Some thoughts about Kitaev materials

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Outline

- 1. A couple random motivations
- 2. Candidate spin liquids in Kitaev materials w/o fields
- 3. Thoughts about thermal Hall transports in fields

I am not intending to explain any specific experiments but provide a different way of thinking.

Iridates (in time order of modern times)

Na₄Ir₃O₈: hyperkagome quantum spin liquid

Na₂IrO₃: alpha-Li₂IrO₃, beta-Li₂IrO₃ "Kitaev materials"

R₂Ir₂O₇: topological insulator, Weyl semimetal, ABL semimetal

A₂IrO₄: candidate for high-Tc superconductor, isostructure with A₂CuO₄

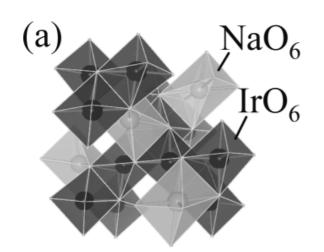
Sr₃Ir₂O₇: metamagnetic transition, isostructure with Sr₃Ru₂O₇

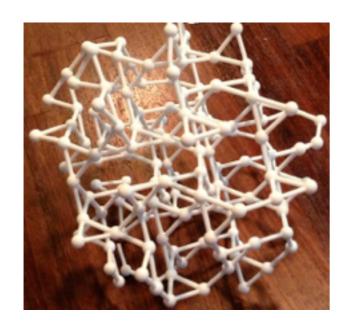
IrO2: pyrochlore lattice spin liquid

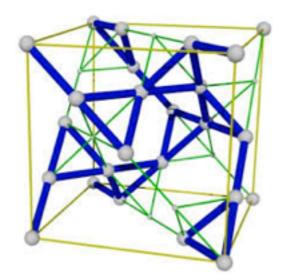
AlrO3 perovskite heterostructure: topological crystalline metal

HLi3Ir2O6, fcc iridates, etc

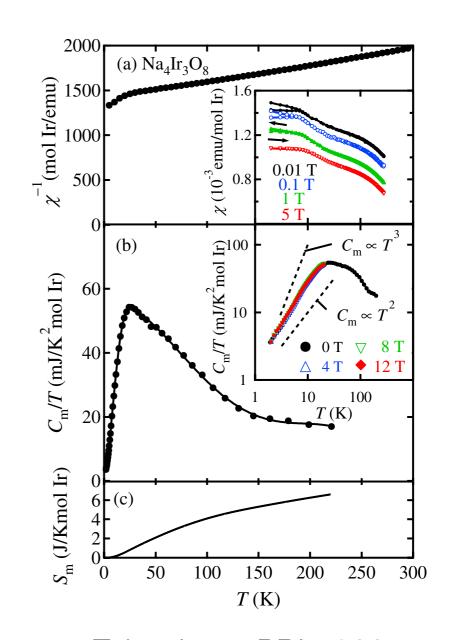
Na₄Ir₃O₈: hyperkagome quantum spin liquid?







hyperkagome

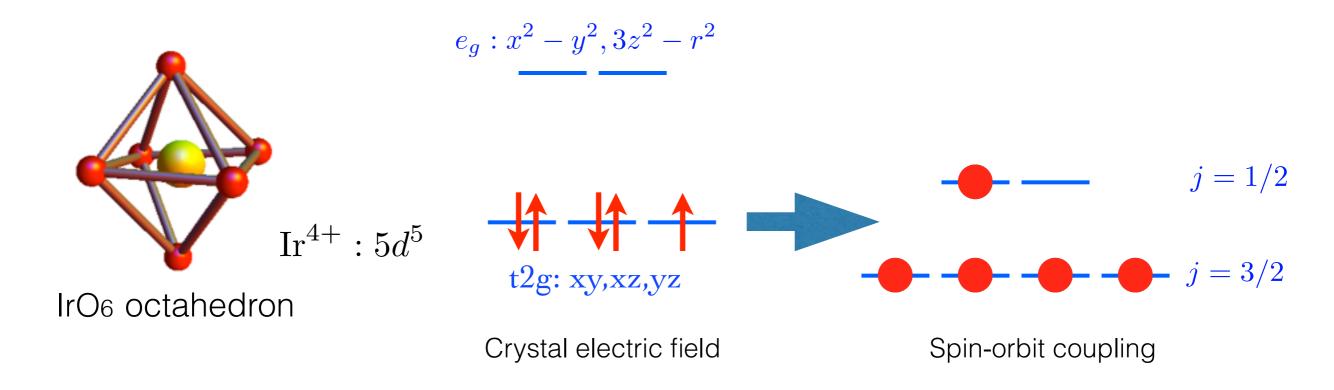


Takagi, etc, PRL, 2007

 $\chi \sim {\rm constant}, \quad C_v/T \sim {\rm constant}$

Why Ir ion behaves as a spin-1/2?

t2g orbitals in octahedral crystal field



$$\langle \{t_{2g}\}|\mathbf{L}|\{t_{2g}\}\rangle = -\mathbf{l}, \quad H_{soc} = -\lambda \mathbf{l} \cdot \mathbf{S}, \quad \mathbf{j} = \mathbf{l} + \mathbf{S}$$

It is interesting to look at how the magnetic moment M = L+2S = -I+2S varies.

