Kitaev magnets

Autumn School on Correlated Electrons
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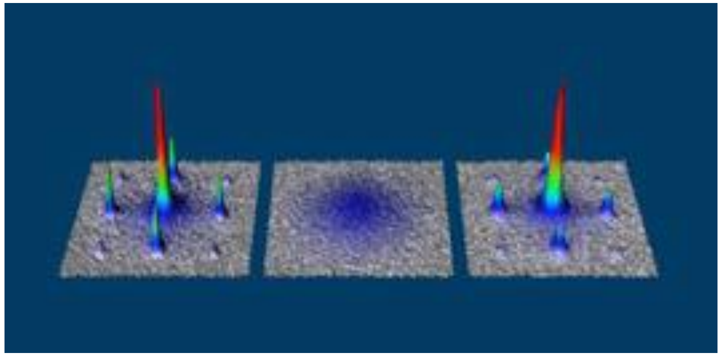
CRC 1238 Control and Dynamics of Quantum Materials

CRC 183 ENTANGLED STATES OF MATTER

Matter – a collective phenomenon

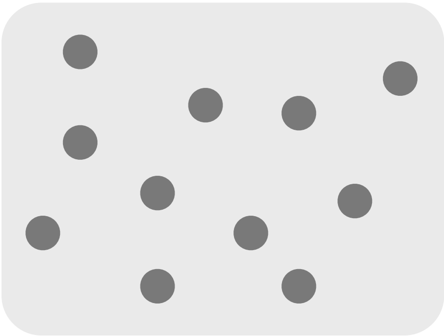
water ice

superconductor



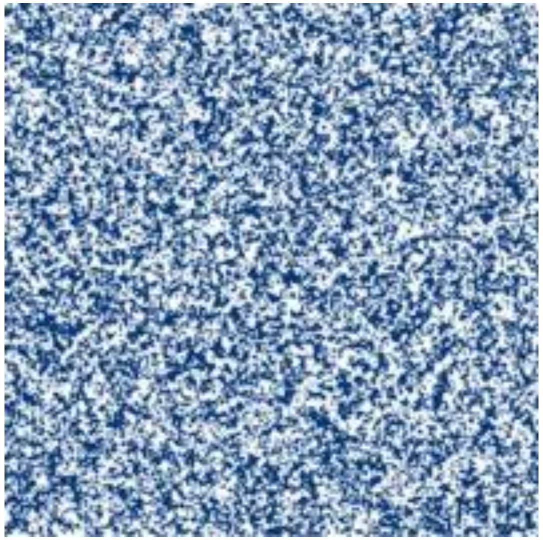
Bose-Einstein condensate

Motivation – a paradigm

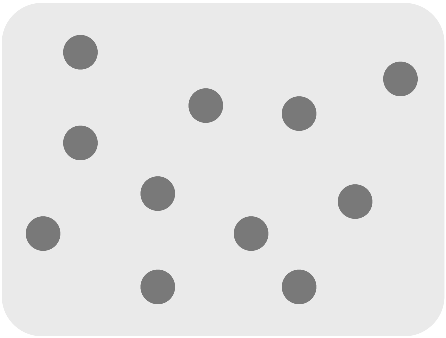


interacting
many-body system

$$\mathcal{H} = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z$$



Motivation – a paradigm



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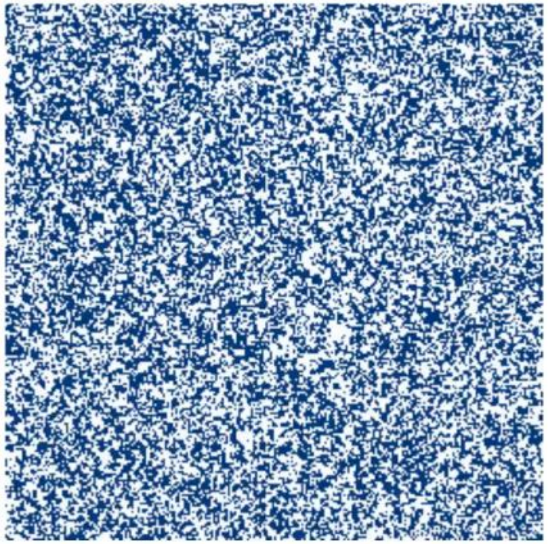
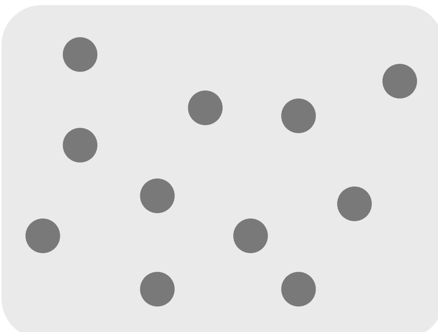


Motivation – a paradigm



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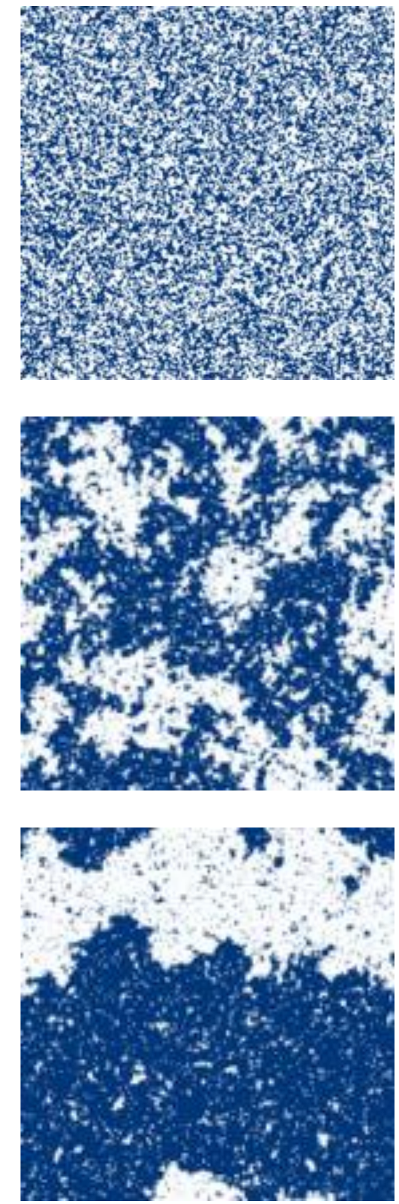
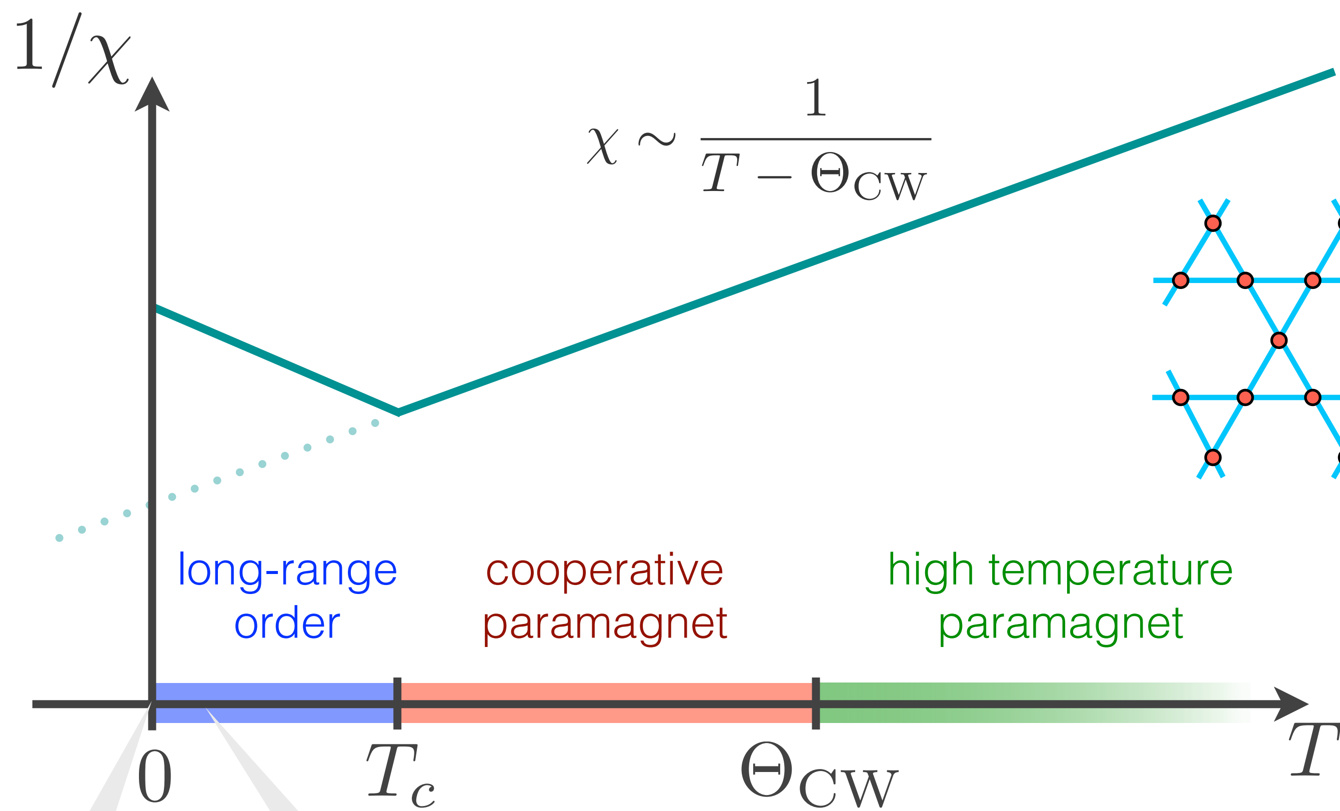


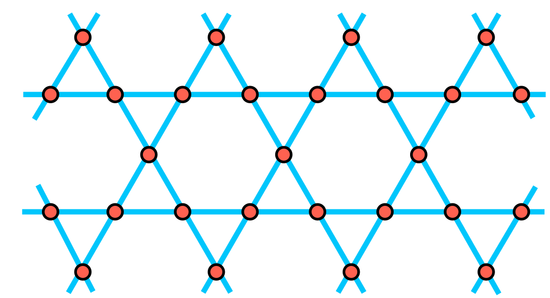
Spontaneous symmetry breaking

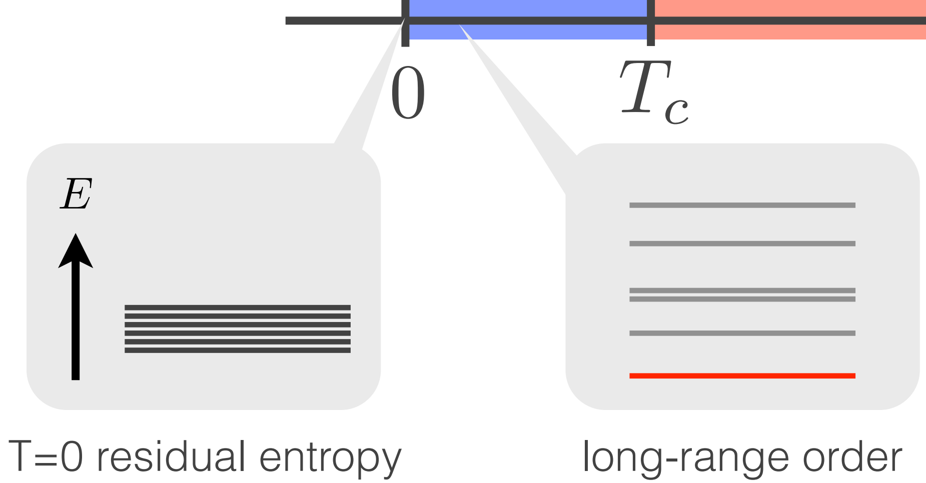
- ground state has **less symmetry** than Hamiltonian
- **local** order parameter
- phase transition / **Landau-Ginzburg-Wilson** theory

Beyond the paradigm – frustrated magnets

Insulating magnets with competing interactions.





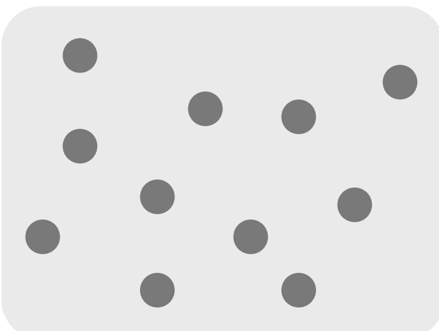


How can we quantify 'frustration' ?

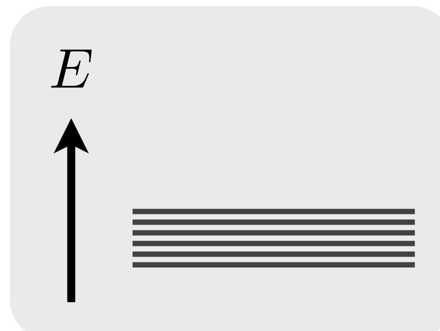
$$f = \frac{\Theta_{\text{CW}}}{T_c}$$

Why we should look for the misfits

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



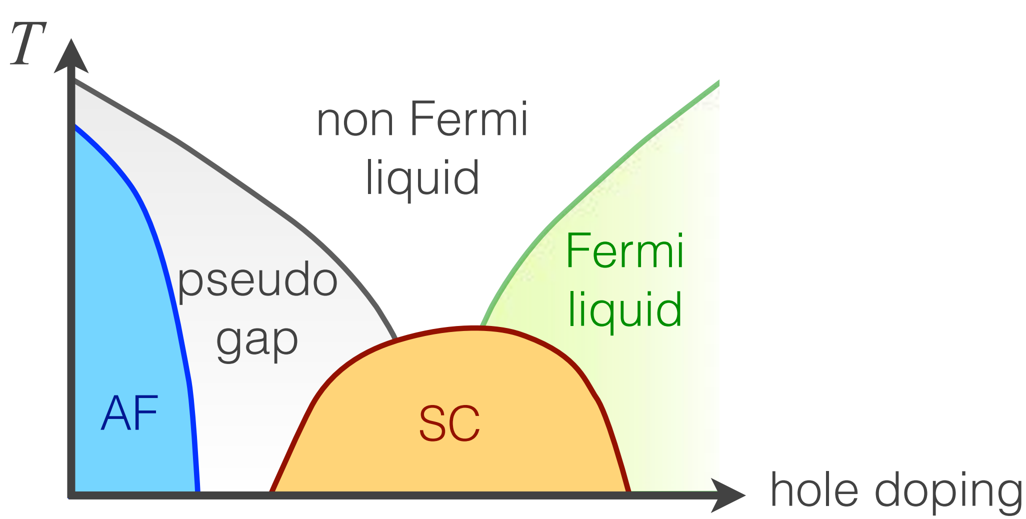
interacting
many-body system



‘accidental’
degeneracy

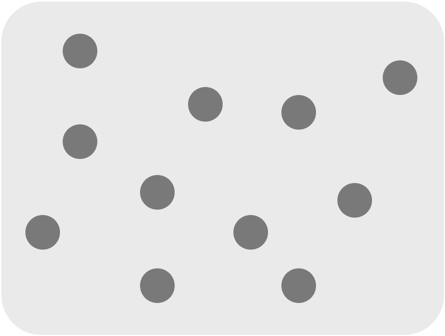
residual effects
select ground state

phase diagram of
cuprate superconductors

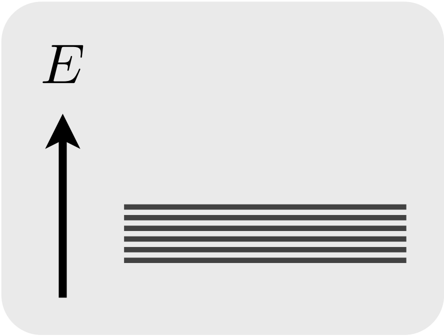


When do interesting things happen?

