Title: Topological phases in Kitaev Materials

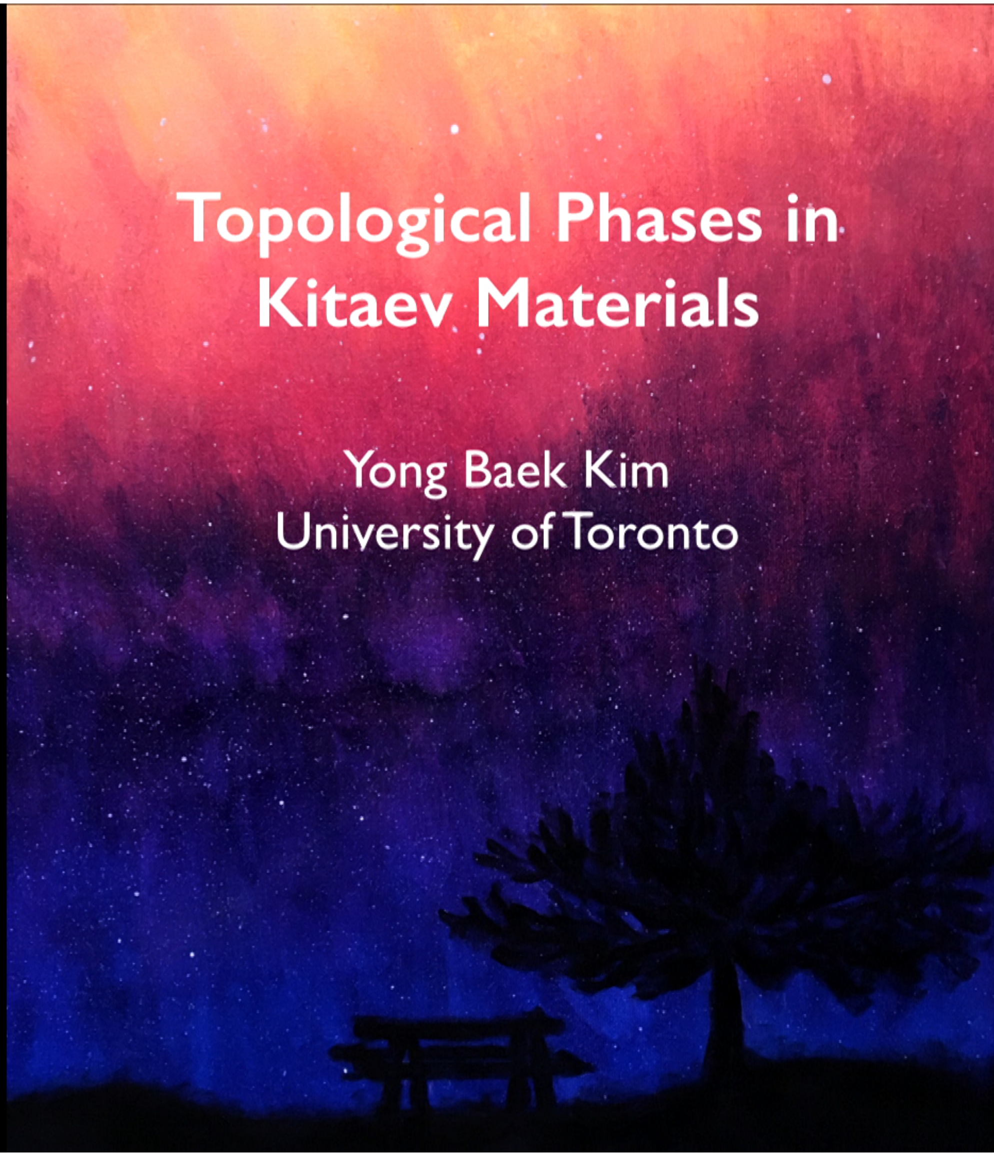
Speakers: Yong-Baek Kim

Collection: Quantum Matter: Emergence & Entanglement 3

Date: April 25, 2019 - 2:45 PM

URL: http://pirsa.org/19040115

Abstract: We discuss recent progress in theory and experiment on emergent topological phases in Kitaev materials. Here the competition between different anisotropic spin-exchange interactions may lead to a number of exotic phases of matter. We investigate possible emergence of quantum spin liquid, topological magnons, and topological superconductivity in two and three dimensional systems. We make connections to existing and future experiments.



Topological Phases in Kitaev Materials

Yong Baek Kim
University of Toronto

CIFAR

NSERC CRSNG

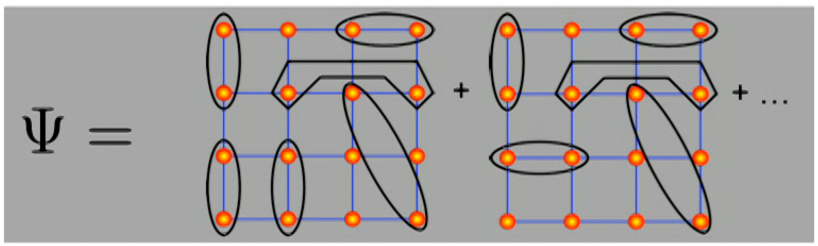
Perimeter Institute
April 25, 2019

Quantum Spin Liquids

Quantum Paramagnet $\langle \mathbf{S} \rangle = 0$

Correlated insulator with no broken translational symmetry

Resonating Valence Bond state (RVB);
Superposition of Valence Bond coverings



P.W.Anderson

Rokhsar-Kivelson

$$|RVB\rangle = \sum_{vb} A_{vb} |vb\rangle$$

$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ Valence Bond

PHYSICS

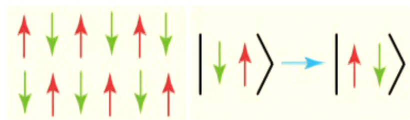
An End to the Drought of Quantum Spin Liquids

Patrick A. Lee

After decades of searching, several promising examples of a new quantum state of matter have now emerged.

Electrons possess magnetic behavior through the quantum mechanical property of spin. The magnetic properties of materials then arise from the collective interaction of electrons on atoms within the crystal. Below a transition temperature, the electron spins of normal magnets "freeze" into an ordered array of magnetic dipoles. Whether the ordering is ferromagnetic (all the dipoles point in the same direction) or antiferromagnetic (the dipoles on adjacent sites point in opposite directions) is determined by the sign and strength of the interaction between the electrons. Early theoretical work has indicated a departure from these ordered states, suggesting that quantum mechanical fluctuations of the spin could be so strong that ordering would be suppressed and the spin ensemble would remain in a liquid-like state, even down to the lowest temperatures. Experimental evidence, which has until recently remained elusive, is emerging in favor of this long-predicted state of quantum matter.

Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA. E-mail: palee@mit.edu



Ordered spins. (Left) Néel's picture of antiferromagnet ordering with an alternate spin-up–spin-down pattern across the lattice. **(Right)** Quantum fluctuations lead to mutual spin flips, which Landau argued would disorder Néel's state.

To understand the controversy surrounding this exotic quantum spin liquid state, it is instructive to go back to the description of antiferromagnetism. Soon after the invention of quantum mechanics, Heisenberg pointed out that electron spins on neighboring atoms can have short-range interaction due to quantum mechanical exchange. Louis Néel

5 SEPTEMBER 2008 VOL 321 SCIENCE

Until ~15 years ago, candidate materials were limited.

Good theoretical models existed (numerically solvable to high accuracy)

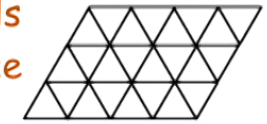
Candidate Materials (selected, as of April 2019)

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$

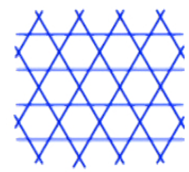
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ — Organic Materials Triangular Lattice

κ-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$

κ-H$_3$(Cat-EDT-TTF)$_2$



Kagome

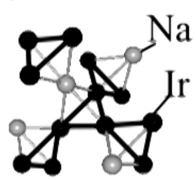


ZnCu$_3$(OH)$_6$Cl$_2$ herbertsmithtite

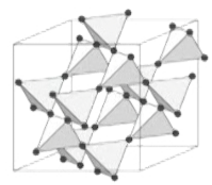
Cu$_3$Zn(OH)$_6$FBr Cu$_4$(OH)$_6$FBr barlowite

Cu$_3$Zn(OH)$_6$FCl Cu$_4$(OH)$_6$FCl claringbullite

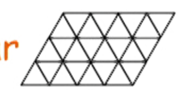
PbCuTe$_2$O$_6$
Na$_4$Ir$_3$O$_8$ hyper-kagome



Yb$_2$Ti$_2$O$_7$
Pr$_2$Zr$_2$O$_7$ pyrochlore



YbMgGaO$_4$ triangular



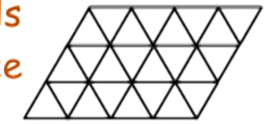
Kitaev Materials honeycomb hyper-honeycomb

Candidate Materials (selected, as of April 2019)

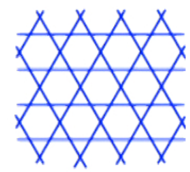
Geometric

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$
κ-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$
κ-H$_3$(Cat-EDT-TTF)$_2$

Organic Materials
Triangular Lattice

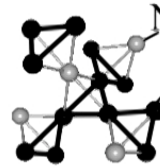


Kagome

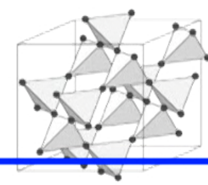


$ZnCu_3(OH)_6Cl_2$ herbertsmithtite
$Cu_3Zn(OH)_6FBr$ $Cu_4(OH)_6FBr$ barlowite
$Cu_3Zn(OH)_6FCl$ $Cu_4(OH)_6FCl$ claringbullite

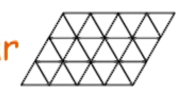
$PbCuTe_2O_6$
$Na_4Ir_3O_8$ hyper-kagome



$Yb_2Ti_2O_7$
$Pr_2Zr_2O_7$ pyrochlore



$YbMgGaO_4$ triangular



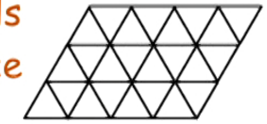
Kitaev Materials honeycomb hyper-honeycomb

Candidate Materials (selected, as of April 2019)

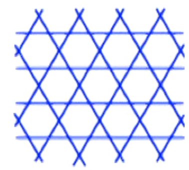
Geometric

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$
κ-(BEDT-TTF)$_2$Ag$_2$(CN)$_3$
κ-H$_3$(Cat-EDT-TTF)$_2$

Organic Materials
Triangular Lattice

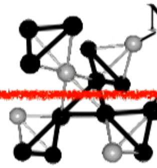


Kagome

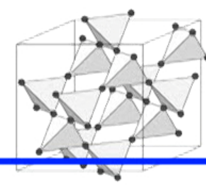


ZnCu$_3$(OH)$_6$Cl$_2$ herbertsmithtite
Cu$_3$Zn(OH)$_6$FBr Cu$_4$(OH)$_6$FBr barlowite
Cu$_3$Zn(OH)$_6$FCl Cu$_4$(OH)$_6$FCl claringbullite

