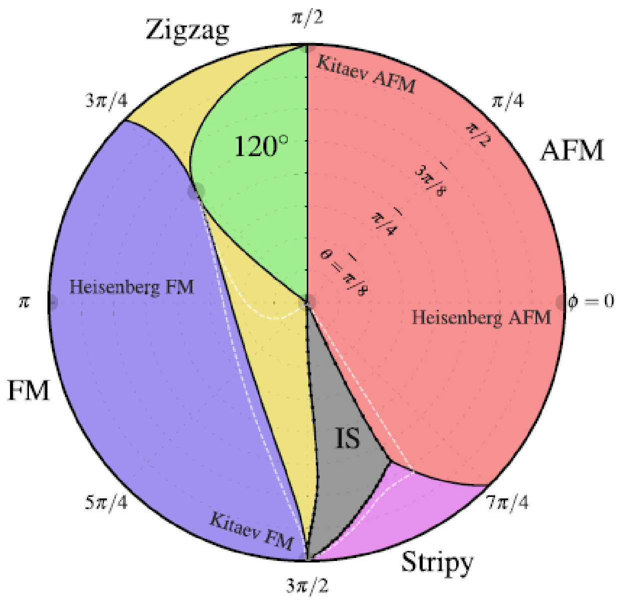
Effect of additional interactions

PRL 112, 077204 (2014) PHYSICAL REVIEW LETTERS week ending 21 FEBRUARY 2014

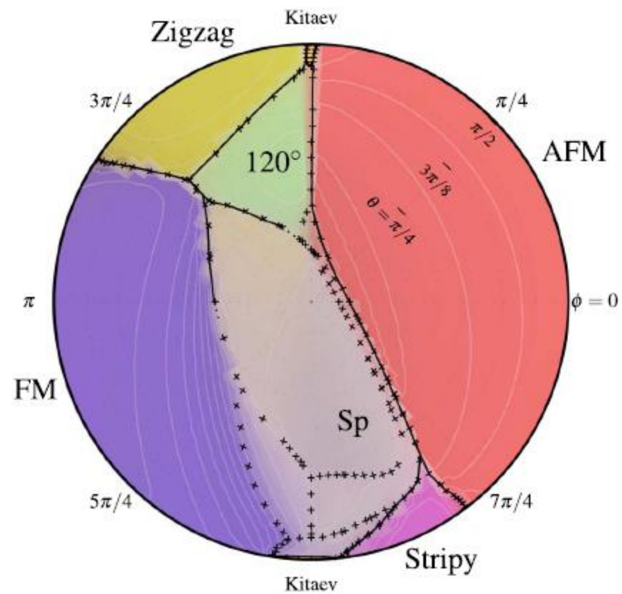
Generic Spin Model for the Honeycomb Iridates beyond the Kitaev Limit

Jeffrey G. Rau,[1] Eric Kin-Ho Lee,[1] and Hae-Young Kee[1,2,*]

$$H = \sum_{\langle ij\rangle \in \alpha\beta(\gamma)} [J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)],$$



(a) Classical phase diagram with $\Gamma > 0$



(a) Phase diagram for $\Gamma > 0$

PHYSICAL REVIEW B 90, 155126 (2014)

Importance of anisotropic exchange interactions in honeycomb iridates: Minimal model for zigzag antiferromagnetic order in Na_2IrO_3

Yuriy Sizyuk,[1,2] Craig Price,[3] Peter Wölfle,[1,4] and Natalia B. Perkins[1,2]

α-$RuCl_3$: quasi - 2D honeycomb material

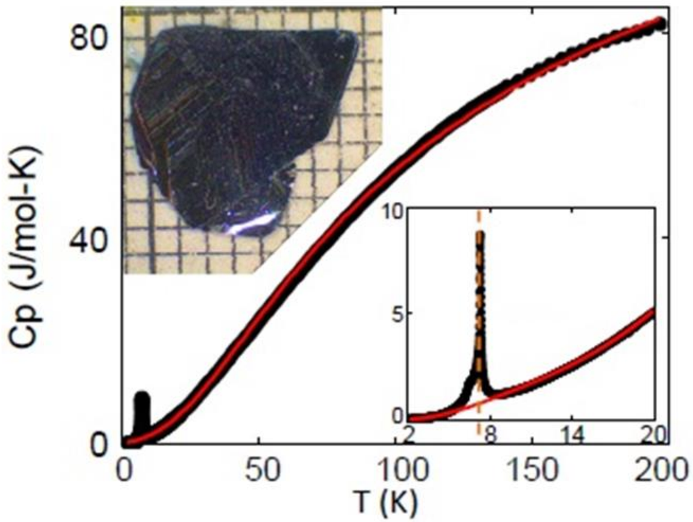
- Honeycomb lattice
- Ru^{3+} in octahedral low spin
- $J_{1/2} \rightarrow J_{3/2}$ transition $\approx$ 200 meV