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

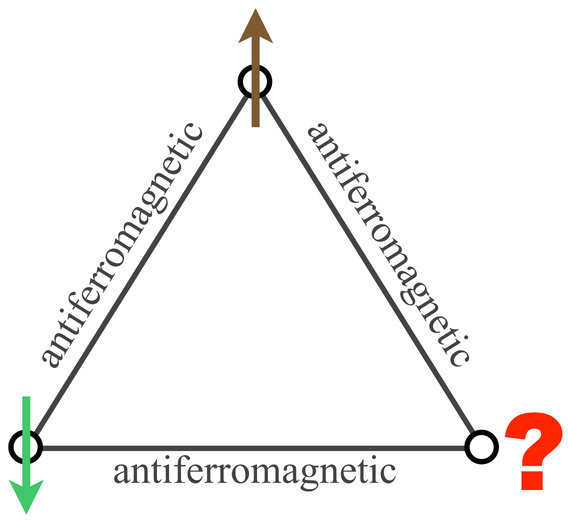
But they are also notoriously difficult to handle, due to

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

classical spin liquids

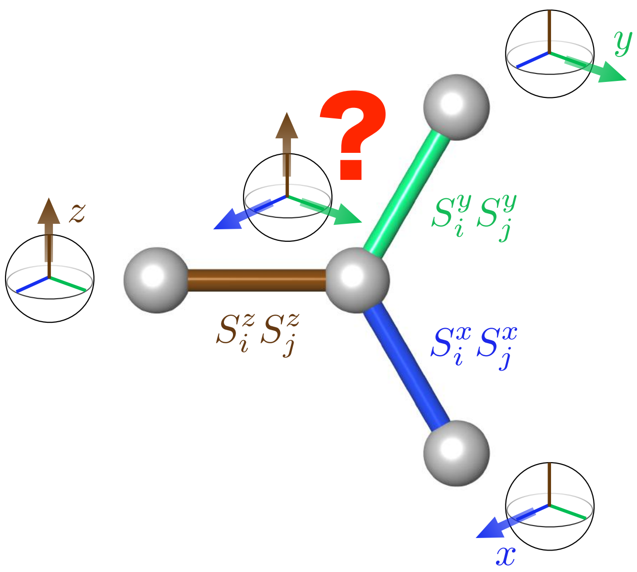
Frustration

Competing interactions lead to frustration.
We will see that frustration can originate interesting spin liquid behavior.



geometric frustration

triangular lattice antiferromagnet
diamond lattice antiferromagnet



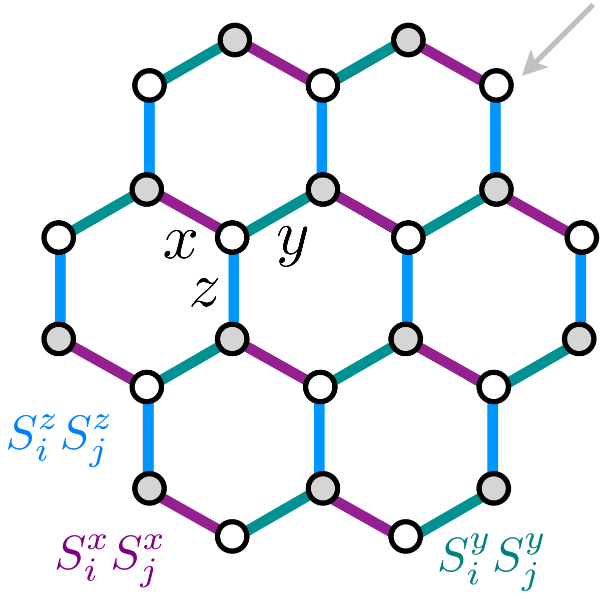
exchange frustration

classical Kitaev model

The Kitaev model

A. Kitaev, Ann. Phys. **321**, 2 (2006)

$\vec{S}_i$ O(3) Heisenberg spins



$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$

Ising-like* interaction

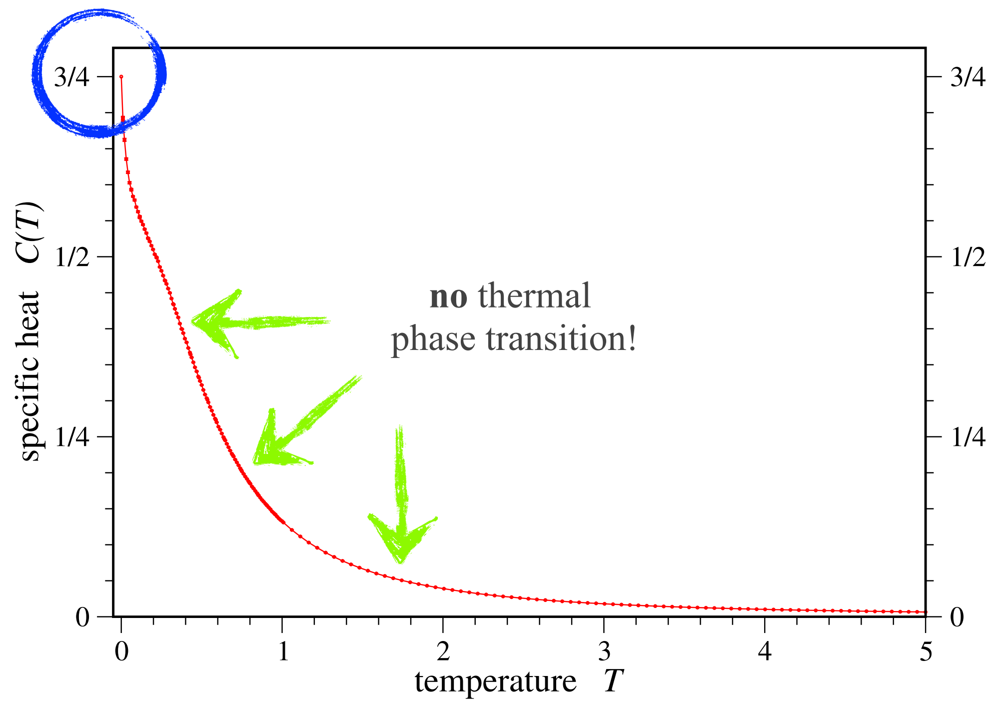
* preferred direction of spin alignment depends on spatial direction of bond

Its **quantum mechanical cousin** is well known for its rare combination of a model of fundamental conceptual importance and an exact analytical solution.

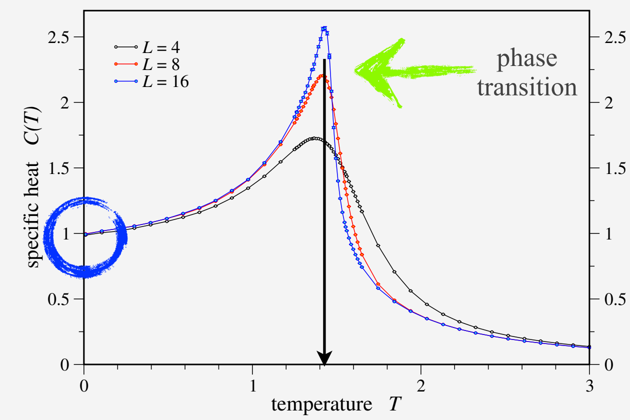
But to a good extent this is also true for the **classical model** (though much less known).

A first step – numerical simulation

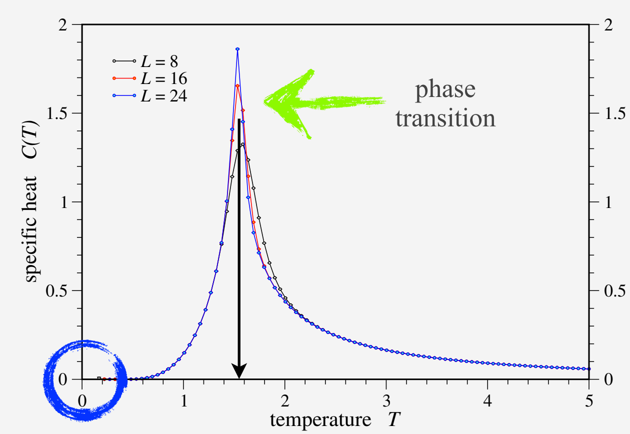
$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$



$$H_{\text{Heisenberg}} = \sum_{\gamma-\text{links}} J_\gamma \vec{S}_i \vec{S}_j$$

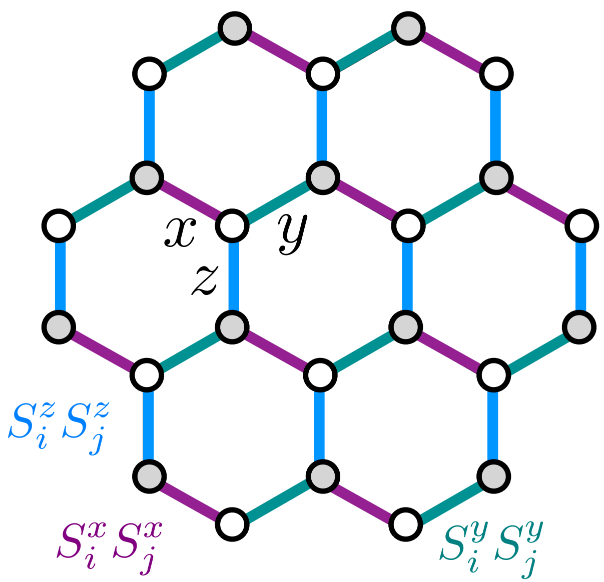


$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$



Frustration in the Kitaev model

Observation: no spin configuration can simultaneously satisfy all exchange terms.

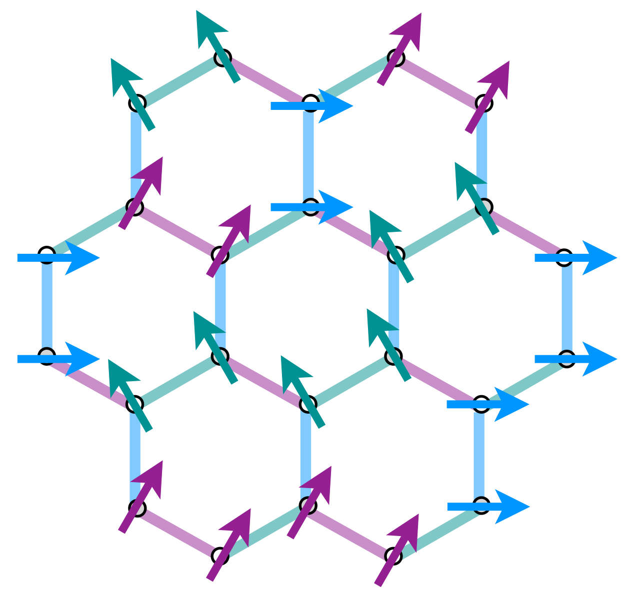


$$H_{\text{Kitaev}} = \sum_{\gamma-\text{links}} J_\gamma S_i^\gamma S_j^\gamma$$

Ising-like* interaction

* preferred direction of spin alignment
depends on spatial direction of bond

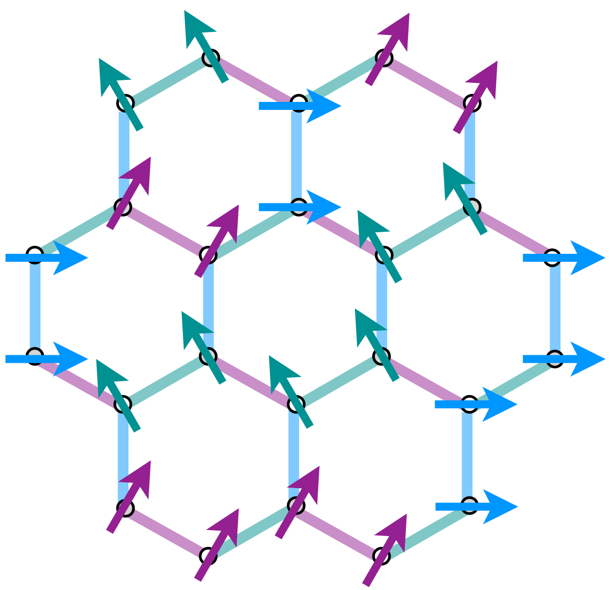
T=0 **spin configuration**



Every spin can minimize its energy by
pointing parallel to precisely one neighbor.

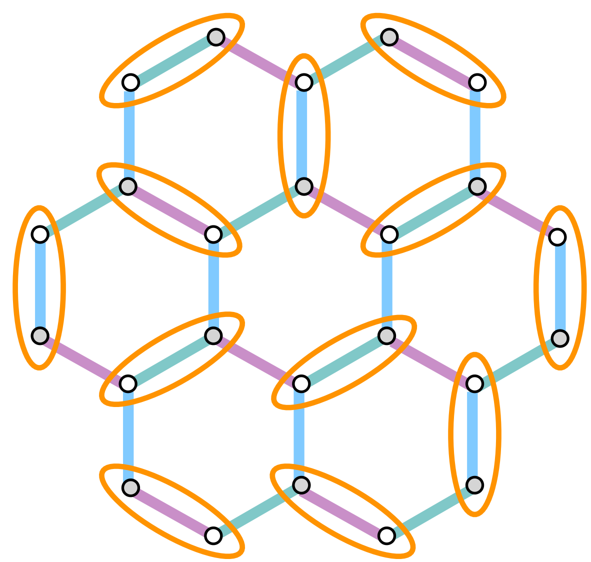
Emergent magnetostatics

T=0 **spin configuration**



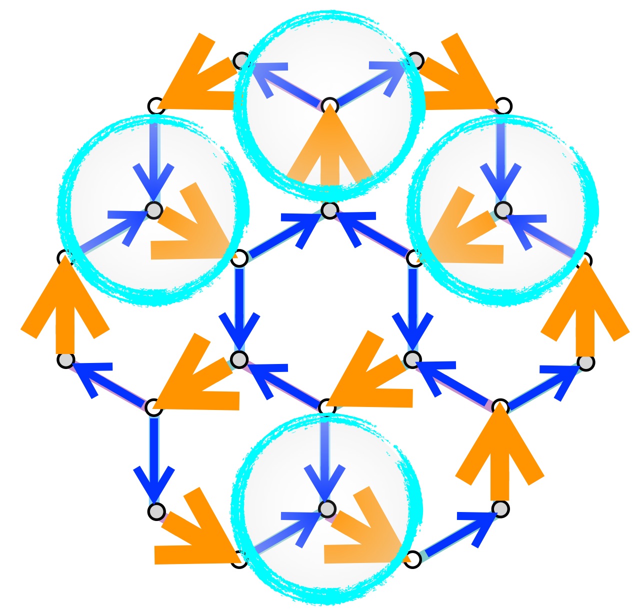
every spin is parallel to *precisely* one neighbor