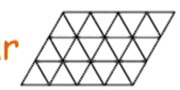
PbCuTe$_2$O$_6$
Na$_4$Ir$_3$O$_8$ hyper-kagome



Yb$_2$Ti$_2$O$_7$
Pr$_2$Zr$_2$O$_7$ pyrochlore



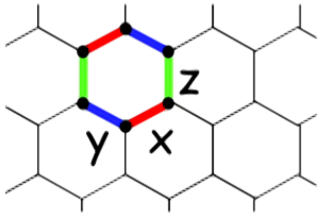
YbMgGaO$_4$ triangular



Kitaev Materials honeycomb hyper-honeycomb

Spin-orbit

Exact Question to the Answer (Kitaev)

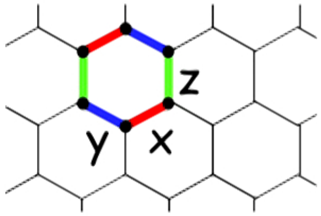


$$\mathcal{H}_{\mathrm{K}} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha \qquad b_i^x b_i^y b_i^z c_i = 1$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions

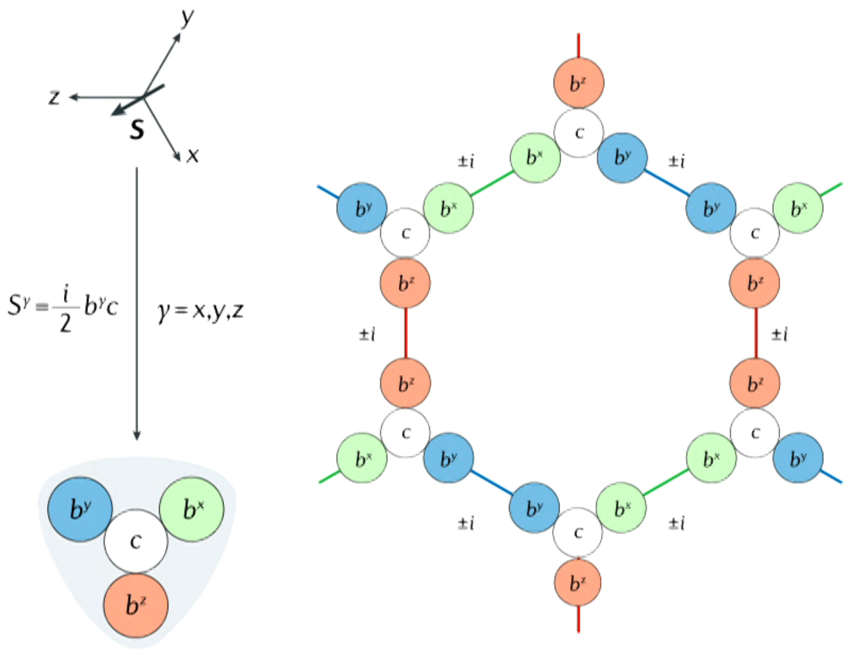
Exact Question to the Answer (Kitaev)



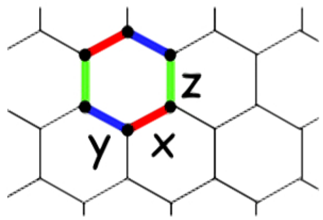
$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha \qquad b_i^x b_i^y b_i^z c_i = 1$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions



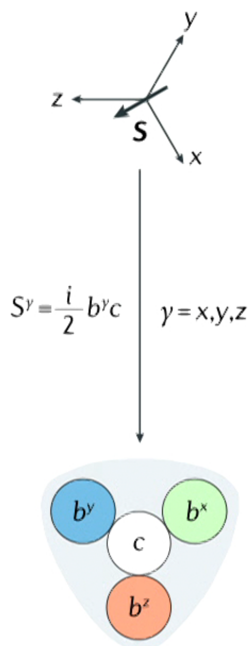
Exact Question to the Answer (Kitaev)

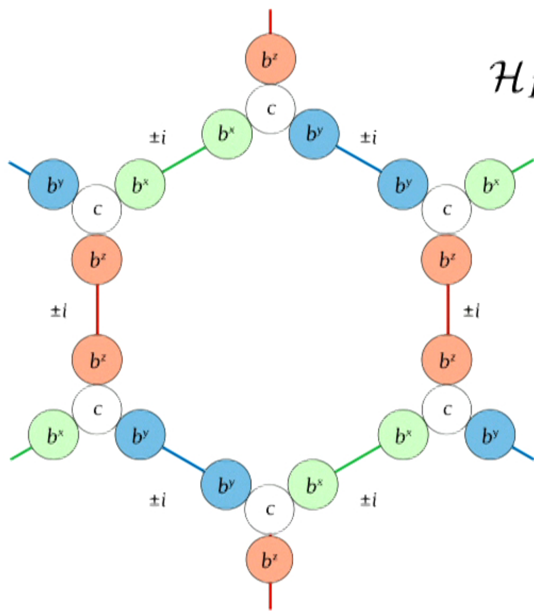


$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha \qquad b_i^x b_i^y b_i^z c_i = 1$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions

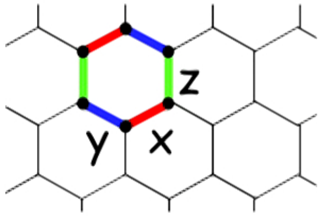




$$\mathcal{H}_K = -\frac{i}{4} \sum_{\alpha-links} u_{ij}^\alpha c_i c_j$$

$$u_{ij}^\alpha = i b_i^\alpha b_j^\alpha$$

Exact Question to the Answer (Kitaev)



$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha \qquad b_i^x b_i^y b_i^z c_i = 1$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

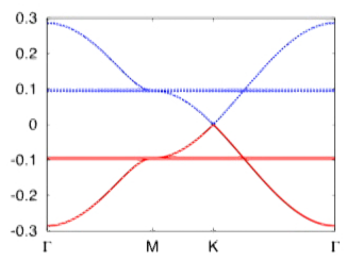
Four Majorana Fermions

$$\mathcal{H}_K = -\frac{i}{4} \sum_{\alpha-links} u_{ij}^\alpha c_i c_j$$

Ground state is in the zero-flux sector

$$W_p = +1$$

$$u_{ij}^\alpha = i b_i^\alpha b_j^\alpha$$



Majorana Fermions with Dirac Dispersion

$$W_p = 2^6 S_1^x S_2^y S_3^z S_4^x S_5^y S_6^z$$

Kitaev Spin Liquid is almost a Superconductor

Making connection to "Superconductor"

$$f_{i\uparrow} = \frac{1}{\sqrt{2}}(c_i + ib_i^z)$$

$$f_{i\downarrow} = \frac{i}{\sqrt{2}}(b_i^x + ib_i^y)$$

$$S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^a f_{i\beta}$$

with $\sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$

Kitaev Spin Liquid is almost a Superconductor

Making connection to "Superconductor"

$$f_{i\uparrow} = \frac{1}{\sqrt{2}}(c_i + ib_i^z) \qquad S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^a f_{i\beta}$$

$$f_{i\downarrow} = \frac{i}{\sqrt{2}}(b_i^x + ib_i^y) \qquad \text{with} \quad \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$$

$$H = \sum_{\langle ij\rangle \in a} \{ f_{i\alpha}^\dagger [T^a]_{\alpha\beta}^{ij} f_{j\beta} + f_{i\alpha} [\Delta^a]_{\alpha\beta}^{ij} f_{j\beta} \}$$

exactly one particle per site (insulator)

Kitaev Spin Liquid is almost a Superconductor

Making connection to "Superconductor"

$$f_{i\uparrow} = \frac{1}{\sqrt{2}}(c_i + ib_i^z) \qquad S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^a f_{i\beta}$$

$$f_{i\downarrow} = \frac{i}{\sqrt{2}}(b_i^x + ib_i^y) \qquad \text{with} \quad \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1$$

$$H = \sum_{\langle ij\rangle \in a} \{ f_{i\alpha}^\dagger [T^a]_{\alpha\beta}^{ij} f_{j\beta} + f_{i\alpha} [\Delta^a]_{\alpha\beta}^{ij} f_{j\beta} \}$$

exactly one particle per site (insulator)

Class BDI
Spin-Triplet
Superconductor
$\langle n_i \rangle = 1$

Hubbard U ==> ∞ ⟶

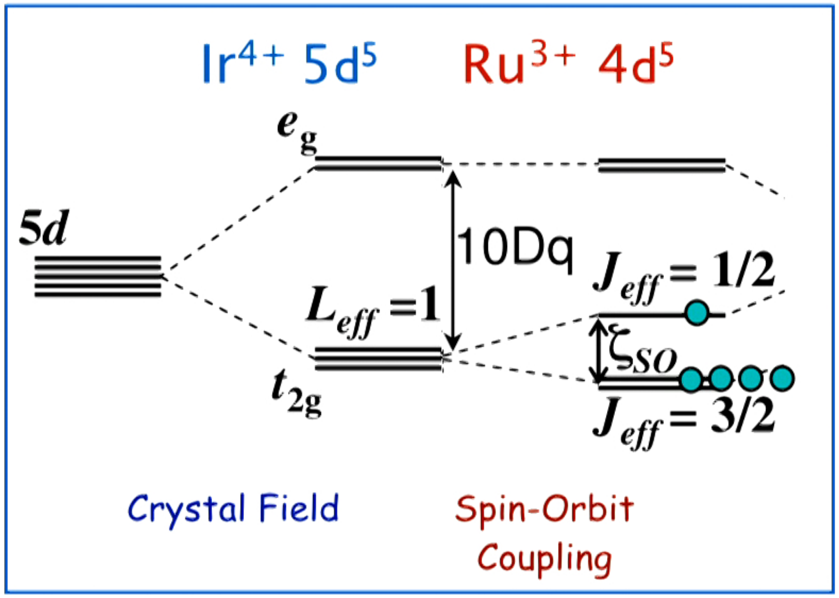
Kitaev Spin Liquid
$n_i = 1$

Kitaev Materials

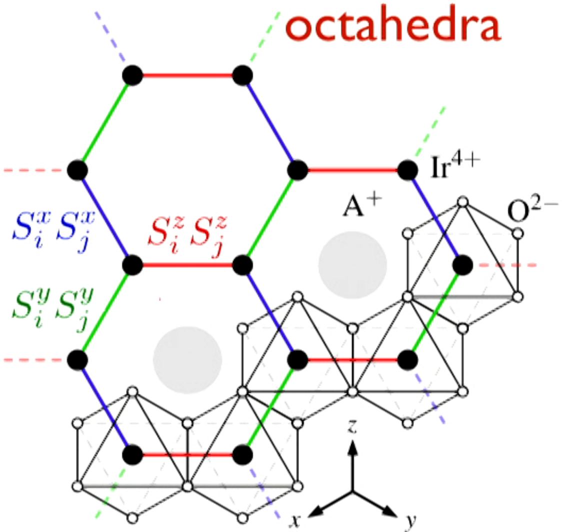
Kitaev Interaction ?