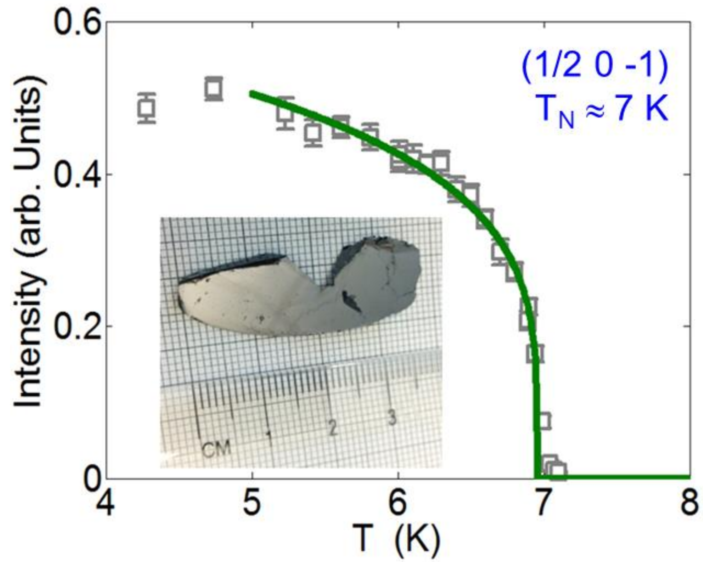
No. 4898 September 14, 1963 NATURE

CHEMISTRY

Anhydrous Ruthenium Chlorides

J. M. FLETCHER
W. E. GARDNER
E. W. HOOPER
K. R. HYDE
F. H. MOORE
J. L. WOODHEAD

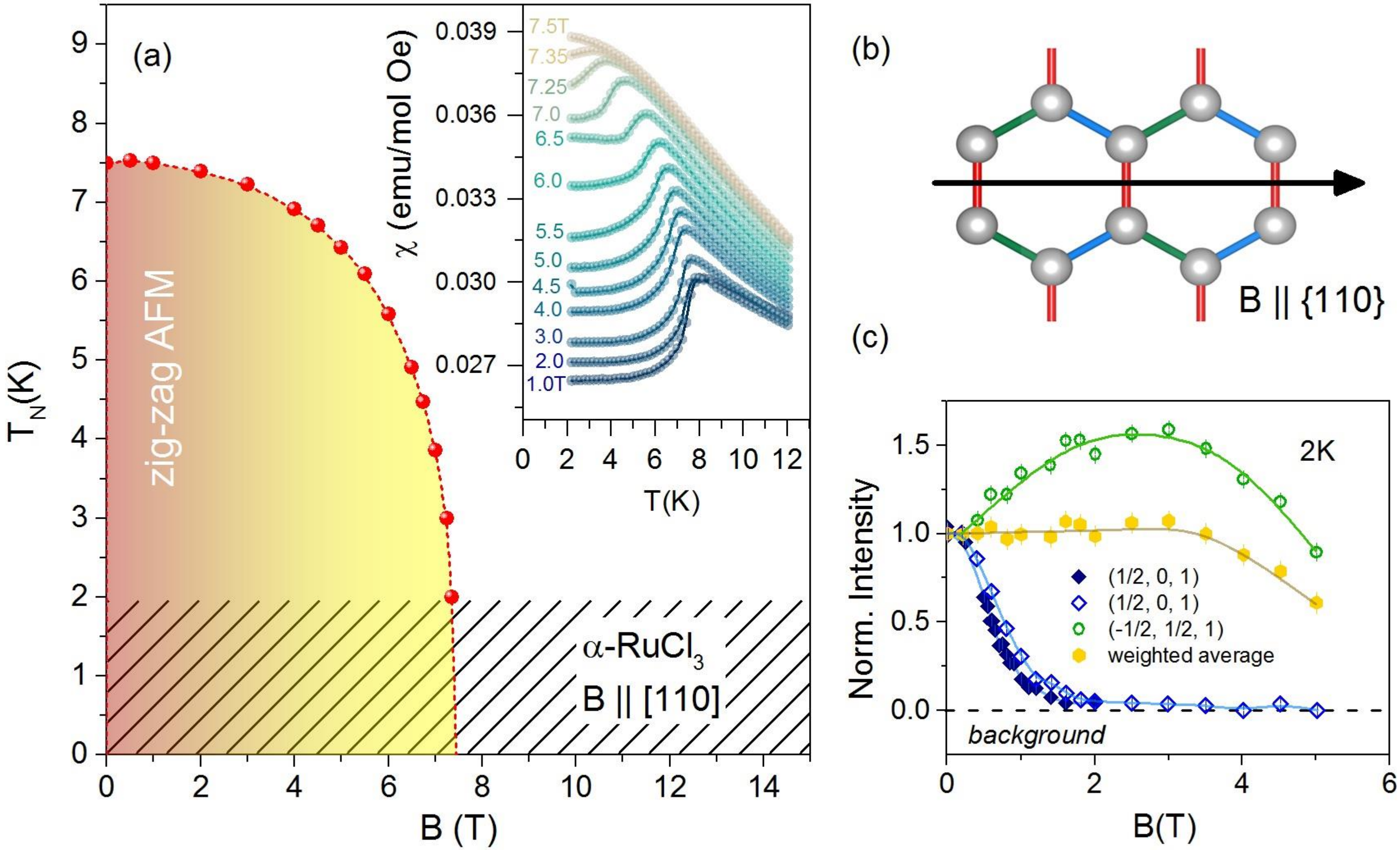




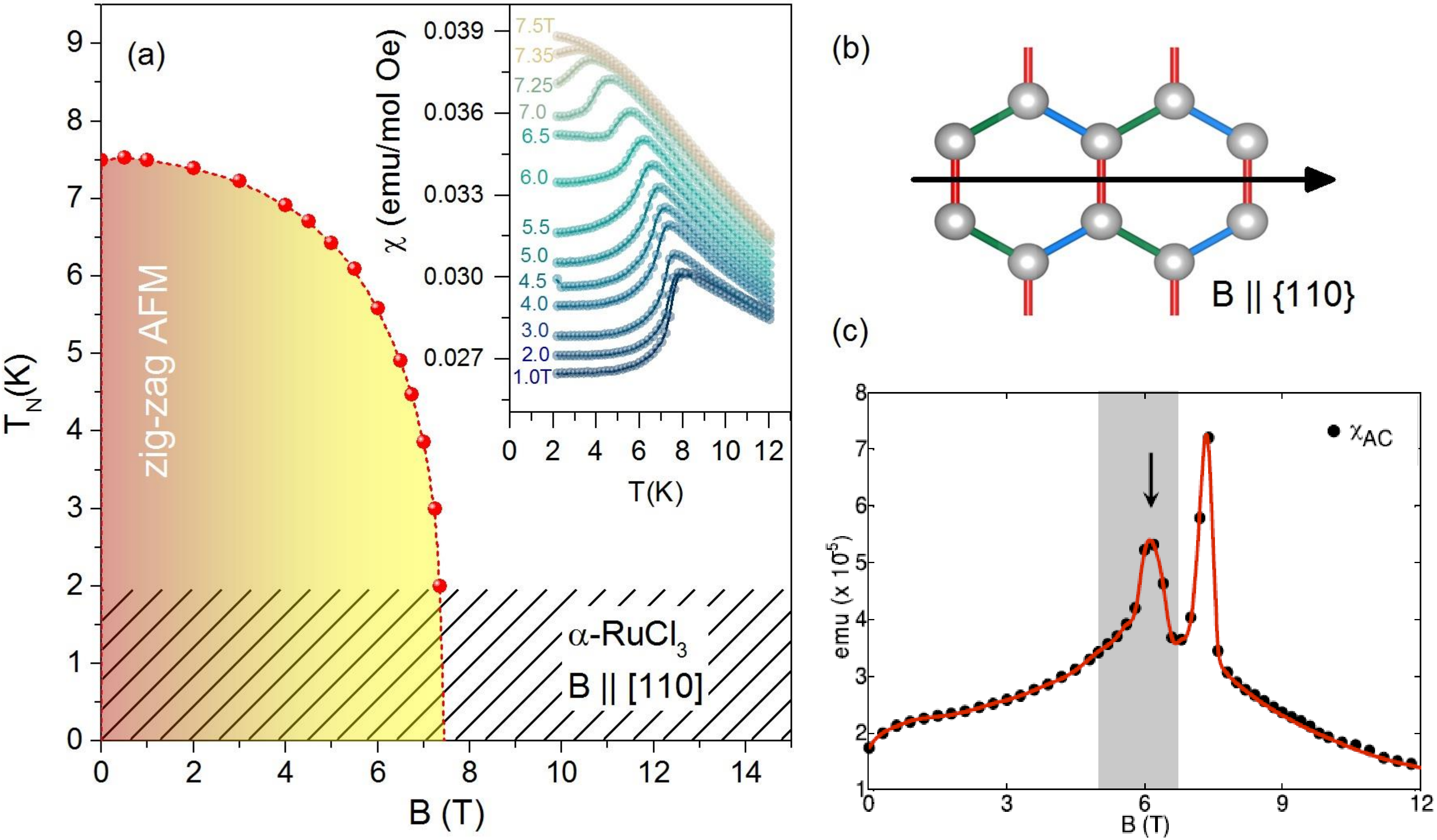
Transition to zig-zag order at T_N = 7 K

Field dependence of T_N

$B_C \approx 7.3$ T



Additional ordered phase 6 – 7.3 T



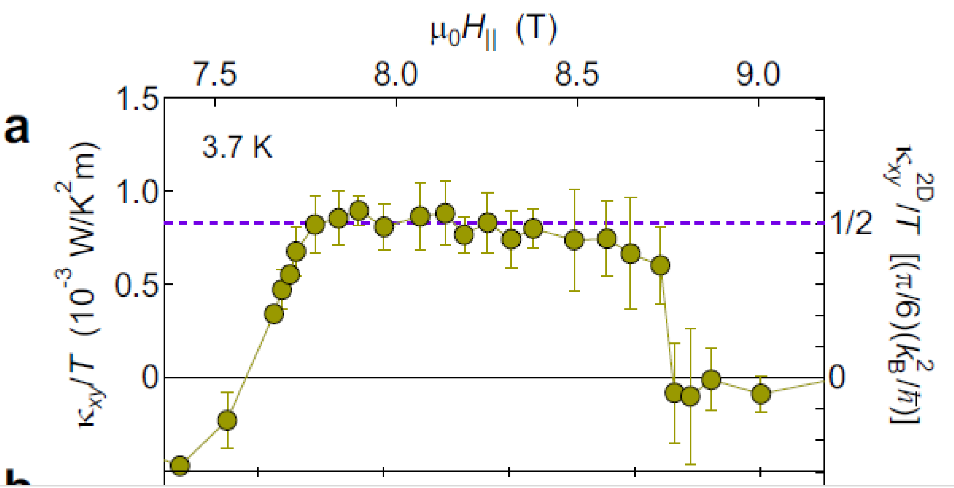
Evidence of fractionalization from thermal Hall ?

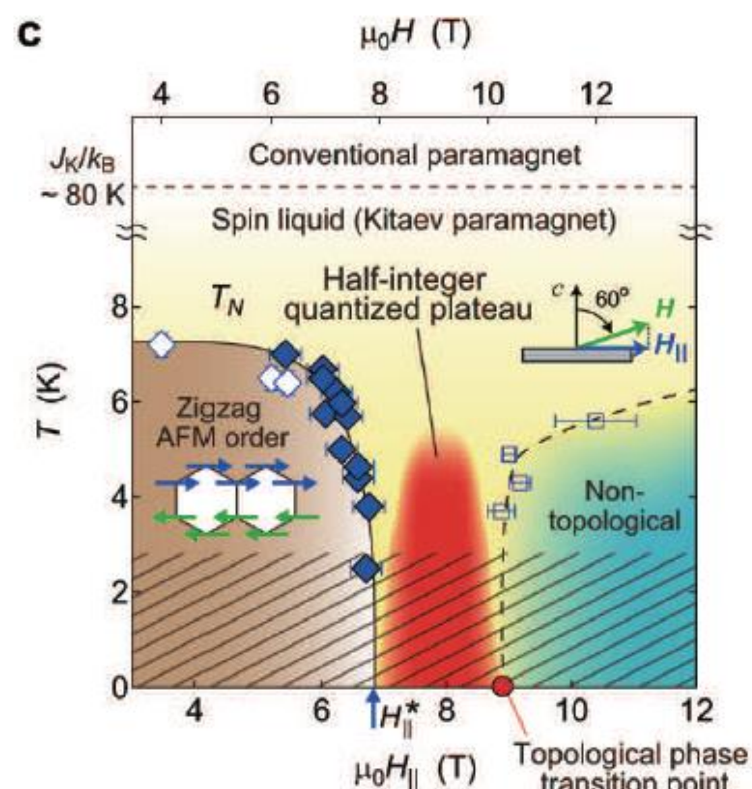
Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid

Y. Kasahara[1], T. Ohnishi[1], N. Kurita[2], H. Tanaka[2], J. Nasu[2], Y. Motome[3], T. Shibauchi[4], and Y. Matsuda[1]

Nature **559**, 227–231 (2018)

κ_{xy}^{2D} reaches a quantum plateau as a function of applied magnetic field. That is, κ_{xy}^{2D}/T attains a quantization value of $(\pi/12)(k_B^2/\hbar)$, which is exactly half of κ_{xy}^{2D}/T in the integer QHE. This half-integer thermal Hall conductance observed in a bulk material is a direct signature of topologically protected chiral edge currents of charge neutral Majorana fermions, particles that are their own antiparticles, which possess half degrees of freedom of conventional fermions [13–16]. These signatures demonstrate the fractionalization of spins into itinerant Majorana fermions and Z_2 fluxes predicted in a Kitaev QSL [1, 3]. Above





Outline

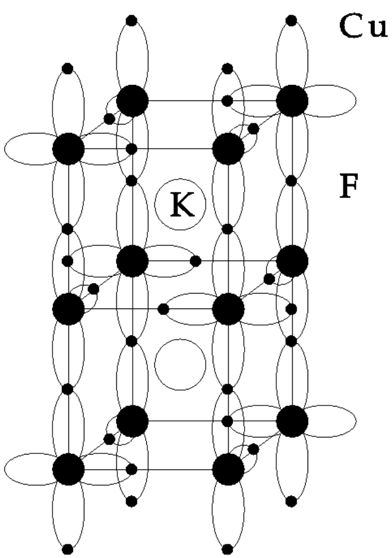
II. Some inelastic neutron scattering
- Magnons and fractional excitations in INS
- Inelastic neutron scattering in α-$RuCl_3$