BTW, SOC is quenched for eg orbitals.

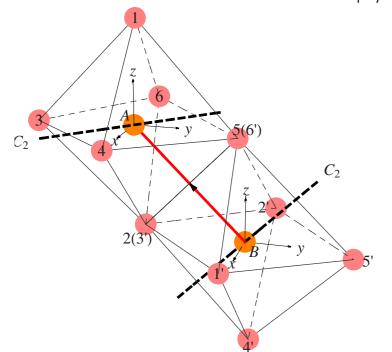
Gang Chen, Balents PRB 2008, B.J. Kim etc, Science 2008, G. Jackeli, Khaliullin PRL 2009

Exchange interaction: direct + indirect via oxygen

Spin-orbit entangled j=1/2 doublet

$$|a\rangle = \frac{1}{\sqrt{3}}(|d_{xy,\uparrow}\rangle + |d_{yz,\downarrow}\rangle + i|d_{zx,\downarrow}\rangle),$$

$$|b\rangle = \frac{1}{\sqrt{3}}(|d_{xy,\downarrow}\rangle - |d_{yz,\uparrow}\rangle + i|d_{zx,\uparrow}\rangle),$$



Surprisingly, direct hopping gives us a Heisenberg model! This is very special especially since orbitals have orientations.

Indirect exchange via oxygen gives highly anisotropic coupling

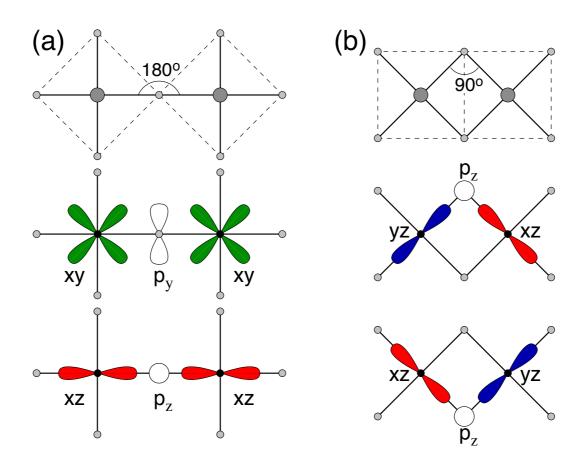
two neighboring IrO6 octahedra: they share 2 oxygens.

$$\mathcal{H}_{AB} = -JS_A^x S_B^x + JS_A^y S_B^y + JS_A^z S_B^z$$

$$= -2JS_A^x S_B^x + J\mathbf{S}_A \cdot \mathbf{S}_B \qquad \text{type-x bond}$$

G Chen, Balents PRB 2008

Honeycomb iridate: Kitaev interaction



$$\mathcal{H}_{ij}^{(\gamma)} = -JS_i^{\gamma}S_j^{\gamma}$$

Kitaev term for gamma bond after including Hund's coupling

G. Jackeli, G Khaliullin PRL 2009 ignited the field of Kitaev materials.

Most Kitaev materials are ordered

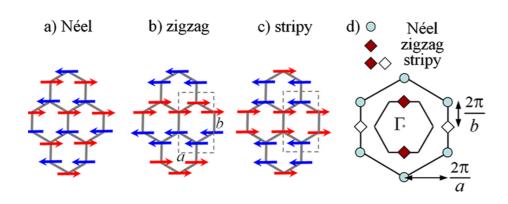
PRL **108,** 127204 (2012)

PHYSICAL REVIEW LETTERS

week ending 23 MARCH 2012

Spin Waves and Revised Crystal Structure of Honeycomb Iridate Na₂IrO₃

S. K. Choi, R. Coldea, A. N. Kolmogorov, T. Lancaster, I. I. I. Mazin, S. J. Blundell, P. G. Radaelli, Yogesh Singh, P. Gegenwart, K. R. Choi, S.-W. Cheong, P. J. Baker, C. Stock, and J. Taylor



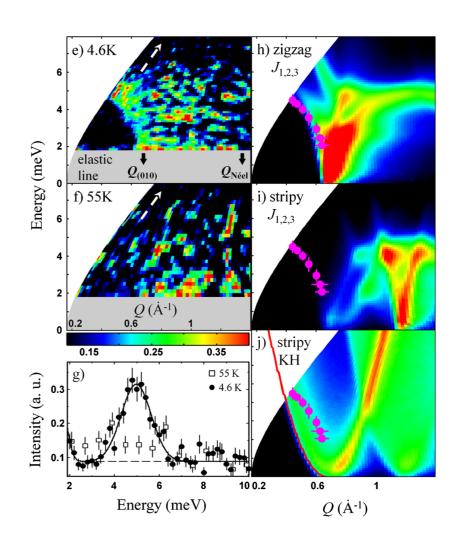
Further extension to RuCl3

PHYSICAL REVIEW B 90, 041112(R) (2014)