$$H = \sum_{\langle ij \rangle \in \gamma} -K S_i^\gamma S_j^\gamma$$

G. Jackeli and G. Khaliullin,
PRL 102, 256403 (2009)



edge sharing octahedra

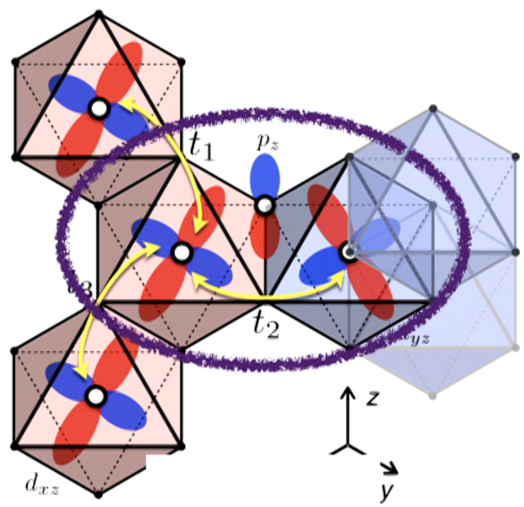


Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

How realistic is the Kitaev model ?

$$H = \sum_{\langle ij \rangle \in \gamma} K S_i^\gamma S_j^\gamma$$

if only the super-exchange via oxygens are considered

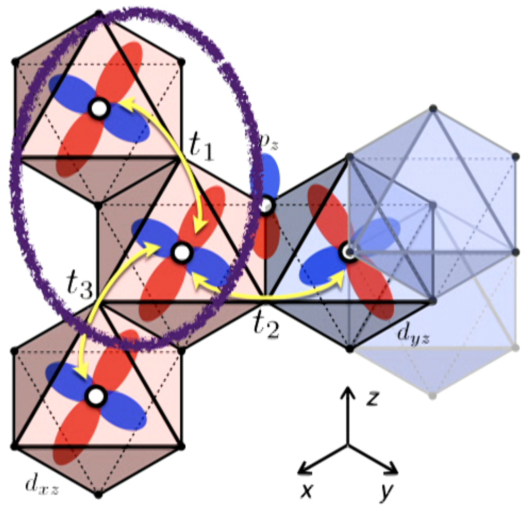


G. Jackeli and G. Khaliullin (2009)

How realistic is the Kitaev model ?

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

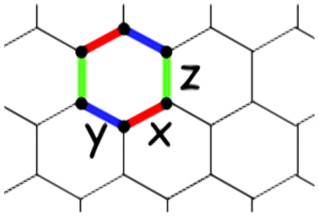
but direct exchange is also important due to large extent of 4d/5d orbitals



G. Jackeli and G. Khaliullin (2009)   J. Rau, E. Lee, H. Y. Kee (2014)

How realistic is the Kitaev model ?

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



$K S_i^x S_j^x + \Gamma[S_i^y S_j^z + S_i^z S_j^y]$ x-bond

$K S_i^y S_j^y + \Gamma[S_i^z S_j^x + S_i^x S_j^z]$ y-bond

$K S_i^z S_j^z + \Gamma[S_i^x S_j^y + S_i^y S_j^x]$ z-bond

How essential/important are
these additional interactions ?

G. Jackeli and G. Khaliullin (2009) J. Rau, E. Lee, H. Y. Kee (2014)

Realization of Kitaev Quantum Spin Liquid ?

2D
Honeycomb

α- Na_2IrO_3

α- Li_2IrO_3

α- $H_3LiIr_2O_6$

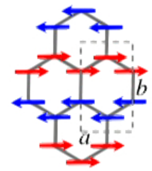
α- $RuCl_3$

β- Li_2IrO_3
3D Hyper-Honeycomb

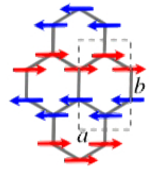
γ- Li_2IrO_3
3D Stripy-Honeycomb

Realization of Kitaev Quantum Spin Liquid ?

2D Honeycomb

	T_N
α- Na_2IrO_3	zig-zag, 14K 
α- Li_2IrO_3	incomm. spiral, 15K
α- $H_3LiIr_2O_6$	no magnetic order (NMR)
α- $RuCl_3$	zig-zag, 7K
β- Li_2IrO_3 (3D Hyper-Honeycomb)	incomm. spiral, 38K
γ- Li_2IrO_3 (3D Stripy-Honeycomb)	incomm. spiral, 38K

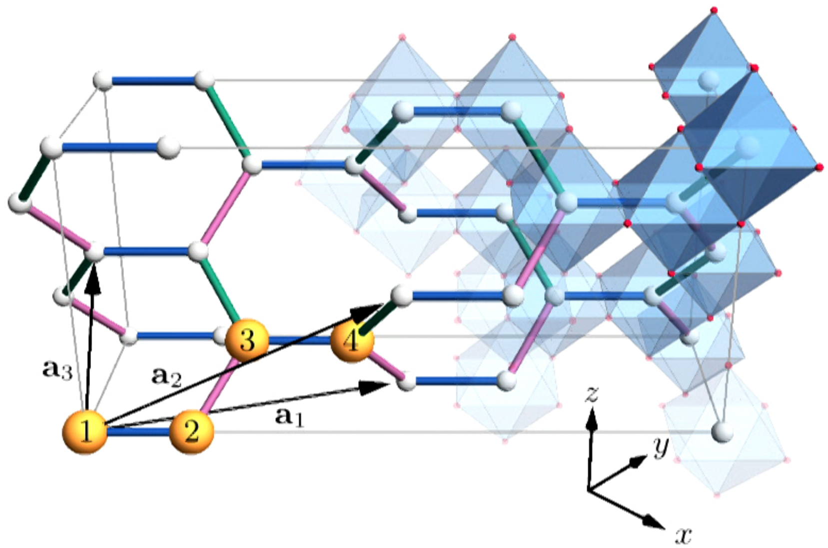
Realization of Kitaev Quantum Spin Liquid ?

2D Honeycomb	T_N	suppressed magnetic order ?	
α- Na_2IrO_3	zig-zag, 14K 		
α- Li_2IrO_3	incomm. spiral, 15K		
α- $H_3LiIr_2O_6$	no magnetic order (NMR)	Hydrogen intercalation	H. Takagi
α- $RuCl_3$	zig-zag, 7K	H_{in} > 8T	
		S. Nagler, Y.-J.Kim, R. Coldea, ...	

β- Li_2IrO_3 3D Hyper-Honeycomb	incomm. spiral, 38K	P > 2.5 GPa	H. Takagi, D. Haskel
γ- Li_2IrO_3 3D Stripy-Honeycomb	incomm. spiral, 38K	P > 1.5 GPa	J. Analytis, D. Haskel

Three-dimensional Hyper-honeycomb Iridates

β-Li_2IrO_3

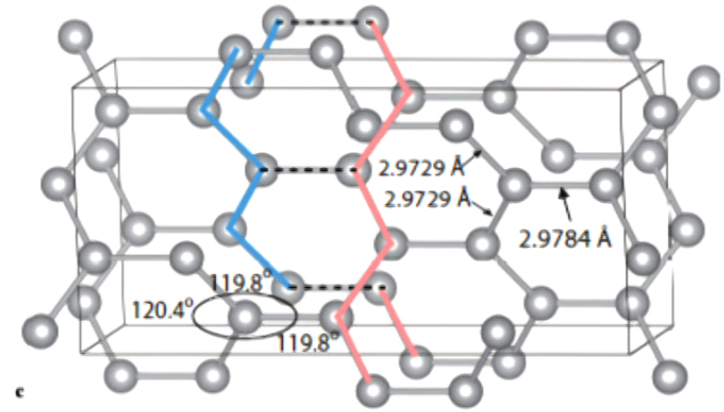


Three dimensional "Hyper-Honeycomb" lattice

β- Li_2IrO_3

H. Takagi (PRL, 2014)

Close to ideal structure



Magnetic order
T_c = 38K

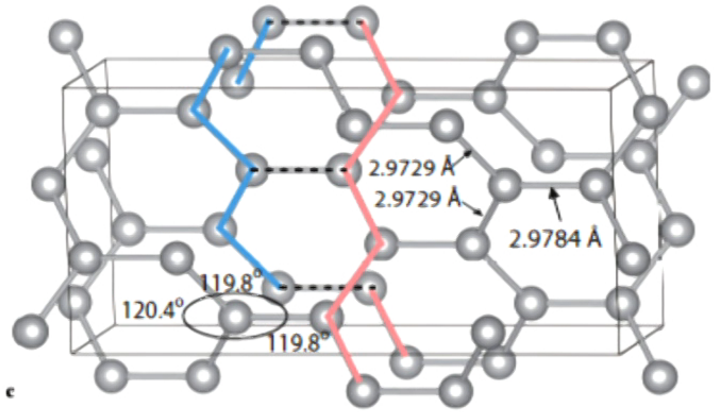
Strong Magnetic Anisotropy

Three dimensional "Hyper-Honeycomb" lattice

β- Li_2IrO_3

H. Takagi (PRL, 2014)

Close to ideal structure

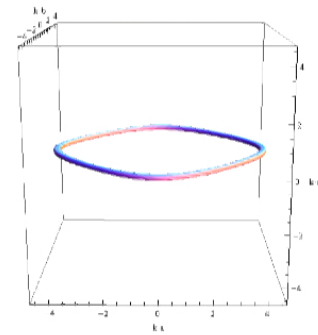


Magnetic order T_c = 38K

Strong Magnetic Anisotropy

Kitaev Model exactly solvable

Nodal Line
Majorana Fermions



S. Mandal and N. Surendran (2009)

E. K.-H. Lee. R. Schaffer, S. Bhattacharjee, YBK (2014)

Classical Analysis

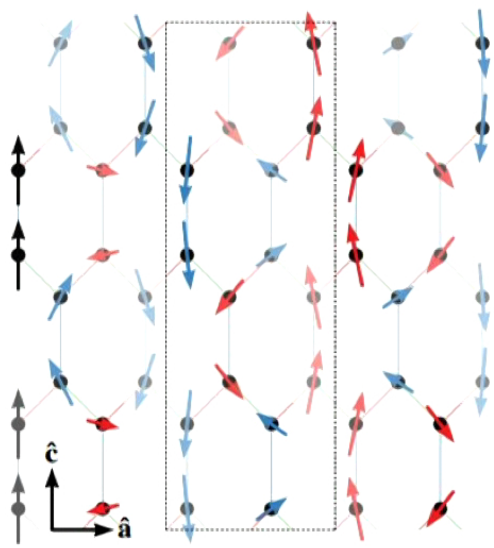
$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$

