Title: Field-driven spin liquids in Kitaev materials

Speakers: Simon Trebst

Series: Condensed Matter

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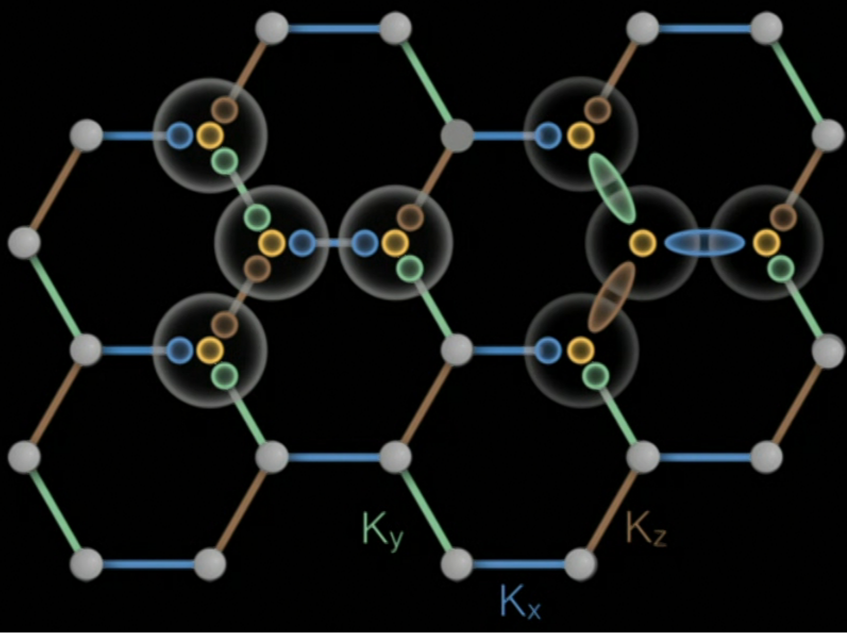
Abstract: Kitaev materials â€” spin-orbit assisted Mott insulators, in which local, spin-orbit entangled j=1/2 moments form that are subject to strong bond-directional interactions â€” have attracted broad interest for their potential to realize spin liquids. Experimentally, a number of 4d and 5d systems have been widely studied including the honeycomb materials Na2IrO3, Î±-Li2IrO3, and RuCl3 as candidate spin liquid compounds â€” however, all of these materials magnetically order at sufficiently low temperatures. In this talk, I will discuss the physics of Kitaev materials that plays out when applying magnetic fields. Experiments on RuCl3 indicate the formation of a chiral spin liquid that gives rise to an observed quantized thermal Hall effect. Conceptually, this asks for a deeper understanding of the physics of the Kitaev model in tilted magnetic fields. I will report on our recent numerical studies that give strong evidence for a Higgs transition from the well known Z2 topological spin liquid to a gapless U(1) spin liquid with a spinon Fermi surface and put this into perspective of experimental studies.

Field-driven phenomena in two-dimensional Kitaev materials

Perimeter Institute
May 2019



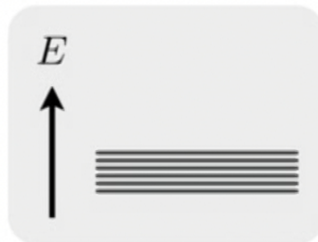
Simon Trebst
University of Cologne

CRC 1238
Control and Dynamics of Quantum Materials

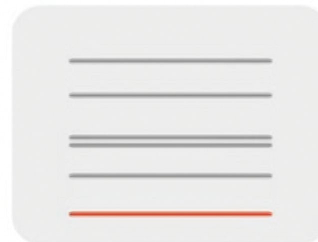
When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of **'accidental' degeneracies**.

interacting
many-body system



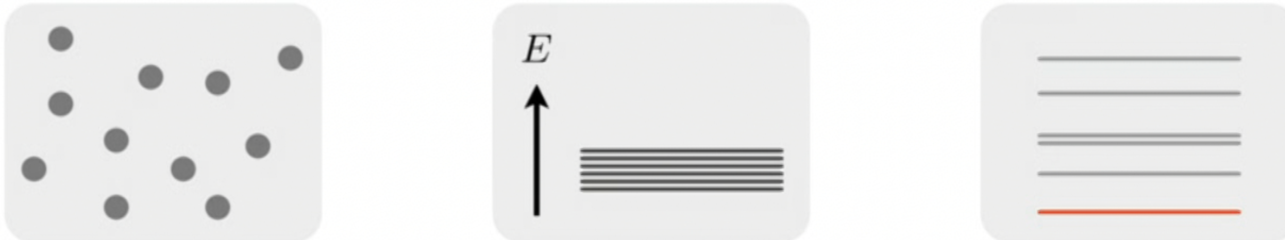
'accidental'
degeneracy



residual effects
select ground state

When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of **‘accidental’ degeneracies**.

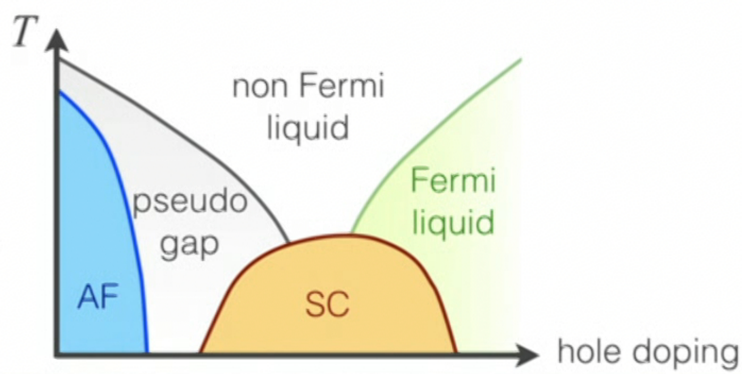


interacting **many-body system**

‘accidental’ **degeneracy**

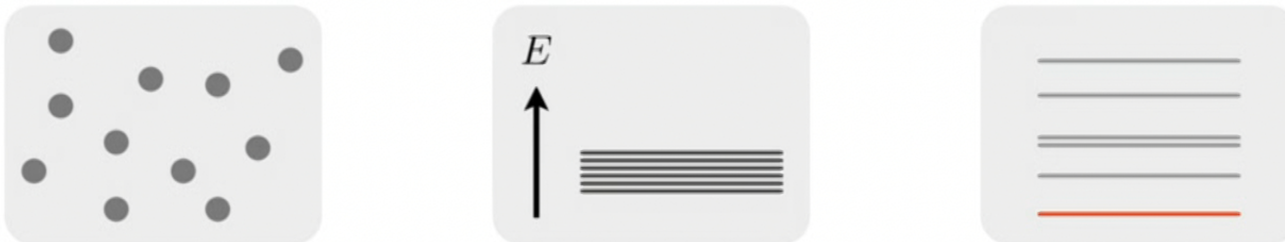
residual effects select ground state

phase diagram of cuprate superconductors



When do interesting things happen?

Some of the most intriguing phenomena in condensed matter physics arise from the splitting of **'accidental' degeneracies**.

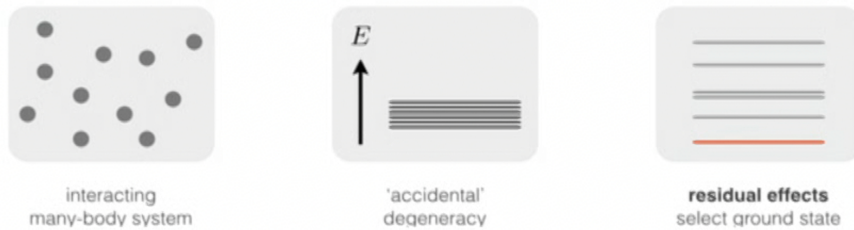


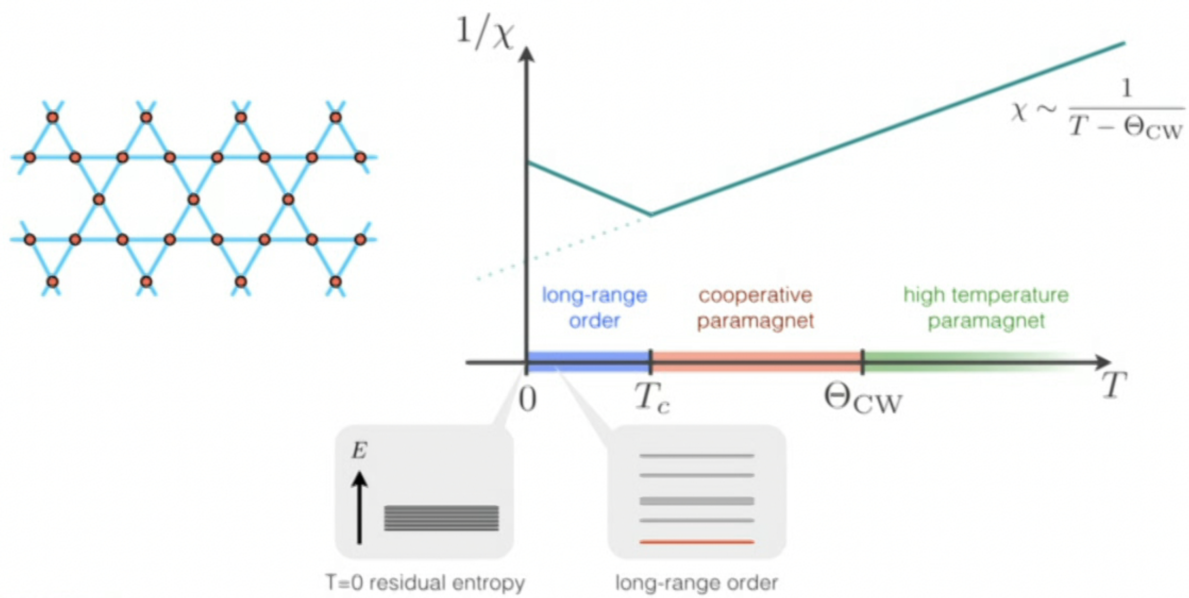
interacting **many-body system** | 'accidental' **degeneracy** | **residual effects** select ground state

But they are also **notoriously difficult** to handle, due to

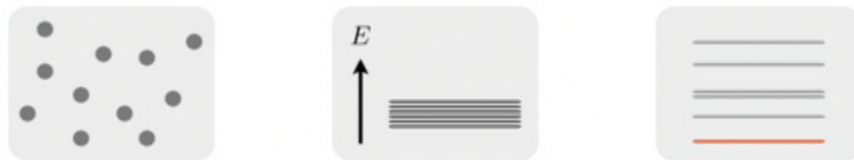
- multiple energy scales
- complex energy landscapes / slow equilibration
- strong coupling
- macroscopic entanglement

Example – frustrated magnets



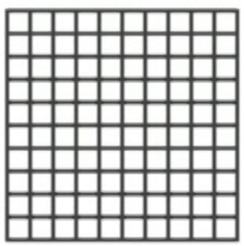


Example – quantum Hall liquids



interacting many-body system | 'accidental' degeneracy | **residual effects** select ground state

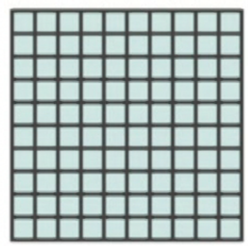
Landau level **degeneracy**



$2\Phi/\Phi_0$

orbital states

integer quantum Hall

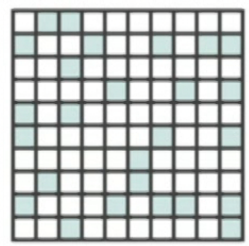


filled level

↓

incompressible liquid

fractional quantum Hall

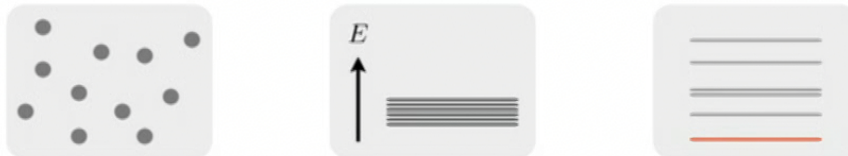


partially filled level

↓ Coulomb repulsion

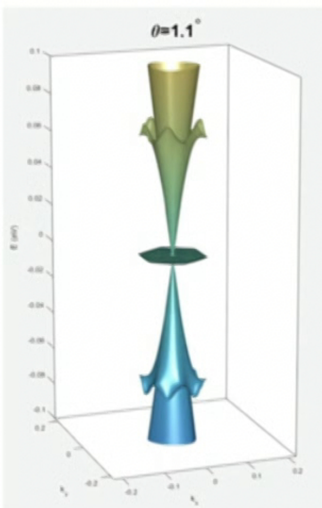
incompressible liquid

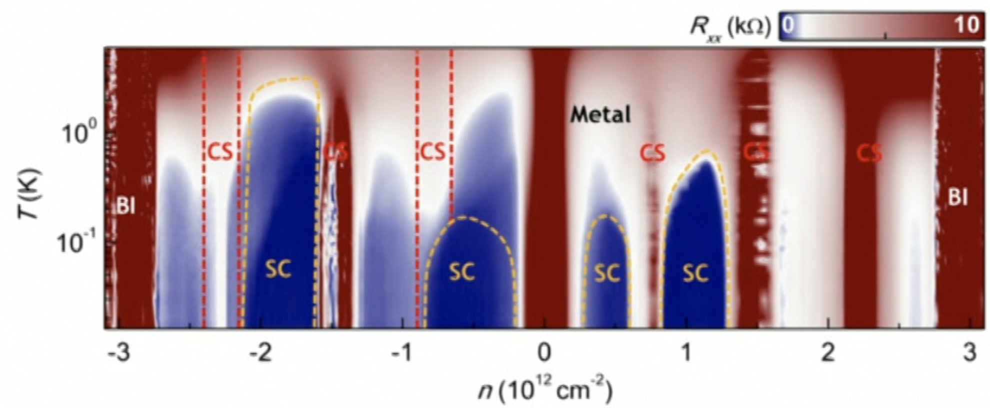
Example – twisted bilayer graphene



interacting many-body system | 'accidental' degeneracy | **residual effects** select ground state

electronic band structure with a **flat band** in twisted bilayer graphene





Efetov group, arXiv:1903.06513

Jarillo-Herrero group, Nature **556**, 43 (April 2018)

Fractionalization

One often concurrent phenomenon in quantum many-body systems is the **emergence of quasiparticles** with **fractional** quantum numbers.