α-RuCl₃: A spin-orbit assisted Mott insulator on a honeycomb lattice

K. W. Plumb, ¹ J. P. Clancy, ¹ L. J. Sandilands, ¹ V. Vijay Shankar, ¹ Y. F. Hu, ² K. S. Burch, ^{1,3} Hae-Young Kee, ^{1,4} and Young-June Kim^{1,*}

Later known to have zig-zag order



More complex interactions

1. Really, 4d/5d electrons are more extended spatially, allowing more distant interactions.

2. More generally, many other symmetry allowed interactions on many neighbors should be there, the selected exchange path only produces limited form of interactions.

Non-Kitaev spin liquids?

If Kitaev did not propose his QSL,

We point out that the Kitaev materials may not necessarily support Kitaev spin liquid. It is well-known that having a Kitaev term in the spin interaction is not the sufficient condition for the Kitaev spin liquid ground state. Many other spin liquids may be stabilized by the competing spin interactions of the systems. We thus explore the possibilities of non-Kitaev spin liquids in the honeycomb Kitaev materials. We carry out a systematic classification of gapped \mathbb{Z}_2 spin liquids using the Schwinger boson representation for the spin variables. The presence of strong spin-orbit coupling in the Kitaev materials brings new ingredients into the projective symmetry group classification of the non-Kitaev spin liquid. We predict the spectroscopic properties of these gapped non-Kitaev spin liquids. Moreover, among the gapped spin liquids that we discover, we identify the spin liquid whose spinon condensation leads to the zig-zag magnetic order that was observed in Na₂IrO₃ and α -RuCl₃. We further discuss the possibility of gapped \mathbb{Z}_2 spin liquid and the deconfined quantum criticality from the zig-zag magnetic order to spin dimerization in pressurized α -RuCl₃.

Yaodong Li, Yang Xu, Yi Zhou, Gang Chen, PRB 2019

SOC-PSG

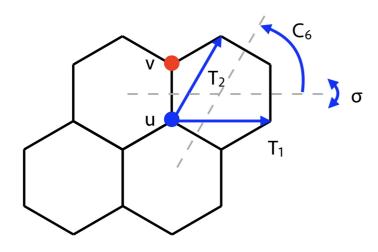


FIG. 1. The honeycomb lattice and its symmetries. Blue/red circles indicate the two sublattices denoted as u/v. The space-group generators are translations T_1 and T_2 , sixfold rotation C_6 around the plaquette center, and horizontal reflection σ through the hexagon center.

bosonic variables. In the Schwinger boson representation, the effective spin S_i on site i is given by $S_i = \frac{1}{2}b_{i\alpha}^{\dagger}\sigma_{\alpha\beta}b_{i\beta}$ where $b_{i\alpha}$ ($\alpha = \uparrow, \downarrow$) is the bosonic spinon operator. The Hilbert space is enlarged due to the introduction of the spinons; to project out unphysical states, the constraint $\sum_{\alpha} b_{i\alpha}^{\dagger} b_{i\alpha} = 1$ on local boson number is imposed. The most general candidate mean-field Hamiltonian for the \mathbb{Z}_2 spin liquids has the following form,

$$H_{\rm MF} = \sum_{\langle ij\rangle,\alpha\beta} (u_{ij,\alpha\beta}^{\rm A} b_{i\alpha}^{\dagger} b_{j\beta} + u_{ij,\alpha\beta}^{\rm B} b_{i\alpha} b_{j\beta} + h.c.) + \sum_{i} \mu_{i} (\sum_{\alpha} b_{i\alpha}^{\dagger} b_{i\alpha} - 1)$$

$$(1)$$

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SOC-PSG

same hexagon center. Under the symmetry operation \mathcal{O} , the bosonic spinon transforms as

$$b_i \to \hat{\mathcal{O}}^{\dagger} b_i \hat{\mathcal{O}} = \mathcal{G}_{\mathcal{O}(i)}^{\mathcal{O}} \, \mathcal{U}_{\mathcal{O}} \, b_{\mathcal{O}(i)} \tag{3}$$

where $\mathcal{G}_{\mathcal{O}(i)}^{\mathcal{O}} = e^{i\phi_{\mathcal{O}}[\mathcal{O}(i)]}$ is a local U(1) gauge transformation, which leaves the spin operators invariant. The gauge transformation is generally nontriv-