$K < 0 \qquad J > 0 \qquad \Gamma < 0$

$$|K| > |\Gamma| \gg J$$

Non-coplanar counter-propagating incommensurate spiral order

EXPERIMENT



$\mathbf{Q}_{\mathrm{exp}} = (0.57, 0, 0)$

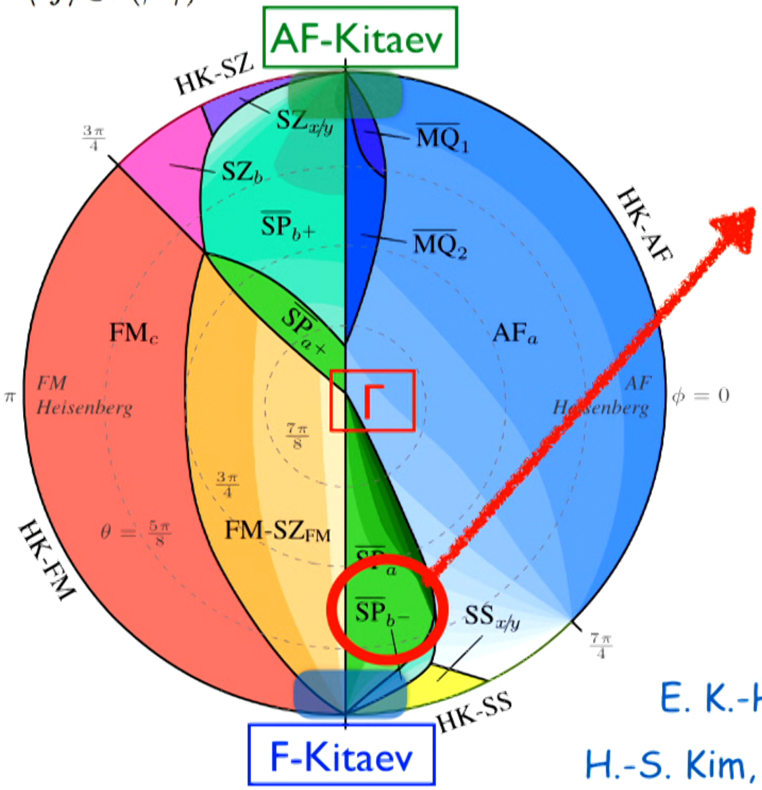
Eric K.-H. Lee, YBK (2014)

Radu Coldea (PRL, PRB, 2014)

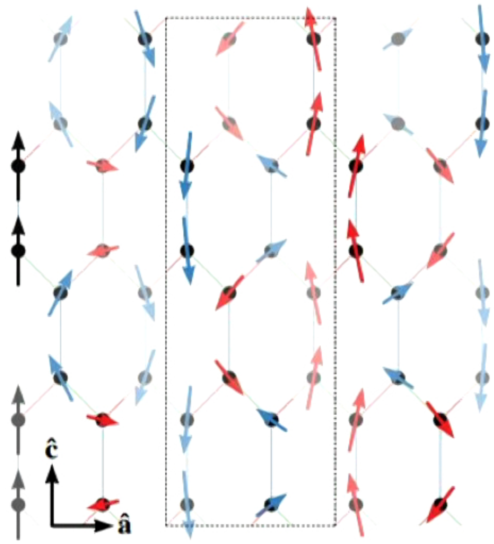
Classical Analysis

$$J = \cos\phi \sin\theta$$
$$K = \sin\phi \sin\theta$$
$$\Gamma = \cos\theta$$

$$H = \sum_{\langle ij \rangle \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$



EXPERIMENT

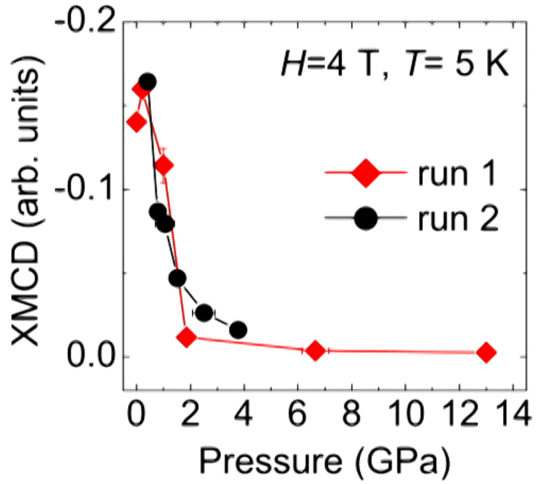


$$\mathbf{Q}_{\mathrm{exp}} = (0.57, 0, 0)$$

E. K.-H. Lee, YBK (2014)

H.-S. Kim, E. K.-H. Lee, YBK (2015)

High Pressure Experiment (H. Takagi, D. Haskel)



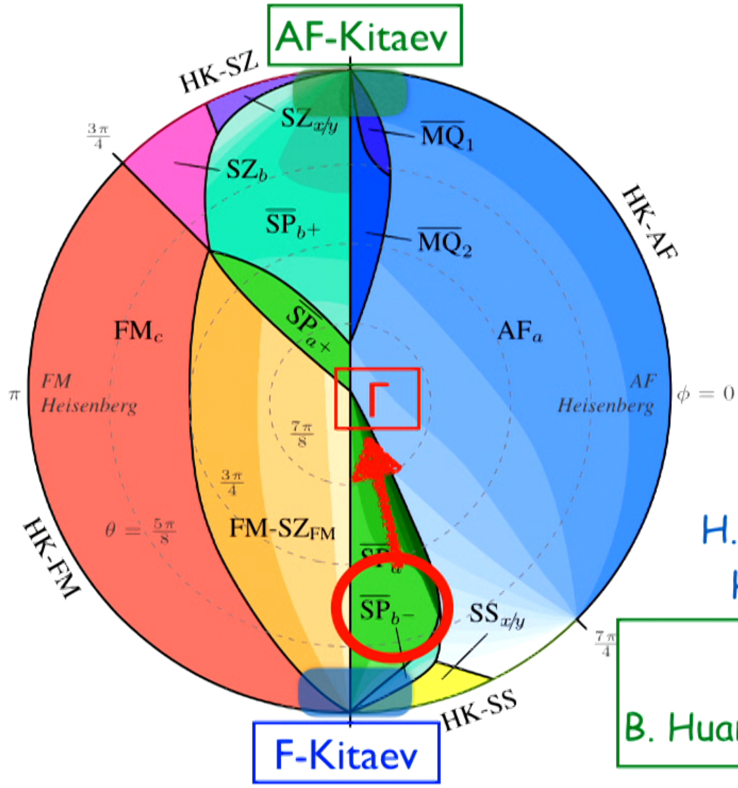
Magnetic order disappear near 2-2.5 GPa

What's the paramagnetic state at P > 2-2.5GPa ?

Structure change at P > 4GPa

Effect of External Pressure (Theory, Ab Initio)

$$H = \sum_{\langle ij\rangle \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)$$



K dominant Low-P

Γ dominant High-P

Highly Frustrated

New Spin Liquid ?

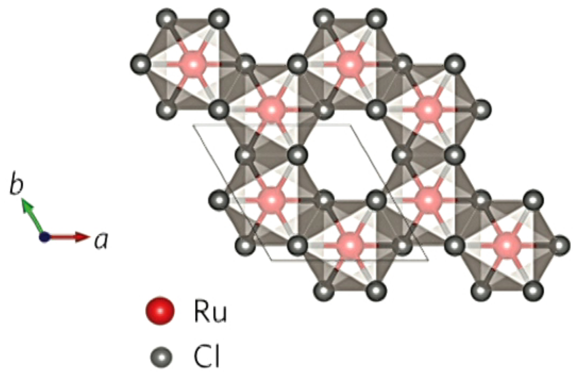
H.-S. Kim, E. K.-H. Lee, YBK (2015)

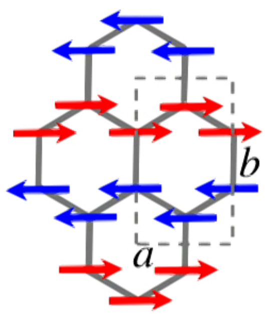
H.-S. Kim, H-Y.Kee, YBK (2016)

Classification

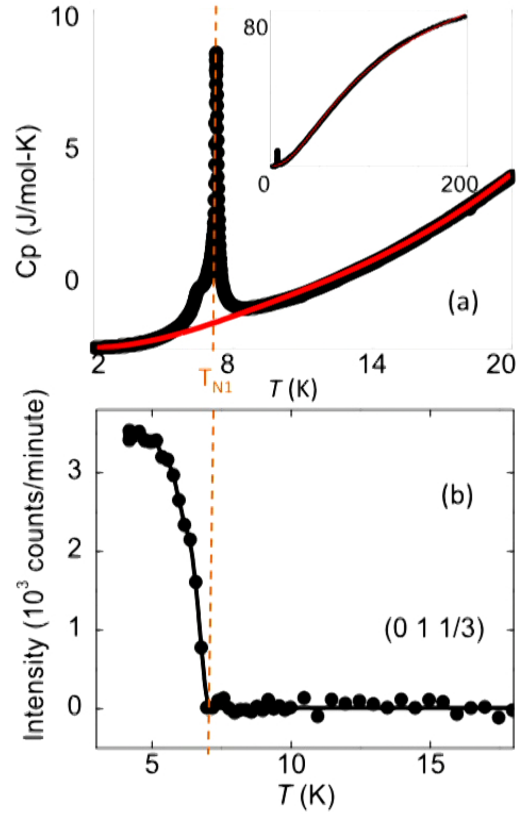
B. Huang, W. Choi, YBK, Y.-M. Lu (2018)

α-$RuCl_3$



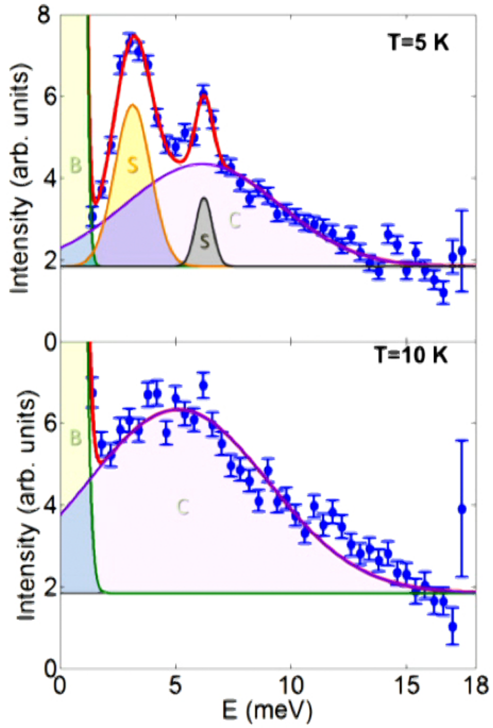


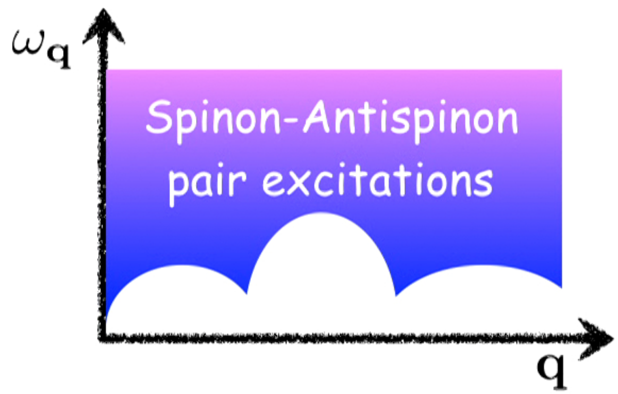
Zig-Zag Order



α- $RuCl_3$ (Y. J. Kim, S. Nagler, R. Coldea ...)

