Topological Magnons in Kitaev Magnets at High Fields

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A revolution in condensed matter started in 1980...

The Integer Quantum Hall effect



K. v. Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980)

http://www.bourbaphy.fr/klitzing.pdf



GATEVOLTAGE

from Kubo formula to Chern number

the same form as Berry curvature (1984).

Can be recast into a topological invariant (Chern number):

Avron, Seiler, Simon (1983) Thouless, Kohmoto, Nightingale, den Nijs (1982)

$$\sigma_H \propto \int_{\mathrm{BZ}} \left(\partial_x \langle n(\mathbf{k}) | \partial_y | n(\mathbf{k}) \rangle - \partial_y \langle n(\mathbf{k}) | \partial_x | n(\mathbf{k}) \rangle \right)$$

n(**k**) is the wave function at momentum **k** in the Brillouin zone.

Topological invariants — geometry

Gauss-Bonnet formula for closed surfaces provides a link between local geometric properties (local curvature K) and global topological properties.

total curvature = Euler characteristic

$$\frac{1}{2\pi} \int_S K \mathrm{d}A = 2(1-g)$$

g is the number of handles (e.g. torus g=1, pretzel g=3)



Topological invariants — Quantum mechanics

$$F_n^{xy}(\mathbf{k}) = \langle \partial_x n(\mathbf{k}) | \partial_y n(\mathbf{k}) \rangle - \langle \partial_y n(\mathbf{k}) | \partial_x n(\mathbf{k}) \rangle$$

Berry curvature, *n*(**k**) is the nth wave function with momentum **k** in the 2D Brillouin zone.

$$C_n = \frac{1}{2\pi i} \int_{\mathrm{BZ}} dk_x dk_y F_n^{xy}$$

The Chern number is a topological invariant. It takes integer values only.

E.g. Integer Quantum Hall Effect and topology:

$$\sigma_{xy} = \frac{e^2}{h}C$$

Philosophy

Band structures may host nontrivial topological invariants with consequences for observable properties

noninteracting

- electrons
- magnons
- light in photonic crystals

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Magnon Chern Insulator

Magnets should have significant spin-orbit coupling and have more than one mode

Unidirectional magnon modes living at edge of 2D magnets protected by topological index

Bulk bands

Katsura, Nagaosa & Lee,. PRL **104**, 066403 (2010). Shindou, Matsumoto, Murakami, & Ohe, PRB **87**, 174427 (2013). Matsumoto, Murakami, PRL **106**, 197202 (2011).



In contrast to electronic cousins:

- Magnon edge states are gapped
- No quantized response except under exceptional circumstances
- Response thermally activated
 - Thermal magnon Hall response (Transverse thermal conductivity: Temperature gradient and magnetic field)
 - Spin Nernst effect (Transverse spin current: Temperature gradient in antiferromagnets

Observation of the Magnon Hall Effect

SCIENCE VOL 329 16 JULY 2010

Y. Onose,^{1,2}* T. Ideue,¹ H. Katsura,³ Y. Shiomi,^{1,4} N. Nagaosa,^{1,4} Y. Tokura^{1,2,4}



The crystal structure of $Lu_2V_2O_7$ and the magnon Hall effect. (A) The V sublattice of $Lu_2V_2O_7$, which is composed of corner-sharing tetrahedra. (B) The direction of the Dzyaloshinskii-Moriya vector on each bond of the tetrahedron. The Dzyaloshinskii-Moriya interaction acts between the *i* and *j* sites. (C) The magnon Hall effect. A wave packet of magnon (a quantum of spin precession) moving from the hot to the cold side is deflected by the Dzyaloshinskii-Moriya interaction playing the role of a vector potential.

$Lu_2V_2O_7$ is a FM insulator

Magnetic field variation of the thermal Hall conductivity of $Lu_2V_2O_7$ at various temperatures. The magnetic field is applied along the [100] direction. The solid lines are guides to the eye.



Thermal Hall conductivity in the frustrated pyrochlore magnet $Tb_2Ti_2O_7$

M. Hirschberger, J. W. Krizan, R. J. Cava, and N. P. Ong Science 348, (2015)

FIG. 3: Curves of the thermal Hall conductivity \varkappa_{xy}/T vs. H in Tb₂Ti₂O₇ (Sample 2). From 140 to 50 K, \varkappa_{XY}/T , is Hlinear (Panel A). Below 45 K, it develops pronounced curvature at large H, reaching its largest value near 12 K. The sign is always "hole-like". Panel B shows the curves below 15 K. A prominent feature is that the weak-field slope $[\varkappa_{xy}/TB]_0$ is nearly T independent below 15 K. Below 3 K, the field profile changes qualitatively, showing additional features that become prominent as $T \rightarrow 0$, namely the sharp peak near 1 T and the broad maximum at 6 T.