$$u_{\mathcal{O}(i)\mathcal{O}(j),\alpha\beta}^{A} = \left(\mathcal{G}_{\mathcal{O}(i)}^{\mathcal{O}}\right)^{*} \mathcal{G}_{\mathcal{O}(j)}^{\mathcal{O}} \left(\mathcal{U}_{\mathcal{O}}^{*}\right)_{\alpha\nu} \left(\mathcal{U}_{\mathcal{O}}\right)_{\beta\lambda} u_{ij,\nu\lambda}^{A}, (4)$$
$$u_{\mathcal{O}(i)\mathcal{O}(j),\alpha\beta}^{B} = \mathcal{G}_{\mathcal{O}(i)}^{\mathcal{O}} \mathcal{G}_{\mathcal{O}(j)}^{\mathcal{O}} \left(\mathcal{U}_{\mathcal{O}}\right)_{\alpha\nu} \left(\mathcal{U}_{\mathcal{O}}\right)_{\beta\lambda} u_{ij,\nu\lambda}^{B}, \tag{5}$$

where we have used the fact that $\mathcal{U}_{\mathcal{O}}$ commutes with $\mathcal{G}^{\mathcal{O}}$. For a general pair of sites (i, j), the above equations are solvable if for each group relation $\mathcal{O}_1\mathcal{O}_2\cdots\mathcal{O}_n=1$, the following identities are satisfied,

$$\mathcal{U}_{\mathcal{O}_{1}}\mathcal{U}_{\mathcal{O}_{2}}\cdots\mathcal{U}_{\mathcal{O}_{n}}\mathcal{G}_{i}^{\mathcal{O}_{1}}\mathcal{G}_{\mathcal{O}_{2}\mathcal{O}_{3}\cdots\mathcal{O}_{n}(i)}^{\mathcal{O}_{2}}\mathcal{G}_{\mathcal{O}_{3}\cdots\mathcal{O}_{n}(i)}^{\mathcal{O}_{3}}\cdots\mathcal{G}_{n}^{\mathcal{O}_{3}}\cdots\mathcal{G}_{n}^{\mathcal{O}_{n}(i)}=\pm 1$$

$$\Leftrightarrow \mathcal{G}_{i}^{\mathcal{O}_{1}}\mathcal{G}_{\mathcal{O}_{2}\mathcal{O}_{3}\cdots\mathcal{O}_{n}(i)}^{\mathcal{O}_{2}}\mathcal{G}_{\mathcal{O}_{3}\cdots\mathcal{O}_{n}(i)}^{\mathcal{O}_{3}}\cdots\mathcal{G}_{n}^{\mathcal{O}_{n}(i)}\cdots\mathcal{G}_{\mathcal{O}_{n}(i)}^{\mathcal{O}_{n}}=\pm 1, \quad (6)$$

where ± 1 is either element of \mathbb{Z}_2 , the invariant gauge group (IGG). The IGG turns out to be the gauge group of the low-energy effective theory of the QSL state^{39,40}. Here, since we are considering \mathbb{Z}_2 QSLs, the IGG should also be \mathbb{Z}_2 . The two lines in Eq. (6) are equivalent because the identity element involves either rotation by 0 or 2π , so $\mathcal{U}_{\mathcal{O}_1}\mathcal{U}_{\mathcal{O}_2}\cdots\mathcal{U}_{\mathcal{O}_n}=\pm 1$, and the group relations constraint only the phases $\phi_{\mathcal{O}}$. Given the defining relations between group generators T_1, T_2, C_6, σ , we can solve for all the possible gauge transformation functions $\phi_{\mathcal{O}}(i)$'s compatible with Eq. (6).

SOC-PSG

\mathbb{Z}_2 QSL	$ \mathcal{G}^{T_1} $	\mathcal{G}^{T_2}	\mathcal{G}^{C_6}	$\mathcal{G}^{\sigma}[u]$	$\mathcal{G}^{\sigma}[v]$
$\mathbb{Z}2A000$	1	1	1	1	1
$\mathbb{Z}2A001$	1	1	i	i	-i
$\mathbb{Z}2A010$	1	1	i	1	1
$\mathbb{Z}2A011$	1	1	-1	i	-i
$\mathbb{Z}2A100$	1	1	i	i	i
$\mathbb{Z}2A101$	1	1	-1	-1	1
$\mathbb{Z}2A110$	1	1	-1	i	i
$\mathbb{Z}2A111$	1	1	-i	-1	1
$\mathbb{Z}2B000$	1	$(-1)^{x}$	$i^{x(x+2y-1)}$	$i^{2x+y(y+1)}$	$i^{2x+y(y+1)}$
$\mathbb{Z}2B001$	1	$(-1)^x$	$i^{x(x+2y-1)+1}$	$i^{2x+y(y+1)+1}$	$i^{2x+y(y+1)-1}$
$\mathbb{Z}2B010$	1	$(-1)^x$	$i^{x(x+2y-1)+1}$	$i^{2x+y(y+1)}$	$i^{2x+y(y+1)}$
$\mathbb{Z}2B011$	1	$(-1)^{x}$	$i^{x(x+2y-1)+2}$	$i^{2x+y(y+1)+1}$	$i^{2x+y(y+1)-1}$
$\mathbb{Z}2B100$	1	$(-1)^x$	$i^{x(x+2y-1)+1}$	$i^{2x+y(y+1)+1}$	$i^{2x+y(y+1)+1}$
$\mathbb{Z}2B101$	1	$(-1)^{x}$	$i^{x(x+2y-1)+2}$	$i^{2x+y(y+1)+2}$	$i^{2x+y(y+1)}$
$\mathbb{Z}2B110$	1	$(-1)^{x}$	$i^{x(x+2y-1)+2}$	$i^{2x+y(y+1)+1}$	$i^{2x+y(y+1)+1}$
$\mathbb{Z}2B111$	1	$(-1)^x$	$i^{x(x+2y-1)+3}$	$i^{2x+y(y+1)+2}$	$i^{2x+y(y+1)}$