Fractionalization

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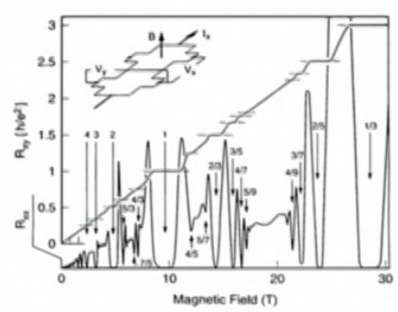
electron fractionalization

Quantum Hall liquids



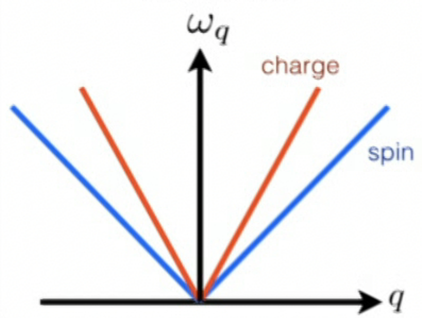
2D

Fractionalization

One often concurrent phenomenon in quantum many-body systems is the **emergence of quasiparticles** with **fractional** quantum numbers.

spin-charge separation

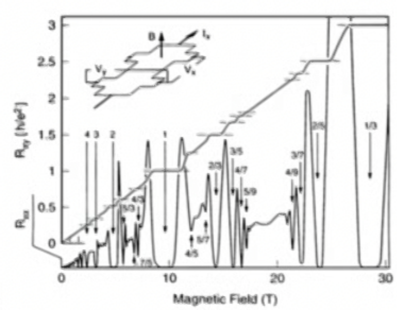
1D metals



1D

electron fractionalization

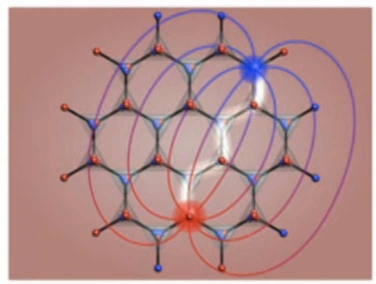
Quantum Hall liquids



2D

magnetic monopoles

Spin ice

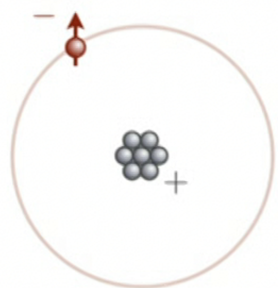


3D

spin-orbit materials

Spin-orbit coupling

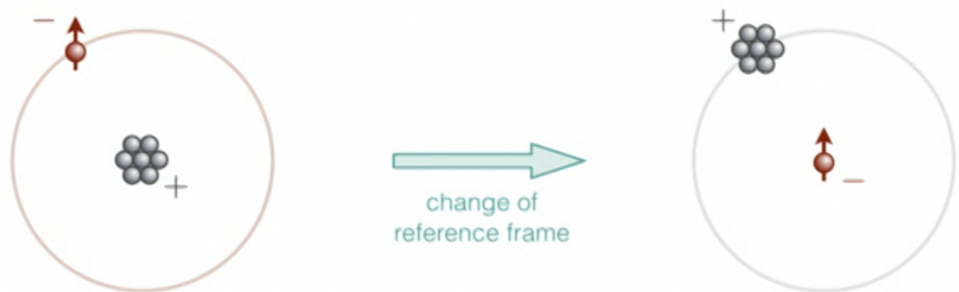
Spin-orbit coupling 101 – quantum mechanics lecture



relativistic correction

Spin-orbit coupling

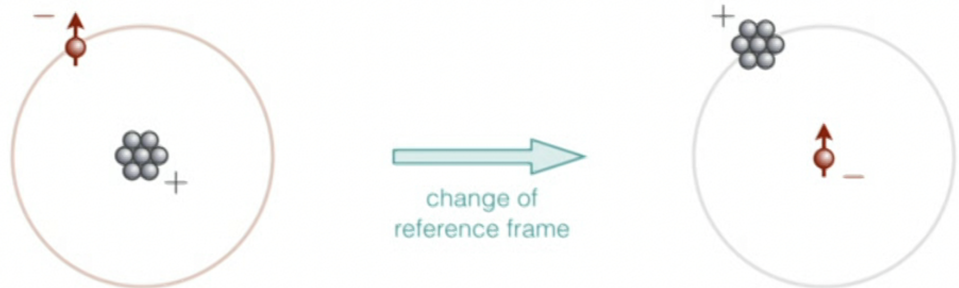
Spin-orbit coupling 101 – quantum mechanics lecture



relativistic correction

Spin-orbit coupling

Spin-orbit coupling 101 – quantum mechanics lecture

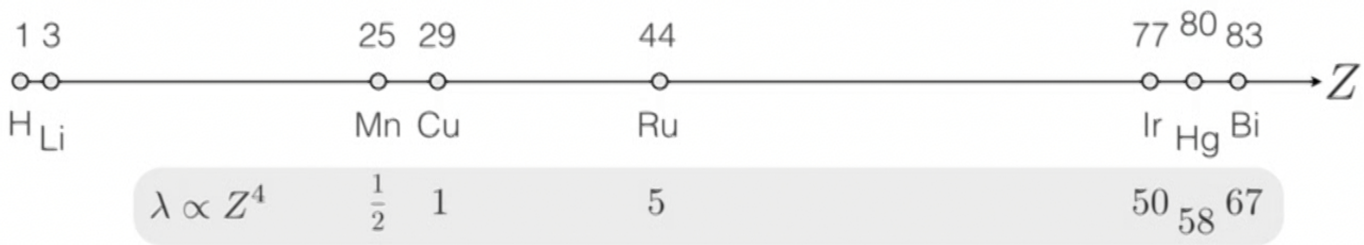


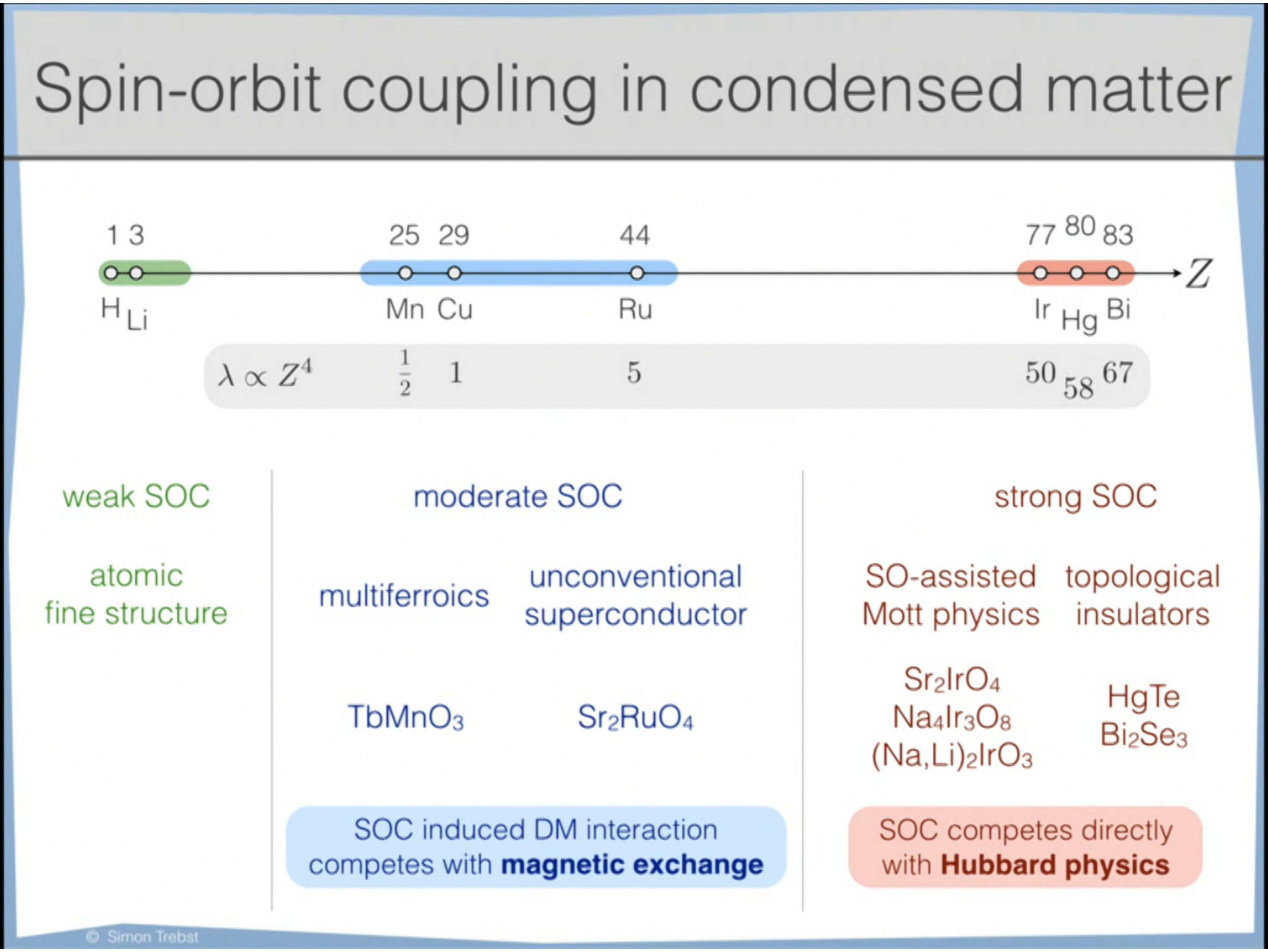
relativistic correction

$$\Delta E = \frac{\lambda}{\hbar^2}\,\vec{l}\cdot\vec{s} = \frac{\lambda}{2}\left[j(j-1) - l(l-1) - s(s-1)\right]$$

$$\lambda = \frac{Ze^2\mu_0\hbar^2}{8\pi m_e^2 r^3} \qquad r \propto 1/Z \qquad \lambda \propto Z^4$$