Thermal Hall Effect of Spin Excitations in a Kagome Magnet

Max Hirschberger, Robin Chisnell, Young S. Lee and N. P. Ong

PRL 115, 106603 (2015)



Emergence of nontrivial magnetic excitations in a spin liquid state of kagome volborthite

Daiki Watanabe, Kaori Sugii, Masaaki Shimozawa, Yoshitaka Suzuki, Takeshi Yajima, Hajime Ishikawa, Zenji Hiroi, Takasada Shibauchi, Yuji Matsuda, Minoru Yamashita

Proc. Natl. Acad. Sci. USA 113, 8653 (2016)



Kitaev Honeycomb Magnetism



Exactly solvable anisotropic exchange model

Ground state is quantum spin liquid with gapless Majorana modes and gapped fluxon excitations

Apply small field perpendicular to plane to enter into chiral spin liquid regime

Kitaev-Heisenberg Model



Condensed matter physicist: Is the Kitaev model physical?

(Chaloupka) + Jackeli + Khaliullin: Yes!

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i,j \rangle_{\gamma}} 2K \mathbf{S}_i^{\gamma} \mathbf{S}_j^{\gamma} - \mathbf{h} \cdot \sum_i \mathbf{S}_i$$

Honeycomb materials with edge sharing oxygen octahedra

- effective J=1/2 in strong spin-orbit coupled ions Ir⁴⁺
- spin orbit coupling gives mechanism for Kitaev exchange to arise
- isotropic exchange can be suppressed relative to Kitaev exchange: destructive interference from 90 degree Ir-O-Ir bonds
- Candidate materials: Na_2IrO_3 and α -RuCl₃

Materials

We need $J_{eff} = 1/2$ moments

 $\alpha - RuCl_3$ Na₂IrO₃

- Both exhibit zero field collinear zigzag magnetic order
- Kitaev exchange thought to play important role in these magnets
- Much still remains to be understood in these magnets
- In particular, nature of excitations above the zero field ordered state in RuCl3 and field evolution
- Long-range order drops away in high field tilted from [111]

Semiclassical Phase Diagram, h || [111]



Magnon condensation

Transition to fully polarized state for [111] field

Quantum effects...phase boundaries renormalized, QSL appear Janssen, Andrade, Vojta (2016/2017)

Semiclassical Phase Diagram, h || [111]



Janssen, Andrade, Vojta Phys. Rev. Lett. **117**, 277202 (2017)

Linear Spin Waves in Field-Polarized Phase

Janssen, Andrade, Vojta (2016/2017)

$$\boldsymbol{\Upsilon}_{\boldsymbol{k}} = (a_{\boldsymbol{k}}, b_{\boldsymbol{k}}, a_{-\boldsymbol{k}}^{\dagger}, b_{-\boldsymbol{k}}^{\dagger}) \ .$$

$$\mathcal{H}_{\rm LSW} = \frac{1}{2} \sum_{\boldsymbol{k} \in \rm BZ} \boldsymbol{\Upsilon}_{\boldsymbol{k}}^{\dagger} \cdot \boldsymbol{\mathsf{H}}_{\rm LSW}(\boldsymbol{k}) \cdot \boldsymbol{\Upsilon}_{\boldsymbol{k}}$$

$$\mathsf{H}_{\mathrm{LSW}}(\boldsymbol{k}) = \begin{pmatrix} \mathsf{A}(\boldsymbol{k}) & \mathsf{B}(\boldsymbol{k}) \\ \mathsf{B}^{\dagger}(\boldsymbol{k}) & \mathsf{A}^{T}(-\boldsymbol{k}) \end{pmatrix} \qquad \begin{aligned} \mathsf{A}(\boldsymbol{k}) = h \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + (3J + 2K)S \begin{pmatrix} -1 & \gamma_{0,\boldsymbol{k}}^{*} \\ \gamma_{0,\boldsymbol{k}} & -1 \end{pmatrix}, \\ \mathsf{B}(\boldsymbol{k}) = 2KS \begin{pmatrix} 0 & \gamma_{1,\boldsymbol{k}}^{*} \\ \gamma_{2,\boldsymbol{k}} & 0 \end{pmatrix}. \end{aligned}$$