TABLE I. List of the gauge transformations associated with the symmetry operations of the 16 \mathbb{Z}_2 QSLs, where (x, y, w) denotes the site in the honeycomb coordinate system.

\mathbb{Z}_2 QSL	u_s^A	u_a^A	u_s^B	u_a^B
$\mathbb{Z}2A000$	$\neq 0$	$\neq 0$	0	0
$\mathbb{Z}2A001$	0	$\neq 0$	$\neq 0$	0
$\mathbb{Z}2A010$	$\neq 0$	$\neq 0$	$\neq 0$	0
$\mathbb{Z}2A011$	0	$\neq 0$	0	0
$\mathbb{Z}2A100$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$\mathbb{Z}2A101$	0	$\neq 0$	0	$\neq 0$
$\mathbb{Z}2A110$	$\neq 0$	$\neq 0$	0	$\neq 0$
$\mathbb{Z}2A111$	0	$\neq 0$	$\neq 0$	$\neq 0$
$\mathbb{Z}2B000$	$\neq 0$	$\neq 0$	0	0
$\mathbb{Z}2B001$	0	$\neq 0$	$\neq 0$	0
$\mathbb{Z}2B010$	$\neq 0$	$\neq 0$	$\neq 0$	0
$\mathbb{Z}2B011$	0	$\neq 0$	0	0
$\mathbb{Z}2B100$	$\neq 0$	$\neq 0$	$\neq 0$	$\neq 0$
$\mathbb{Z}2B101$	0	$\neq 0$	0	$\neq 0$
$\mathbb{Z}2B110$	$\neq 0$	$\neq 0$	0	$\neq 0$
$\mathbb{Z}2B111$	0	$\neq 0$	$\neq 0$	$\neq 0$

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Spinon condensation

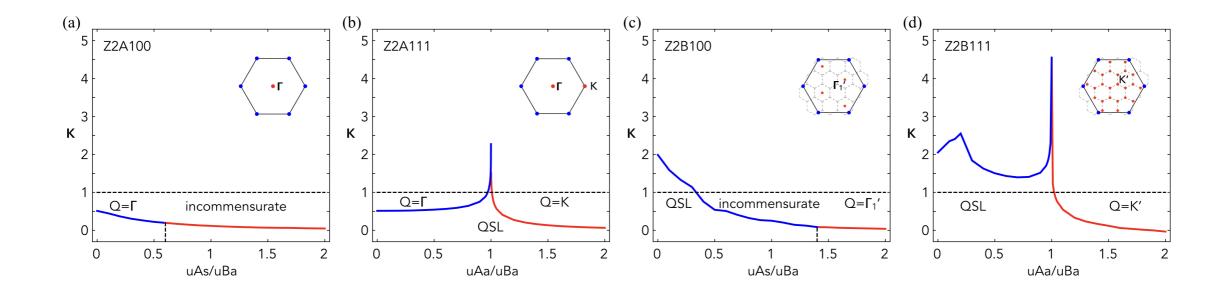


FIG. 2. The phase diagrams for representative mean-field Hamiltonians. Here κ is the average boson density, defined to be $\sum_{i,\alpha} \langle b_{i\alpha}^{\dagger} b_{i\alpha} \rangle / N_{\text{site}}$, and \mathbf{Q} is the position in Brillouin zone of the spinon band minimum. In (a) and (c), we choose $u_a^A/u_s^A=0.6$ and $u_s^B=0$, and in (b) and (d) we choose $u_s^B=0$. The solid line marks the phase boundary between magnetic ordered state (above solid line) and the \mathbb{Z}_2 QSL states (below solid line). Here we use different colors for solid lines to indicate different ordered states above the solid lines. The choice of the momenta can be found in Appendix A.