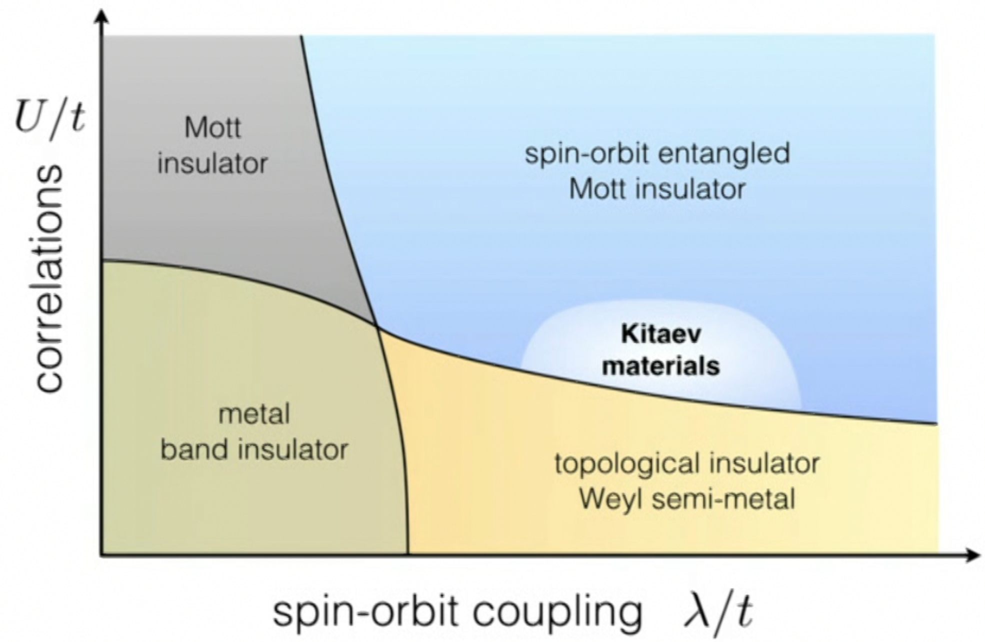
Spin-orbit coupling in condensed matter




Spin-orbit coupling in condensed matter
1 3
25 29
44
77 80 83
Z
H Li
Mn Cu
Ru
Ir Hg Bi
$\lambda \propto Z^4$ $\frac{1}{2}$ 1 5 50 58 67
weak SOC
atomic fine structure
moderate SOC
multiferroics
unconventional superconductor
$TbMnO_3$
Sr_2RuO_4
SOC induced DM interaction competes with **magnetic exchange**
strong SOC
SO-assisted Mott physics
topological insulators
Sr_2IrO_4
$Na_4Ir_3O_8$
$(Na,Li)_2IrO_3$
HgTe
Bi_2Se_3
SOC competes directly with **Hubbard physics**
© Simon Trebst

4d/5d transition metal compounds

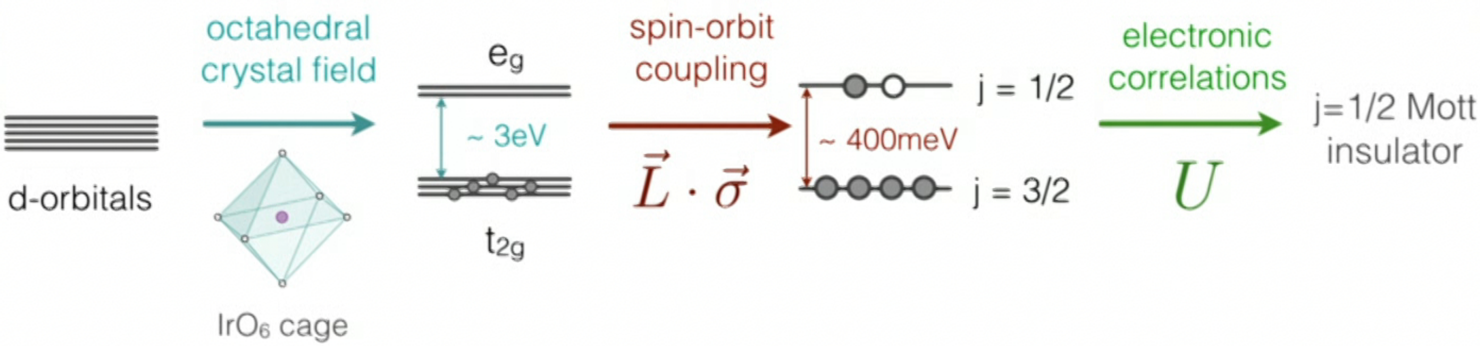
Transition metal oxides with **partially filled 4d/5d shells** exhibit an intricate interplay of **spin-orbit coupling**, **electronic correlations**, and **crystal field effects** resulting in a **broad variety of metallic and insulating states**.



W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Annual Review of Condensed Matter Physics 5, 57 (2014).

j=1/2 Mott insulators

most common **Iridium valence** Ir^{4+} $(5d^5)$

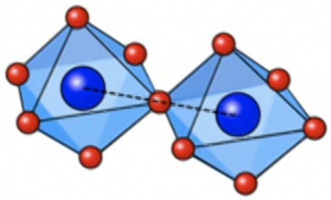


Why are these spin-orbit entangled j=1/2 Mott insulators **interesting?**

spin-orbit entangled Mott insulators

Why are these spin-orbit entangled j=1/2 Mott insulators **interesting?**

corner-sharing

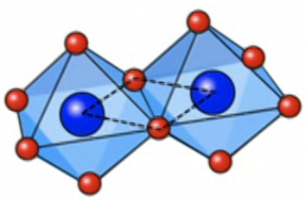


Sr_2IrO_4

exhibits cuprate-like magnetism
superconductivity?

B.J. Kim et al. PRL 101, 076402 (2008)
B.J. Kim et al. Science 323, 1329 (2009)

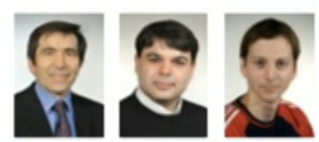
edge-sharing



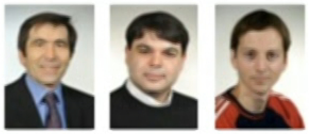
$(Na,Li)_2IrO_3$
$RuCl_3$
$H_2LiIr_2O_6$
Cu_2IrO_3
...

exhibit Kitaev-like magnetism
spin liquids?

G. Jackeli and G. Khaliullin, PRL 102, 017205 (2009)
J. Chaloupka, G. Jackeli, and G. Khaliullin, PRL 105, 027204 (2010)



bond-directional exchange



G. Jackeli and G. Khaliullin, PRL 102, 017205 (2009)
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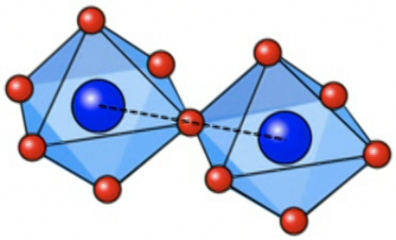
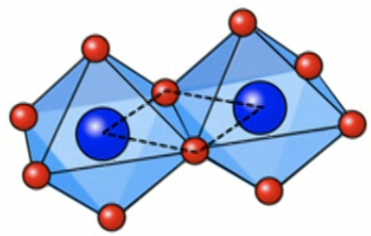
corner-sharing



Sr_2IrO_4

Heisenberg exchange

edge-sharing

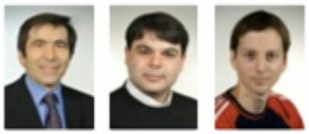


$(Na,Li)_2IrO_3$
$RuCl_3$

Heisenberg-Kitaev exchange

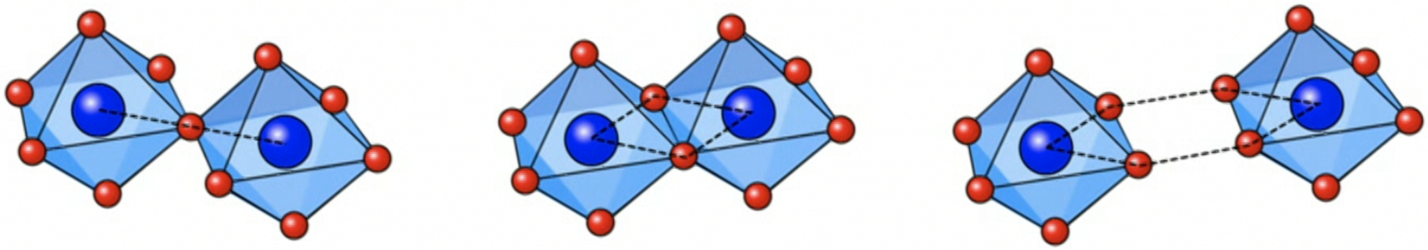
$$H = -\sum_{\gamma-\text{bonds}} J\,\mathbf{S}_i\mathbf{S}_j + K\,S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

bond-directional exchange



G. Jackeli and G. Khaliullin, PRL 102, 017205 (2009)
J. Chaloupka, G. Jackeli, and G. Khaliullin, PRL 105, 027204 (2010)

corner-sharing | **edge**-sharing | "**parallel edge**"-sharing



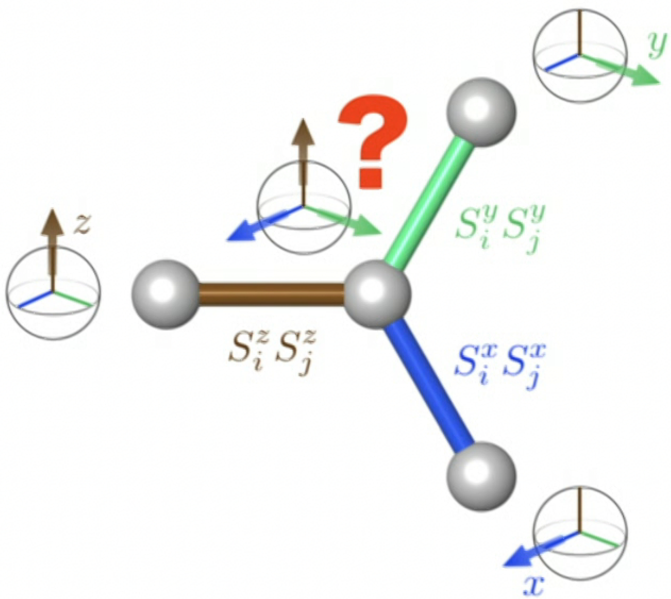
Sr_2IrO_4 | $(Na,Li)_2IrO_3$, $RuCl_3$ | $Ba_3IrTi_2O_9$

Heisenberg exchange | Heisenberg-Kitaev exchange

$$H = -\sum_{\gamma-\mathrm{bonds}} J\,\mathbf{S}_i\mathbf{S}_j + K\,S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

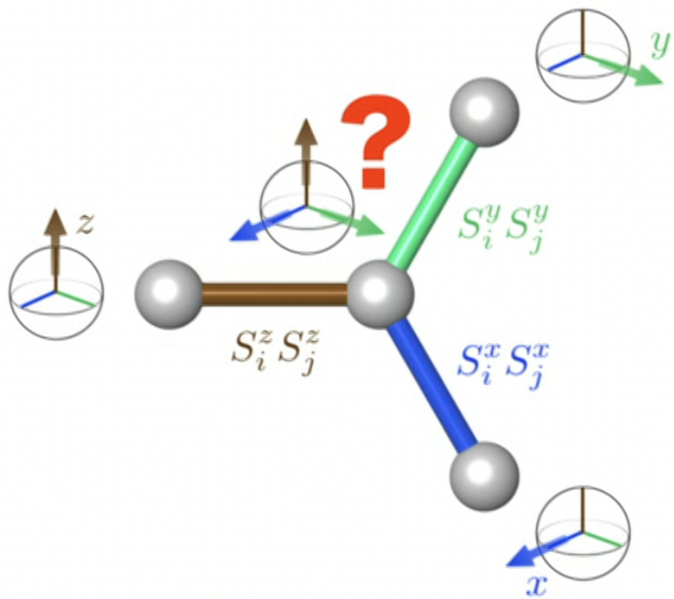
exchange frustration

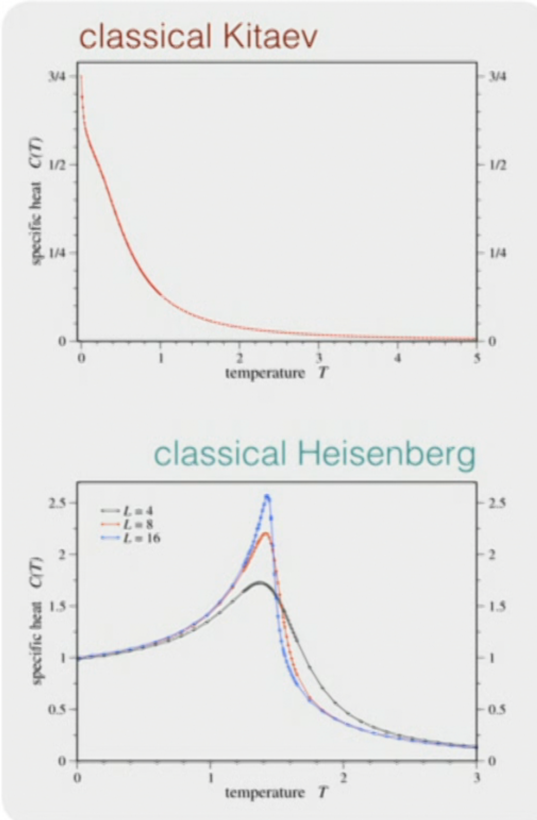
$$H = - \sum_{\gamma-\text{bonds}} J\, \mathbf{S}_i \mathbf{S}_j + K\, S_i^\gamma S_j^\gamma$$



exchange frustration

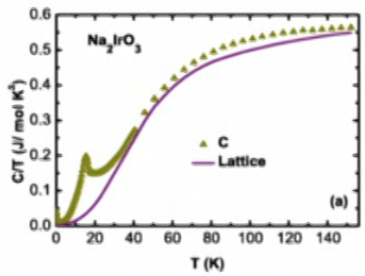
$$H = -\sum_{\gamma-\text{bonds}} J\,\mathbf{S}_i\mathbf{S}_j + K\; S_i^\gamma S_j^\gamma$$



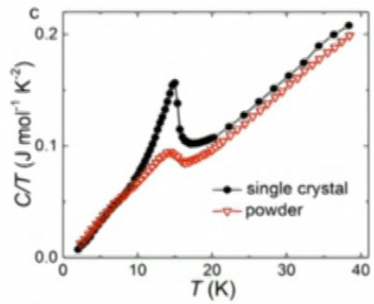


Kitaev materials – really?