Two magnon bands (two spins in the unit cell), the pairing terms B(*k*) opens a gap between the bands

$$\begin{split} \gamma_{0,\mathbf{k}} &= \frac{1}{3} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{x}}} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{y}}} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{z}}}), \\ \gamma_{1,\mathbf{k}} &= \frac{1}{3} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{x}} - (2\pi\mathbf{i}/3)} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{y}} + (2\pi\mathbf{i}/3)} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{z}}}), \\ \gamma_{2,\mathbf{k}} &= \frac{1}{3} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{x}} + (2\pi\mathbf{i}/3)} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{y}} - (2\pi\mathbf{i}/3)} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}_{\mathbf{z}}}), \\ \delta_{x} &= (0,1), \delta_{y} = \left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right), \delta_{z} = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \end{split}$$

Linear spin wave dispersions



Kitaev Points and Topological Magnons

Focus on antiferromagnetic Kitaev point

Threshold field h=4

Flat band condensation, localized modes -> degenerate classical manifold



Magnon bands have Chern number +1 and -1

Topology across Kitaev-Heisenberg



Mapping from $\vartheta \rightarrow \vartheta + \pi$ leaves the spin wave spectrum invariant as measured from threshold field

Except for isolated points, whole of polarized phase has topological bands

Comparing linear spin wave and ED



Comparing magnetization and excitations in ED



Strong quantum fluctuations in the collinear, polarized state

Comparing linear spin wave and ED



Canonical transformation

$$\mathsf{H}_{\mathrm{LSW}}(\boldsymbol{k}) = \begin{pmatrix} \mathsf{A}(\boldsymbol{k}) & \mathsf{B}(\boldsymbol{k}) \\ \mathsf{B}^{\dagger}(\boldsymbol{k}) & \mathsf{A}^{T}(-\boldsymbol{k}) \end{pmatrix} \qquad \qquad \mathsf{A}(\boldsymbol{k}) = h \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + (3J + 2K)S \begin{pmatrix} -1 & \gamma_{0,\boldsymbol{k}}^{*} \\ \gamma_{0,\boldsymbol{k}} & -1 \end{pmatrix},$$
$$\qquad \qquad \mathsf{B}(\boldsymbol{k}) = 2KS \begin{pmatrix} 0 & \gamma_{1,\boldsymbol{k}}^{*} \\ \gamma_{2,\boldsymbol{k}} & 0 \end{pmatrix}.$$

effective model in 1/h to reduce the anomalous term

$$\begin{aligned} \mathcal{H}_{\mathrm{eff}} &= e^{\mathcal{W}} \mathcal{H} e^{-\mathcal{W}} = \mathcal{H} + [\mathcal{W}, \mathcal{H}] + \frac{1}{2} [\mathcal{W}, [\mathcal{W}, \mathcal{H}]] + \cdots \\ \mathcal{W} &= \frac{KS}{h} \sum_{\mathbf{k} \in \mathrm{BZ}} \left(\gamma_{1,\mathbf{k}}^* a_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger} - \gamma_{1,\mathbf{k}} a_{\mathbf{k}} b_{-\mathbf{k}} \right), \\ \mathrm{effective mag}_{\mathrm{model with neal}} \\ \mathrm{A}_{\mathrm{eff}}(\mathbf{k}) &= \mathrm{A}(\mathbf{k}) - \frac{2K^2S^2}{h} \left(\begin{array}{c} \gamma_{1,\mathbf{k}}^* \gamma_{1,\mathbf{k}} & 0 \\ 0 & \gamma_{2,\mathbf{k}}^* \gamma_{2,\mathbf{k}} \end{array} \right), \\ \mathrm{B}_{\mathrm{eff}}(\mathbf{k}) &= -\frac{K(3J+2K)S^2}{h} \left(\begin{array}{c} \gamma_{0,\mathbf{k}} \gamma_{1,\mathbf{k}}^* + \gamma_{0,\mathbf{k}}^* \gamma_{2,\mathbf{k}} & -2\gamma_{1,\mathbf{k}}^* \\ -2\gamma_{2,\mathbf{k}} & \gamma_{0,\mathbf{k}} \gamma_{1,\mathbf{k}}^* + \gamma_{0,\mathbf{k}}^* \gamma_{2,\mathbf{k}} \end{array} \right), \end{aligned}$$

effective magnon hopping odel with nearest neighbor nd complex next-neighbor hopping (DM interaction)