Proximate orders

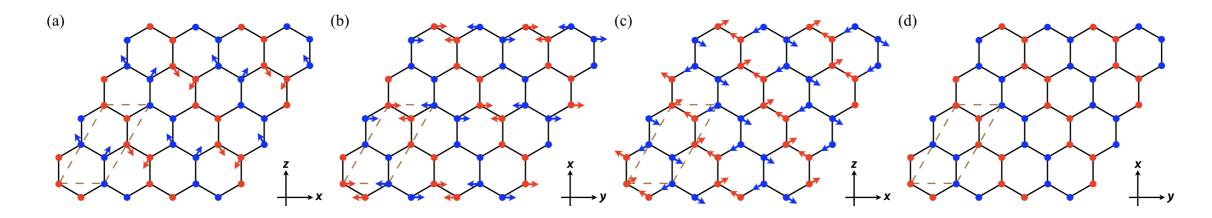


FIG. 4. (Color online.) The magnetic order for a $\mathbb{Z}2B100$ state. We have split the components in x-z plane and along y-direction for clarity. Blue and red sites are the antiferromagnetically aligned chains along the direction prependicular to $2\mathbf{Q}$. The gray dashed lines denote the enlarged unit cell. The parameters of the Hamiltonian are the same as in Fig. 3. In (a) and (b), we have chosen $|z_1^{\mathbf{Q}}| = |z_2^{\mathbf{Q}}|$, and $\arg z_2 - \arg z_1 = \pi/3$. In (c) and (d), we depict the order for $|z_2^{\mathbf{Q}}| = 0$. Notice that in the latter case the magnetic order is completely in the x-z plane.

Spinon continua and symmetry enrichment

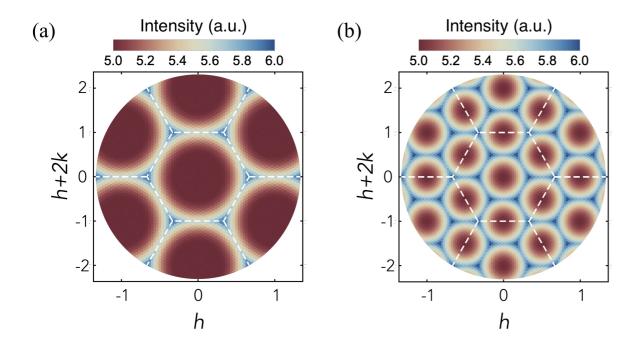


FIG. 3. (Color online.) Intensity plot of lower excitation edges of $\mathcal{S}(\mathbf{q},\omega)$ for the (a) $\mathbb{Z}2A100$ and (b) $\mathbb{Z}2B100$ states. We have chosen $u_s^A=2,\ u_a^A=1.2,\ u_s^B=0,\ u_a^B=1$ (see Tab. II and Appendix B for definitions of the parameters). The white dashed lines mark the Brillouin zone boundary.

of spinon variables. In inelastic neutron scattering experiments, one neutron flip event creates a spin-1 excitation, and the energy-transfer of the neutron is shared between a pair of spin-1/2 spinons,

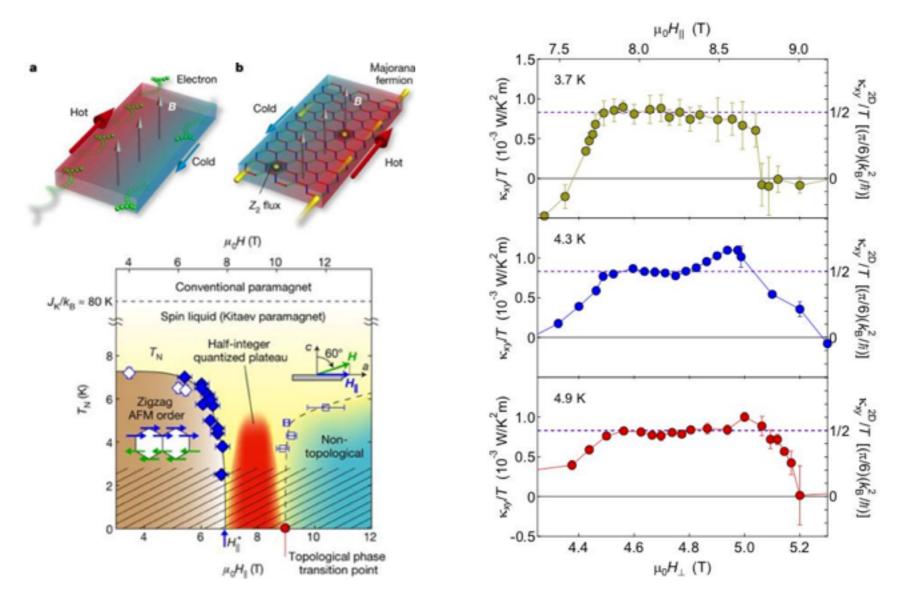
$$\boldsymbol{q} = \boldsymbol{k}_1 + \boldsymbol{k}_2, \tag{13}$$

$$\Omega(\mathbf{q}) = \omega(\mathbf{k}_1) + \omega(\mathbf{k}_2). \tag{14}$$

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Even the zero-field state is ordered, the finite field regime can be gapped Kitaev spin liquid.