dimer covering



every site is part of *precisely* one dimer

divergence-free field



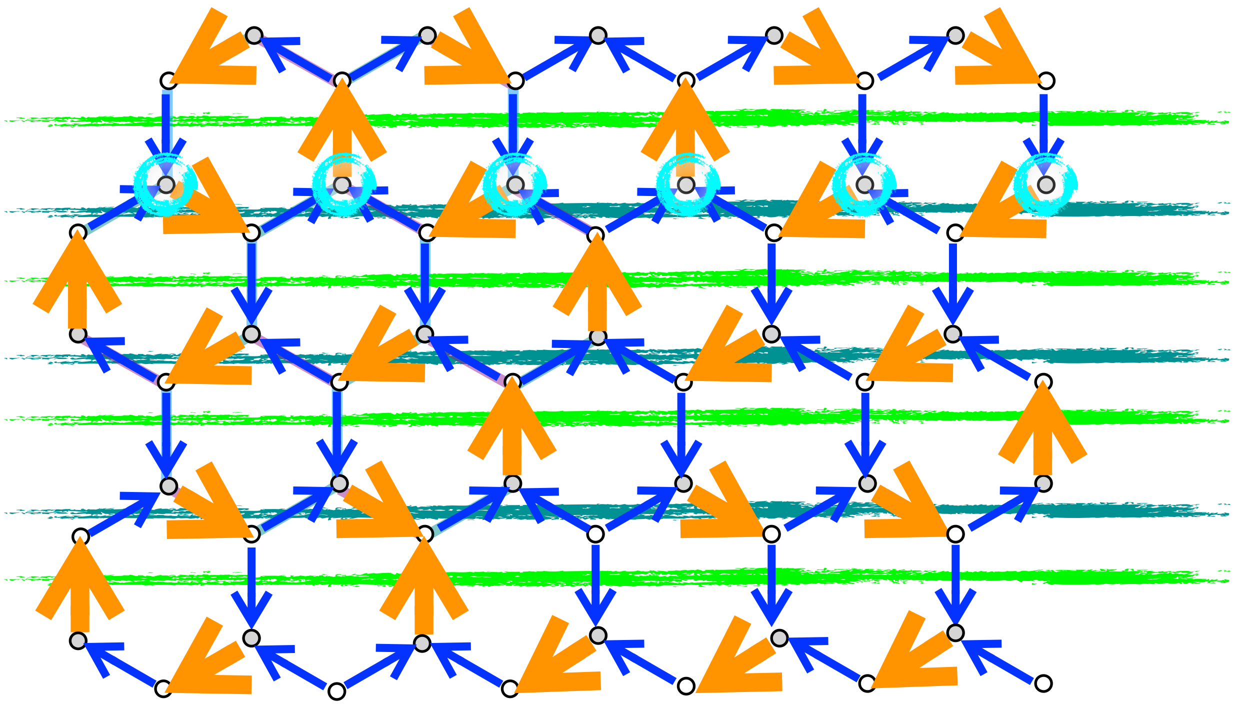
$$\mathrm{div}\ \vec{B} = 0$$

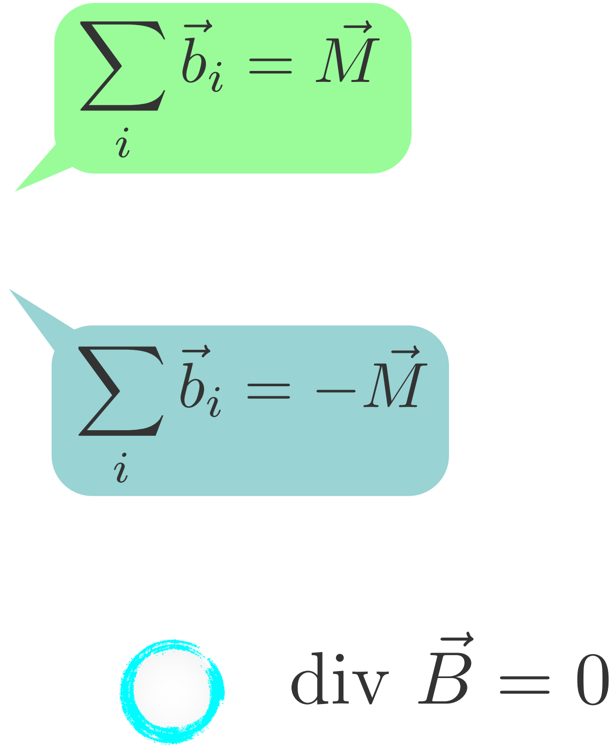
$= \hat{e}_{ij}$

$= -\hat{e}_{ij}/2$

Long-range correlations

divergence-free field



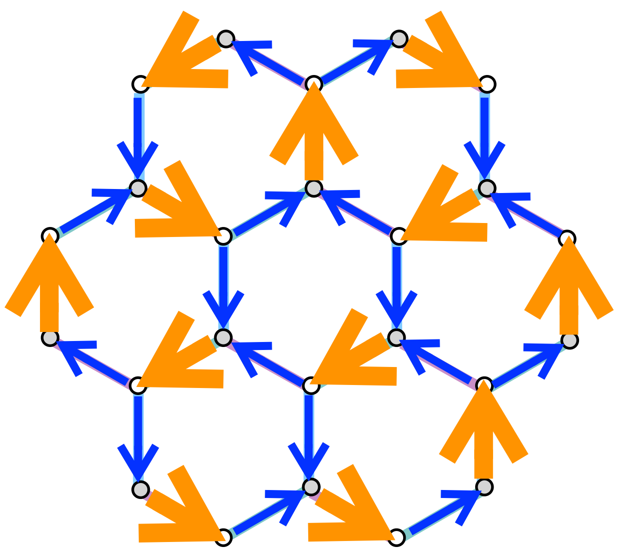


An immediate consequence from the strictly enforced **local constraint** of a divergence-free field is the emergence of **long-range correlations**.

Emergent magnetostatics – Coulomb phase

look also at D.A. Huse et al., Phys. Rev. Lett. 91, 167004 (2003)

divergence-free field



$$\mathrm{div}\ \vec{B} = 0$$

 $= \hat{e}_{ij}$

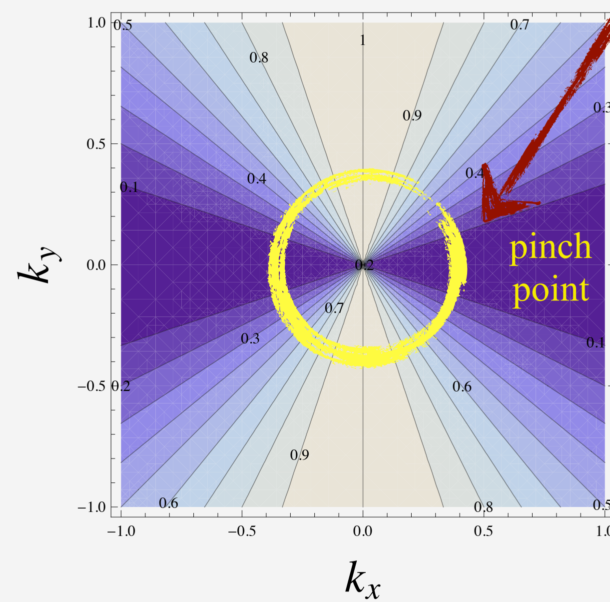
 $= -\hat{e}_{ij}/2$

dimer-dimer correlations

$$\langle n(\vec{r})n(0)\rangle \propto \frac{1}{r^2}$$

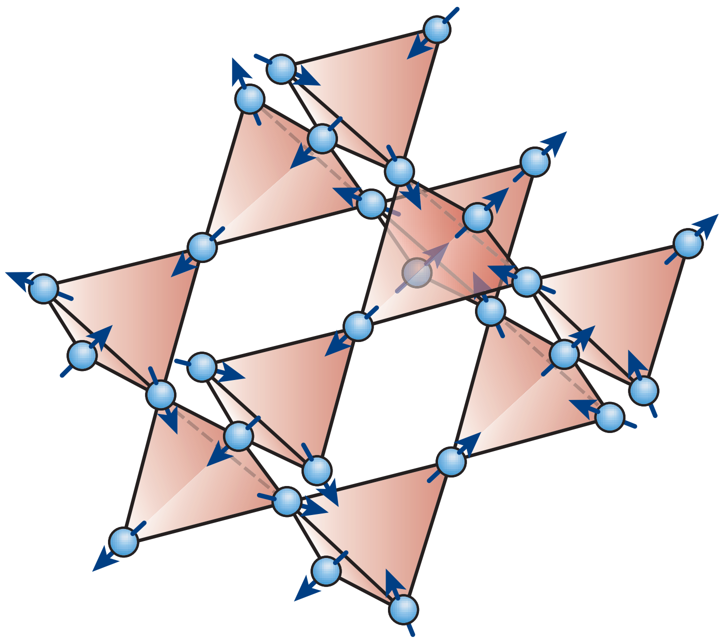
Coulomb phase

... and in Fourier space



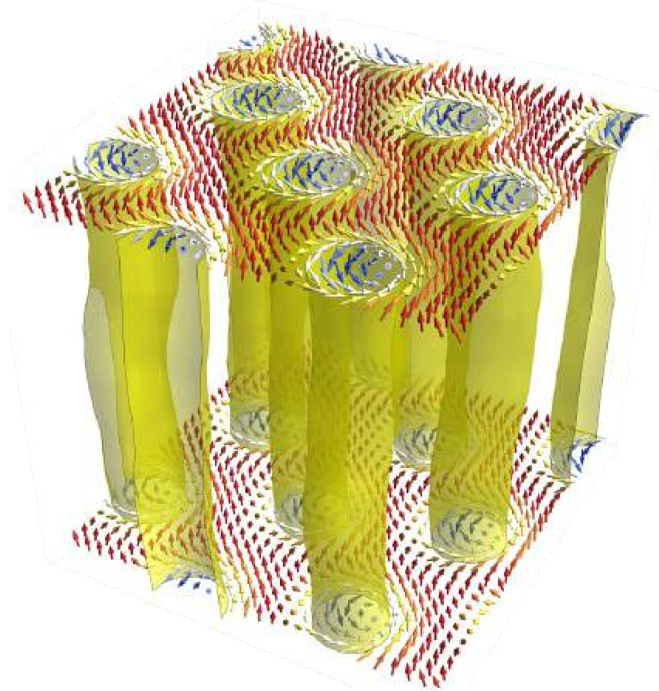
Emergent magnetostatics – Coulomb phase

Such analogies to electromagnetism have also been exploited to discuss the frustrated magnetism in **spin ice** materials and the physics of **skyrmion lattices** in chiral magnets.



spin ice on the pyrochlore lattice

Moessner group
MPI-PKS Dresden

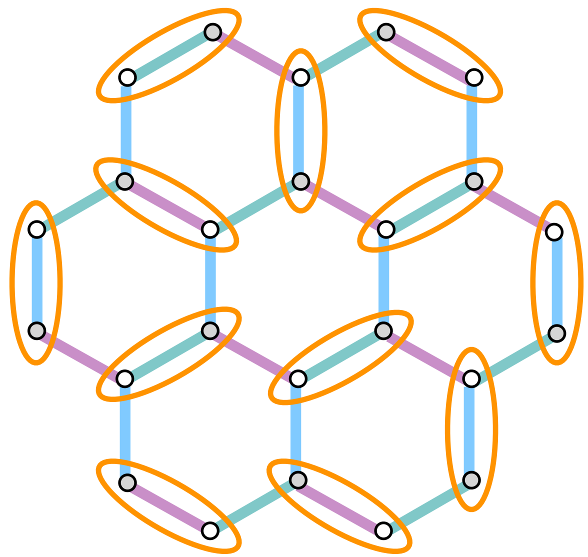


skyrmion lattice in MnSi

Rosch group
University of Cologne

degeneracy – the imprint of frustration

dimer covering



every site is part of
precisely one dimer

The number of dimer coverings
for the hexagonal lattice grows as

$$Z \propto 1.402581^N$$

degeneracy @ $T = 0$

(for periodic boundary conditions)

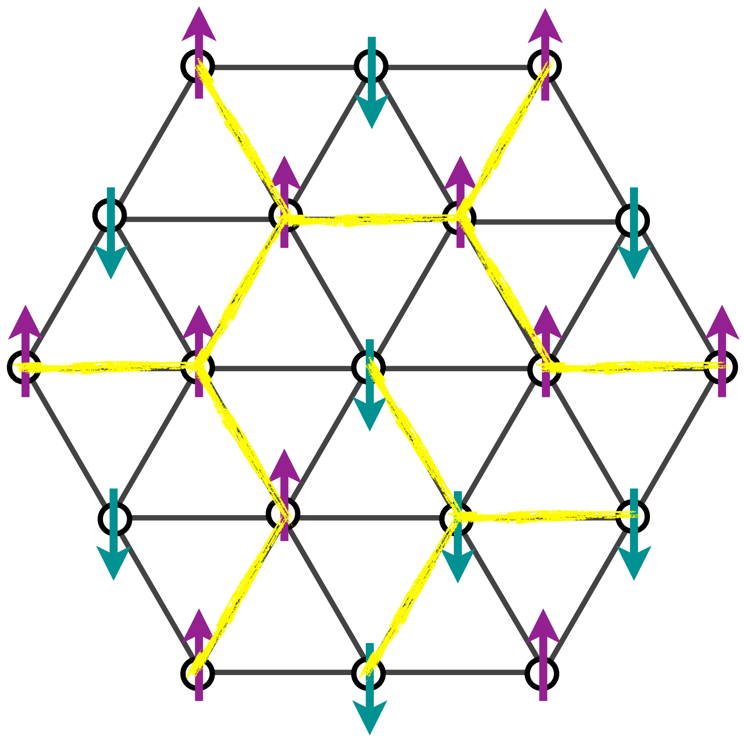
G.H. Wannier, Phys. Rev. 79, 357 (1950)
P.W. Kasteleyn, J. Math. Phys. 4, 287 (1963)
V. Elser, J. Phys. A: Math. Gen 17, 1509 (1984)

At **finite temperature**
this degeneracy will be immediately lifted.
Monomer defects are introduced (and screened).