$KCuF_3$ – a one dimensional S=1/2 HAFC

•Tetragonal structure

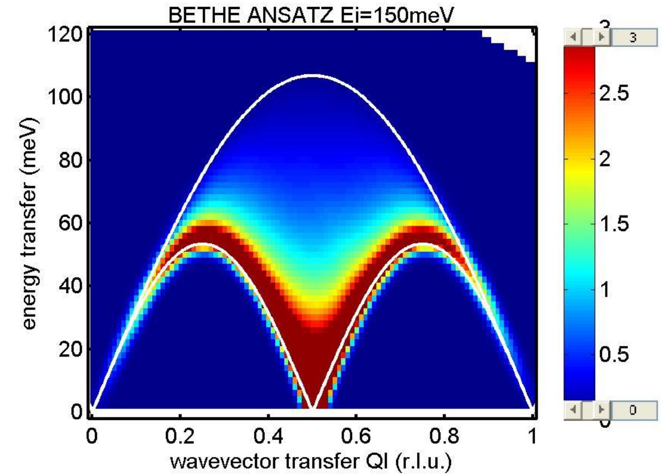
•Chains of Cu^{2+} ions along *c* axis

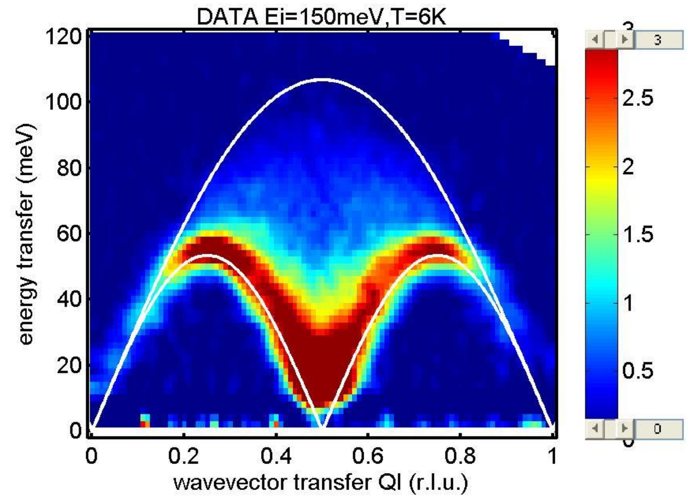
•"Orbitally ordered"



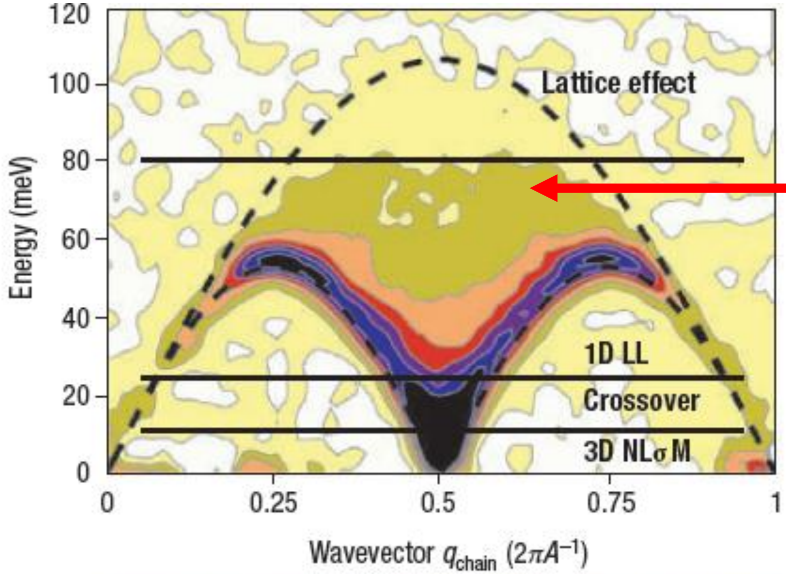
- Heisenberg AF chains of S=1/2 Cu^{2+} ions
- Inter-chain coupling leads to 3D AF order at T_N = 39 K

- Above T_N the response follows that expected for the isolated S=1/2 chain – which is much different from that predicted for classical spins

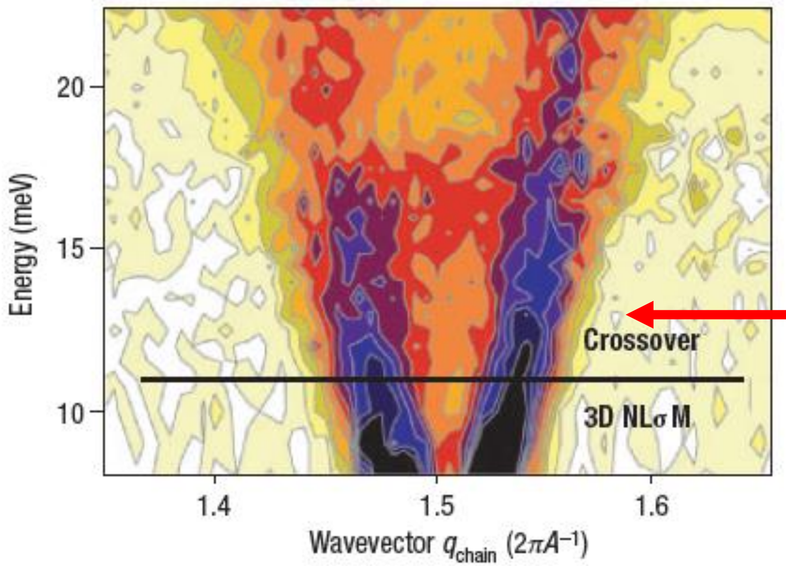




Energy dependence of the response below T_N

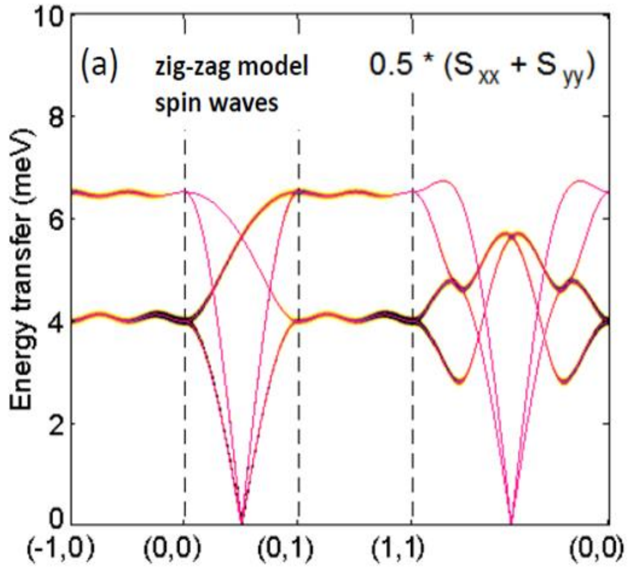


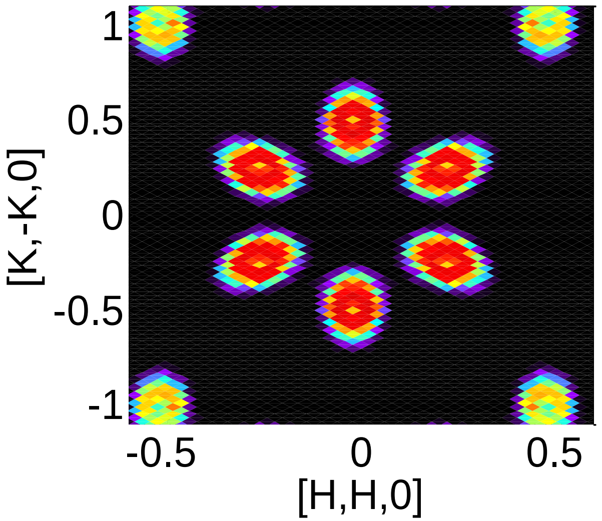
3 fold degenerate



2 fold degenerate

Expectations for spin waves in a zigzag state

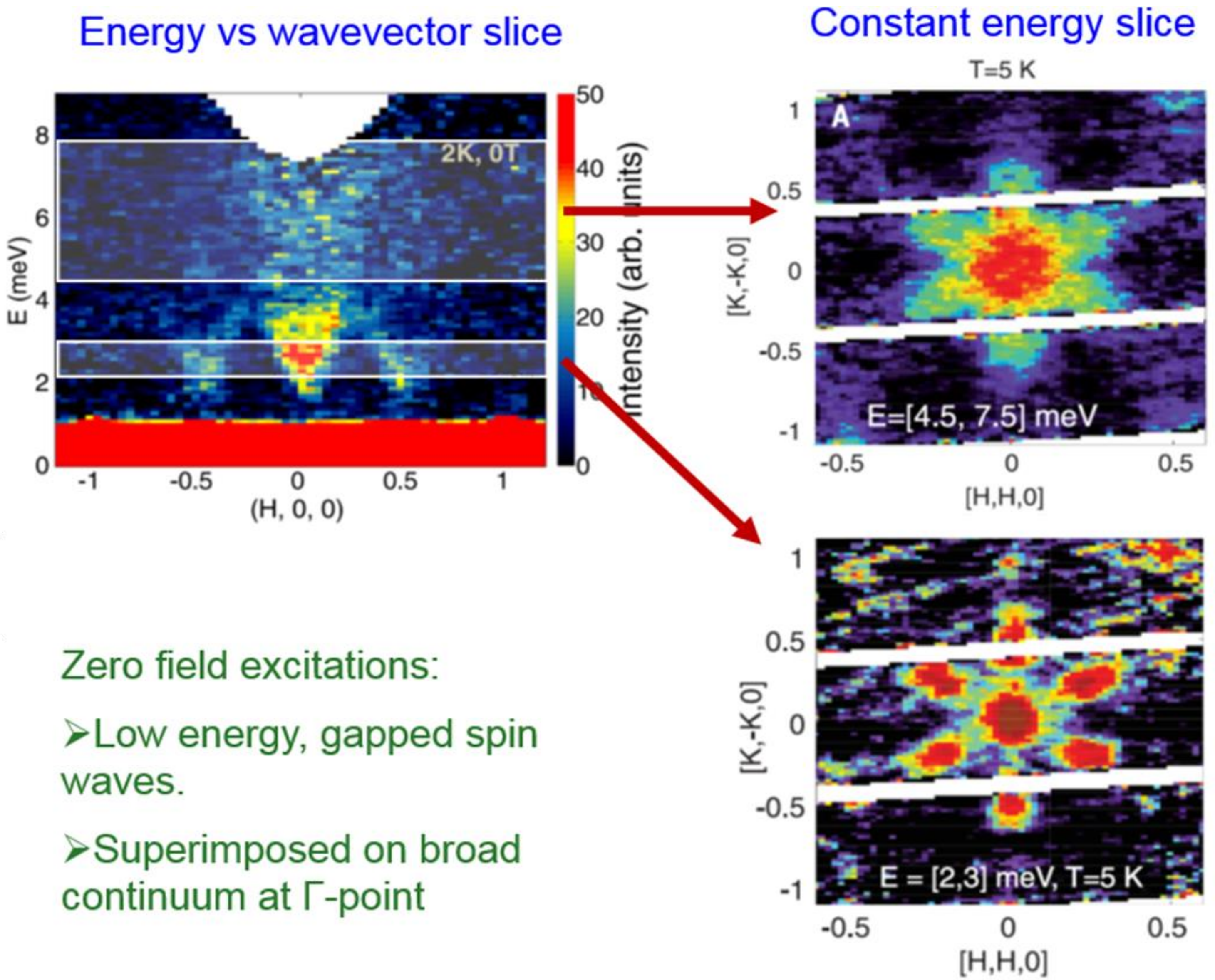




- Dispersion minima at ordering wavevectors (M points)
- Low energy constant E slices show cone shaped dispersion surfaces around the M points
- Less general, but true for Heisenberg-Kitaev model:

  Γ points show flat modes sharp in energy

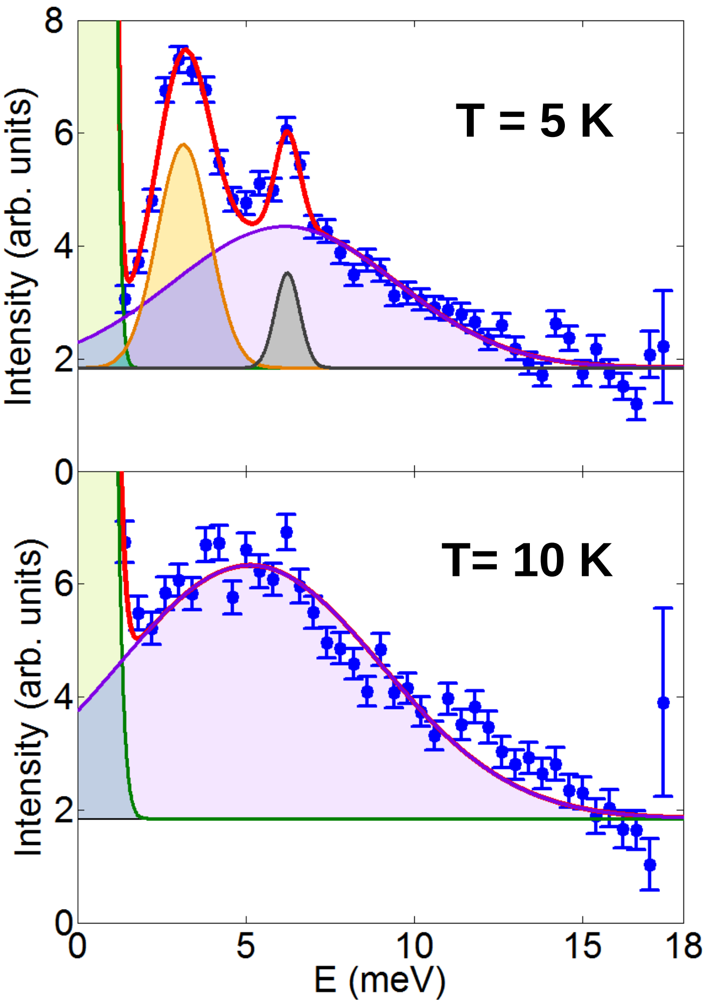
α-$RuCl_3$ single crystal - INS

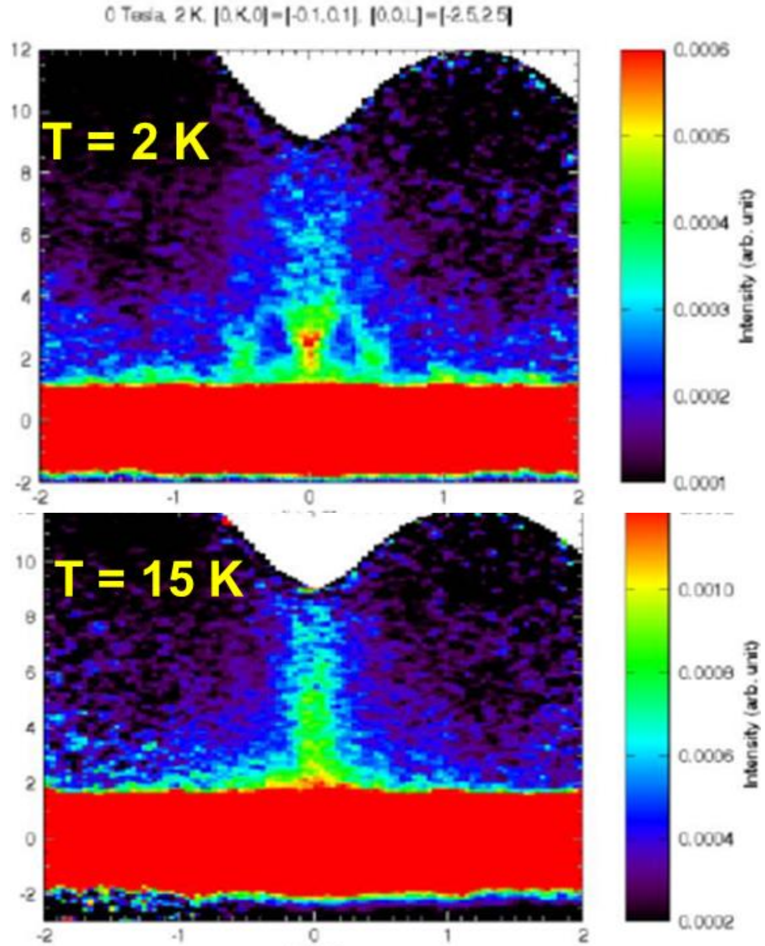


Zero field excitations:

- Low energy, gapped spin waves.
- Superimposed on broad continuum at Γ-point

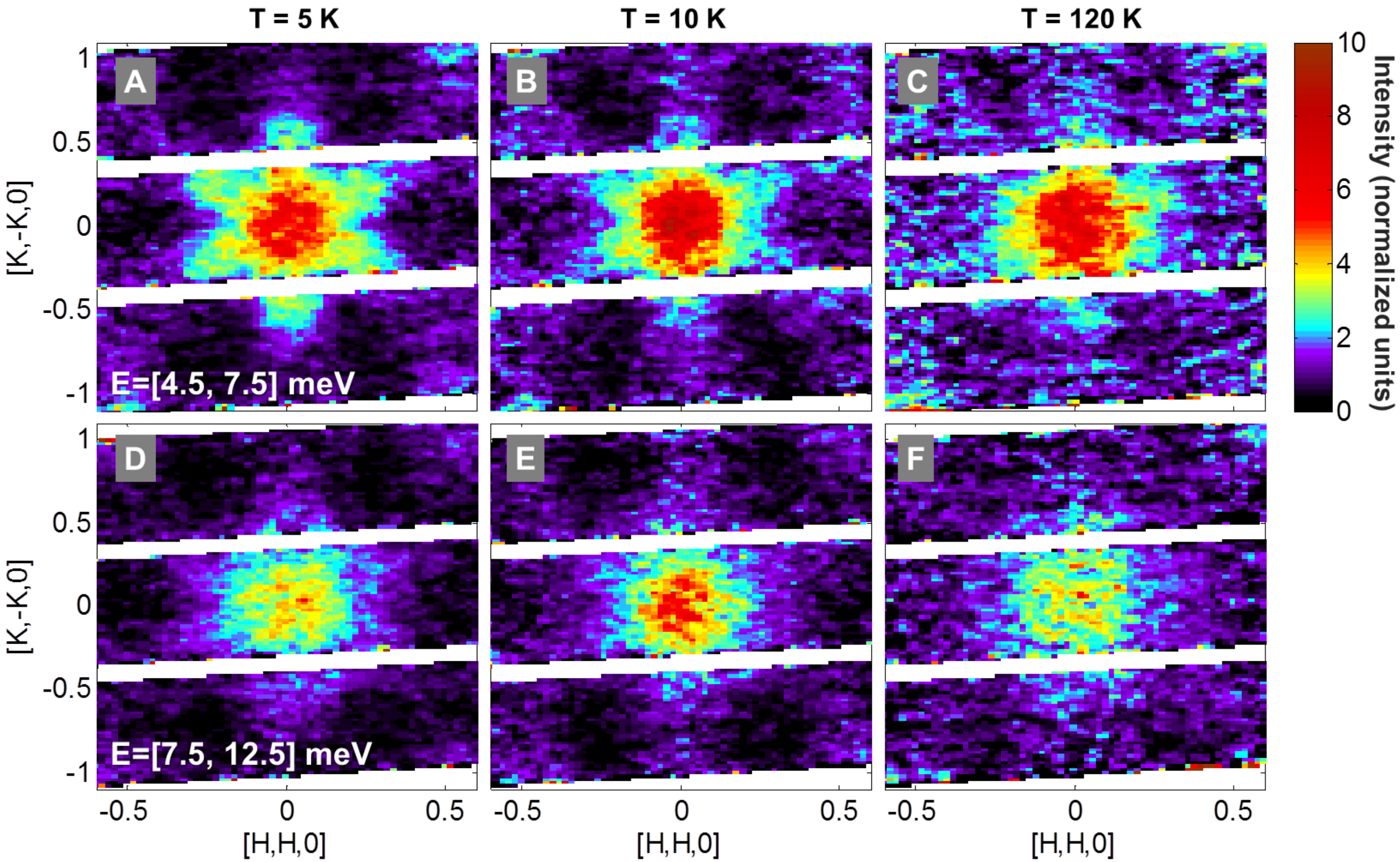
Experiment: Γ point signal inconsistent with SW





- At $T_N \approx 7$ K the spin waves disappear throughout the Brillouin zone
- Above T_N the continuum near the Γ point persists

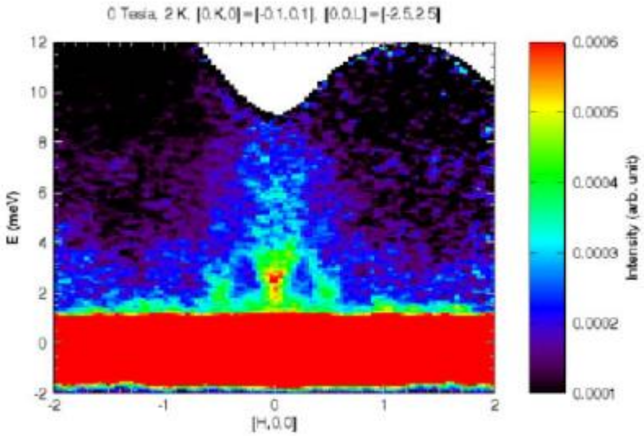
Q,T dependence of the continuum scattering



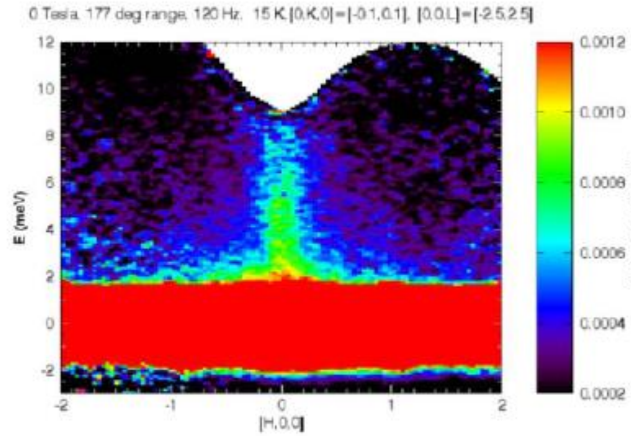
- circular column centered on H=K=0, extending to higher energies
- at low T, moderate energy SW peaks and column merge and scattering resembles a six pointed star
- scattering persists to high T

How does field affect the magnetic excitations?