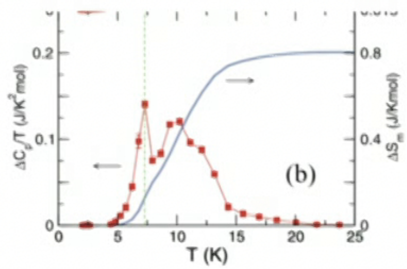
Na_2IrO_3



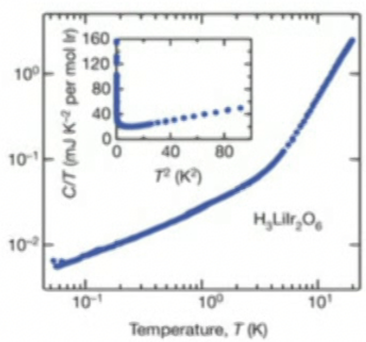
Li_2IrO_3



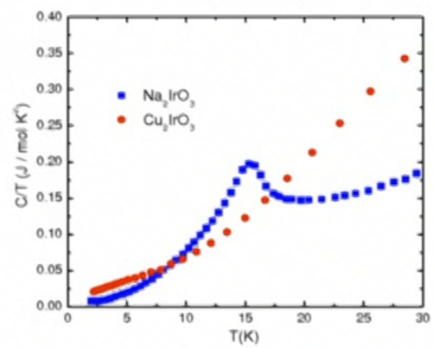
$RuCl_3$



$H_2LiIr_2O_6$



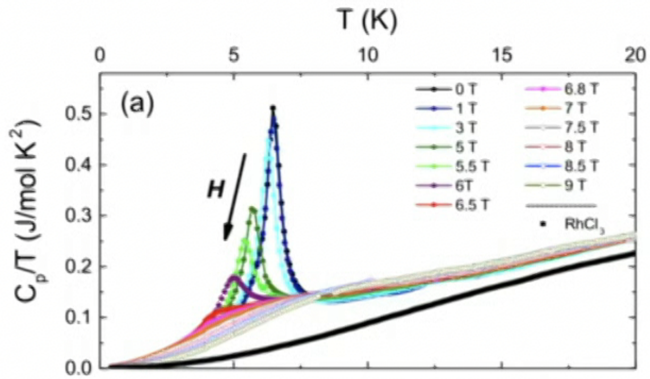
Cu_2IrO_3



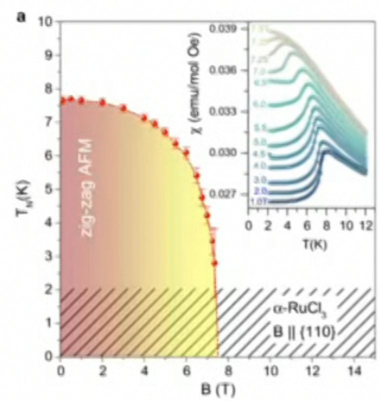
Candidate materials tend to exhibit **magnetic ordering** at low T.

Spin liquids?!

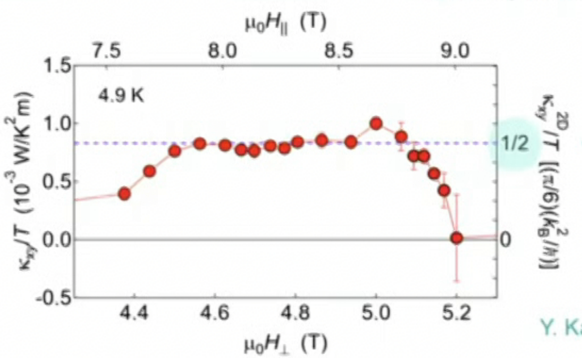
Something interesting happens for **$RuCl_3$ in a magnetic field**.



A. U. B. Wolter et al., PRB **96**, 041405(R) (2017)



A. Banerjee et al., npj Quantum Mater. **3**, 8 (2018)

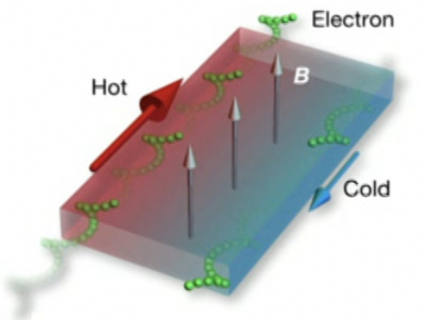


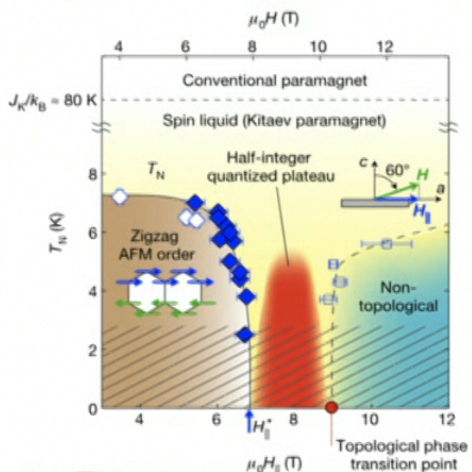
half-integer quantized
thermal Hall effect

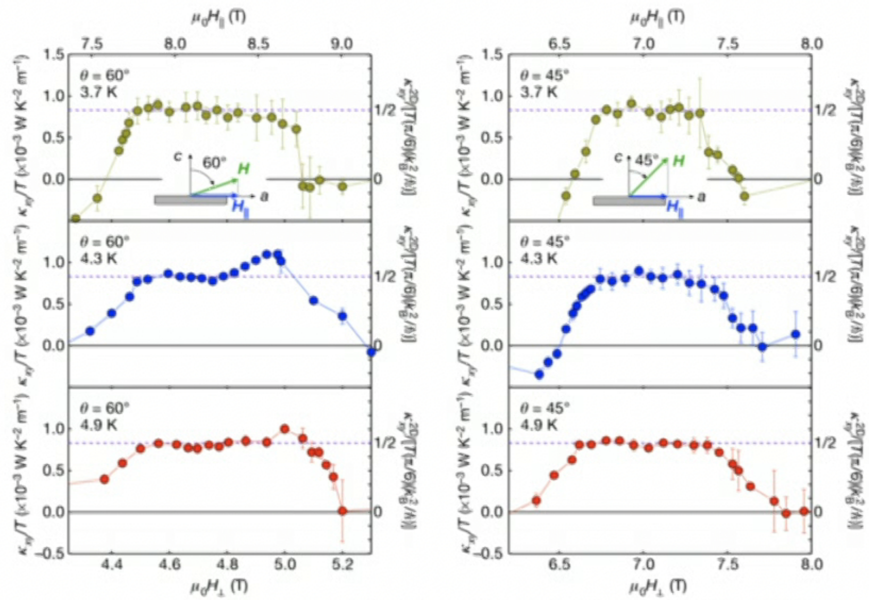
Y. Kasahara et al., Nature **559**, 227-231 (2018)

quantum Hall 4.0

Something interesting happens for **$RuCl_3$ in a magnetic field**.







Y. Kasahara et al., Nature **559**, 227-231 (2018)

Why does this work in the presence of phonons?

Y. Vinkler-Aviv & A. Rosch, PRX **8**, 031032 (2018)

M. Ye, G. Halász, L. Savary, and L. Balents, PRL **121**, 147201 (2018)

Kitaev spin liquids

magnetic field effects

Ciarán Hickey

Kitaev spin liquids

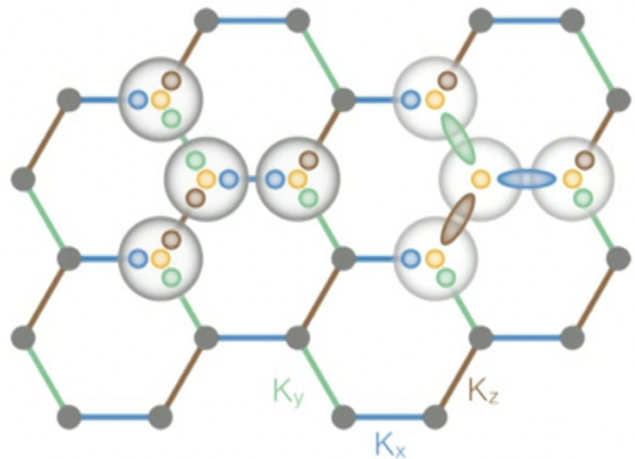
magnetic field effects

Kitaev model

$$\mathcal{H} = - \sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$

Represent spins in terms of four **Majorana fermions**

$$S_i^\gamma = i \; c_i \; c_i^\gamma$$



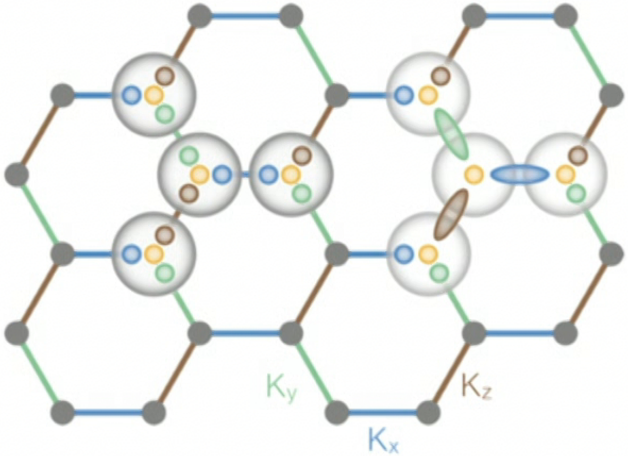
Kitaev model

$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$

Represent spins in terms of four **Majorana fermions**

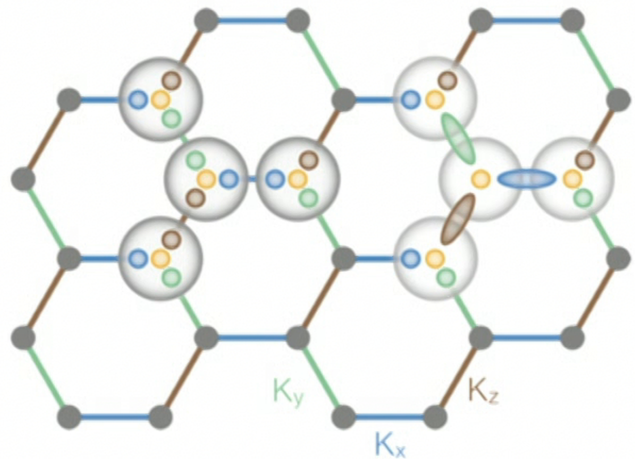
$$S_i^\gamma = i \; c_i \; c_i^\gamma$$

$$S_i^\alpha \to S_i^\alpha \qquad c_i^\alpha \to e^{-i\phi_i} c_i^\alpha \qquad c_i \to e^{i\phi_i} c_i$$