Canonical transformation

High field effective Hamiltonian is the famous Haldane model



Chern number

For large fields, we can neglect the anomalous part B_{eff}, and work only with A_{eff} normal part describing the hopping of the magnon:

$$A_{eff}(k) = A(k) - \frac{2K^2S^2}{h} \begin{pmatrix} \gamma_{1,k}^*\gamma_{1,k} & 0\\ \gamma_{2,k}^*\gamma_{2,k} \end{pmatrix}$$

$$= d_0(k) + \frac{1}{2}d(k) \cdot \vec{\sigma}$$

$$M(k) = \begin{pmatrix} (3J+2K)S(\gamma_{0,k}^*+\gamma_{0,k})\\ i(3J+2K)S(\gamma_{0,k}^*-\gamma_{0,k})\\ -\frac{2K^2S^2}{h} \begin{pmatrix} \gamma_{1,k}^*\gamma_{1,k} - \gamma_{2,k}^*\gamma_{2,k} \end{pmatrix} \end{pmatrix}.$$

Finite Chern number if the surface of the d(k) vector has a finite volume around the origin (skyrmion).
When K = 0 or 3 J + K = 0 the Chern number is 0.
$$K = 0 \text{ or } 3 \text{ J + } K = 0 \text{ the Chern number is } 0.$$

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Chern number and skyrmions : arbitrary spin

Berry curvature

$$F_{n}^{xy}(\mathbf{k}) = \partial_{x} \langle n(\mathbf{k}) | \partial_{y} | n(\mathbf{k}) \rangle - \partial_{y} \langle n(\mathbf{k}) | \partial_{x} | n(\mathbf{k}) \rangle}{= 2i \sum_{m \neq n} \operatorname{Im} \frac{\langle n | (\partial_{x}H) | m \rangle \langle m | (\partial_{y}H) | n \rangle}{(E_{n} - E_{m})^{2}}.$$
Hamiltonian (Zeeman levels)

$$H(\mathbf{k}) = J\mathbf{1} - \mathbf{d}(\mathbf{k}) \cdot \mathbf{Q}$$

$$H(\mathbf{k}) | n \rangle = [J - nd(\mathbf{k})] | n \rangle$$

$$[Q^{\alpha}, Q^{\beta}] = i\varepsilon_{\alpha\beta\gamma}Q^{\gamma} \operatorname{SU}(2) \operatorname{algebra}$$

$$F_{n}^{xy}(\mathbf{k}) = 2i \sum_{\alpha,\beta} \frac{\partial_{x}d^{\alpha}(\mathbf{k})\partial_{y}d^{\beta}(\mathbf{k})}{d^{2}(\mathbf{k})} \sum_{m \neq n} \operatorname{Im} \frac{\langle n | Q^{\alpha} | m \rangle \langle m | Q^{\beta} | n \rangle}{(n - m)^{2}}$$

$$= 2i \sum_{\alpha,\beta} \frac{\partial_{x}d^{\alpha}(\mathbf{k})\partial_{y}d^{\beta}(\mathbf{k})}{d^{2}(\mathbf{k})} \operatorname{Im} (\langle n | Q^{\alpha} | n + 1 \rangle \langle n + 1 | Q^{\beta} | n \rangle + \langle n | Q^{\alpha} | n - 1 \rangle \langle n - 1 | Q^{\beta} | n \rangle)$$

$$\vdots \qquad \text{the Berry curvature is proportional to}$$

$$= in\hat{\mathbf{d}}(\mathbf{k}) \cdot (\partial_{y}\hat{\mathbf{d}}(\mathbf{k}) \times \partial_{x}\hat{\mathbf{d}}(\mathbf{k})$$

$$C_{n} = \frac{1}{2\pi i} \int dk_{x}dk_{y}F_{n}^{xy} = -2nN_{s}$$
The Chern number of the *n*-th band is 2n times the number of

skyrmions -> 2n edge states

Kitaev—Heisenberg— Γ — Γ' model



Symmetry of Kitaev materials allows two further nearest neighbor exchange couplings

 $\mathcal{H}_x = 2K\mathsf{S}_1^x\mathsf{S}_2^x + J\mathsf{S}_1\cdot\mathsf{S}_2 + \Gamma\left(\mathsf{S}_1^z\mathsf{S}_2^y + \mathsf{S}_1^y\mathsf{S}_2^z\right)$ $+ \Gamma'\left(\mathsf{S}_1^x\mathsf{S}_2^y + \mathsf{S}_1^x\mathsf{S}_2^z + \mathsf{S}_1^y\mathsf{S}_2^x + \mathsf{S}_1^z\mathsf{S}_2^x\right)$

In fully polarized phase, can map any point in full phase diagram into Kitaev-Heisenberg model at some field

$$K \to K + \Gamma - \Gamma' ,$$

$$J \to J - \Gamma ,$$

$$h \to h - 3\Gamma S - 6\Gamma' S$$

So whole paramagnetic region is topological except for isolated surfaces

Can topological magnons exist in materials?