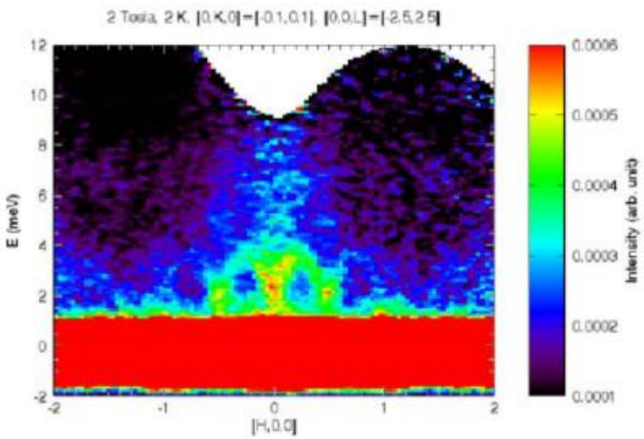
2K, 0T



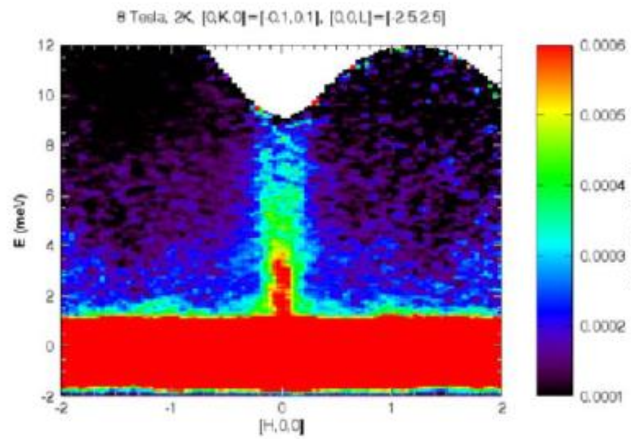
15K, 0T



2K, 2T



2K, 8T



Npj Quantum Materials **3**, 8 (2018).