Kitaev model

$$\mathcal{H} = - \sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$



Represent spins in terms of four **Majorana fermions**

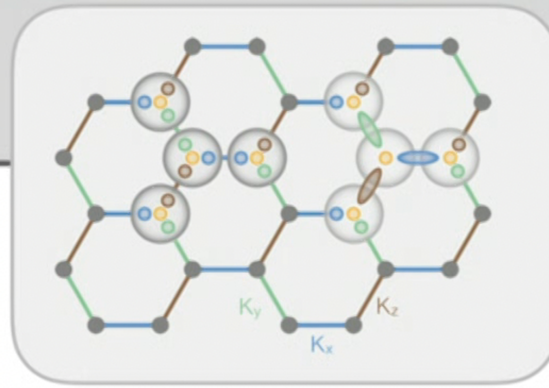
$$S_i^\gamma = i \; c_i \; c_i^\gamma$$

$$S_i^\alpha \to S_i^\alpha \qquad c_i^\alpha \to e^{-i\phi_i} c_i^\alpha \qquad c_i \to e^{i\phi_i} c_i$$

$$(c_i)^2 = 1 \to (e^{i\phi_i} c_i)^2 = 1 \qquad e^{i\phi_i} = \pm 1$$

Z_2 redundancy

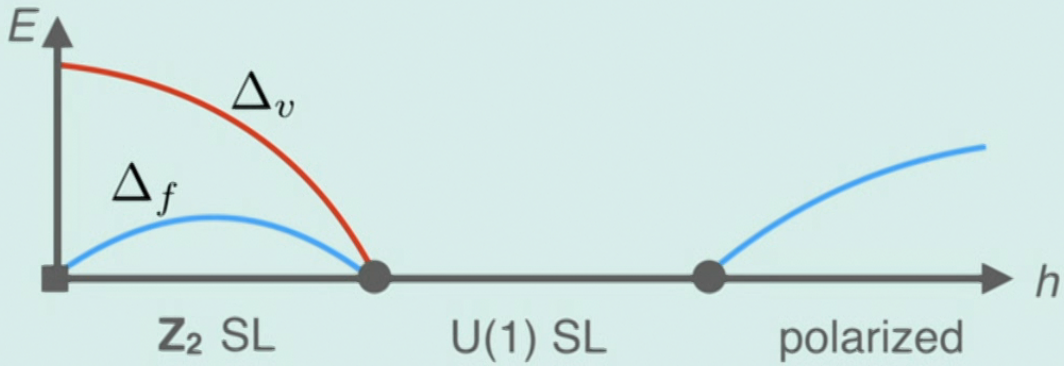
Kitaev spin liquids



$$\mathcal{H} = - \sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$

Kitaev spin liquids are textbook examples of **$\mathbf{Z_2}$ spin liquids.**

For strong magnetic fields, this picture no longer holds.
The Kitaev model exhibits a **gauge transition** to a **U(1) spin liquid.**



Kitaev model – magnetic field effects

$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

Z. Zhu, I. Kimchi, D.Sheng, & L. Fu,
PRB **97**, 241110 (2018)

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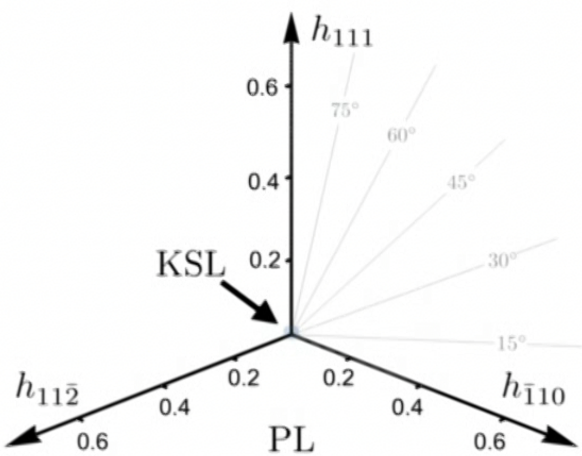
FM Kitaev coupling



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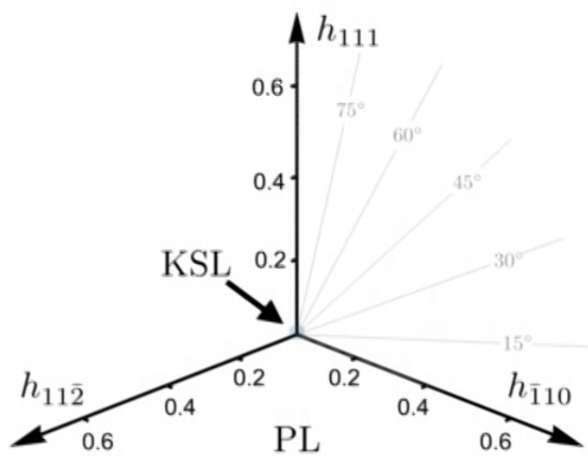
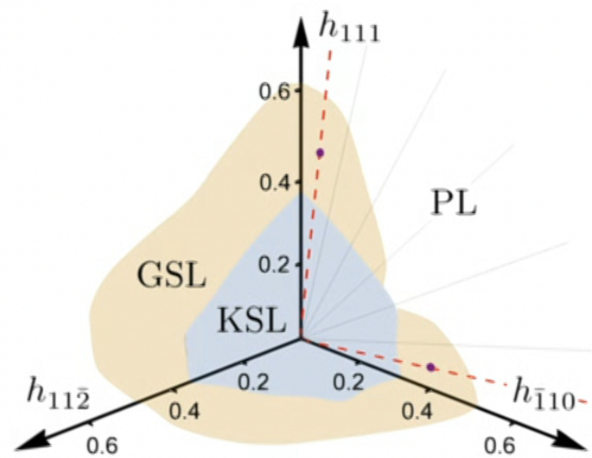
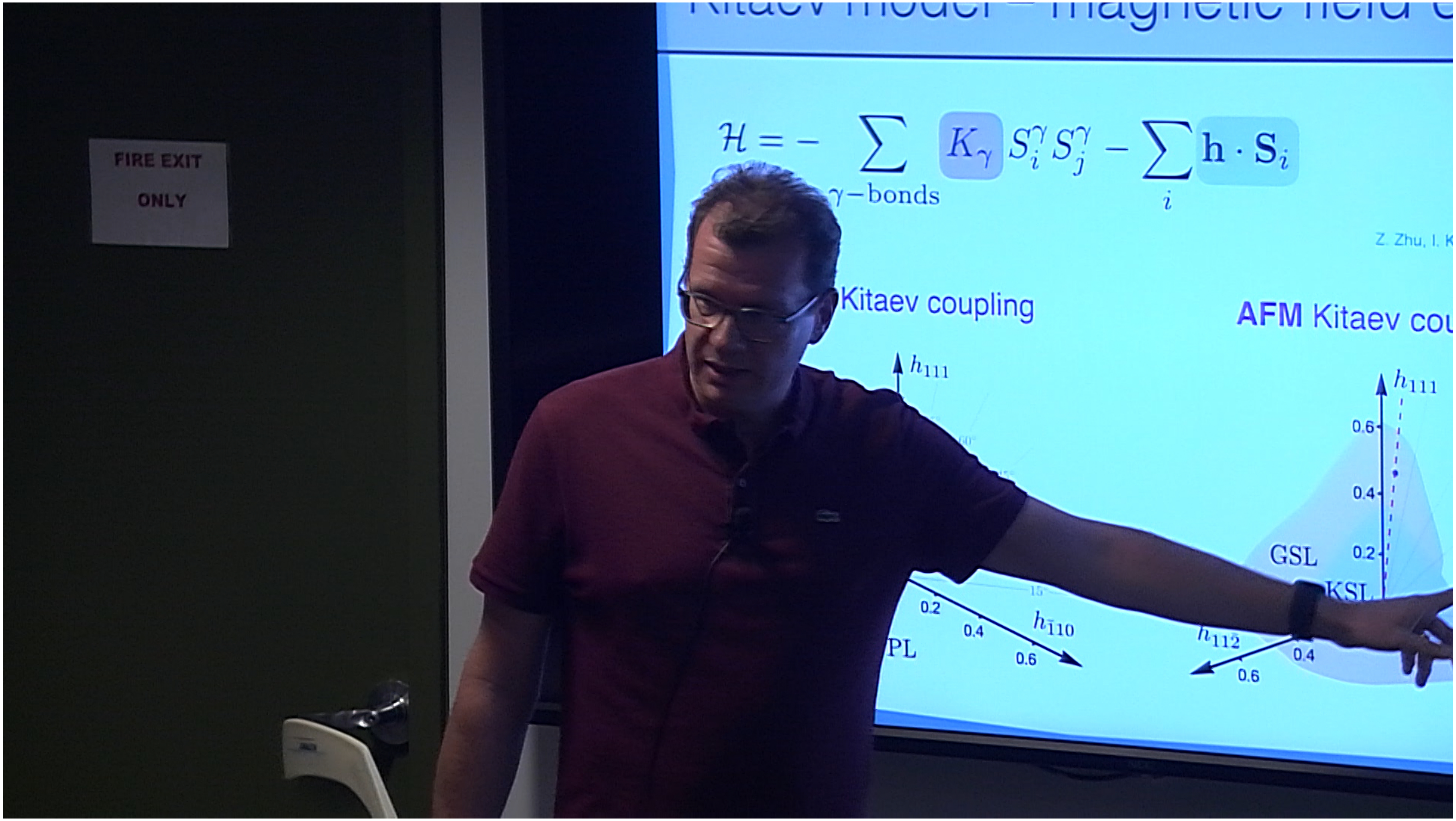


AFM Kitaev coupling




FIRE EXIT
ONLY
$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h}\cdot\mathbf{S}_i$
Z. Zhu, I. K
Kitaev coupling
AFM Kitaev cou
h_{111}
$h_{\bar{1}10}$
$h_{11\bar{2}}$
GSL
KSL
PL
0.2
0.4
0.6

Kitaev model – magnetic field effects

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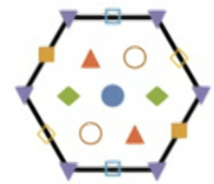
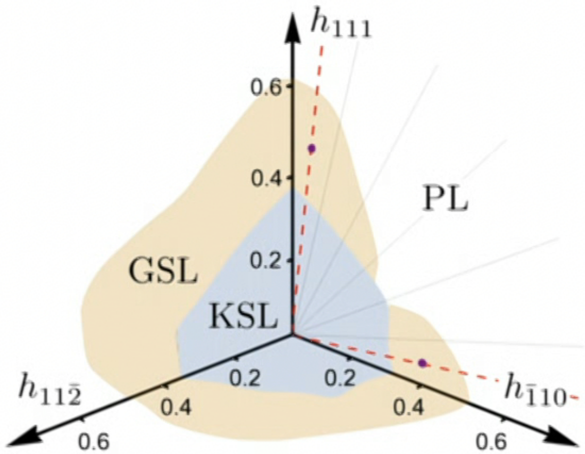
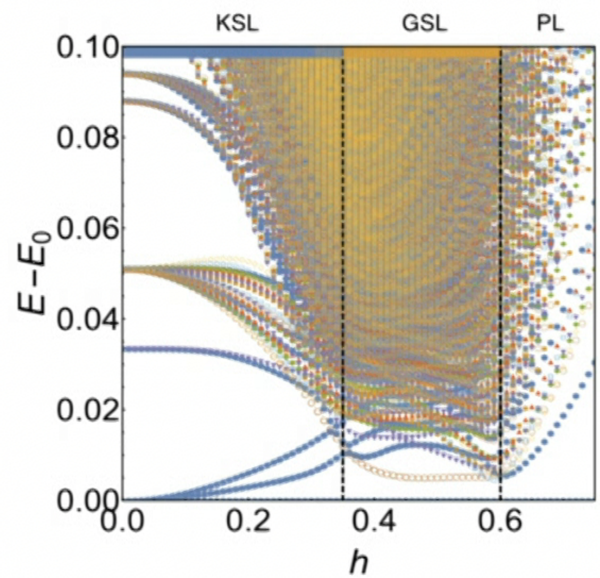


AFM Kitaev coupling





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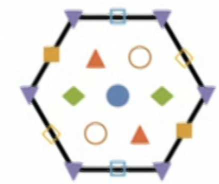

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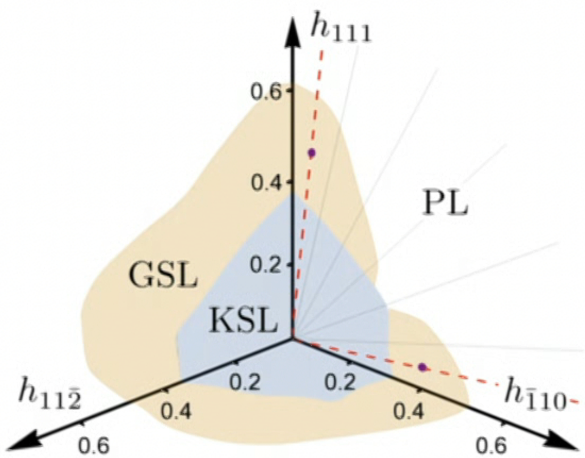

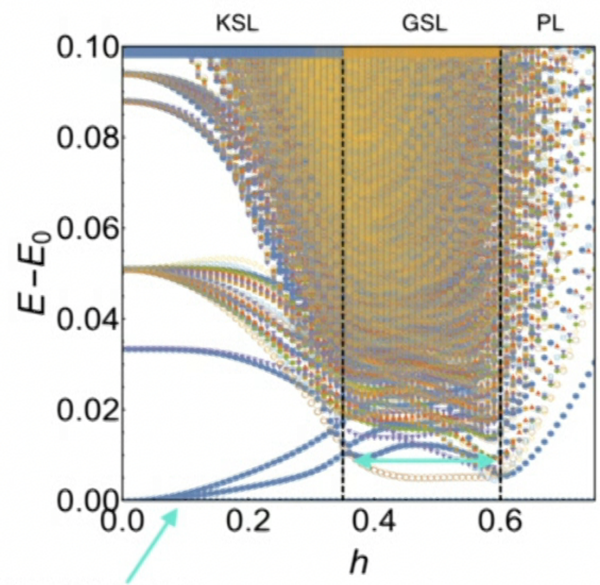

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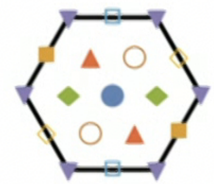