→ screened Coulomb phase
= high-temperature paramagnet

Triangular lattice Ising model

G.H. Wannier, Phys. Rev. 79, 357 (1950)



$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$

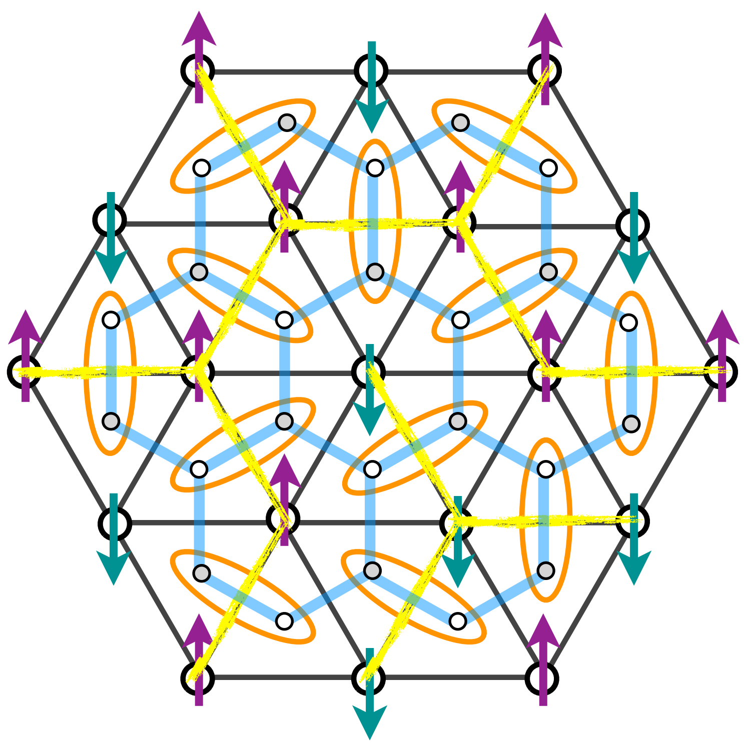
antiferromagnetic

T=0 **spin configuration**

precisely one frustrated bond per triangle

Triangular lattice Ising model

G.H. Wannier, Phys. Rev. 79, 357 (1950)



$$H_{\text{Ising}} = \sum_{\gamma-\text{links}} J_\gamma S_i^z S_j^z$$

antiferromagnetic

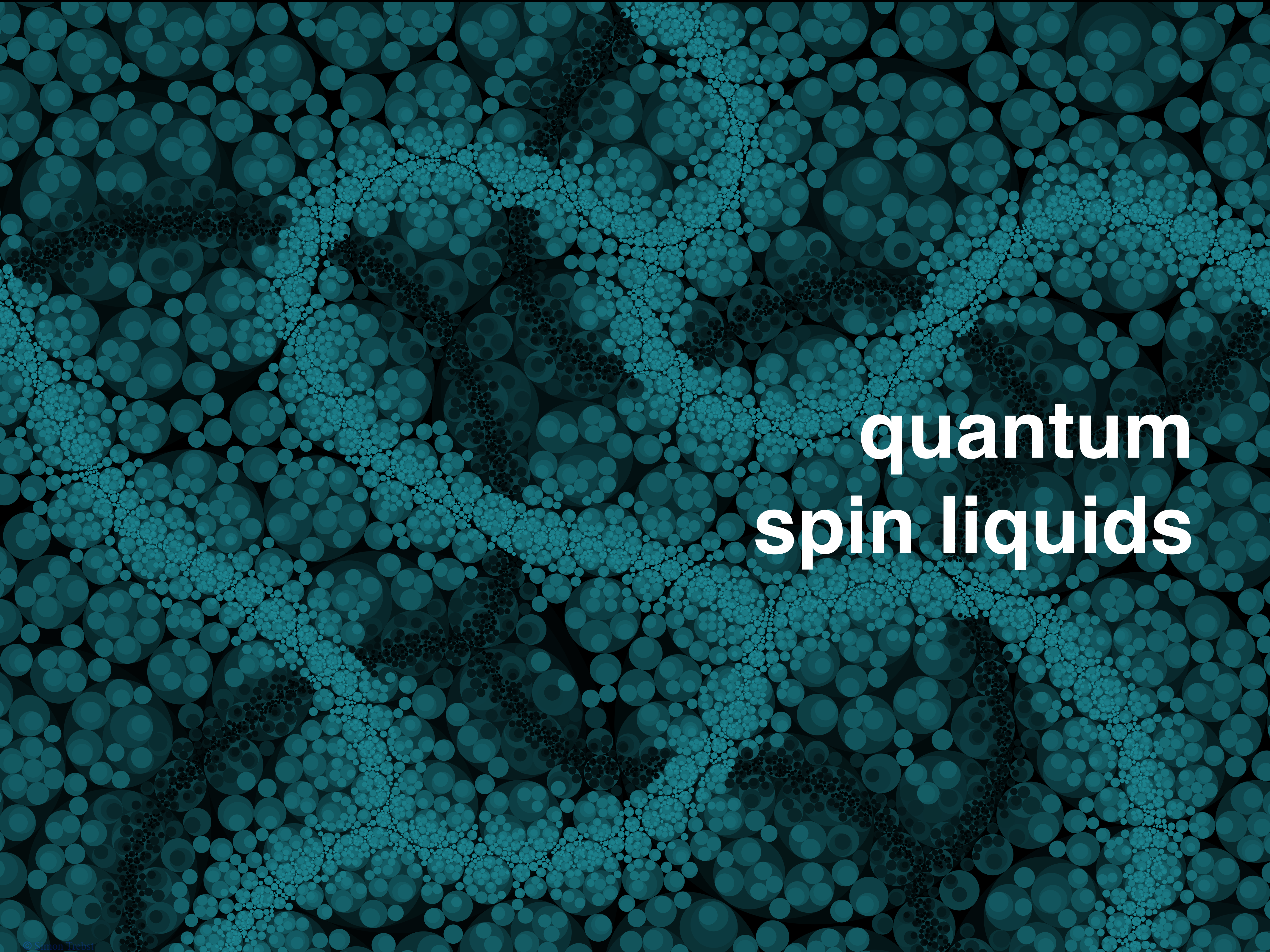
T=0 **spin configuration**

precisely one frustrated bond per triangle

T=0 **dual dimer configuration**

precisely one dimer per site on dual honeycomb lattice

→ $Z \propto 1.402581^N$ degenerate spin configurations → Coulomb correlations $\langle S^z(\vec{r}) S^z(0) \rangle \propto \frac{1}{r^2}$


quantum
spin liquids
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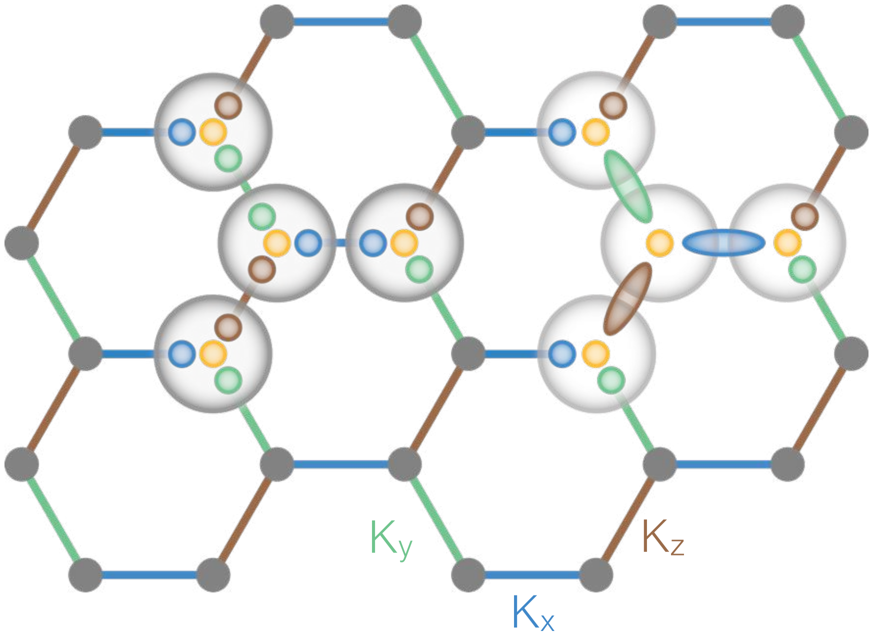
Kitaev model

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



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

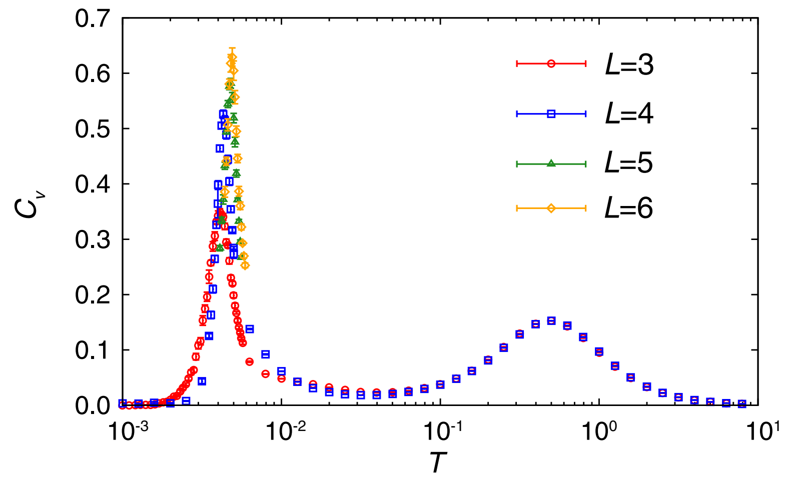
$$\sigma^\alpha = i a^\alpha c$$

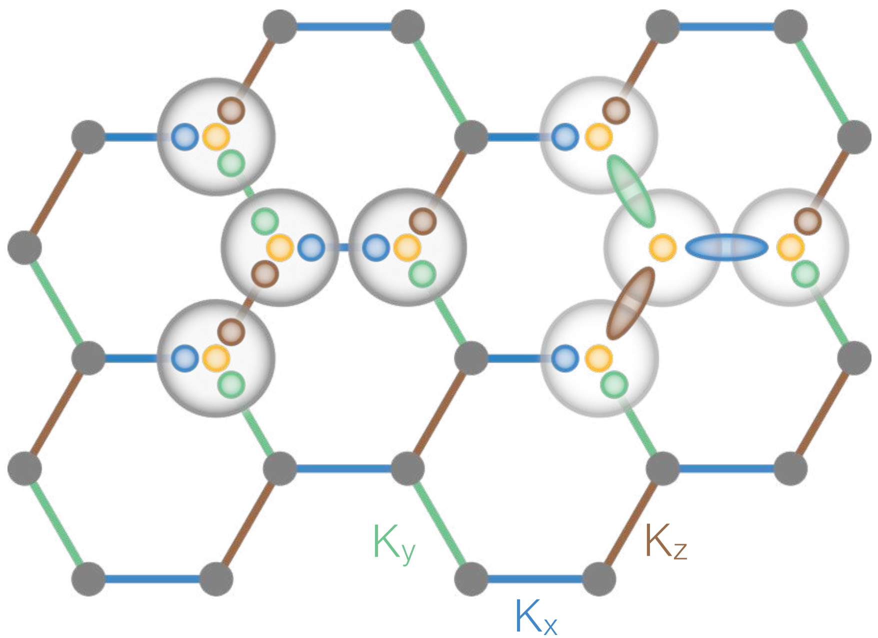
Bond operators

$$\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$$

realize a $\mathbf{Z_2}$ **gauge field**

Kitaev model





The Z_2 **gauge fields** are **static** degrees of freedom.

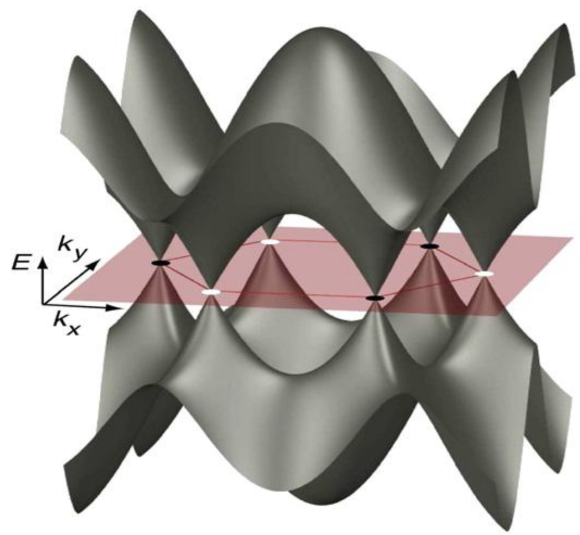
Generically, one has to find its **gapped ground-state** configuration via educated guesses, Monte Carlo sampling, or for some lattices via Lieb's theorem.

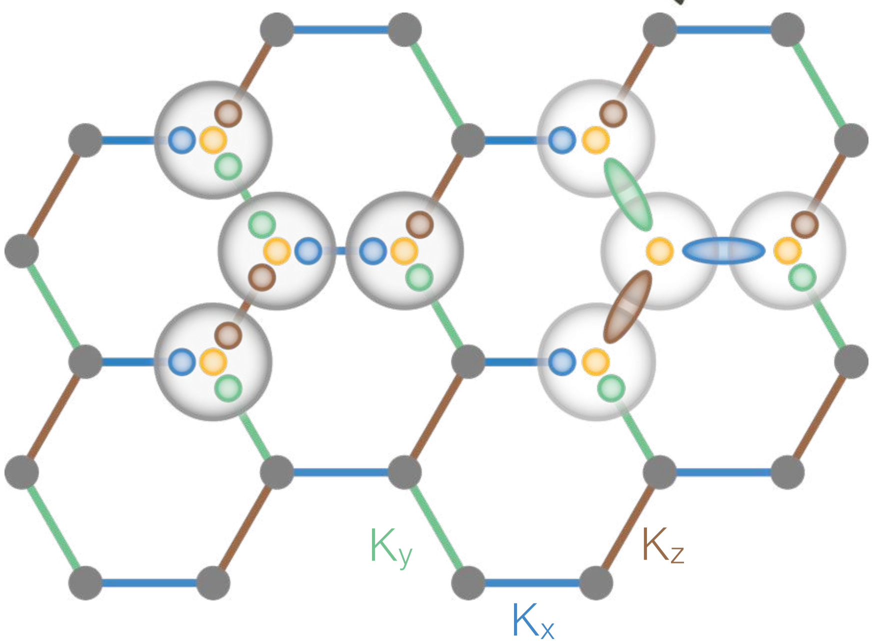
Bond operators

$$\hat{u}_{jk} = i a_j^\alpha a_k^\alpha$$

realize a Z_2 **gauge field**

Kitaev model





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

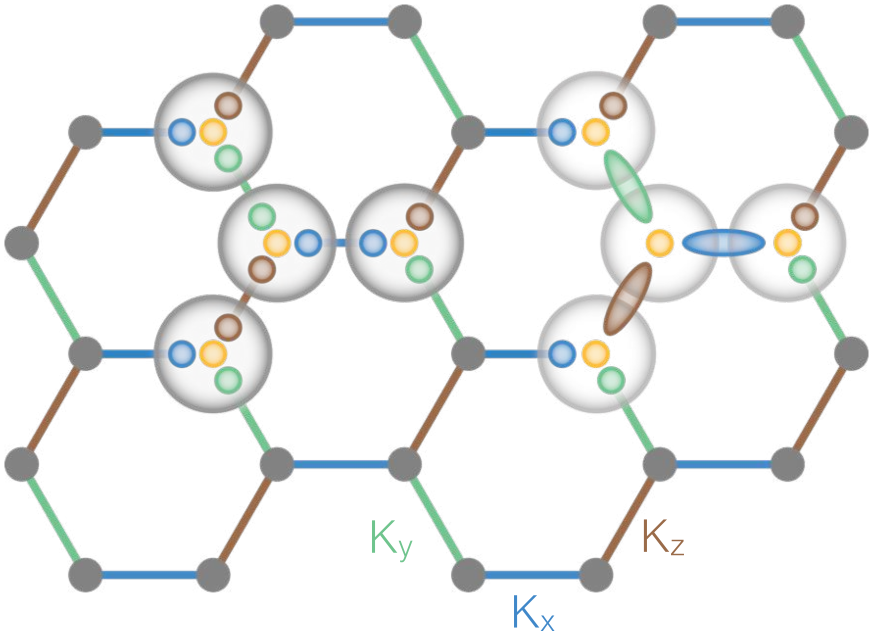
$$\sigma^{\alpha} = i a^{\alpha} c$$

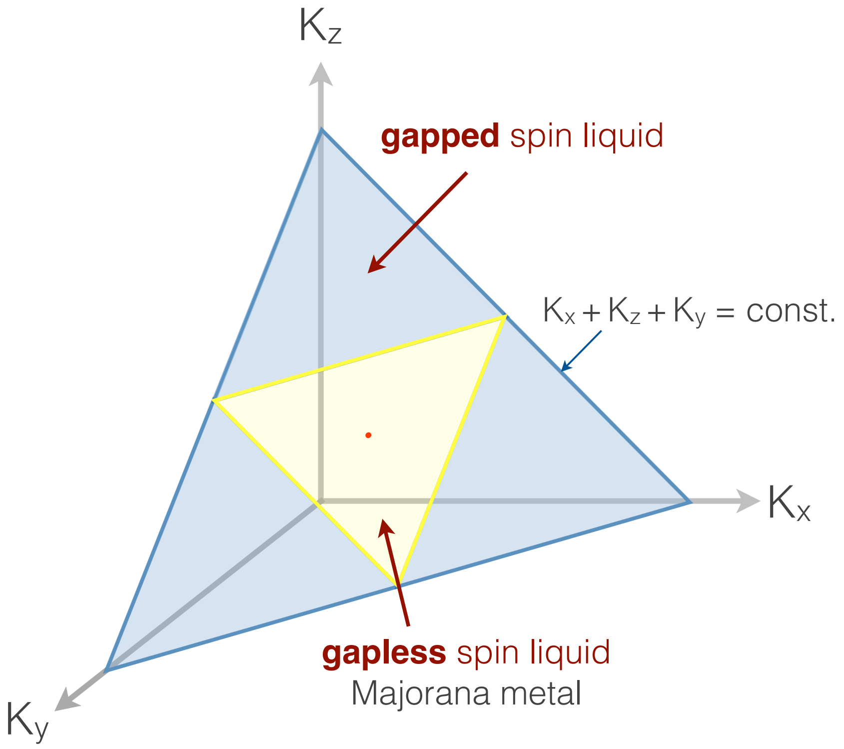
The emergent **Majorana fermions** are **itinerant** degrees of freedom.