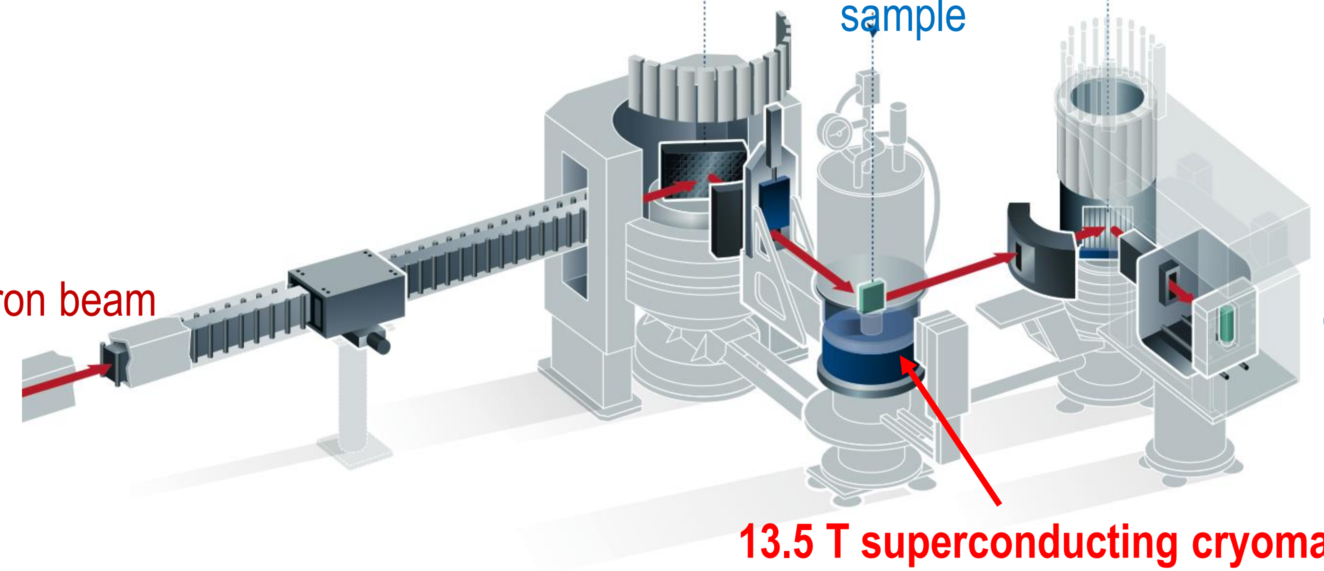
Outline

III. Recent results

- Higher fields and 3rd dimension
- Magnetocaloric effect and T- B phase diagram

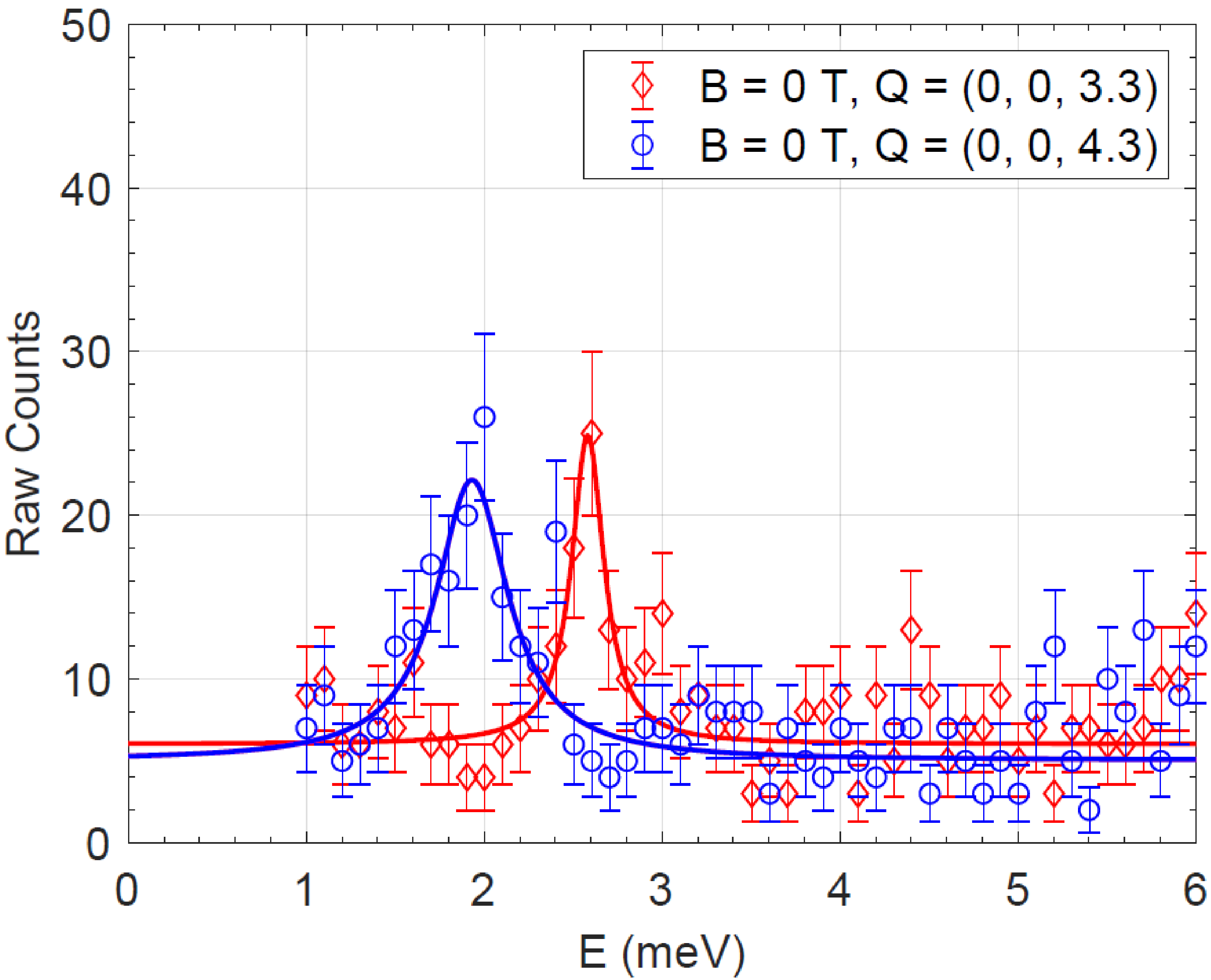
C. Balz et al., arXiv:1903.00056

FLEXX triple-axis-spectrometer

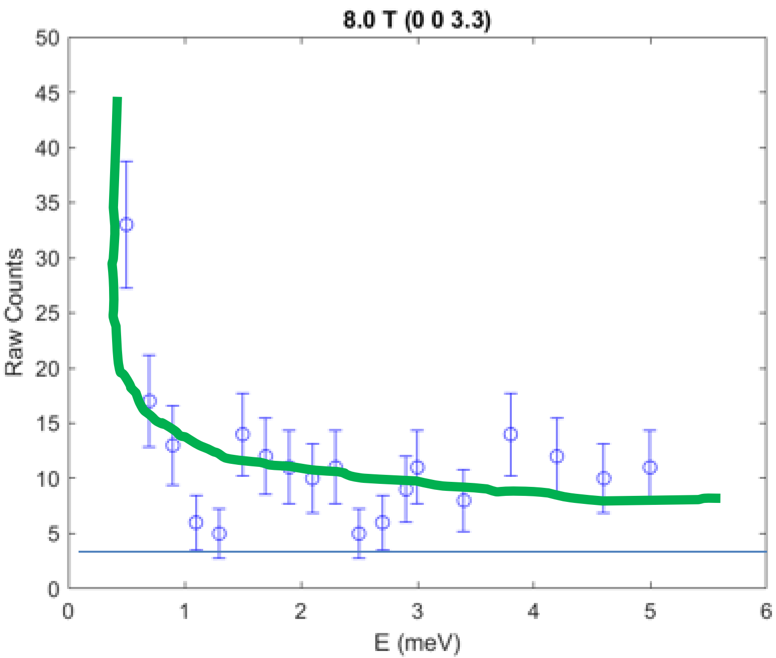


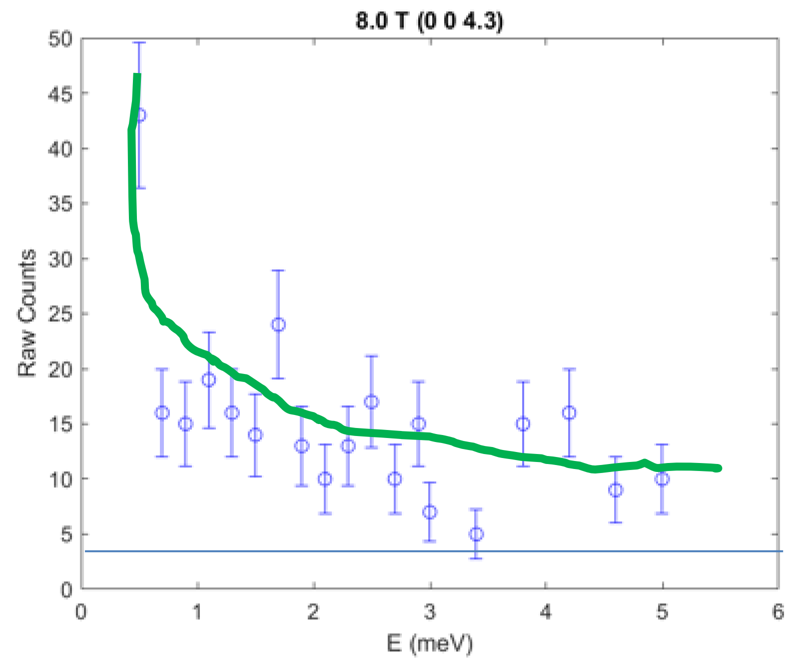
K. Habicht et al., EPJ Web of Conferences 83, 03007 (2015)

