Possible Kitaev spin liquid physics and topological transitions in $\alpha$-RuCl$_3$
Outline

I. Kitaev’s model
   • Quick reminder of possible relevance to materials
   • Basics of $\alpha$-RuCl$_3$

II. Some inelastic neutron scattering
   • Magnons and fractional excitations in INS
   • Inelastic neutron scattering in $\alpha$-RuCl$_3$

III. Recent results
   • Higher fields and 3$^{rd}$ dimension
   • Magnetocaloric effect and T- B phase diagram
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arXiv:1903.00056

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I. Kitaev’s model
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Kitaev’s model on honeycomb lattice – a special QSL

Anyons in an exactly solved model and beyond

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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
  \[ \rightarrow \text{quantum spin liquid} \] ground state

Fig. 3. Three types of links in the honeycomb lattice.
Majorana: $a = a^\dagger \sim (f + f^\dagger)$
Kitaev interactions in materials

See also:

d⁵ in low spin octahedral configuration

strong spin-orbit coupling

edge-sharing octahedra

\[ J=3/2 \] (4)

\[ J=1/2 \] (2)

\[ \lambda_L \cdot S \]

strong field limit
\[ S=1/2, L_{\text{eff}}=1 \]
e.g. \((5d^5)\) Ir⁴⁺
\((4d^5)\) Ru⁴⁺
Zigzag Magnetic Order in the Iridium Oxide \( \text{Na}_2\text{IrO}_3 \)

Jiří Chatoupka,\textsuperscript{1,2} George Jackeli,\textsuperscript{1,*} and Giniyat Khaliullin\textsuperscript{1}

\[ \mathcal{H}_{ij}^{(\gamma)} = 2K S_i^\gamma S_j^\gamma + JS_i \cdot S_j. \]
Effect of additional interactions

Generic Spin Model for the Honeycomb Iridates beyond the Kitaev Limit

Jeffrey G. Ran, Eric Kin-Ho Lee, and Hae-Young Kee

\[ H = \sum_{\langle i,j \rangle} \left[ J \vec{S}_i \cdot \vec{S}_j + KS_i^\alpha S_j^\alpha + \Gamma(S_i^\beta S_j^\beta + S_i^\beta S_j^\alpha) \right], \]

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

Importance of anisotropic exchange interactions in honeycomb iridates: Minimal model for zigzag antiferromagnetic order in Na$_2$IrO$_3$

Yuriy Sireyk, Craig Price, Peter Wölfle, and Natalia B. Perkins

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

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. Kasahara¹, T. Ohnishi¹, N. Kurita², H. Tanaka², J. Nasu², Y. Motome³, T. Shibauchi⁴, and Y. Matsuda¹

$k^{2D}_{xy}$ reaches a quantum plateau as a function of applied magnetic field. That is, $k^{2D}_{xy}/T$ attains a quantization value of $(π/12)(k_B^2/\hbar)$, which is exactly half of $k^{2D}_{xy}/T$ 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

![Graph and diagram showing the relationship between $μ_0H_\parallel (T)$ and $κ^{2D}_{xy}$, with a focus on the quantization behavior at 3.7 K.](image)
II. Some inelastic neutron scattering

- Magnons and fractional excitations in INS
- Inelastic neutron scattering in $\alpha$-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 $T_N$
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:
  $\Gamma$ 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: $\Gamma$ 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 $\Gamma$ 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?

Npj Quantum Materials 3, 8 (2018).
III. Recent results

- Higher fields and 3\textsuperscript{rd} 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

\[ B = 0 \text{ T}, \quad Q = (0, 0, 3.3) \]

\[ B = 0 \text{ T}, \quad Q = (0, 0, 4.3) \]
Constant Q scans, $B > 7.3$ T
Constant Q scans, $B > 9\ T$

- $B = 13.5\ T$, $Q = (0, 0, 3.3)$
- $B = 13.5\ T$, $Q = (0, 0, 4.3)$

The graph shows the raw counts of energy (E) in meV for different magnetic fields and momentum transfer (Q) values.
Dispersion along L

Takeaway:
L dependence consistent with antiferromagnetic interlayer interaction (unit cell has 3 layers)
Recall B dependence of line shape

(a) $B = 0 \, T$

(b) $B = 8 \, T$

(c) $B = 13.5 \, T$
B dependence of $\Gamma$ point gap from INS

C. Balz et al.,

![Graph showing the dependence of the $\Gamma$ point gap on magnetic field](image-url)
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 $\alpha$-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 $\alpha$-RuCl$_3$

Neutron scattering experiments:
- C. Balz et al., arXiv:1903.00056

Others:
- A. N. Ponomaryov et al., PRB 96, 241107(R), (2017).