Generically, they form a **gapless** collective state – a **Majorana metal**.

Kitaev model

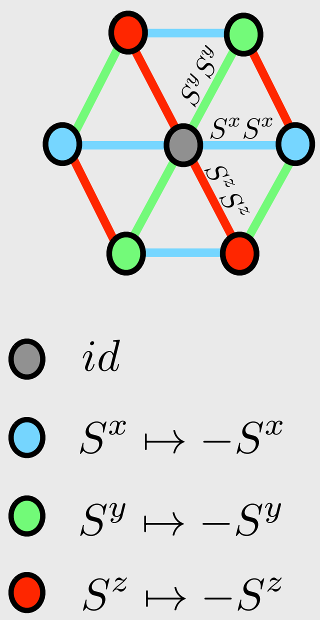
$$H = - \sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$





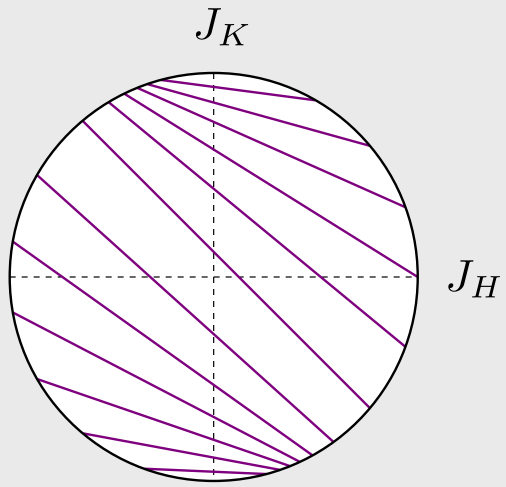
Heisenberg-Kitaev model

$$H = \sum_{\gamma-\text{bonds}} \cos\varphi\ \mathbf{S}_i\mathbf{S}_j + \sin\varphi\ S_i^\gamma S_j^\gamma$$



Klein duality

- **mapping** between pairs of points (on left and right half-circle)
- **basis transformation** involves spin-rotations on four sublattices
- preserves **symmetry** of Hamiltonian, four SU(2) symmetric points



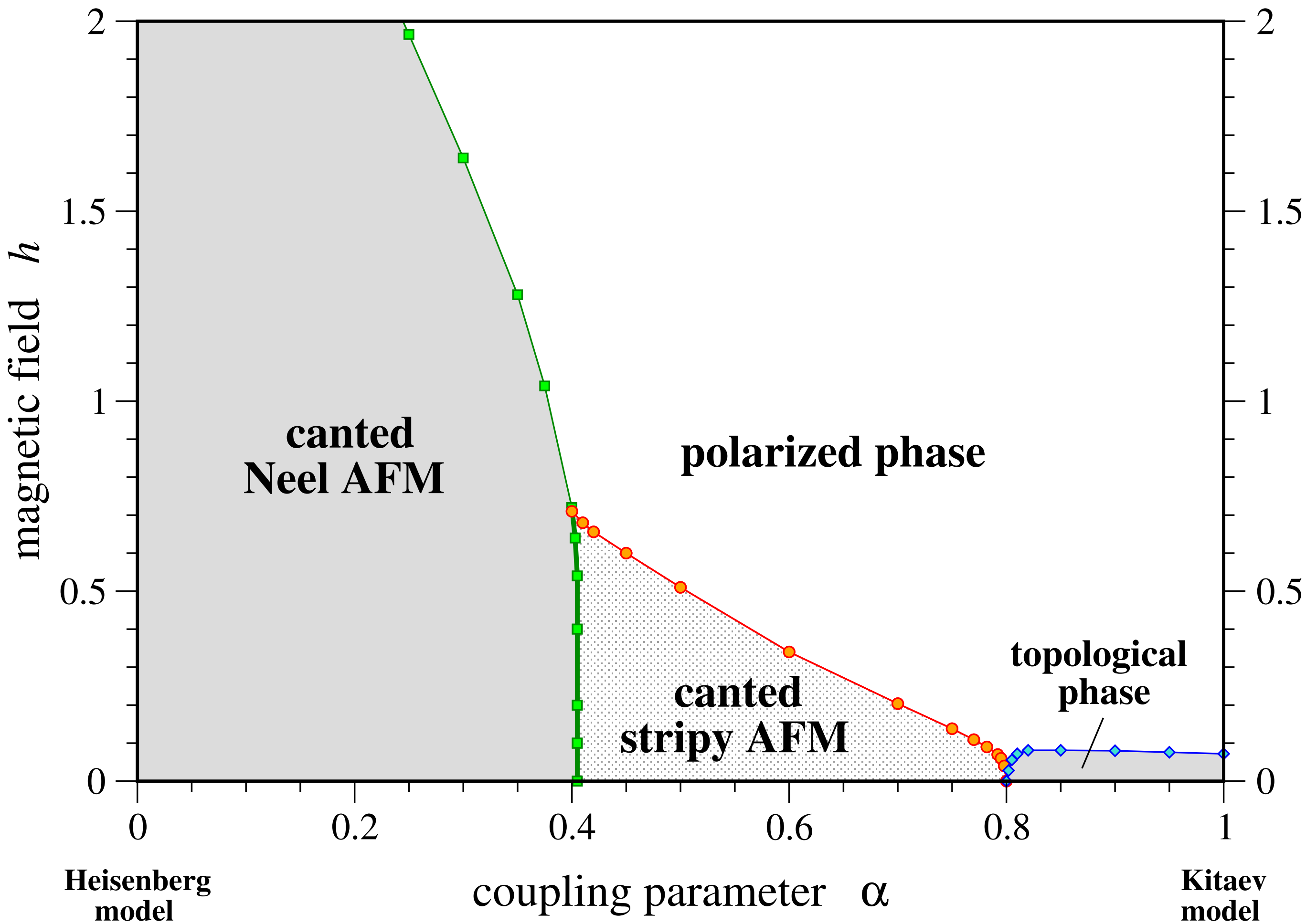
$$\tilde{J}_H = -J_H \qquad \tilde{J}_K = 2J_H + J_K$$

G. Khaliullin, Prog. Theor. Phys. Suppl. 160, 155 (2005)

Magnetic field & topological order

$$H = (1-\alpha)\sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - 2\alpha \sum_{\gamma-\text{bonds}} S_i^\gamma S_j^\gamma + \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

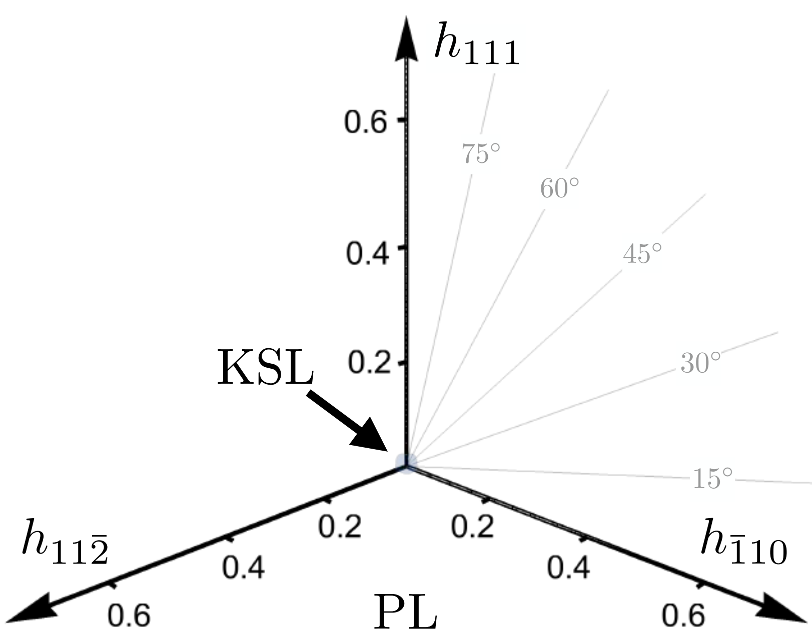
H.-C. Jiang, Z.-C. Gu, X.-L. Qi, ST, PRB **83**, 245104 (2011).



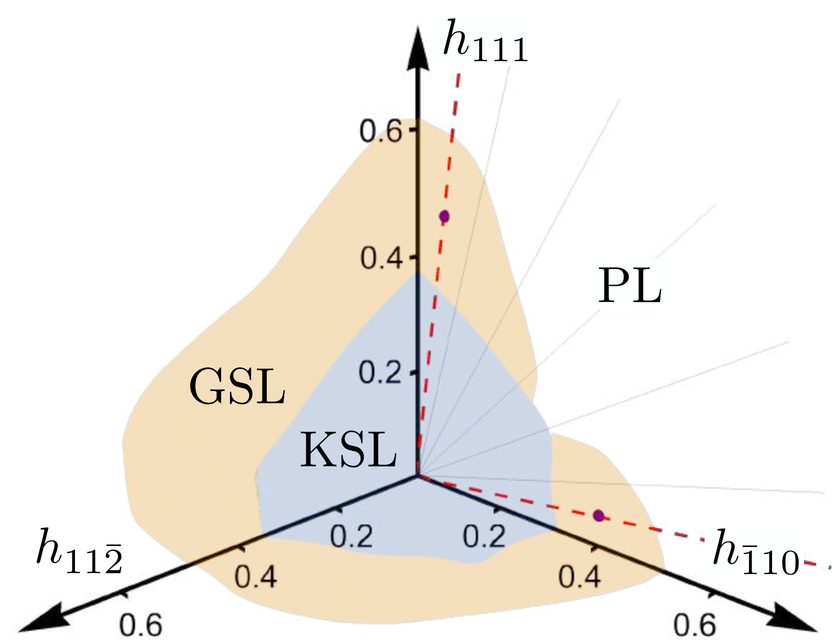
Kitaev model – magnetic field effects

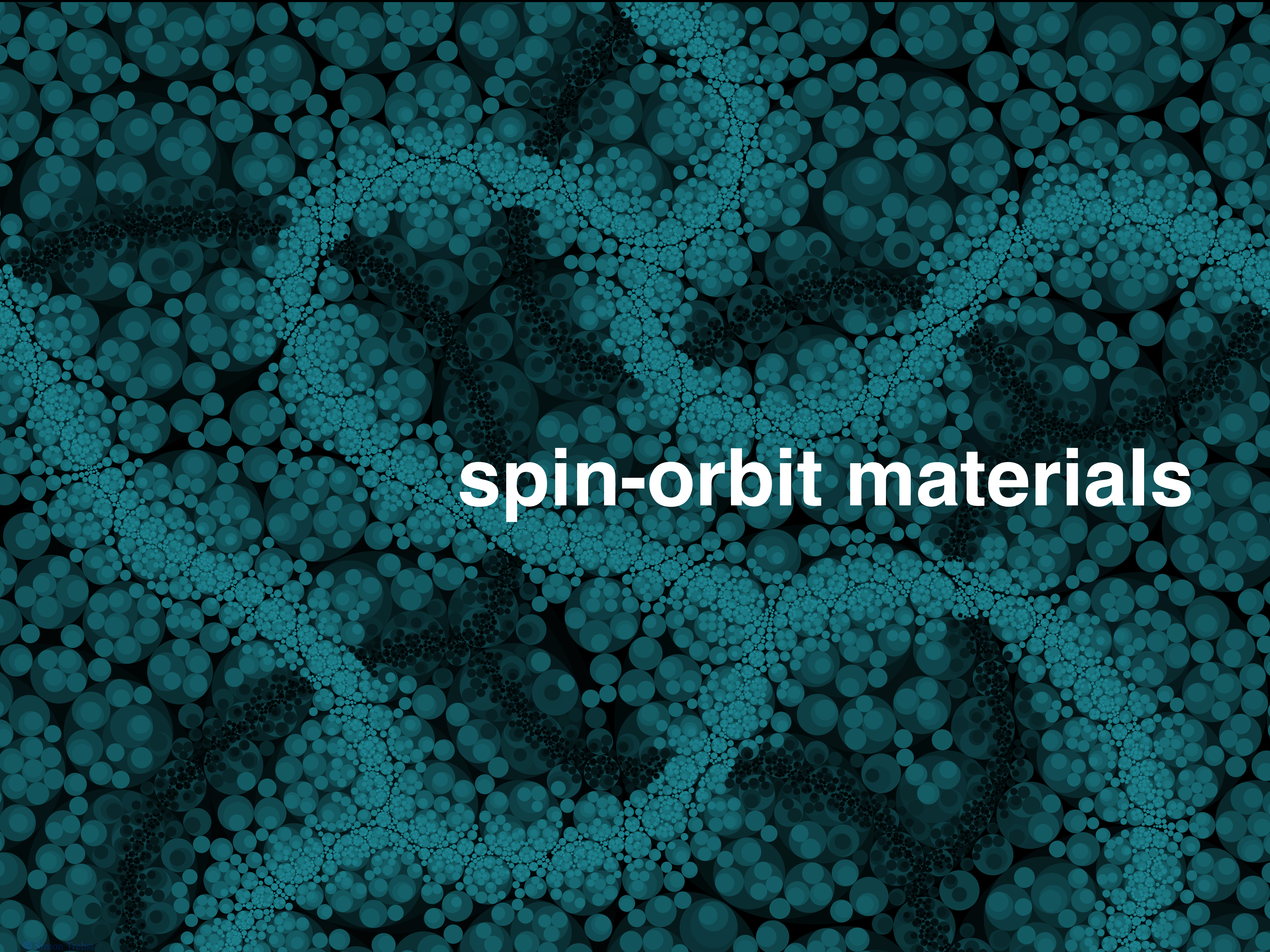
$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma S_i^\gamma S_j^\gamma - \sum_i \mathbf{h}\cdot\mathbf{S}_i$$