Spinon Continuum ?



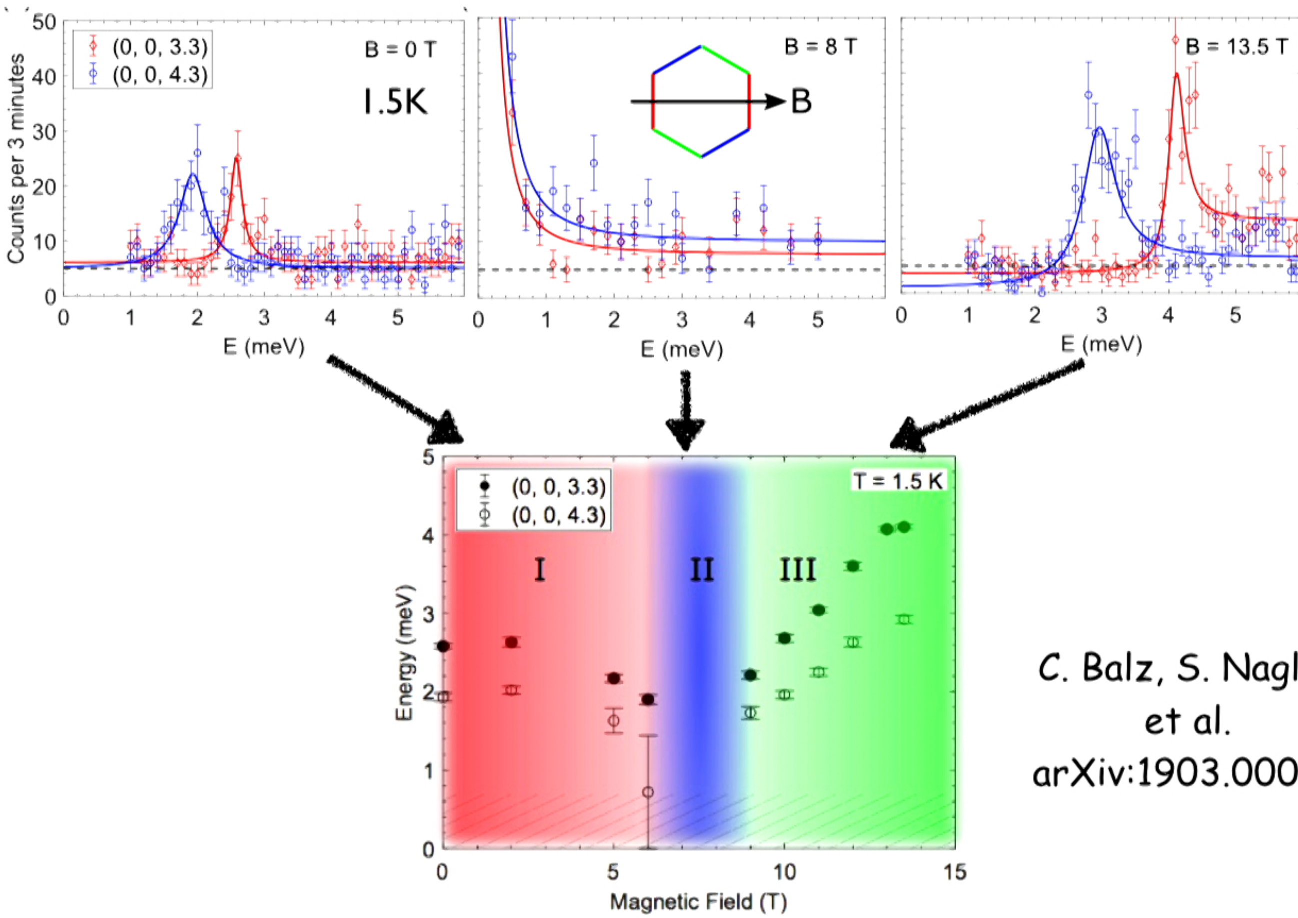


Well-defined dispersion -->

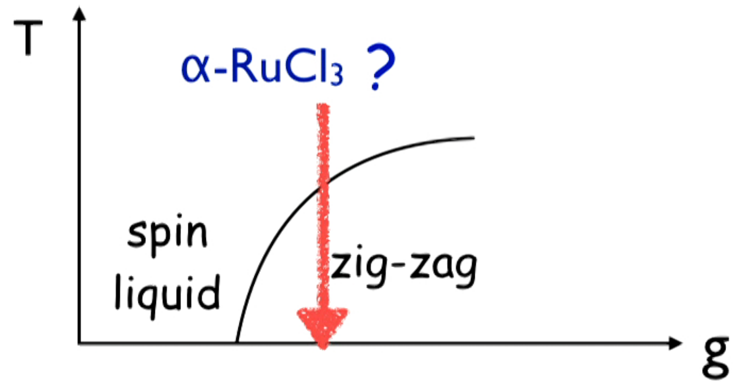
Threshold energy for pair excitations

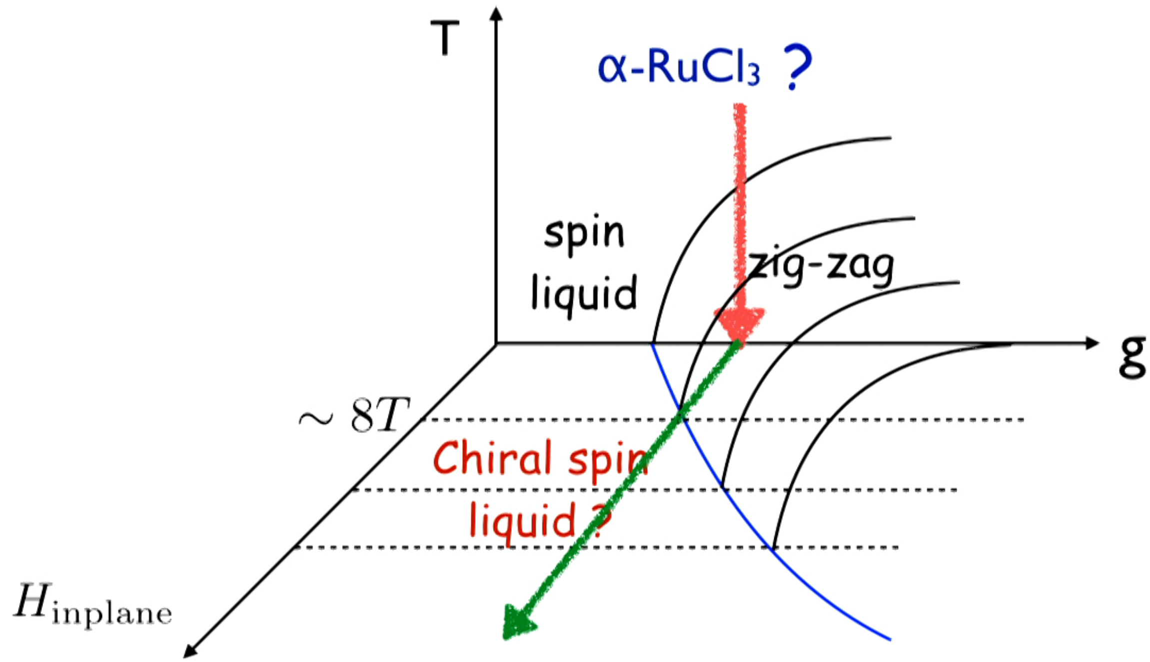
A. Banerjee, S. Nagler et al. (2016)

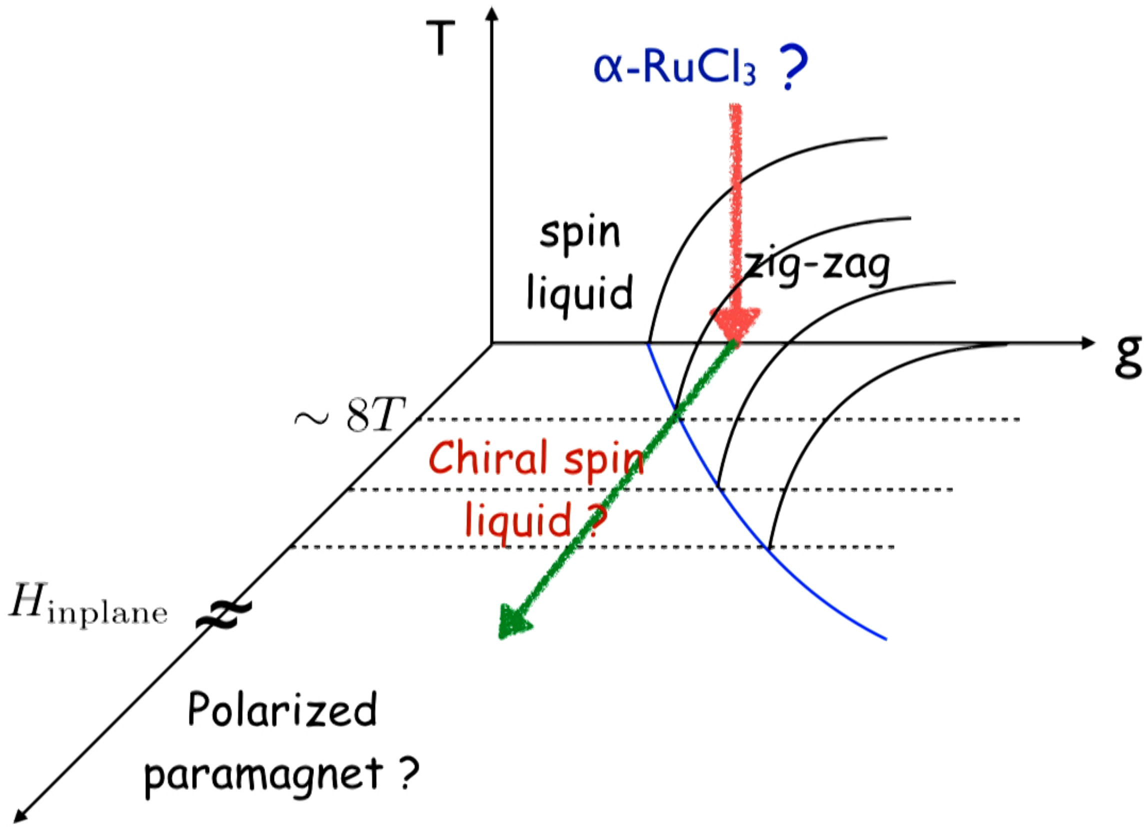
Field-induced Paramagnet: Spin Liquid ?