How about finite field? Quantized thermal Hall effect in RuCl3?



Yuji Matsuda's group

Again, I am not trying to explain expts.

Numerics

ARTICLE

https://doi.org/10.1038/s41467-019-08459-9

OPEN

Emergence of a field-driven U(1) spin liquid in the Kitaev honeycomb model

Ciarán Hickey 1 & Simon Trebst 1

Model. We start our discussion by considering the pure Kitaev honeycomb model in the presence of a uniform magnetic field of arbitrary orientation, defined by the Hamiltonian

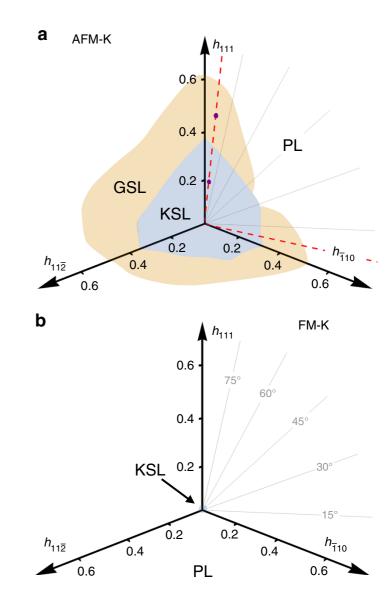
$$H_{\pm} = \pm K \sum_{\langle i,j \rangle \in \gamma} S_i^{\gamma} S_j^{\gamma} - \sum_i \mathbf{h} \cdot \mathbf{S}_i, \tag{1}$$

C. Hickey and S. Trebst, Emergence of a field-driven U(1) spin liquid in the Kitaev honeycomb model, Nat. Commun. **10**, 530 (2019).

H.-C. Jiang, C.-Y. Wang, B. Huang, and Y.-M. Lu, Field induced quantum spin liquid with spinon Fermi surfaces in the Kitaev model, arXiv:1809.08247.

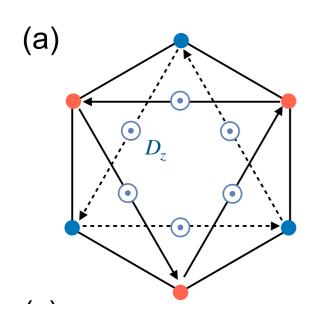
L. Zou and Y.-C. He, Field-induced neutral Fermi surface and QCD₃-Chern-Simons quantum criticalities in Kitaev materials, arXiv:1809.09091.

F Pollmann's group, Trivedi's group



one can understand from pair breaking picture. maybe not U(1) QSL according to Chong Wang

Dzyaloshinskii-Moriya interaction



$$\sin \phi = \frac{1}{2} \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \times \boldsymbol{S}_3.$$

Dzyaloshinskii-Moriya interaction is prohibited. However, the second neighbor Dzyaloshinskii-Moriya interaction is allowed by symmetry since the second neighbor magnetic bonds have no inversion center. According to Moriya's rules⁵¹, there are components of D_{ij} perpendicular to the planes with strength D_z as schematically depicted in Fig. 4(a) and all the in-plane components vanish when the honeycomb plane is a mirror plane of the crystal structure. Therefore, a representative Dzyaloshinskii-

Moriya interaction of the honeycomb lattice Mott insulator up to second neighbor has the form,

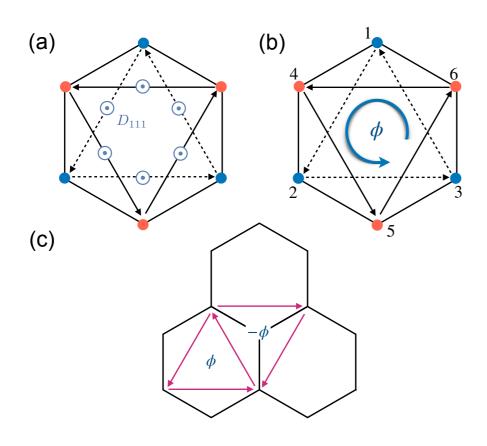
$$H_{\rm DM} = \sum_{\langle \langle i,j \rangle \rangle} \boldsymbol{D}_{ij} \cdot \boldsymbol{S_i} \times \boldsymbol{S_j}. \tag{11}$$

For example, it has been estimated¹⁸ that a large second neighbor Dzyaloshinskii-Moriya term $|\mathbf{D}_{ij}| > 4 \text{ meV}$ for the Kitaev material α -Li₂IrO₃, which is usually not considered in the literatures.