FM Kitaev coupling



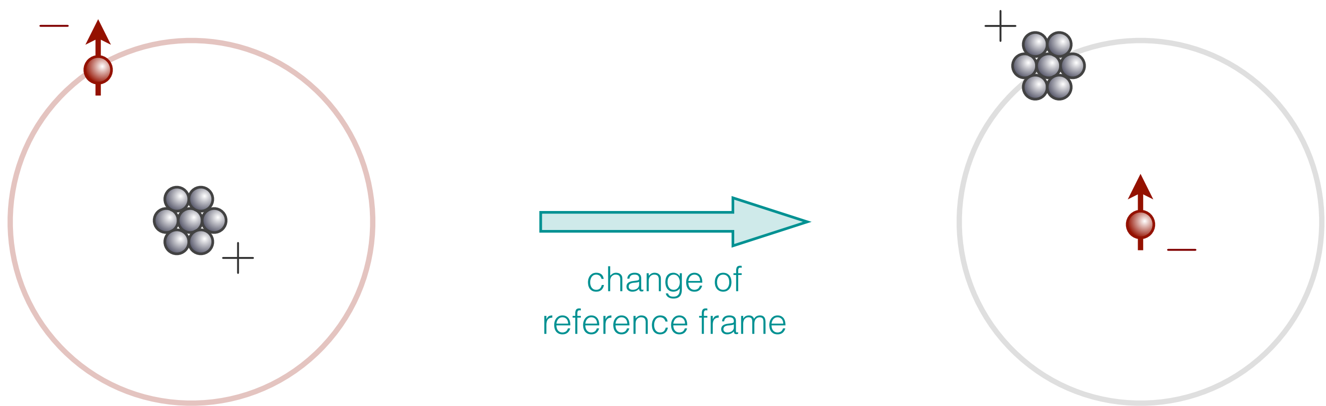
AFM Kitaev coupling




spin-orbit materials
© Simon Trebst

Spin-orbit coupling

Spin-orbit coupling 101 – quantum mechanics lecture

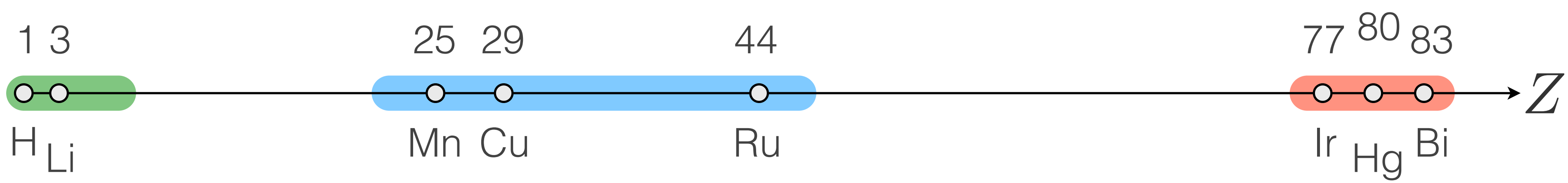


relativistic correction

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

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

Spin-orbit coupling in condensed matter

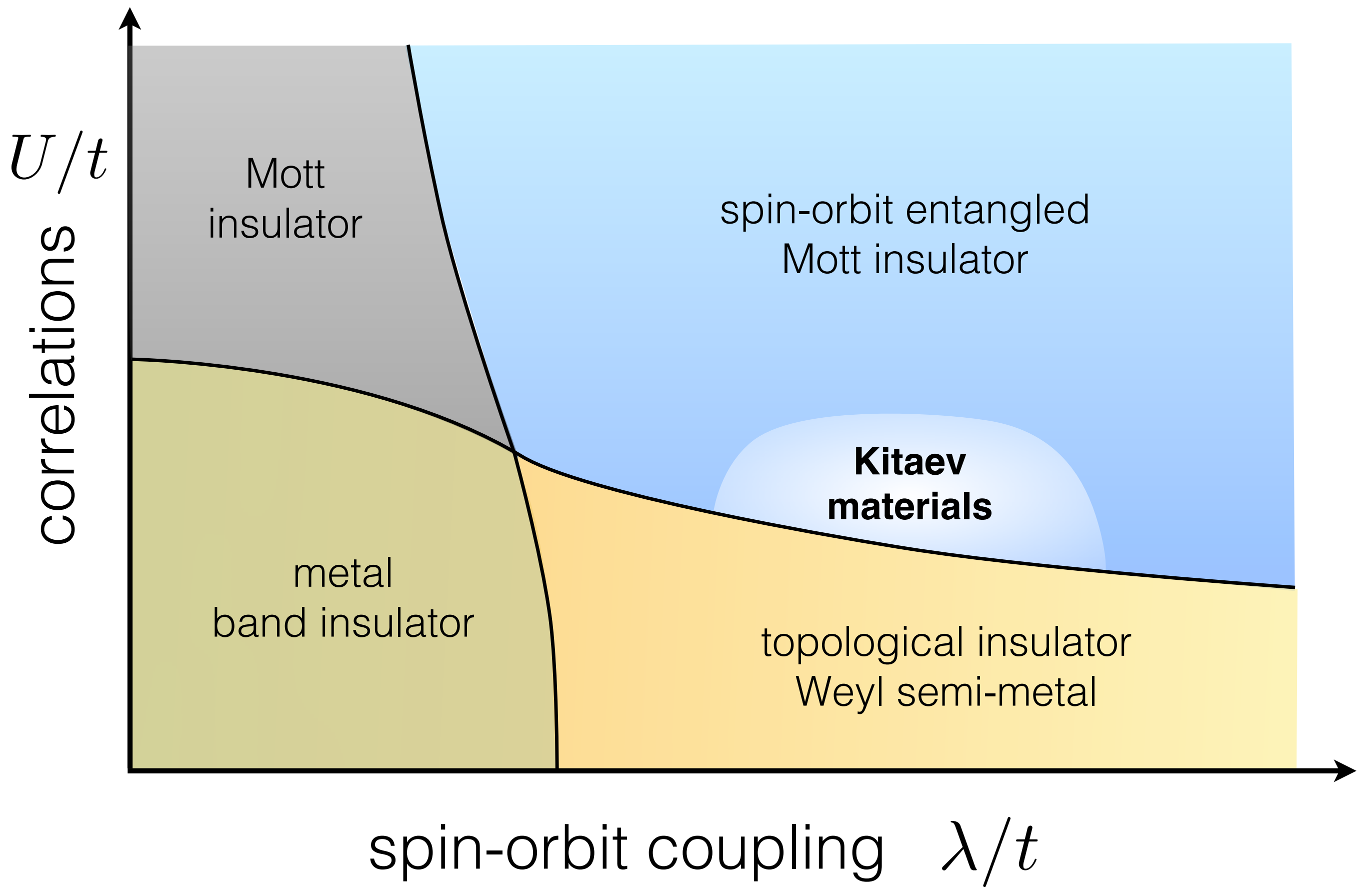


$\lambda \propto Z^4$ $\frac{1}{2}$ 1 5 50 58 67

weak SOC	moderate SOC		strong SOC	
atomic fine structure	multiferroics	unconventional superconductor	SO-assisted Mott physics	topological insulators
	$TbMnO_3$	Sr_2RuO_4	Sr_2IrO_4 $Na_4Ir_3O_8$ $(Na,Li)_2IrO_3$	HgTe Bi_2Se_3
	SOC induced DM interaction competes with **magnetic exchange**		SOC competes directly with **Hubbard physics**	

4d/5d transition metal compounds

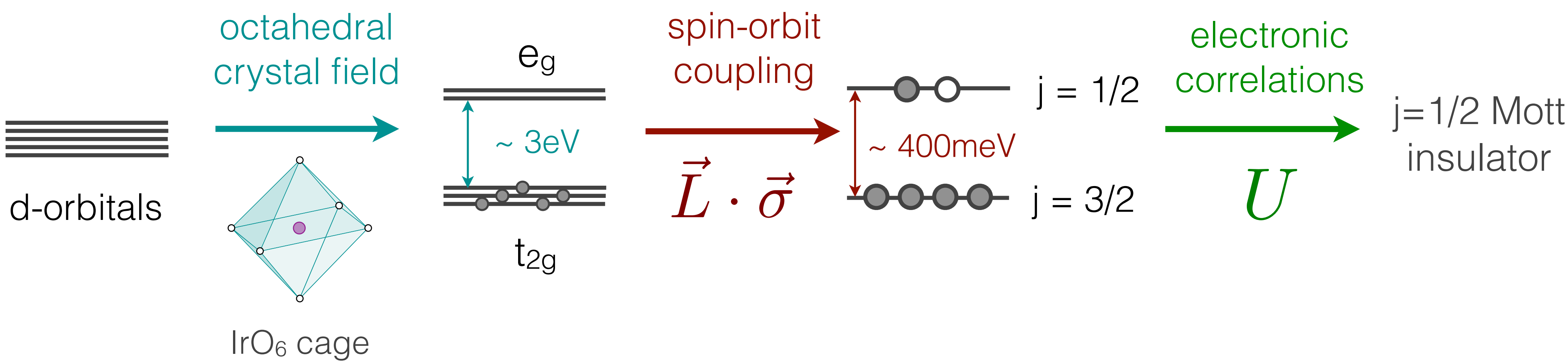
Transition metal oxides with **partially filled 4d/5d shells** exhibit an intricate interplay of **spin-orbit coupling**, **electronic correlations**, and **crystal field effects** resulting in a **broad variety of metallic and insulating states**.



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+} $(5d^5)$

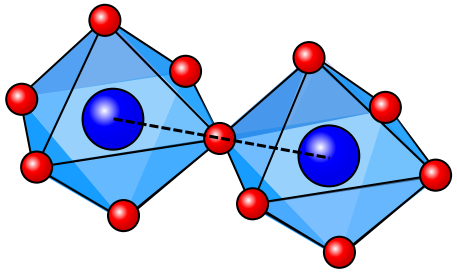


Why are these spin-orbit entangled j=1/2 Mott insulators **interesting?**

spin-orbit entangled Mott insulators

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

corner-sharing

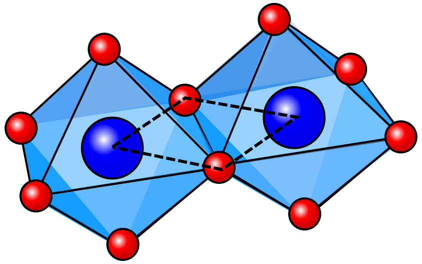


Sr_2IrO_4

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

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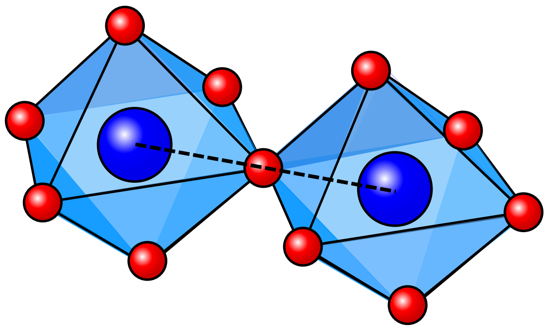
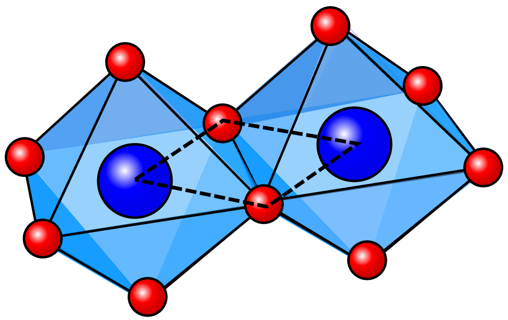


Sr_2IrO_4

Heisenberg exchange

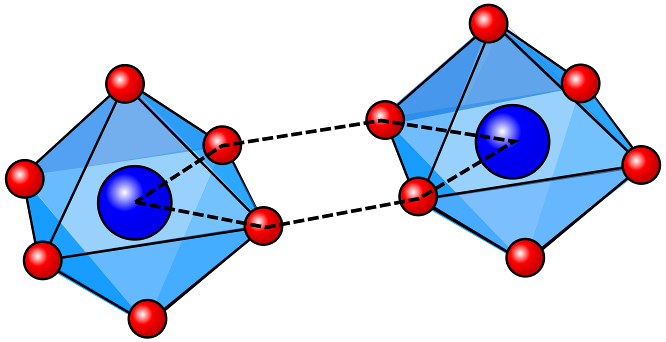
edge-sharing



$(Na,Li)_2IrO_3$
$RuCl_3$

Heisenberg-Kitaev exchange

“**parallel edge**”-sharing



$Ba_3IrTi_2O_9$

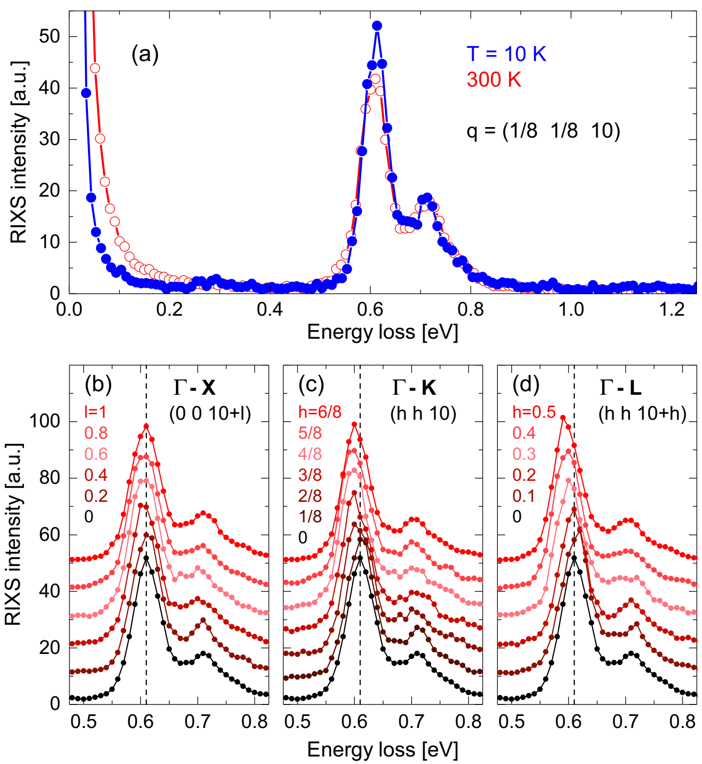
$$H = - \sum_{\gamma-\text{bonds}} J\, \mathbf{S}_i \mathbf{S}_j + K\, S_i^\gamma S_j^\gamma + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right)$$

spin-orbit entangled moments

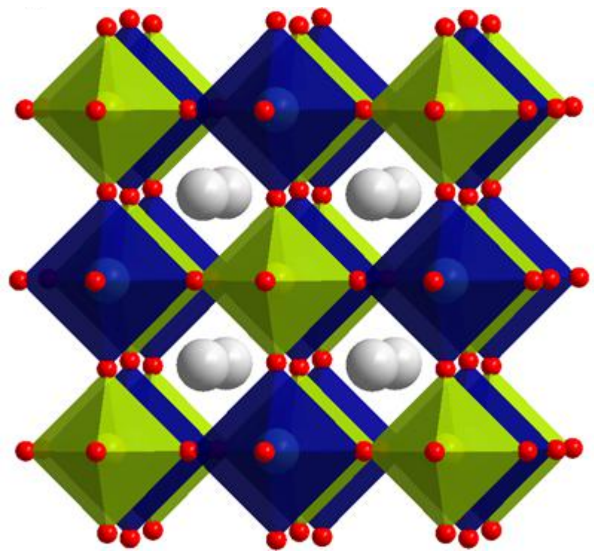
Ba_2CeIrO_6

Revelli *et al.*, PRB **100**, 085139 (2019)

The double perovskite Ba_2CeIrO_6
is the **best j=1/2 system** we have ever seen,
but not really a "Kitaev material".