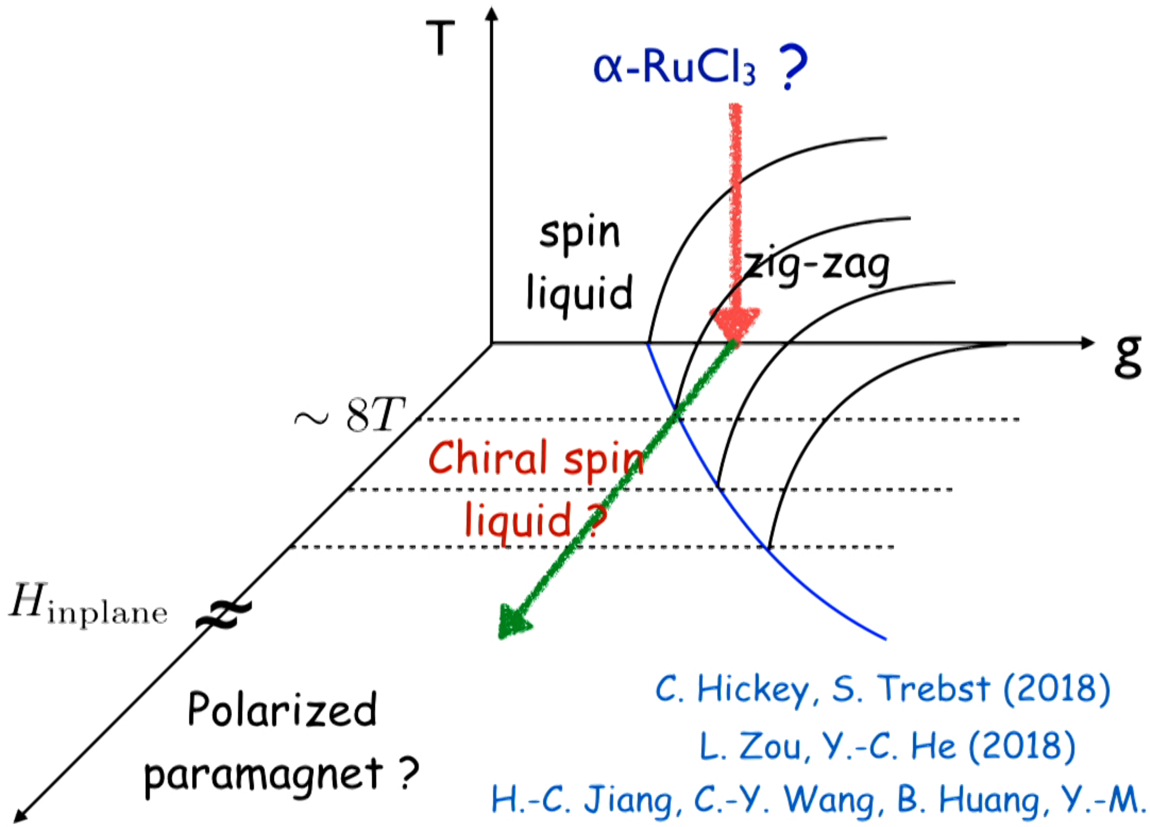


C. Balz, S. Nagler et al. arXiv:1903.00056


T
α-RuCl3 ?
spin liquid
zig-zag
g

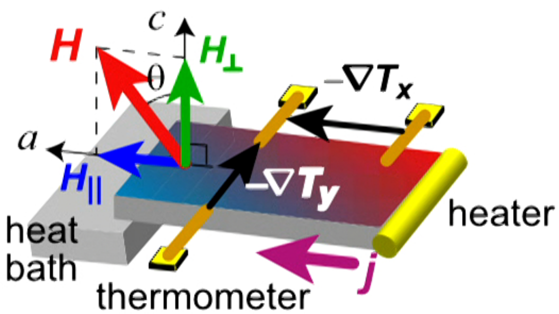

T
α-RuCl3 ?
spin
liquid
zig-zag
g
~ 8T
Chiral spin
liquid ?
H inplane

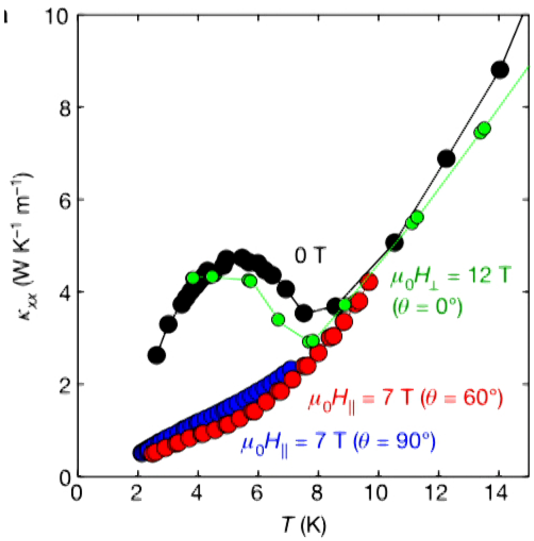

T
α-RuCl₃ ?
spin
liquid
zig-zag
g
$\sim 8T$
Chiral spin
liquid ?
$H_{\rm inplane}$
Polarized
paramagnet ?



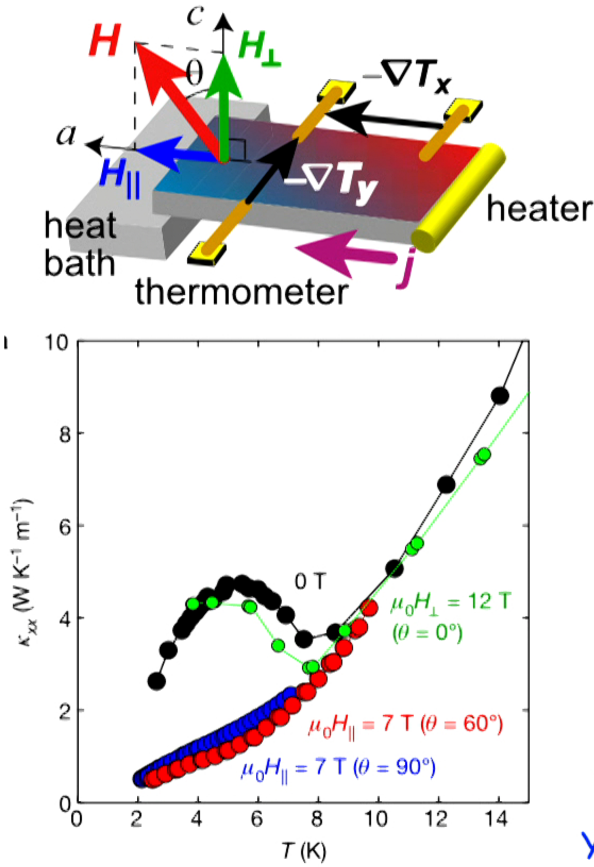
C. Hickey, S. Trebst (2018)
L. Zou, Y.-C. He (2018)
H.-C. Jiang, C.-Y. Wang, B. Huang, Y.-M. Lu (2018)
(AF-Kitaev, 111 magnetic field)

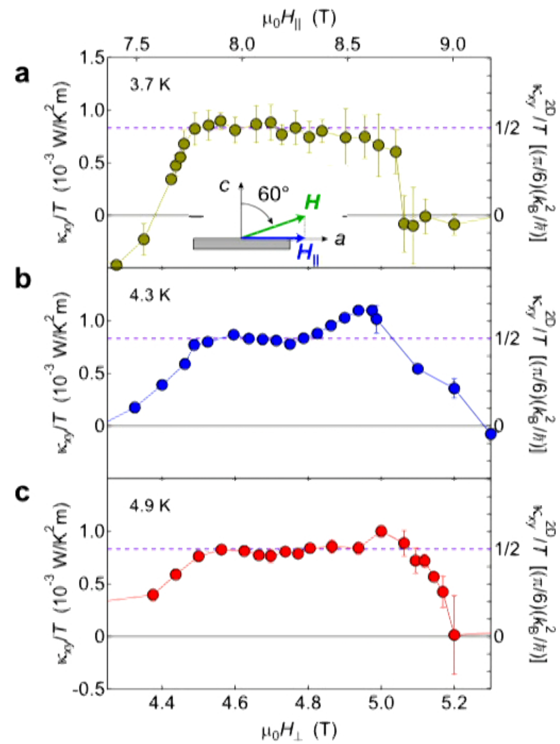
Field-induced Paramagnet: Spin Liquid ?





Field-induced Paramagnet: Spin Liquid ?

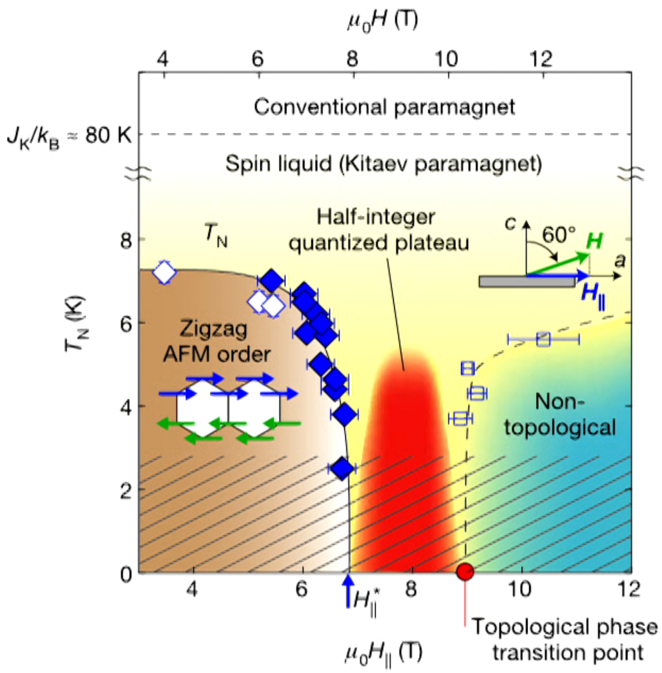


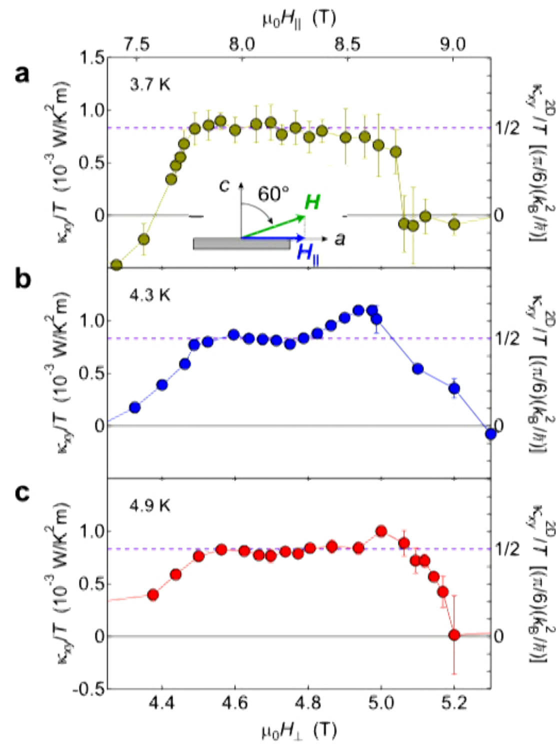


Quantized Thermal Hall Conductivity

Y. Kasahara, … Y. Matsuda et al. (2017, 2018)

Field-induced Paramagnet: Spin Liquid ?