Thermal Hall signatures of non-Kitaev spin liquids in honeycomb Kitaev materials

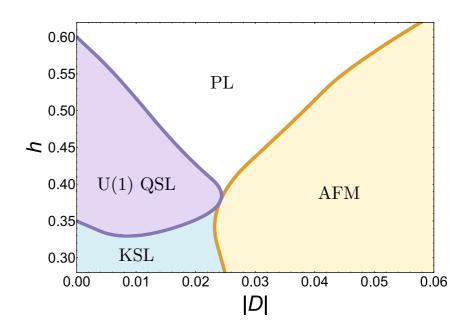
Yong Hao Gao¹, Ciarán Hickey², Tao Xiang^{3,4}, Simon Trebst², and Gang Chen⁵

PR research 2019



$$H = \sum_{\langle ij\rangle\in\gamma} KS_i^{\gamma}S_j^{\gamma} + \sum_{\langle\langle i,j\rangle\rangle} \mathbf{D}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i.$$
(18)

In Fig. 6 we show the resulting phase diagram, with the U(1) spin liquid region stable up to a maximal Dzyaloshinskii-Moriya interaction of about $|\boldsymbol{D}| \sim 0.025 K$. We should



With more generic interactions in RuCl3, can this state be realized in finite field?

Thermal Hall effect

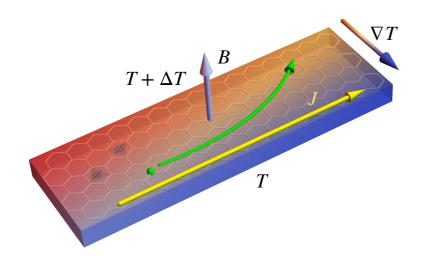


FIG. 1. (Color online.) The schematic plot of the thermal Hall effect of charge-neutral spinons under the external magnetic field in honeycomb Kitaev materials with the spinon Fermi surface state.

$$\sin \phi = \frac{1}{2} \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \times \boldsymbol{S}_3.$$

[Wen, Wilczek, Zee, PRB, 1989]

$$\kappa_{xy} = -\frac{1}{T} \int d\epsilon (\epsilon - \mu)^2 \frac{\partial f(\epsilon, \mu, T)}{\partial \epsilon} \sigma_{xy}(\epsilon).$$
 (15)

Here $f(\epsilon, \mu, T) = 1/[e^{\beta(\epsilon-\mu)} + 1]$ is the Fermi-Dirac distribution and the derivate of the distribution function $\partial f(\epsilon, \mu, T)/\partial \epsilon$ indicates that the integral dominates around the Fermi energy. Moreover,

$$\sigma_{xy}(\epsilon) = -\frac{1}{\hbar} \sum_{\mathbf{k}, \xi_{n, \mathbf{k}} < \epsilon} \Omega_{n, \mathbf{k}}$$
 (16)

$$\Omega_{n\mathbf{k}} = -2\operatorname{Im}\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_x} | \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \rangle$$

Thermal Hall effects

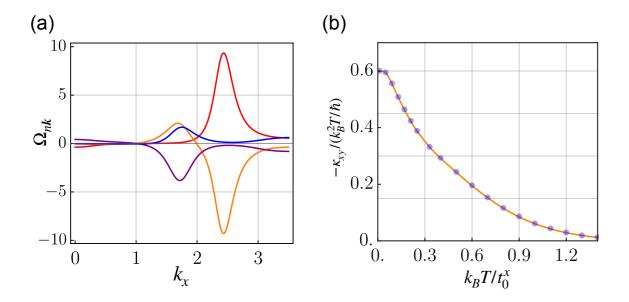


FIG. 6. (a) Berry curvatures for different energy bands and all the parameters are set as in Fig. 5. The red (orange, purple, blue) line is for the first/lowest (second, third, fourth) spinon band. (b) The corresponding evaluation of the thermal Hall conductivity as a function of temperature.

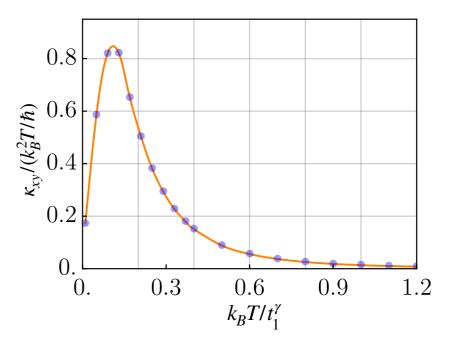


FIG. 8. The actual evaluation of the thermal Hall conductivity for Dirac spin liquid as a function of temperature at the gauge flux $\phi = \pi/10$, here t_2 is set as 0.4 t_1^{γ} .

Summary

Kitaev material is interesting on its own, and may bring more physics beyond Kitaev physics due to the spin-orbit entanglement and anisotropic interactions.