Constant Q scans, zero field

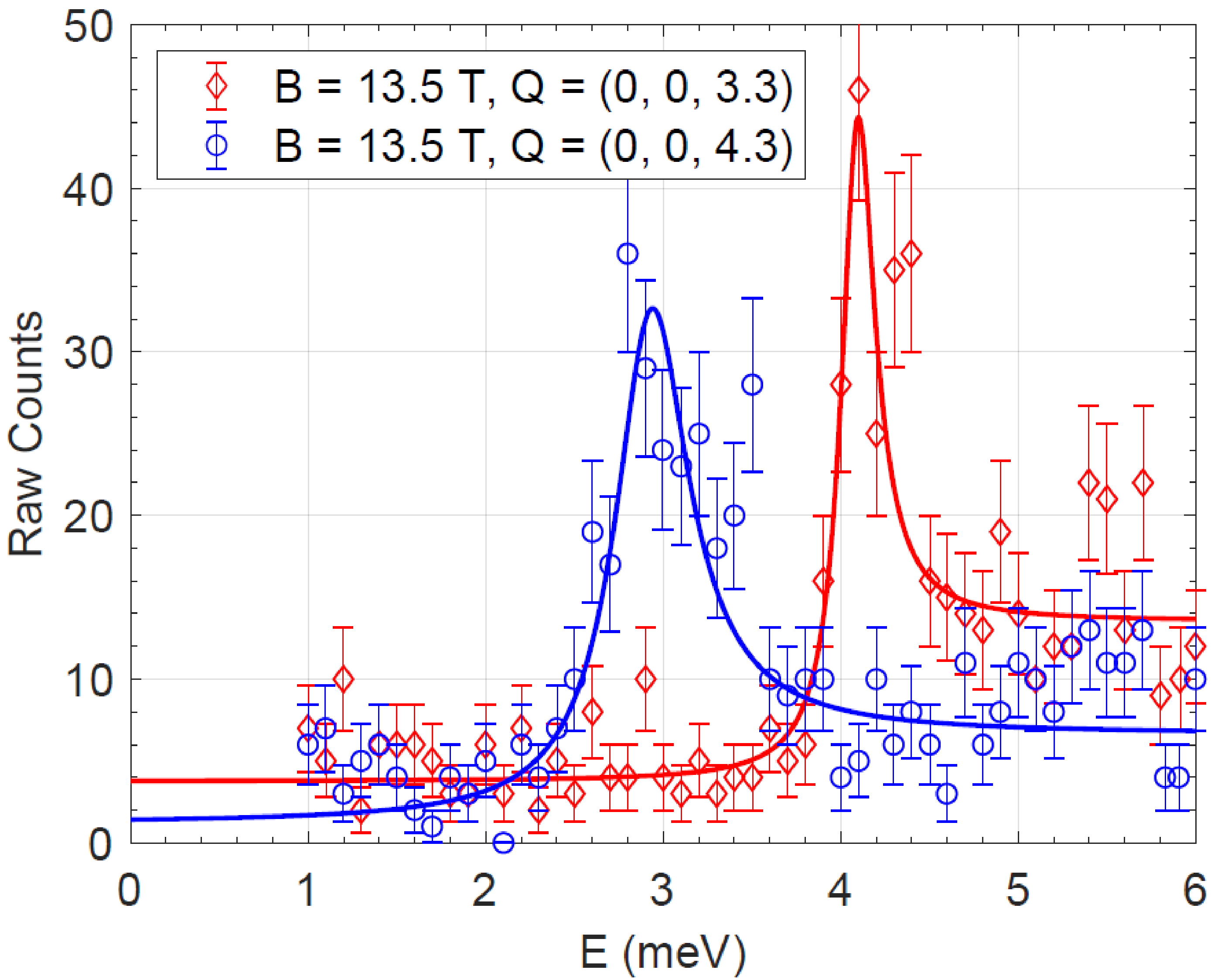


Constant Q scans, B > 7.3 T

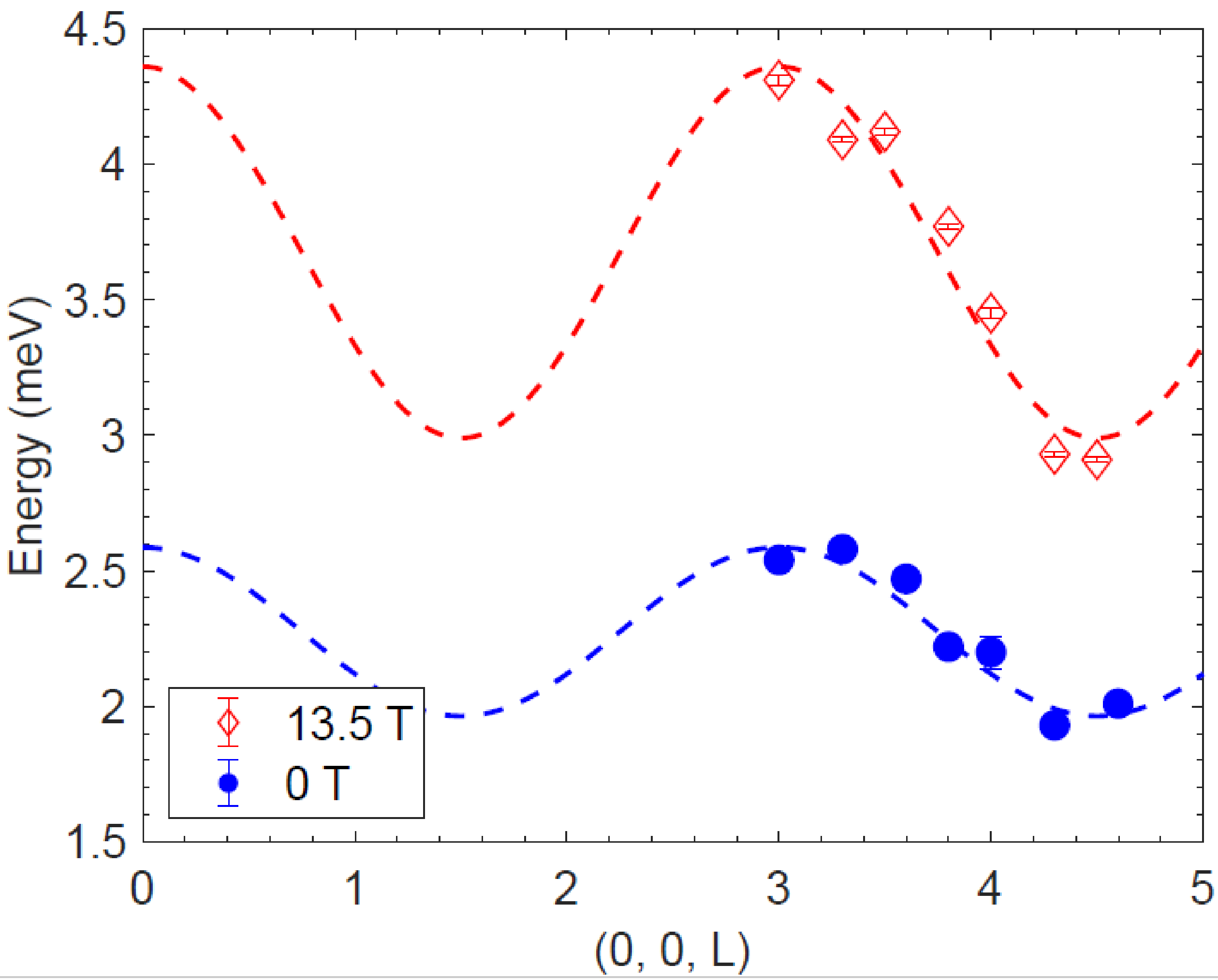




Constant Q scans, B > 9 T



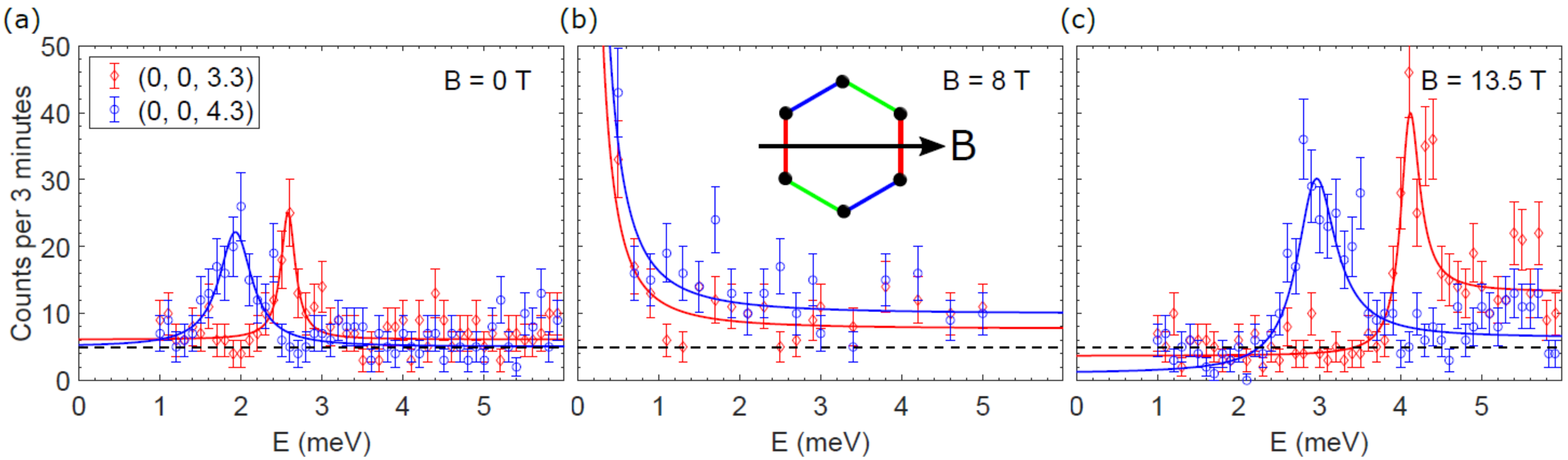
Dispersion along L



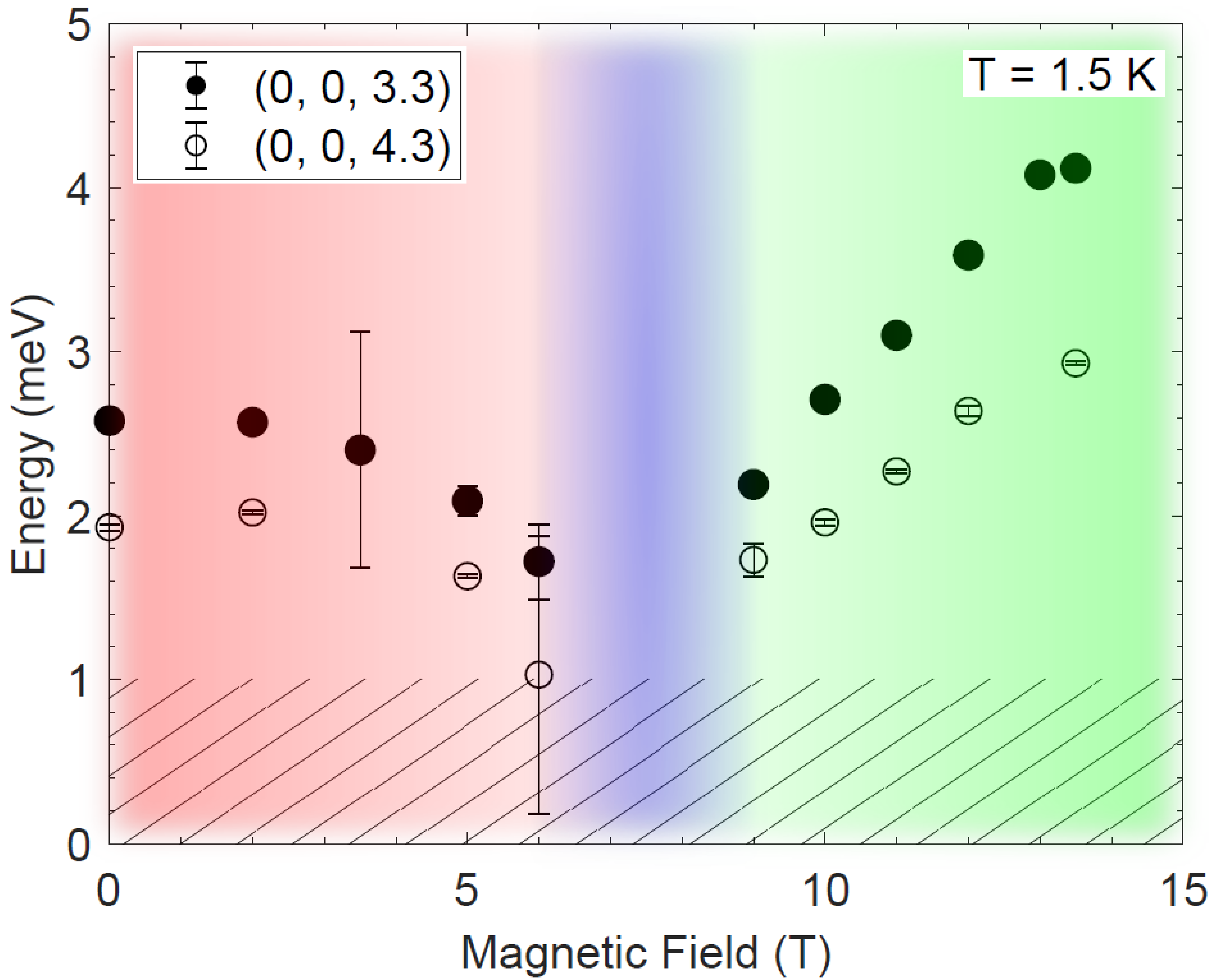
Takeaway:

L dependence consistent with antiferromagnetic interlayer interaction (unit cell has 3 layers)