RIXS experiments



- pristine j=1/2 physics

$$|0\rangle = 0.991\left|\frac{1}{2}, \frac{1}{2}\right\rangle - 0.130\left|\frac{3}{2}, \frac{1}{2}\right\rangle$$

- frustrated FCC magnetism, but Kitaev interaction relieves frustration

- strong magneto-elastic effect

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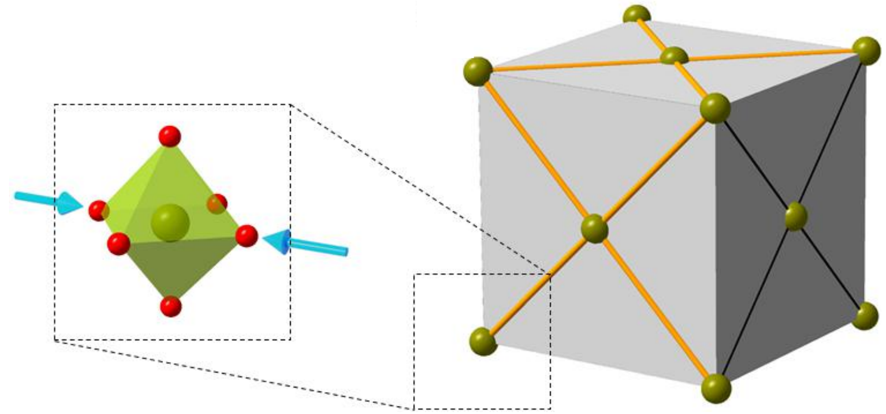

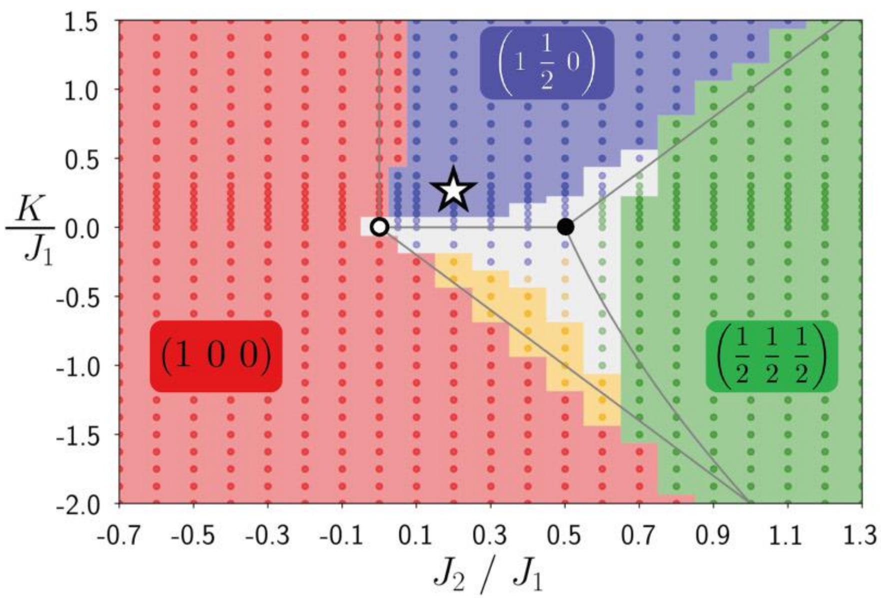

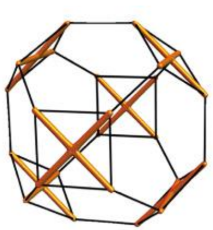

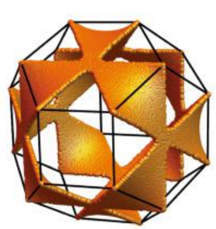

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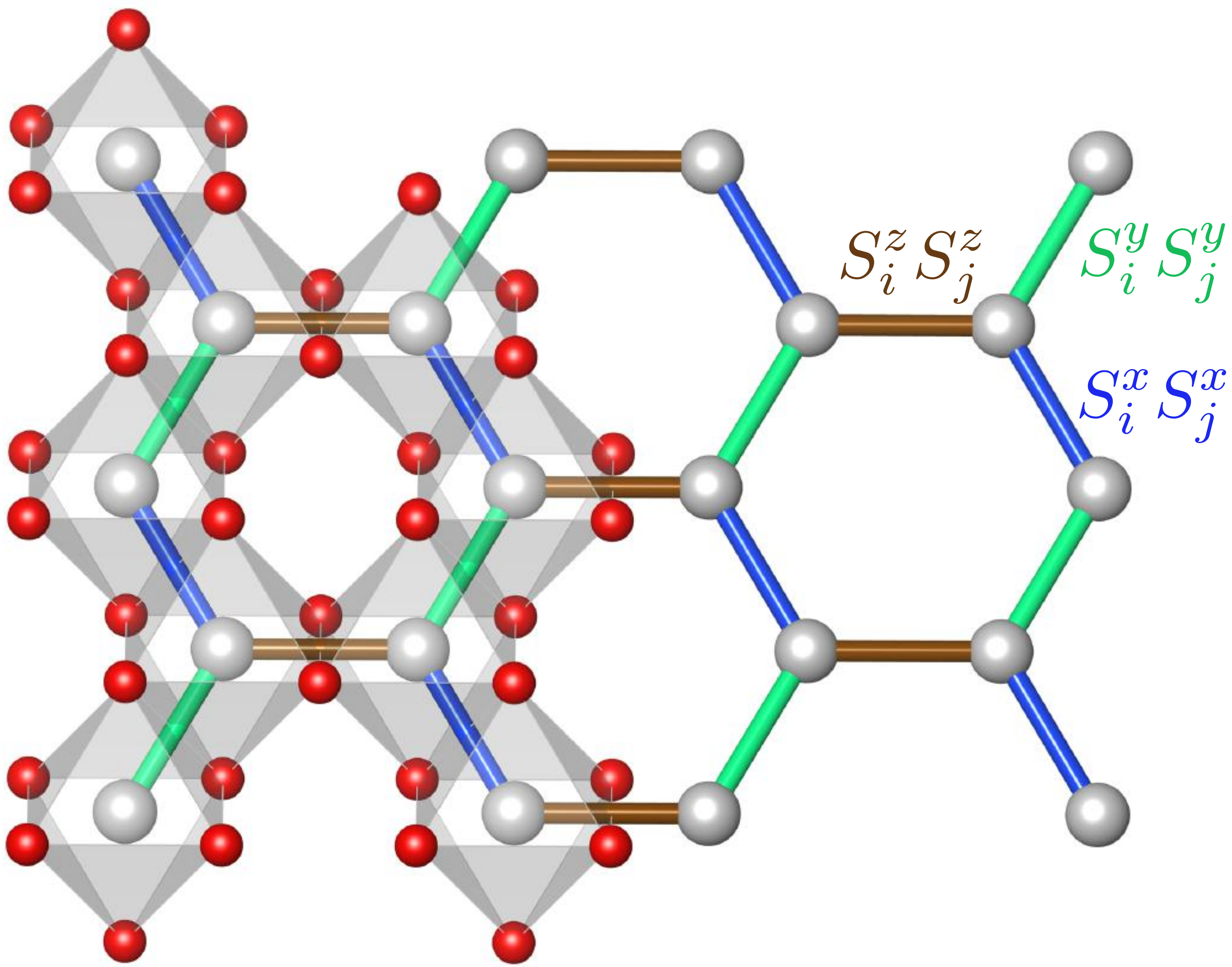
honeycomb Kitaev materials

proximate spin liquids

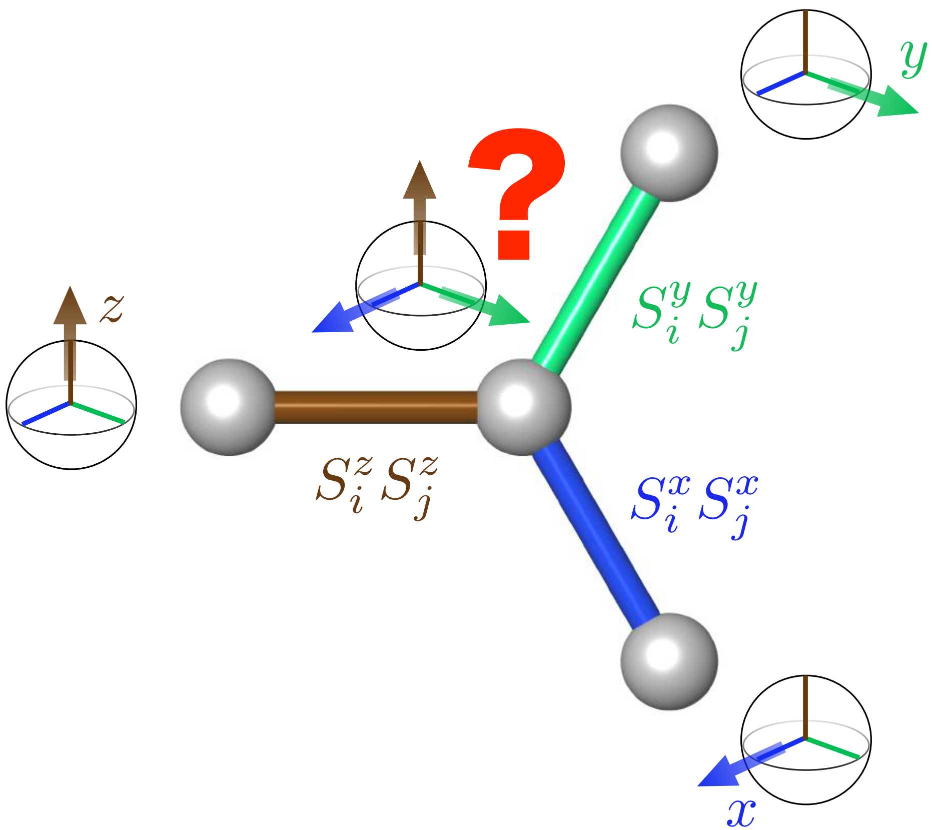
honeycomb Kitaev materials

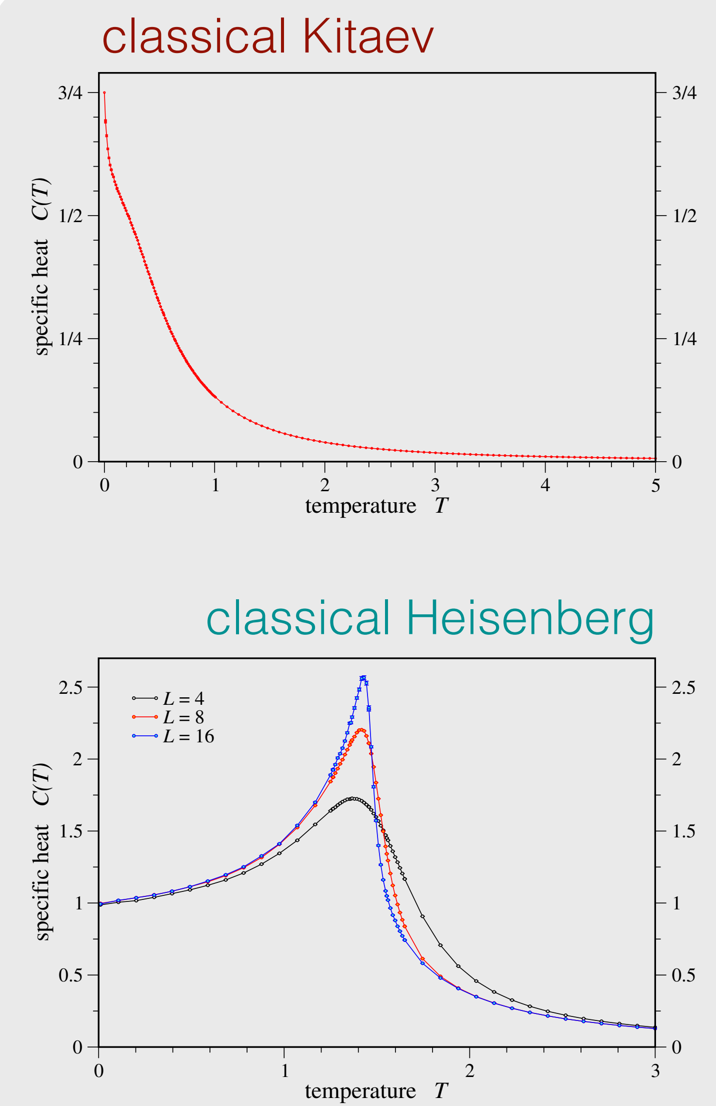
Na_2IrO_3, α-Li_2IrO_3, $RuCl_3$, $H_2LiIr_2O_6$



exchange frustration

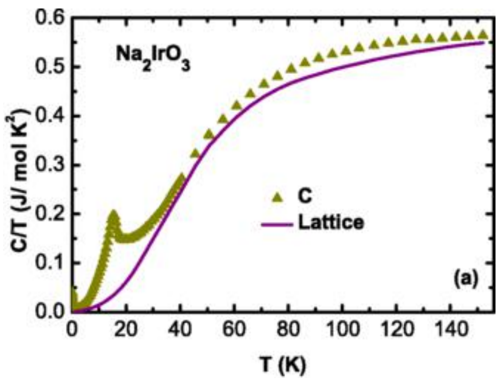
$$H = -\sum_{\gamma-\text{bonds}} J\,\mathbf{S}_i\mathbf{S}_j + K\,S_i^\gamma S_j^\gamma$$



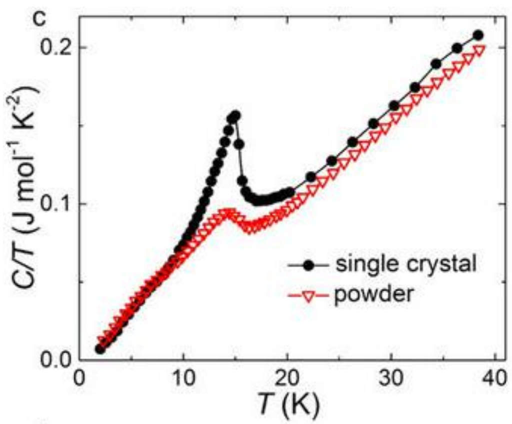


Kitaev materials – really?