Magnon-Magnon Interactions

Magnon-magnon interactions from Holstein-Primakoff beyond 1/S

$$\mathcal{H}_{3} = \frac{1}{2} \sum_{\boldsymbol{k}_{\mu}} V_{3}(\boldsymbol{k}_{1}, \boldsymbol{k}_{2}, \boldsymbol{k}_{3}) (a_{\boldsymbol{k}_{1}}^{\dagger} a_{\boldsymbol{k}_{2}}^{\dagger} a_{\boldsymbol{k}_{3}} + \text{h.c.}) + \dots$$

Generally number non-conserving terms

Single particle picture may not survive in any detail



Four-magnon terms to same order.

The Death of Topological Magnons?

Kagome ferromagnet with Dzyaloshinskii-Moriya exchange



Topological Magnons Live?



Methods I: Perturbation Theory

Compute Green's function

$$\vec{\mathsf{G}}(\vec{k},\omega) = \left[(\omega + i0^+)\vec{\eta} - \vec{\mathsf{M}}(\vec{k}) - \vec{\Sigma}_{\vec{\mathsf{M}}}(\vec{k},\omega) \right]^{-1},$$

formally to one order beyond linear spin wave theory



Self-consistent approach

Renormalize $\vec{M}(\vec{k})$ by including static parts of Hartree-Fock self-energy

Use this to evaluate self-energy in omega.

Get the various components of dynamical structure factor

$$S(\boldsymbol{k},\omega) \equiv \sum_{\alpha} \sum_{a,b} \langle \mathsf{S}^{\alpha}_{a}(-\boldsymbol{k},-\omega) \mathsf{S}^{\alpha}_{b}(\boldsymbol{k},\omega) \rangle$$
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Methods II: DMRG + tMPO

- DMRG on long cylinder with periodic boundary conditions and few unit cells around
- Time evolution on matrix product state after flipping spin to get dynamical structure factor
- This work is first benchmark of technique with perturbation theory



Bulk Spin Waves



Bulk Spin Waves: AFM Kitaev



Bulk Spin Waves: Ferromagnetic Kitaev



Bulk Spin Waves: AFM vs FM Kitaev



Slab Geometry and High Fields

Does the chiral edge state survive?

h=3

AFM Kitaev



Slab Geometry to Lower Fields



AFM Kitaev h=4

AFM Kitaev h=2 (threshold field for LSW)

Slab Geometry to Lower Fields



FM Kitaev h=2

Thermal Hall Conductivity

Chern bands in electrons \longrightarrow quantum Hall effect transverse heat current $\kappa^{xy} = \frac{1}{\beta} \sum_{n} \int_{BZ} d^2 \mathbf{k} \ c_2(\rho_n) \frac{F_n^{xy}(\mathbf{k})}{i}$ $\rho_n = \frac{1}{e^{\omega_n \beta} - 1}$ $c_2(\rho) = \int_0^{\rho} dt \ \ln^2(1 + t^{-1})$

> thermal Hall effect in bosons: linear response (Kubo formula) formalism Katsura et al., PRL **104**, 066403 (2010), Matsumoto et al PRL **106** 197202, (2011)

Thermal Hall Effect in the Kitaev model



FM Kitaev point (S=1/2), K=-1

h=0.01,0.02,0.05,0.1,0.2, 0.5,1,2,3,4 to be read in the arrow direction.

Unusual thermal Hall effect in a Kitaev spin liquid candidate a-RuCl3

Y. Kasahara, K. Sugii, T. Ohnishi, M. Shimozawa, M. Yamashita, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda

arXiv:1709.10286



Large Thermal Hall Effect in α-RuCl3: Evidence for Heat Transport by Kitaev-Heisenberg Paramagnons

R. Hentrich, M. Roslova, A. Isaeva, T. Doert, W. Brenig, B. Büchner, C. Hess

arXiv:1803.08162







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

Y. Kasahara, T. Ohnishi, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda

arXiv:1805.05022



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

Y. Kasahara et al., arXiv:1805.05022

 $\kappa_{xy}^{2D}/T = q(\pi/6)(k_B^2/\hbar).$

also expected in time-reversal-symmetrybroken topological superconductors

FIG. 3. Half-integer thermal Hall conductance plateau. a-d, Thermal Hall conductivity κ_{xy}/T in tilted

Topological Magnons: an Outlook

- Range of topological band structures possible in magnon systems
- Chern numbers can arise in spin-orbit coupled systems with symmetric or antisymmetric exchange
- Interactions potentially important but magnetic field tuning offers way to render them negligible in certain systems
- Thermal Hall effect is first set of experiments to explore

Thank you for your attention