$$\kappa_{xy}^{2D}/T = q(\pi/6)(k_B^2/\hbar)$$
$$q = 1/2$$

Quantized Thermal Hall Conductivity

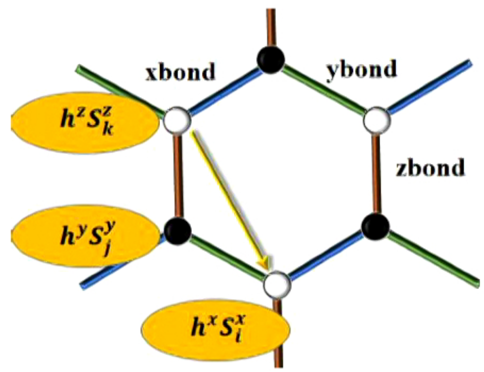
Y. Kasahara, ... Y. Matsuda et al. (2017, 2018)

Chiral spin liquid in magnetic field

A. Kitaev (2006)   Non-abelian quasiparticles, gapped bulk

$$\mathcal{H}_Z = -2\sum_{i,\alpha} S_i^\alpha h^\alpha,$$

$$\mathcal{H}^{(3)} \sim -\frac{8h^x h^y h^z}{K^2}\sum_{i,j,k} S_i^x S_j^y S_k^z,$$



Majorana mass gap $\Delta_0 \sim 4h^x h^y h^z/K^2$

Majorana chiral edge mode

$$\kappa_{xy}^{2D}/T = q(\pi/6)(k_B^2/\hbar) \quad q = 1/2$$

half-quantization
in thermal Hall conductivity

Too good to be true ?

1) Very small Hall angle

$$\frac{\kappa_{xy}}{\kappa_{xx}} \sim 10^{-3}$$

Much larger bulk thermal conduction

Presumably due to phonons

Bulk and edge not well separated ?

Too good to be true ?

1) Very small Hall angle

$$\frac{\kappa_{xy}}{\kappa_{xx}} \sim 10^{-3}$$

Much larger bulk thermal conduction

Presumably due to phonons

Bulk and edge not well separated ?

M. Ye, G. Halasz, L. Savary, L. Balents (2018)

Y. Vinkler-Aviv, A. Rosch (2018)

Majorana mode and phonons can exchange energy at the edge

Coupling between Majorana and phonons help to make the Hall effect observable

Quantization is good w.r.t. phonon temperature

Too good to be true ?

2) Other significant interactions

$$H = \sum_{\langle\langle\langle ij \rangle\rangle\rangle} J_3^{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{\langle ij \rangle,\gamma} K^\gamma S_i^\gamma S_j^\gamma + \sum_{\langle ij \rangle,\gamma} \sum_{\alpha,\beta\neq\gamma} \Gamma^\gamma [S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha]$$

Ab Initio Modeling

Bond	J_n	K_n	ξ_n	Γ_n	Γ'_n	ζ_n
X_1, Y_1	-1.4	**-7.5**	+0.2	**+5.9**	-0.8	+0.2
Z_1	-2.2	**-5.0**	–	**+8.0**	-1.0	–
X_2, Y_2	-0.1	-0.6	+0.1	+0.6	+0.6	+0.1
Z_2	+0.1	-0.9	–	+0.6	+0.3	–
X_3,Y_3	**+3.0**	-0.1	0.0	-0.1	-0.1	-0.1
Z_3	**+2.4**	+0.3	–	-0.1	-0.1	–

Nearest-Neighbour K < 0

Nearest-Neighbour Γ > 0

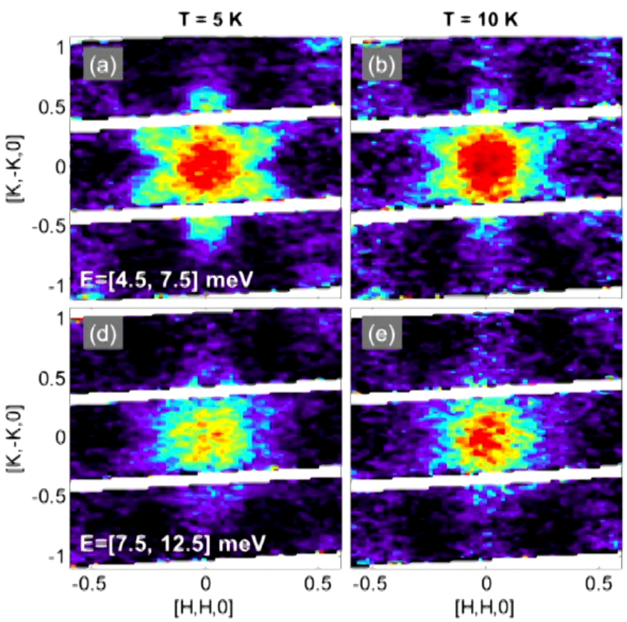
|K| ~ |Γ|

Third-Neighbour J_3 > 0

Zig-Zag magnetic order

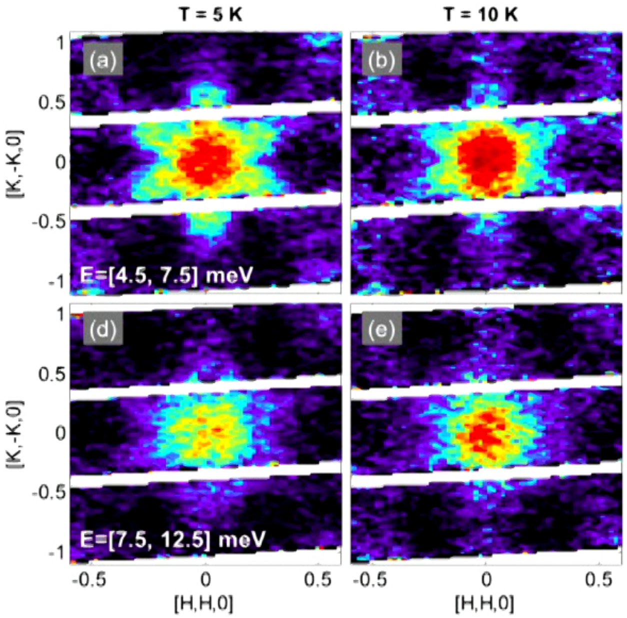
Winter, Li, Jeschke, Valenti (2016)

"Star Shape" continuum



A. Banerjee, S. Nagler et al. (2016)

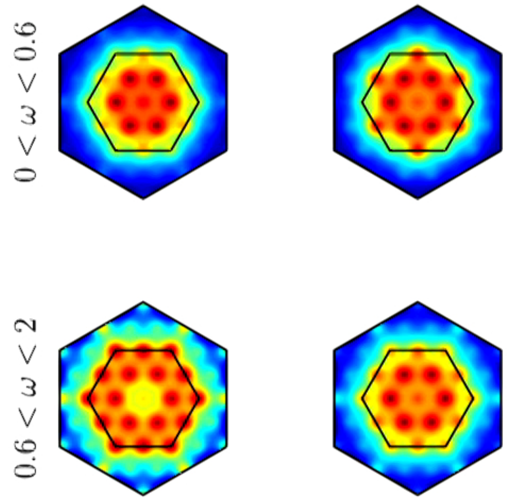
"Star Shape" continuum



A. Banerjee, S. Nagler et al. (2016)

Dynamical Structure Factor (K-Γ model, 24-site ED)

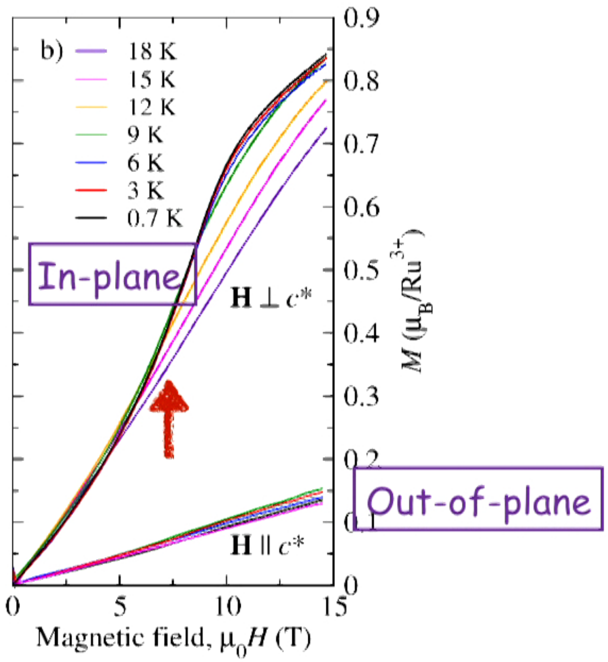
Kitaev model $\Gamma/|K| \sim 0.6$



$K < 0, \Gamma > 0$

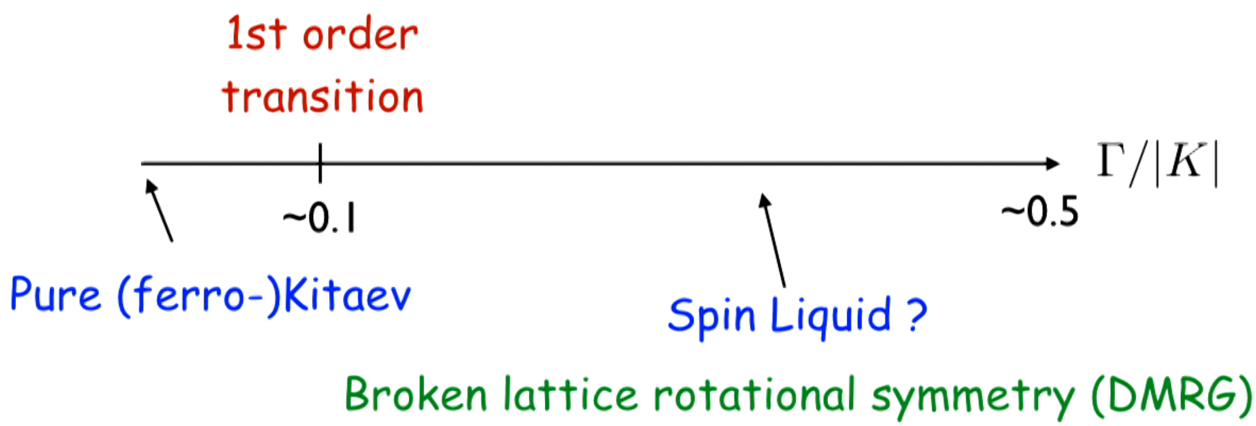
M. Gohlke, G. Wachtel,
Y. Yamaji, F. Pollmann, YBK, (2017)