Recall B dependence of line shape



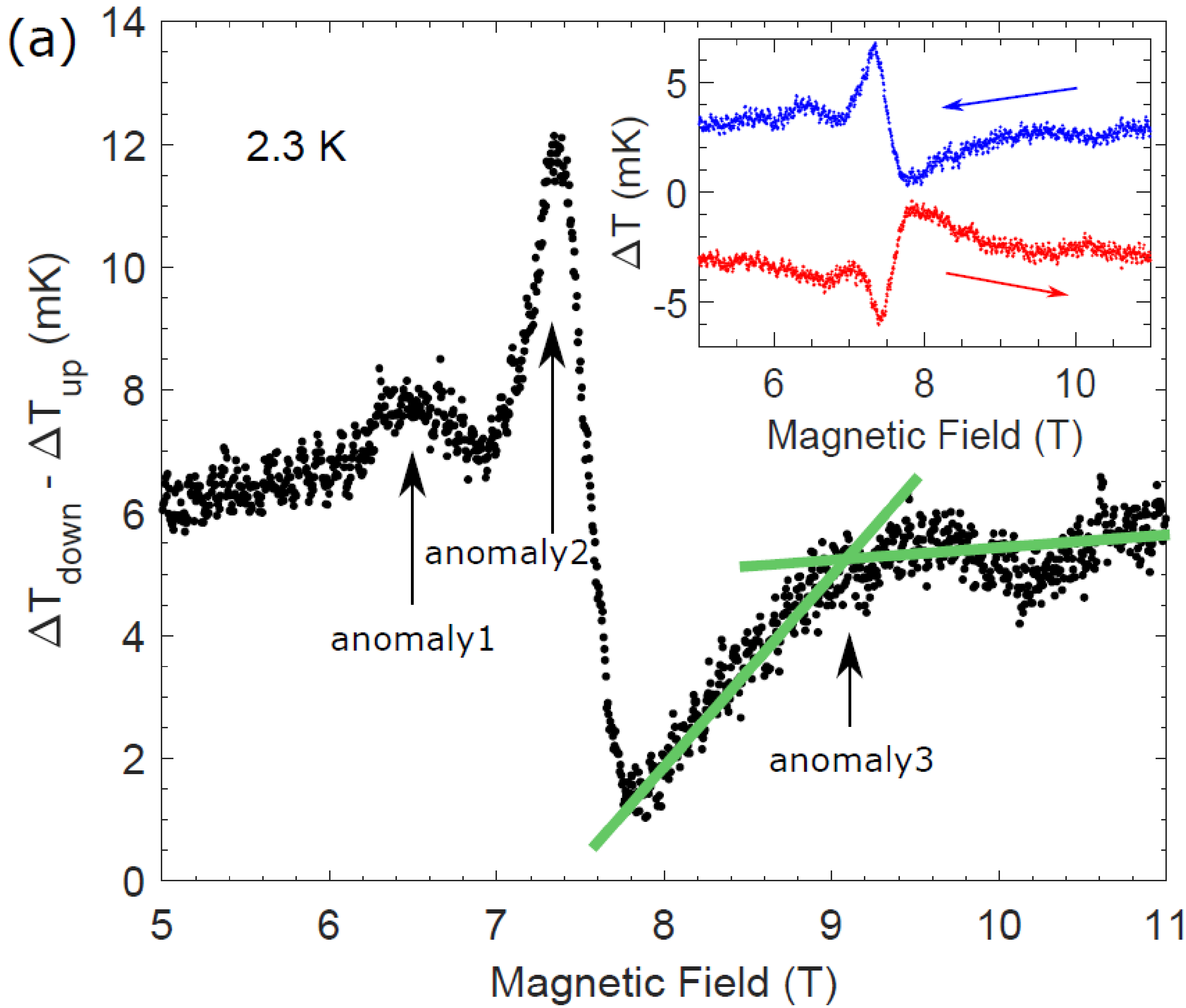
B dependence of Γ point gap from INS



C. Balz *et al.*,

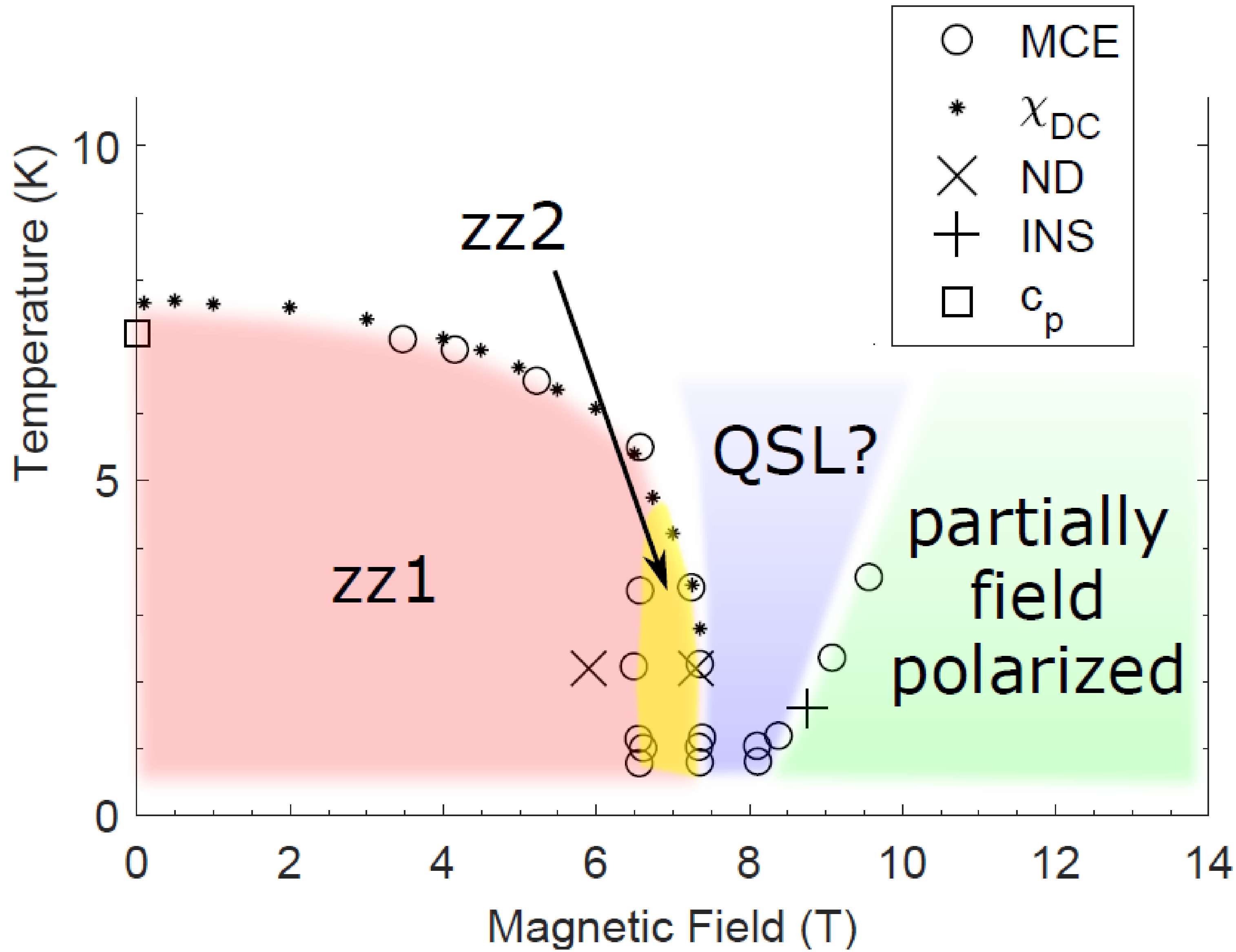
Magnetocaloric Effect

Y. Takano group

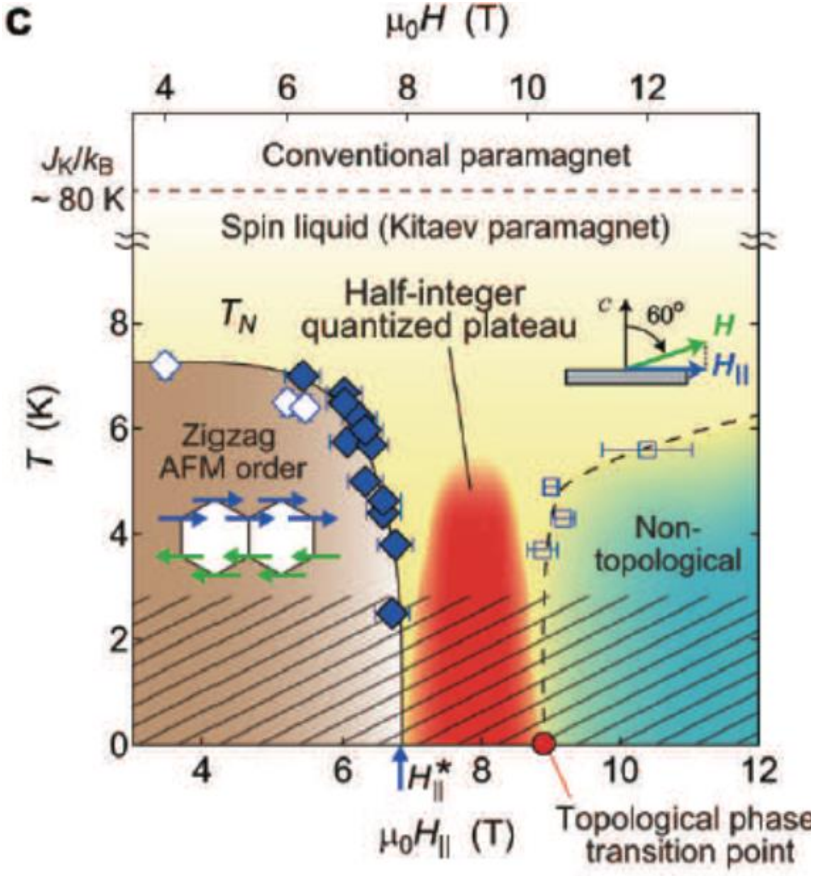


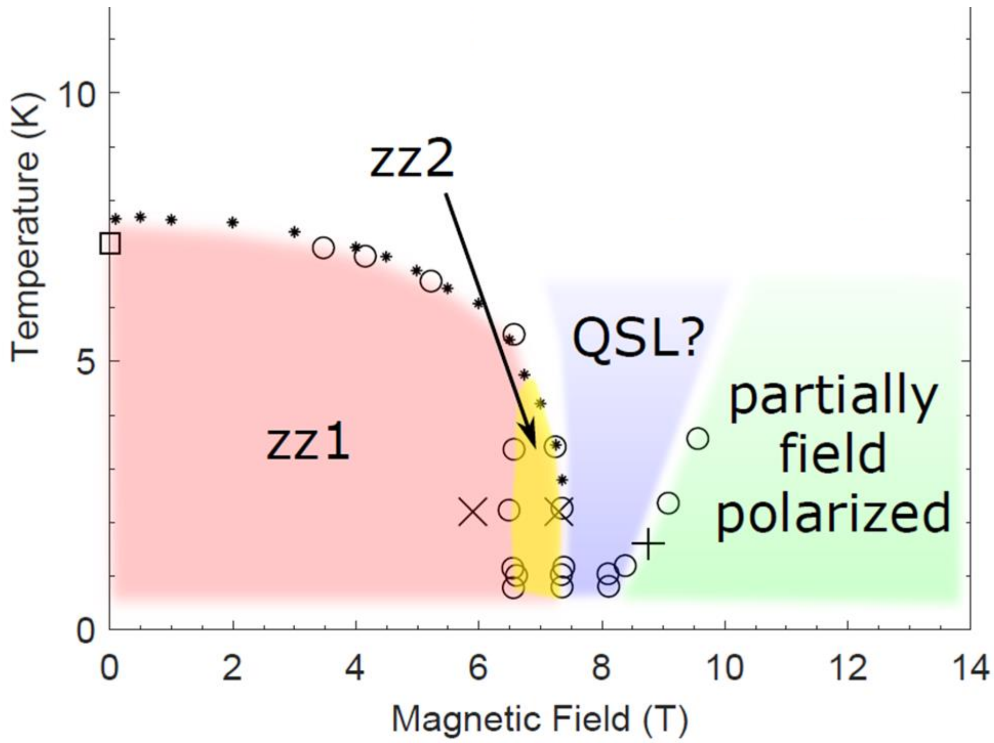
$$\Delta T \propto -T\left(\frac{\partial M}{\partial T}\right)_H \Delta H$$

More complete phase diagram



Comparison with Kasahara *et al.* phase diagram





Some conclusions

- Inelastic neutron scattering in α-$RuCl_3$ is consistent with fractional excitations
- An external magnetic field applied in-plane leads to a magnetically disordered state, with a higher field transition to a state that seems to be partially polarized and supports magnons
- The intermediate field state is consistent with a QSL

References on α-$RuCl_3$

Neutron scattering experiments:

- A. Banerjee *et al.* Nature Materials **15**, 733(2016).
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- A. Banerjee *et al.* SCIENCE **356**, 1055 (2017).
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Others:

- M. Ziatdinov *et al.* Nat. Comm. **7**, 13774 (2016).
- A. Samarakoon *et al.* PRB **96**, 134408 (2017).
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- A. N. Ponomaryov *et al*., PRB **96**, 241107(R), (2017).
- R. Hentrich *et al*., PRL **120**, 117204 (2018).