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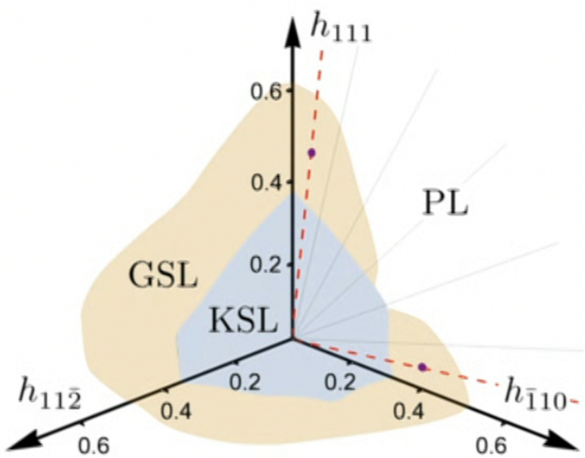

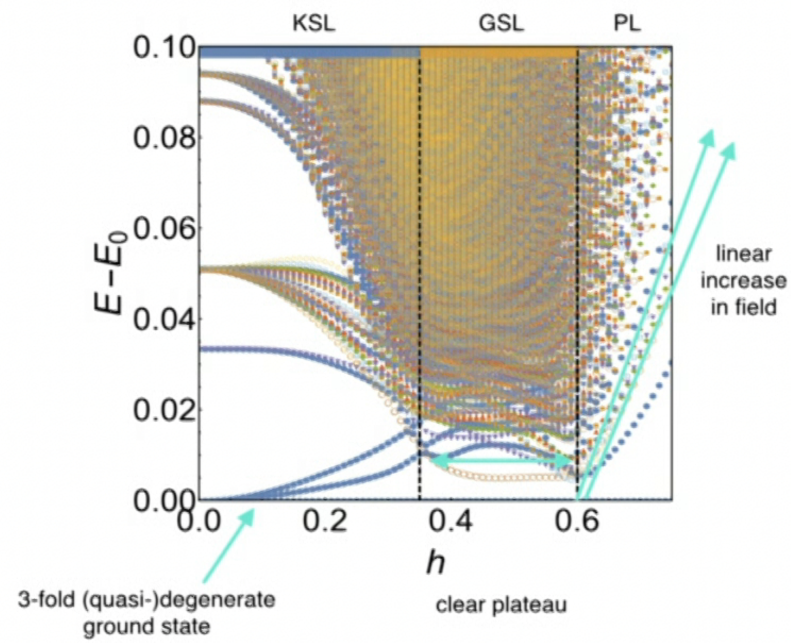

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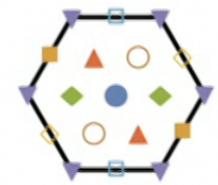


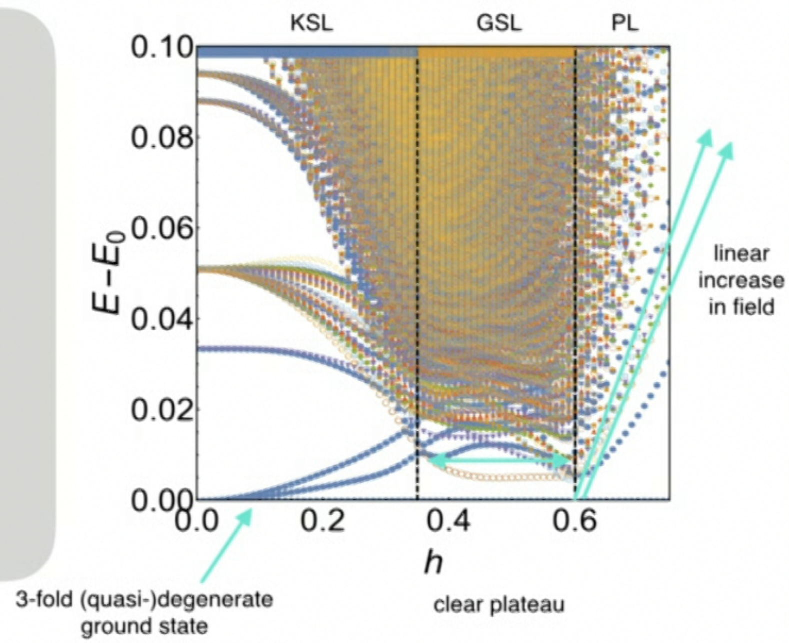
modular matrices

$$S = \begin{pmatrix} 0.50 & 0.71 & 0.50 \\ 0.71 & 0.00 & -0.71 \\ 0.50 & -0.71 & 0.50 \end{pmatrix}$$

Ising TQFT

$$S = \begin{pmatrix} 0.46 & 0.74 & 0.47 \\ 0.71 & 0.04e^{-0.91i} & -0.70 \\ 0.49 & -0.67e^{0.02i} & 0.58e^{-0.13i} \end{pmatrix}$$

numerical result



Kitaev model – magnetic field effects

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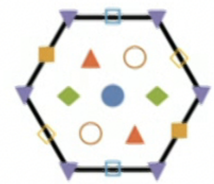
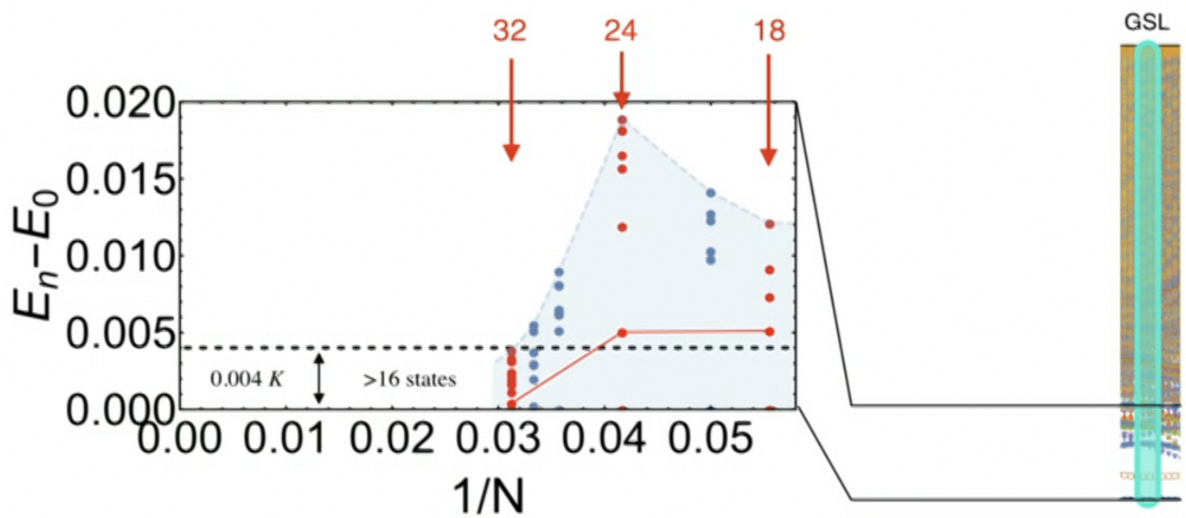
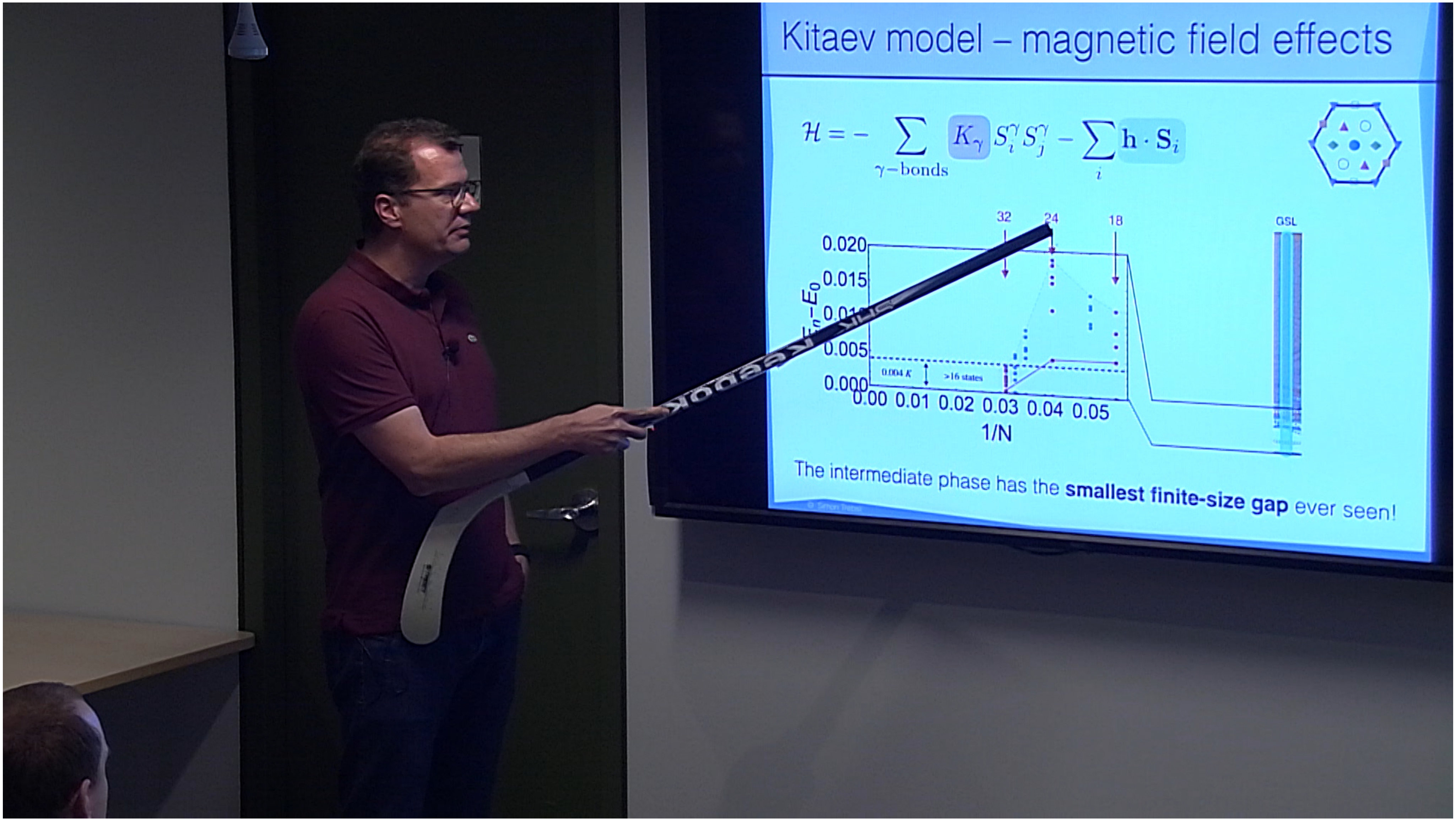




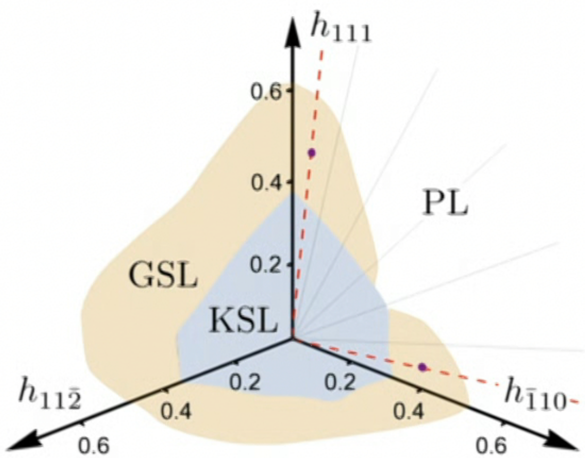
The intermediate phase has the **smallest finite-size gap** ever seen!