Large magnetic anisotropy



Experiment [R. Coldea] (2015)

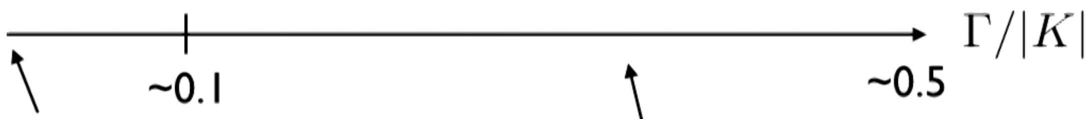
$$H = \sum_{\langle jk \rangle, \alpha\beta(\gamma)} K S_j^\gamma S_k^\gamma + \Gamma (S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha)$$



M. Gohlke, G. Wachtel, Y. Yamaji, F. Pollmann, YBK, (2017)

$$H = \sum_{\langle jk \rangle, \alpha\beta(\gamma)} K S_j^\gamma S_k^\gamma + \Gamma (S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha)$$

1st order transition



Pure (ferro-)Kitaev

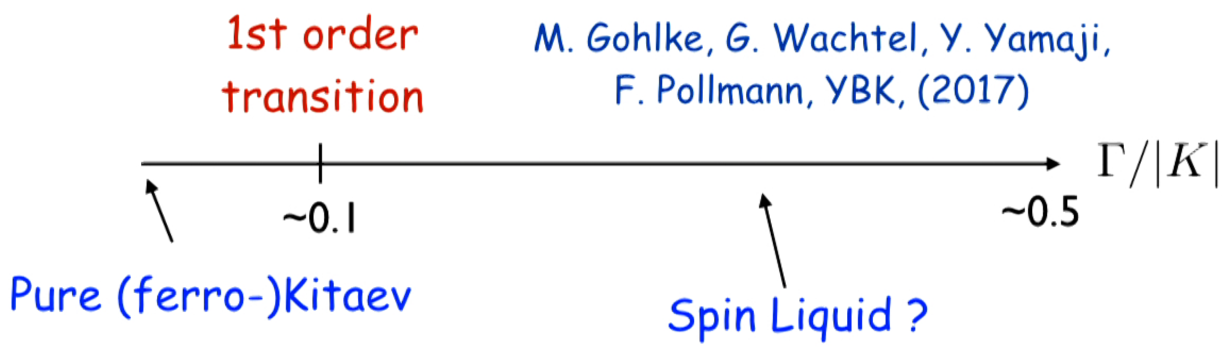
Spin Liquid ?

Broken lattice rotational symmetry (DMRG)

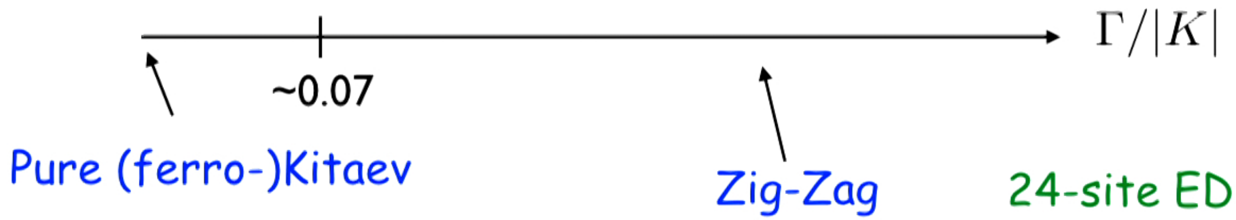
Addition of small J_3 leads to Zig-Zag order for $\Gamma/|K| > 0.1$

M. Gohlke, G. Wachtel, Y. Yamaji, F. Pollmann, YBK, (2017)

$$H = \sum_{\langle jk \rangle, \alpha\beta(\gamma)} K S_j^\gamma S_k^\gamma + \Gamma(S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha)$$



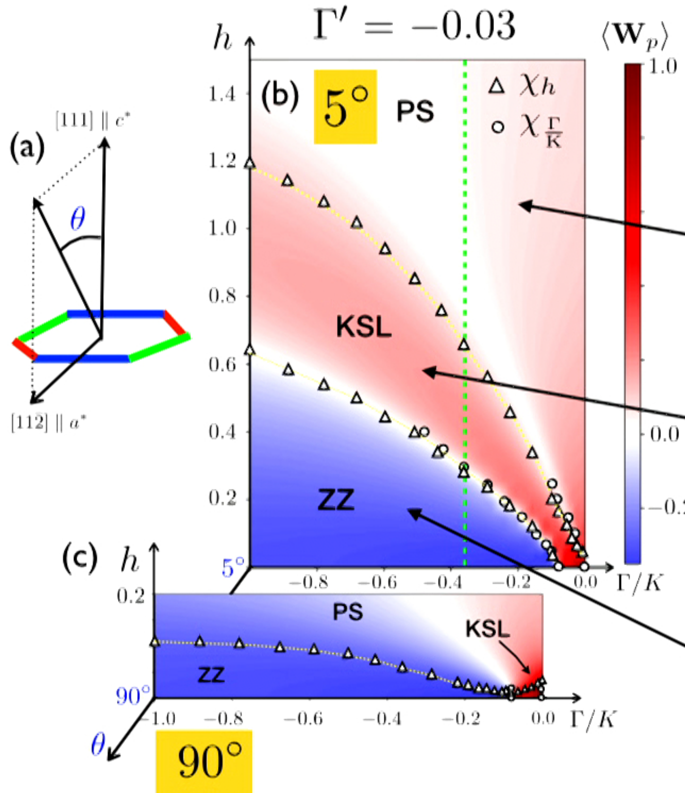
$$+\Gamma'(S_j^\alpha S_k^\gamma + S_j^\gamma S_k^\alpha + S_j^\beta S_k^\gamma + S_j^\gamma S_k^\beta) \qquad \Gamma' = -0.03$$



J. S. Gordon, A. Catuneabum E. S. Sorensen, H.-Y.Kee (2019)

$$H = \sum_{\langle jk \rangle, \alpha\beta(\gamma)} K S_j^\gamma S_k^\gamma + \Gamma(S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha) + \Gamma'(S_j^\alpha S_k^\gamma + S_j^\gamma S_k^\alpha + S_j^\beta S_k^\gamma + S_j^\gamma S_k^\beta)$$

can arise due to trigonal distortion



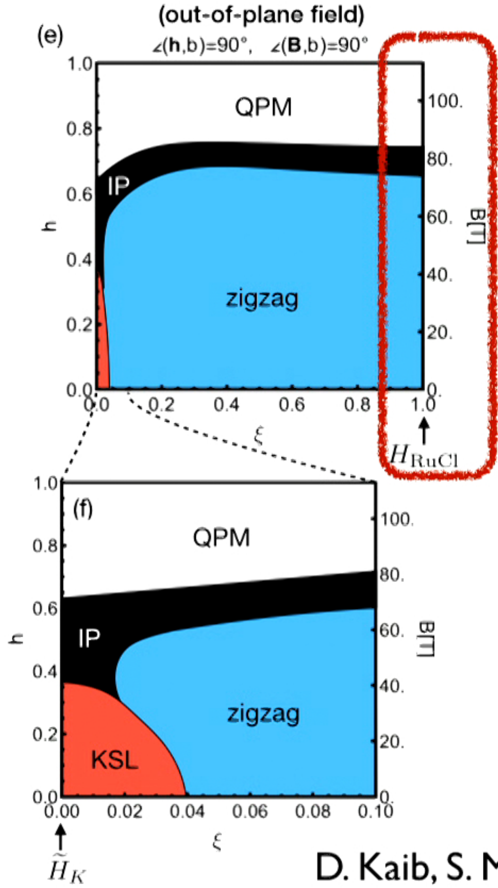
Polarized paramagnet

Chiral spin liquid ?

small Γ' induces Zig-Zag order

J. S. Gordon, A. Catuneau, E. S. Sorensen, H.-Y.Kee (2019)

In contrast, … Ab initio Model



[111] field (perpendicular to 2D plane)

24-site Exact Diagonalization

There is an intermediate phase

But it is not connected to the Kitaev (chiral) spin liquid

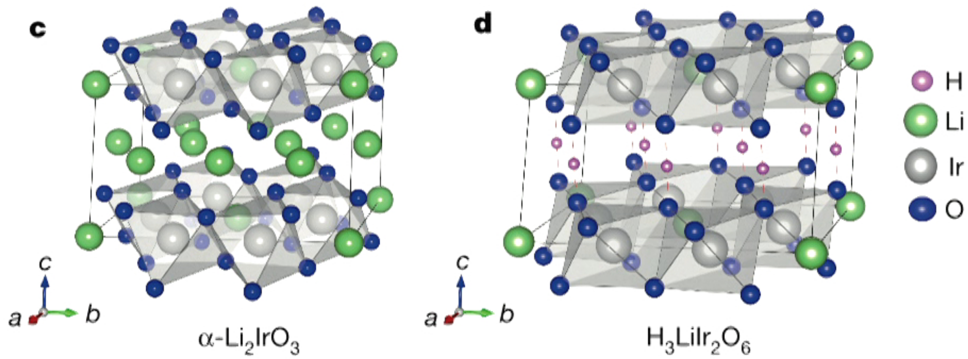
It disappears as soon as the magnetic field is tilted away from [111] direction

D. Kaib, S. M. Winter, and R. Valentí (2019), arXiv:1904.01025

15 FEBRUARY 2018 | VOL 554 | NATURE | 341

A spin–orbital–entangled quantum liquid on a honeycomb lattice

K. Kitagawa[1]*, T. Takayama[2]*, Y. Matsumoto[2], A. Kato[1], R. Takano[1], Y. Kishimoto[3], S. Bette[2], R. Dinnebier[2], G. Jackeli[2,4] & H. Takagi[1,2,4]



$$a = 5.1633(2)\mathring{A} \qquad a = 5.3489(8)\mathring{A}$$

$$b = 8.9294(3)\mathring{A} \qquad b = 9.2431(14)\mathring{A}$$

$$c = 5.1219(2)\mathring{A} \qquad c = 4.8734(6)\mathring{A}$$

enlogated a/b

Reduced interlayer spacing