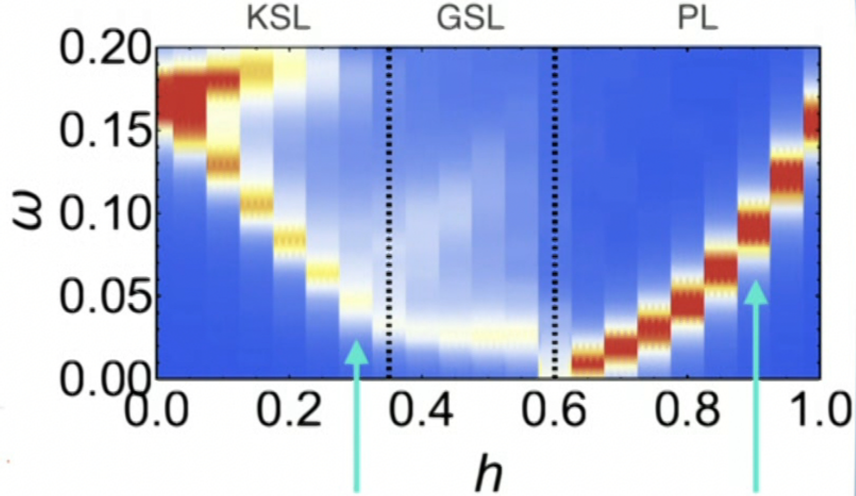

Kitaev model – magnetic field effects
$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$
32
24
18
GSL
0.020
0.015
0.005
0.000
0.004 K
>16 states
0.00 0.01 0.02 0.03 0.04 0.05
1/N
The intermediate phase has the **smallest finite-size gap** ever seen!

dynamical structure factor

$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

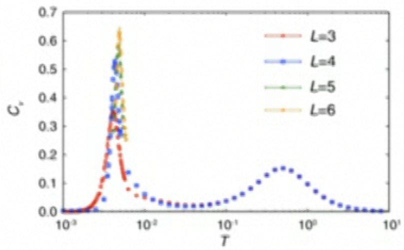
AFM Kitaev coupling

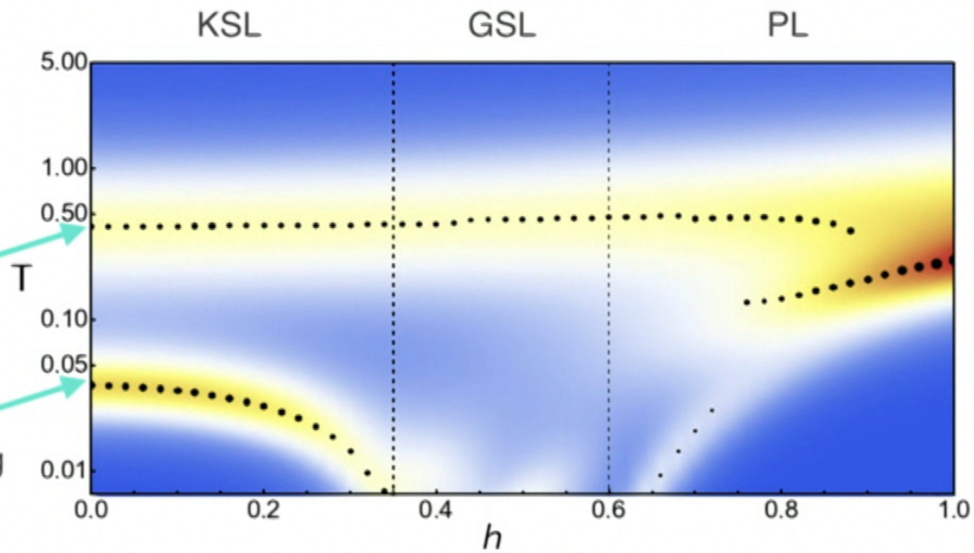




specific heat

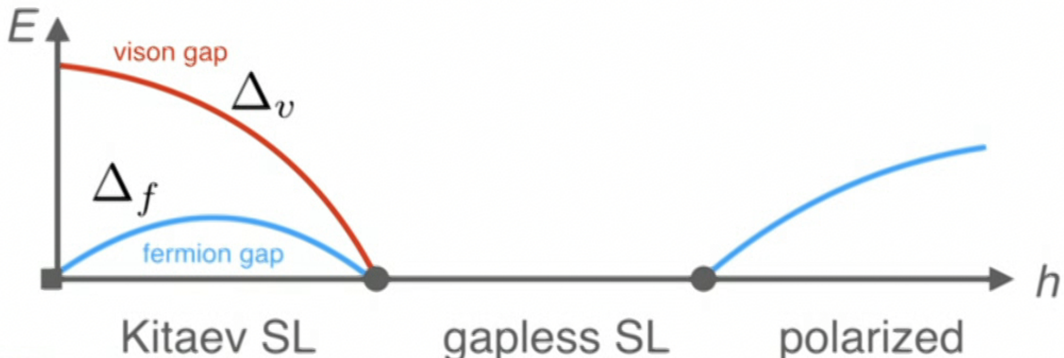
$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h}\cdot\mathbf{S}_i$$





Kitaev unHiggsed!

Synopsis: for strong magnetic fields, the Kitaev model exhibits a **Higgs transition** to a gapless U(1) spin liquid.



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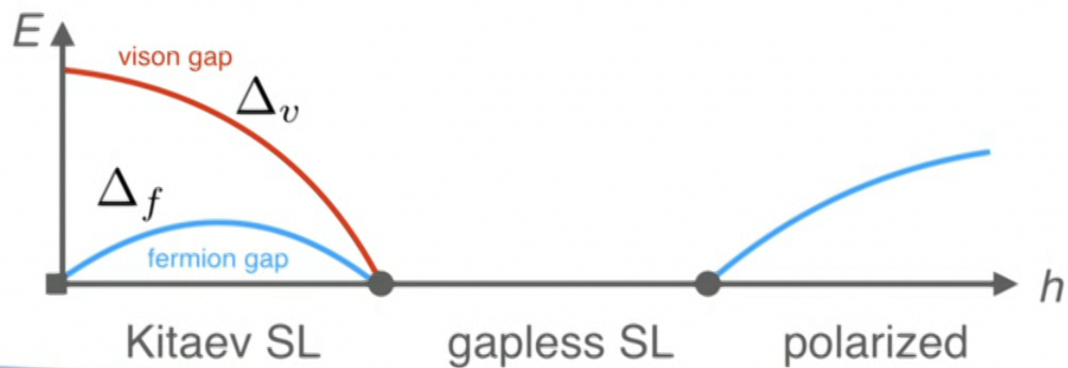
Represent spins in terms of **complex fermions** $S_i^\alpha = f_{i,\mu}^\dagger \sigma_{\mu\nu}^\alpha f_{i,\nu}$

F. J. Burnell and C. Nayak, PRB **84**, 125125 (2011)

fermions	gapped topological SC	gapless Fermi surface	gapped trivial insulator



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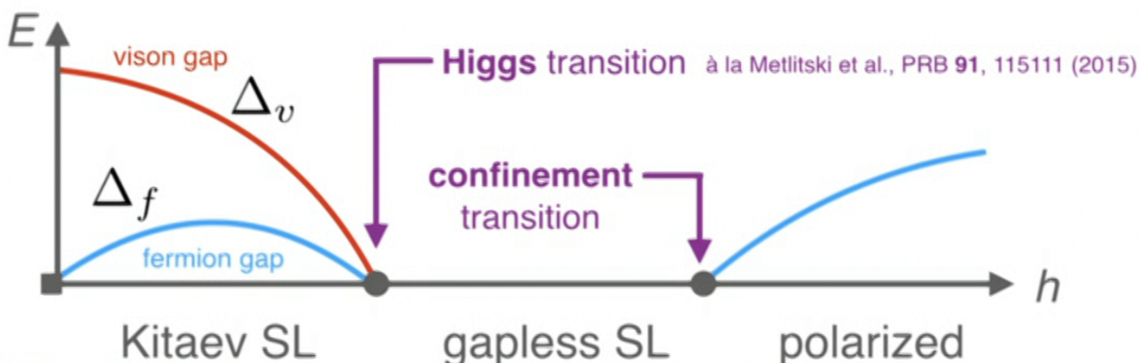
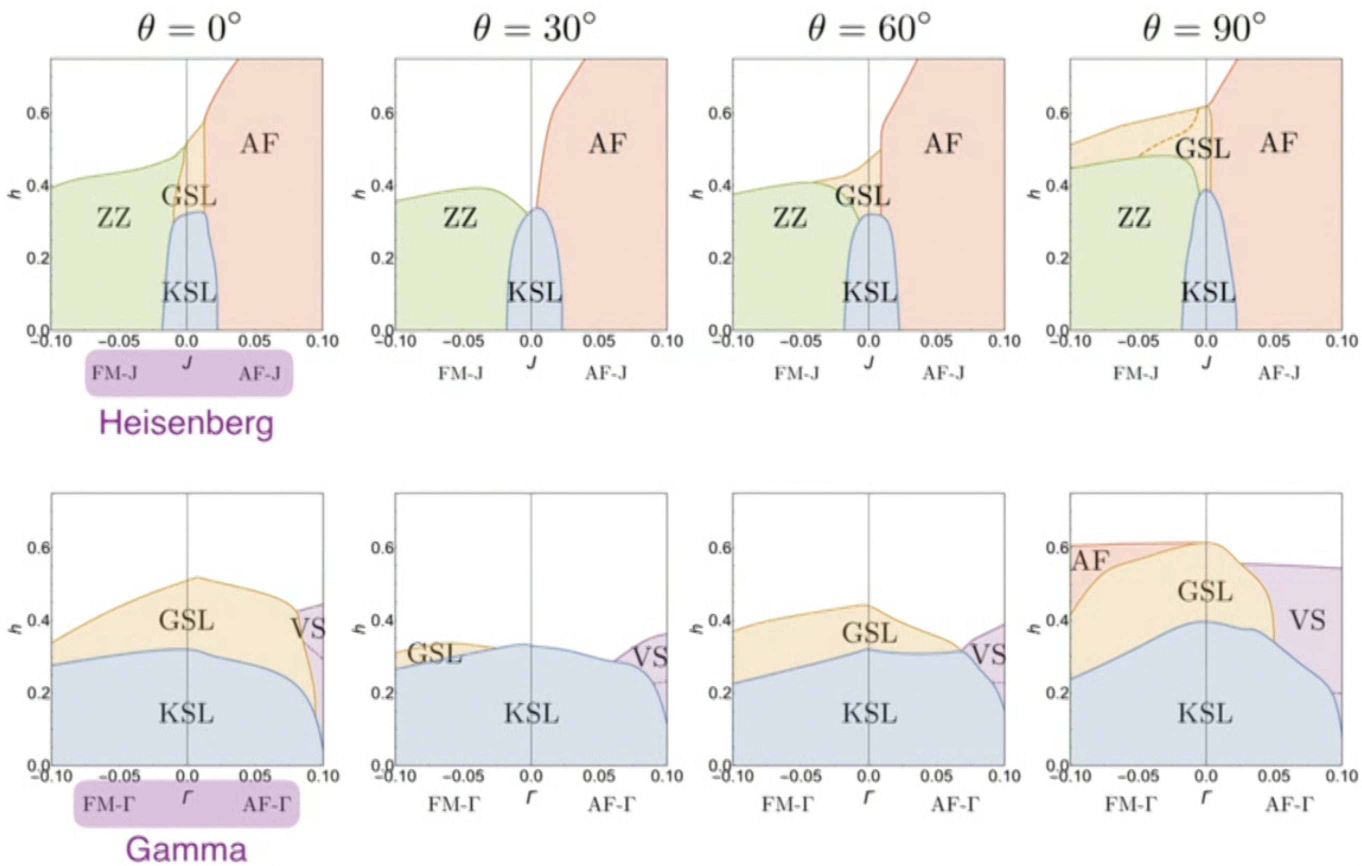
fermions	gapped topological SC	gapless Fermi surface	gapped trivial insulator
gauge field	Z_2 (Higgsed)	U(1)	U(1) [confined]



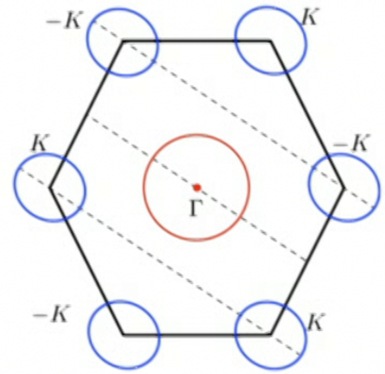
Stability of U(1) spin liquid



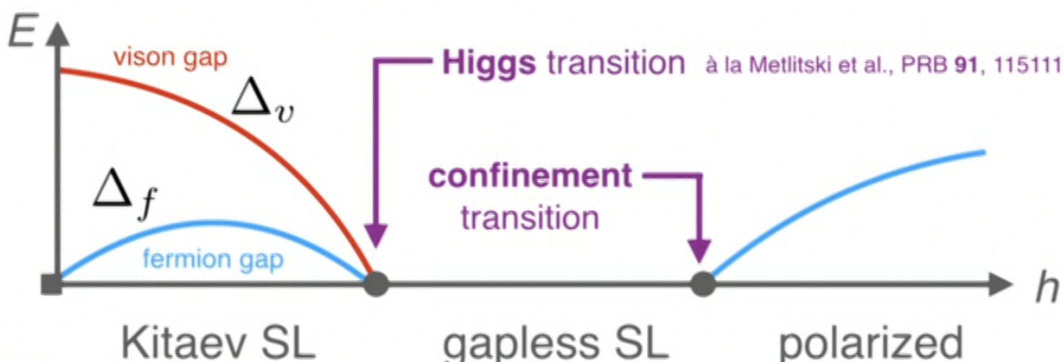
projective symmetry group (PSG)

State	$G_{\tilde{M}_h}(x_1, x_2, s)$	$G_{C_6}(x_1, x_2, s)$	Stable FS?
Kitaev Z_2	$(-1)^s e^{-\mathrm{i}\frac{\pi}{4}\tau_z}$	$(-1)^s e^{\mathrm{i}\frac{\pi}{3}\frac{\tau_x+\tau_y+\tau_z}{\sqrt{3}}}$	N/A
$U1A_{k=0}$	$e^{\mathrm{i}\frac{3\pi}{4}\tau_z}$	$e^{-\mathrm{i}\frac{\pi}{6}\tau_z}$	Yes
$U1B_{k=2}$	1	$\mathrm{i}\tau_x \cdot e^{\mathrm{i}\frac{\pi}{3}(1-2s)\tau_z}$	No
$U1B_{k=4}$	1	$\mathrm{i}\tau_x \cdot e^{\mathrm{i}\frac{\pi}{3}(2s-1)\tau_z}$	No

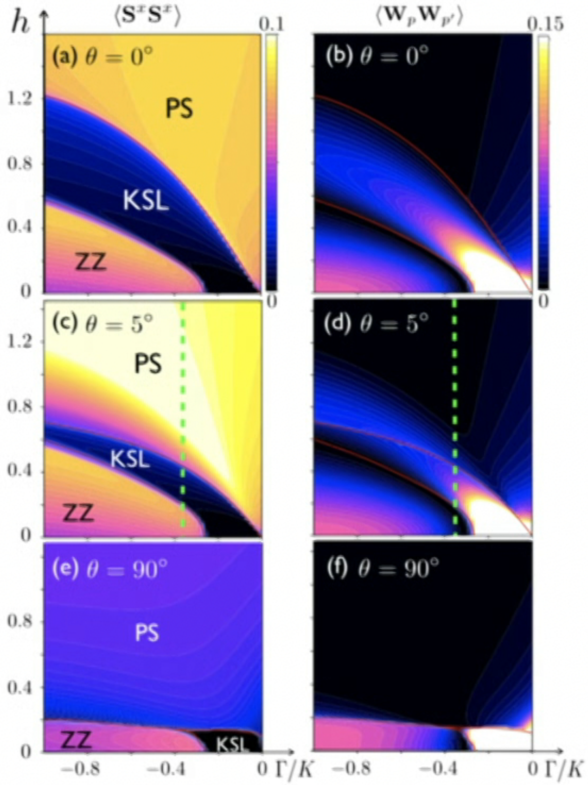
Hong-Chen Jiang, Wang, Huang & Yuan-Ming Lu, arXiv:1809.08247



Liujun Zou and Yin-Chen He, arXiv:1809.09091



Microscopic relevance to $RuCl_3$



AFM off-diagonal coupling

Gordon, Catuneanu, Sørensen & Kee, arXiv:1901.09943

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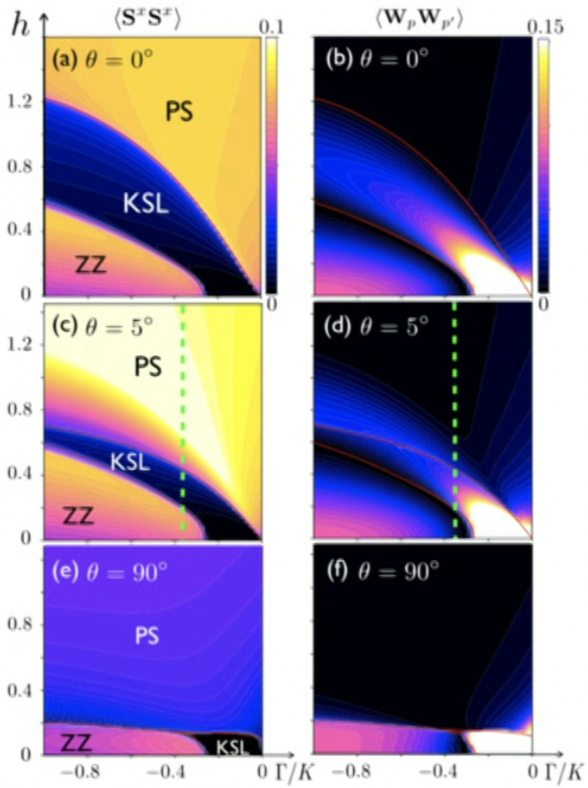

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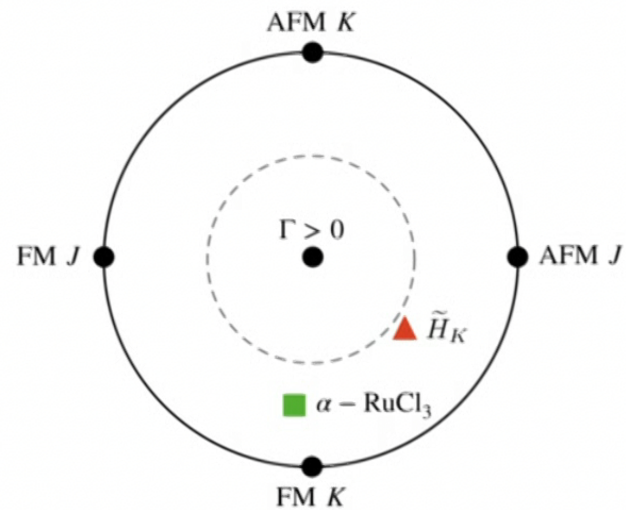
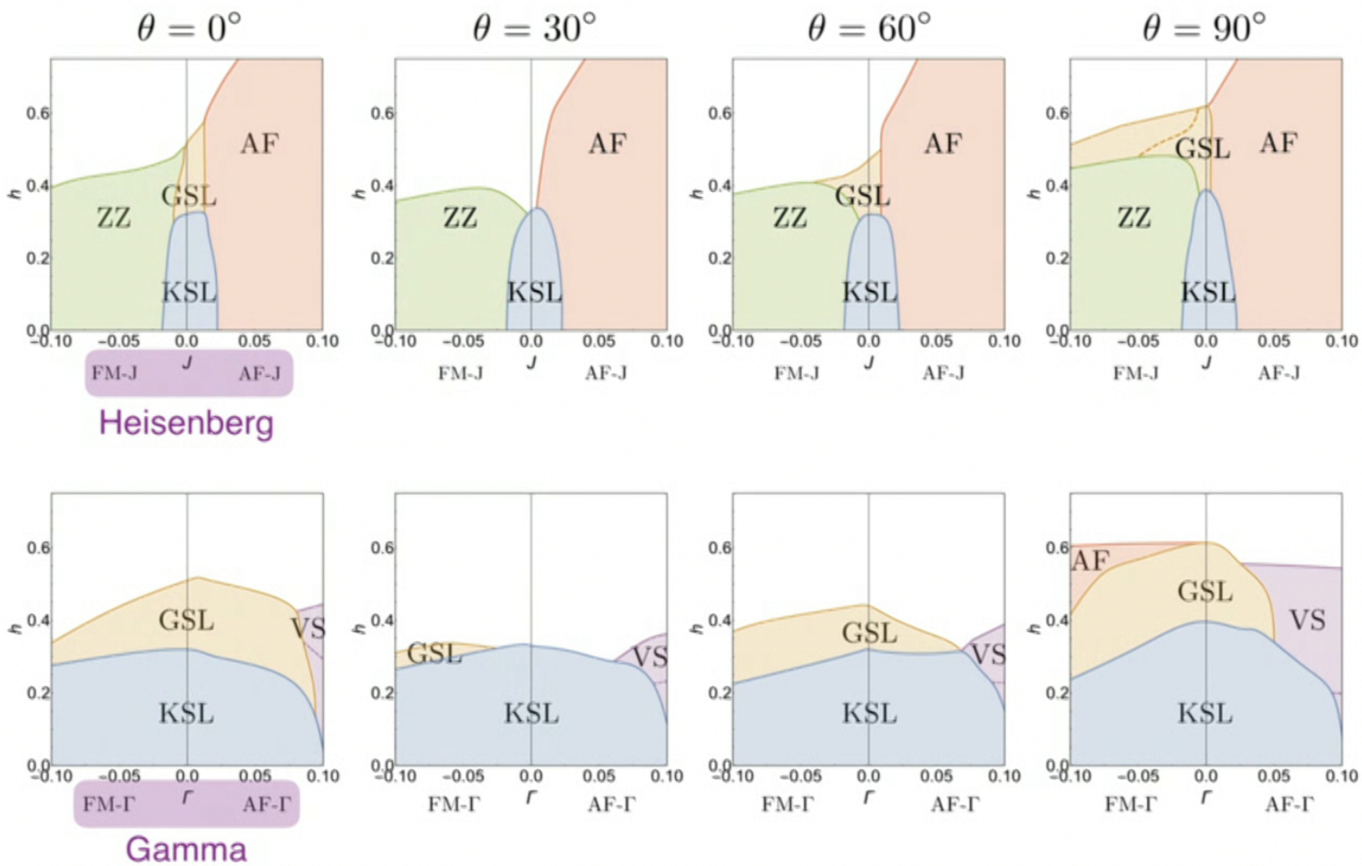


"hidden" AFM Kitaev model

(via Klein duality)

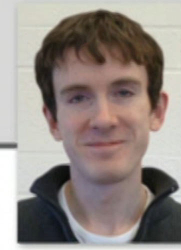
Kaib, Winter & Valenti, arXiv:1904.01025

Higgsed U(1) spin liquid?



Summary

C. Hickey and ST
Nature Comm. **10**, 530 (2019)



$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

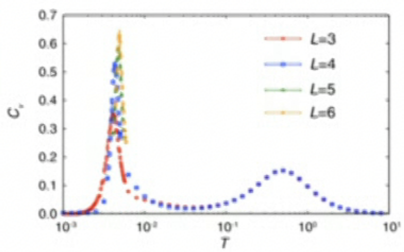
Kitaev spin liquids are textbook examples of **Z_2 spin liquids.**

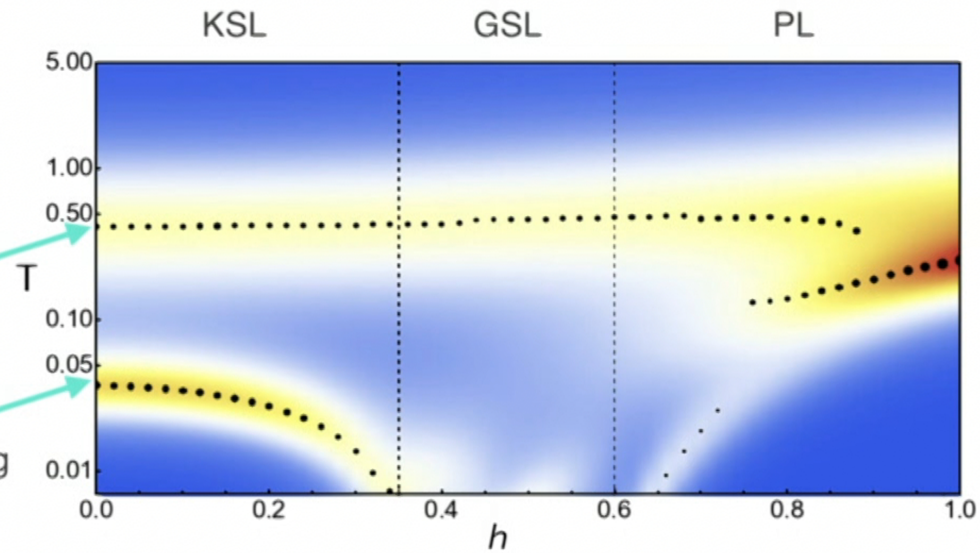
For AFM Kitaev couplings and strong magnetic fields,
a **Higgs transition** to a gapless **U(1) spin liquid** occurs.

The U(1) spin liquid is probably the generic high-field phase, and **parent phase** to the KSLs, but also all kinds of magnetic order.

specific heat

$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$





fractionalization
crossover

Z_2 flux ordering