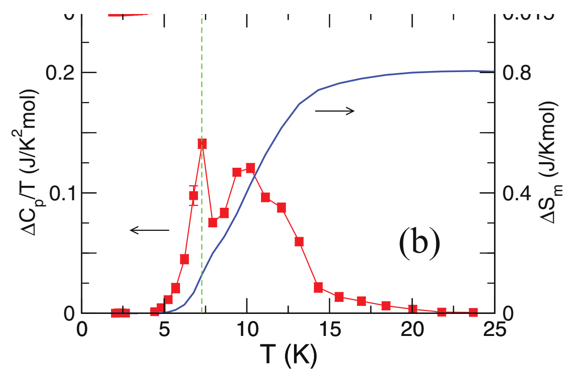
Na_2IrO_3



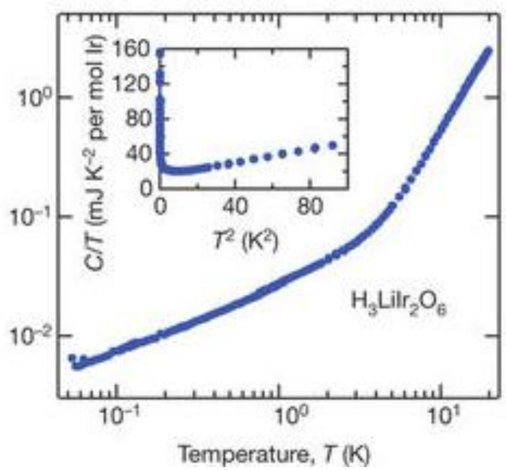
Li_2IrO_3



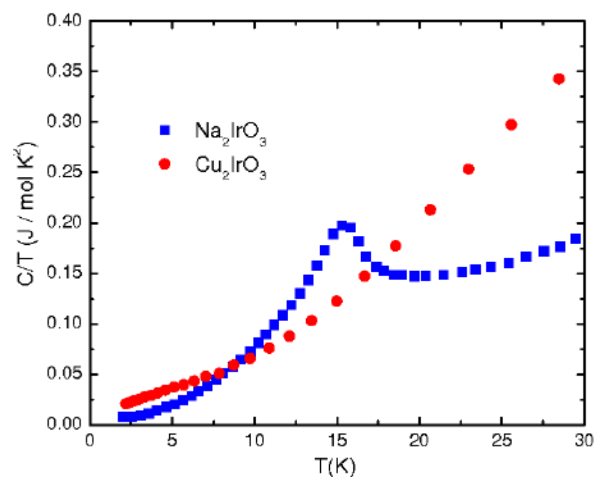
$RuCl_3$



$H_2LiIr_2O_6$



Cu_2IrO_3



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

honeycomb Kitaev materials

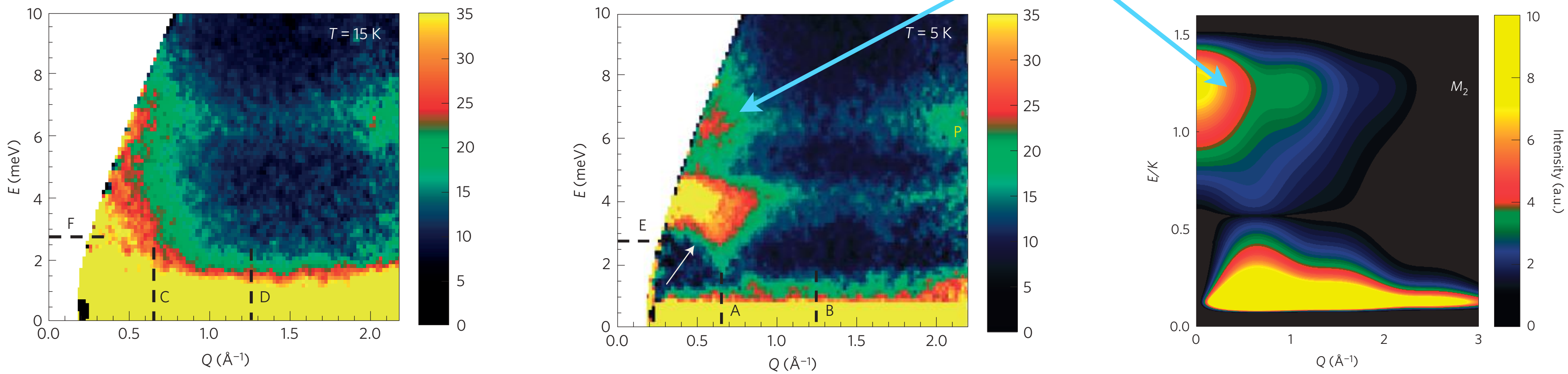
	magnetic moment $\mu_{\mathrm{eff}}/\mu_{\mathrm{B}}$	ordering temperature T_{N}	Curie-Weiss temperature Θ_{CW}
Na_2IrO_3	1.79(2)	15 K zig-zag order	-125 K
α-Li_2IrO_3	1.83(5)	15 K counterrotating spirals	-33 K
$RuCl_3$	2.2	7 K zig-zag order	-150 K
$H_2LiIr_2O_6$	?	—	?

$RuCl_3$

neutron scattering

Banerjee *et al.*, Nature Materials 4604 (2016)

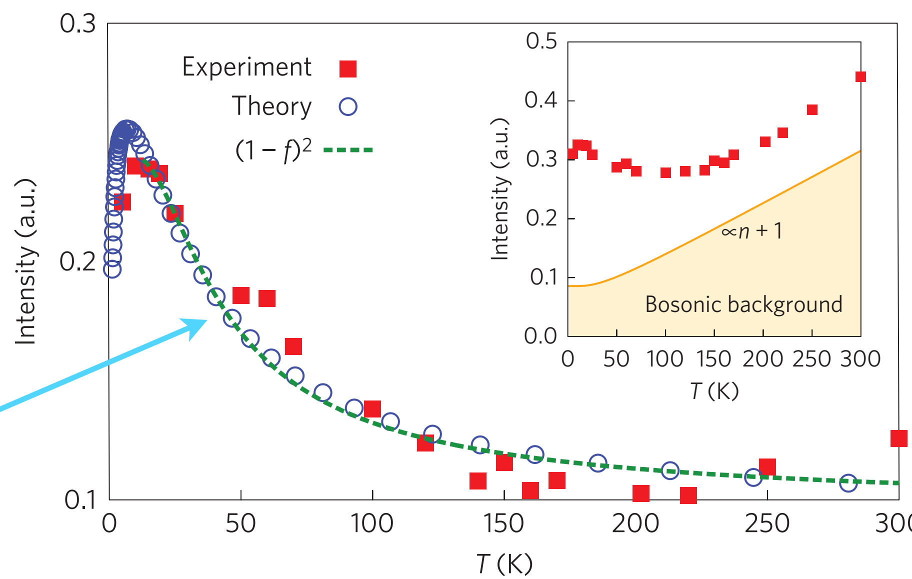
broad **scattering continuum**



Raman scattering

Nasu *et al.*, Nature Physics **12**, 912 (2016)
Sandilands *et al.*, PRL **114**, 147201 (2015)

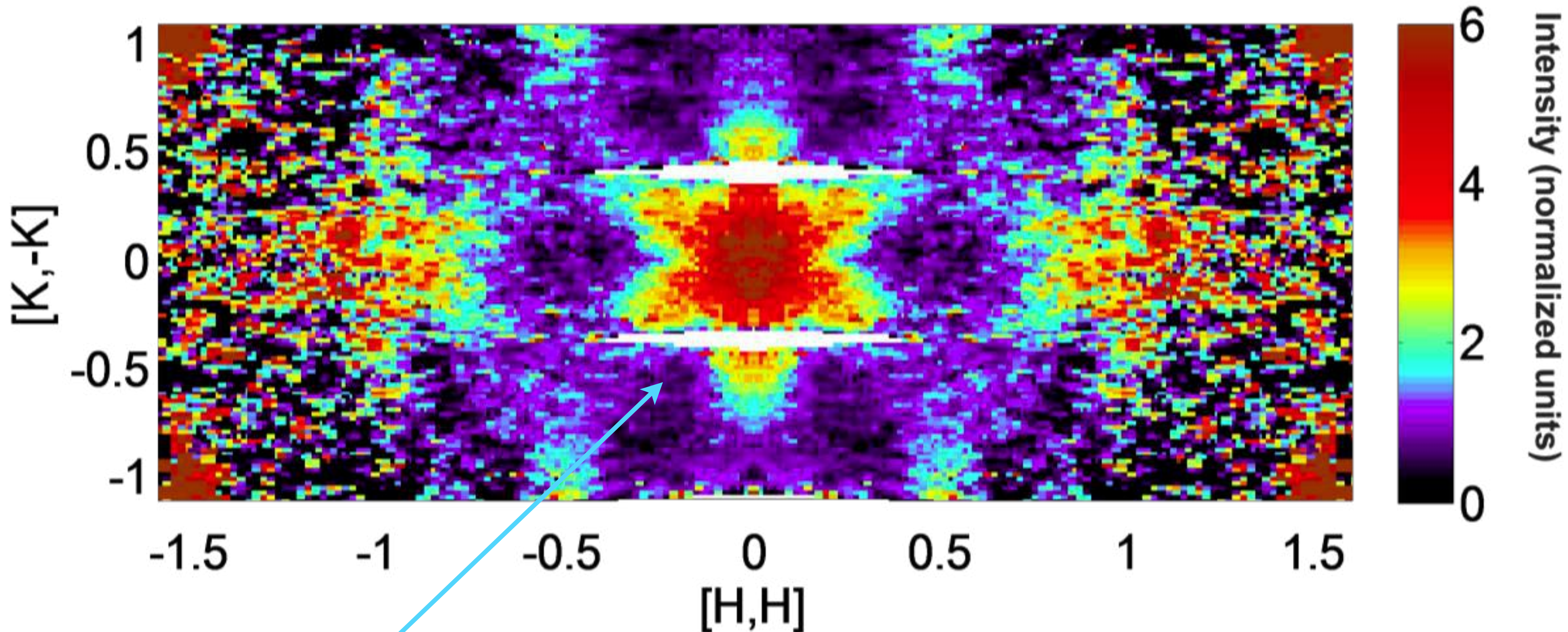
fermionic contribution



RuCl$_3$

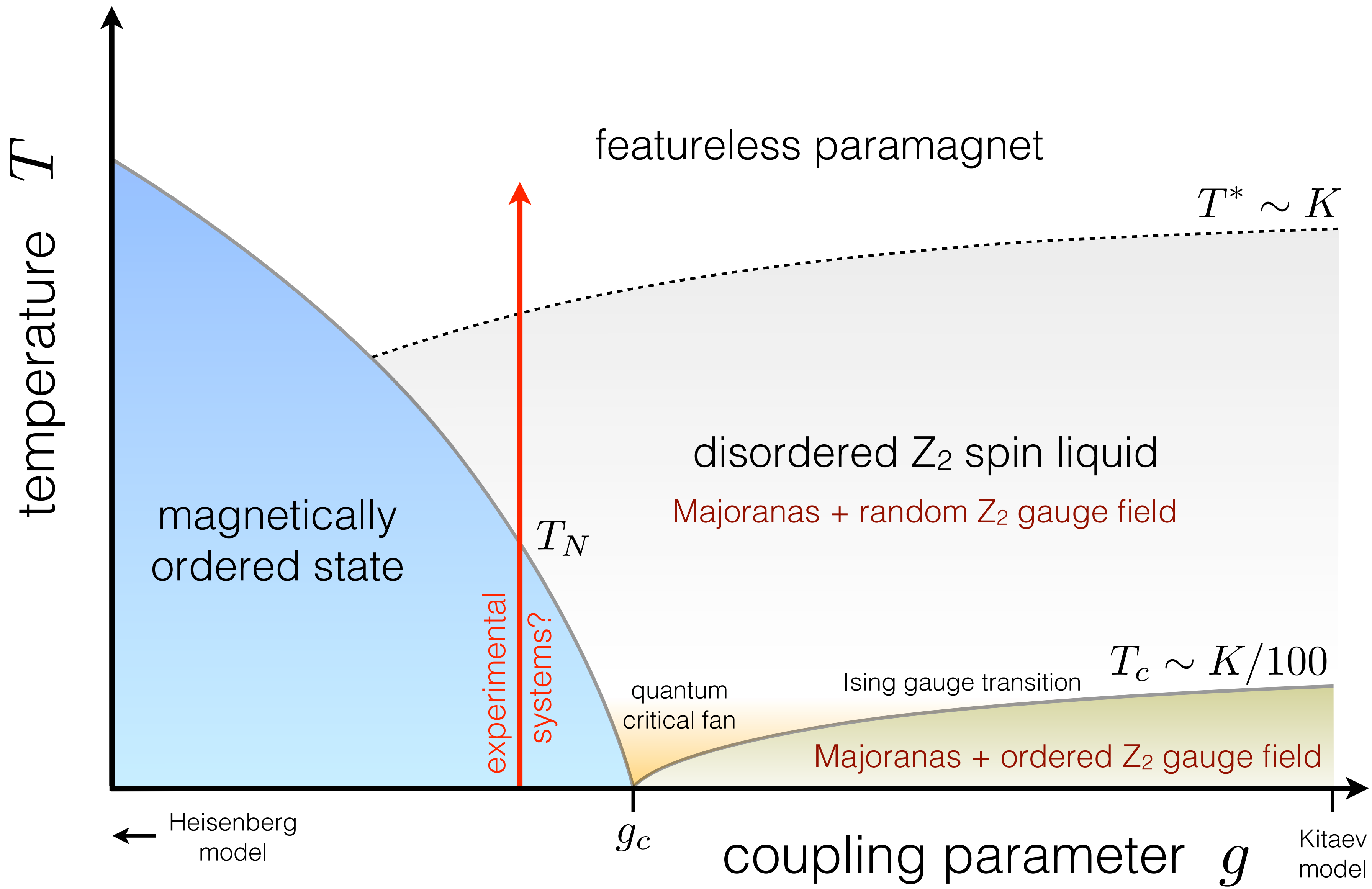
neutron scattering

Banerjee *et al.*, Nature Materials 4604 (2016)



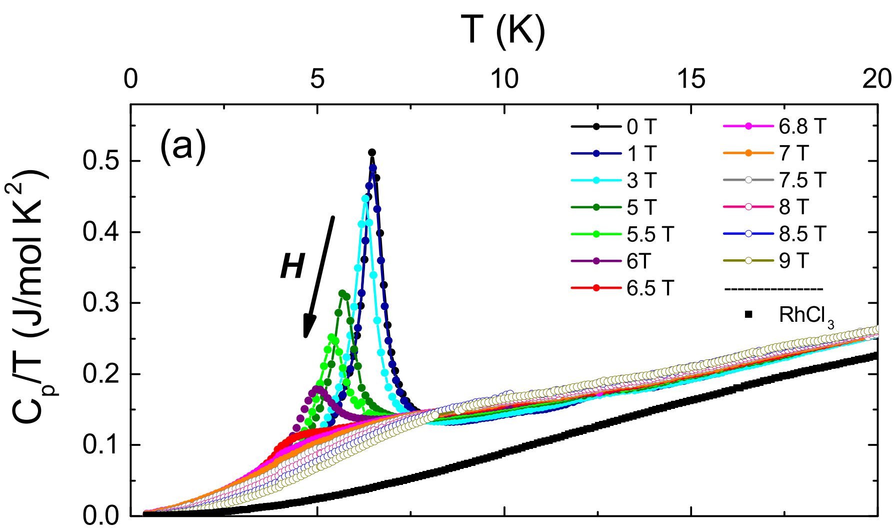
star-like feature arises from
interplay of spin-wave and spin liquids physics
at intermediate energy scales.

Proximate spin liquids

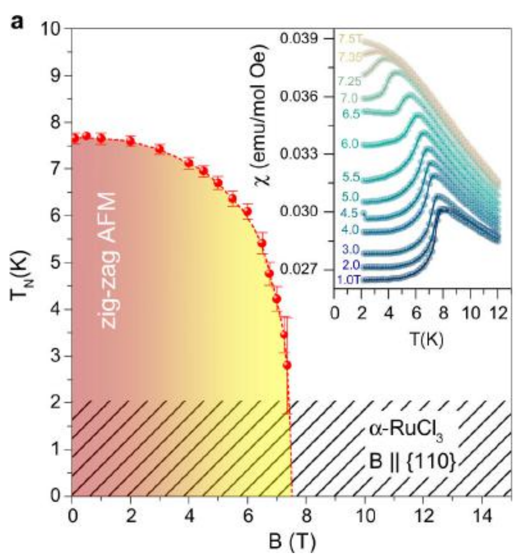


Spin liquids?!

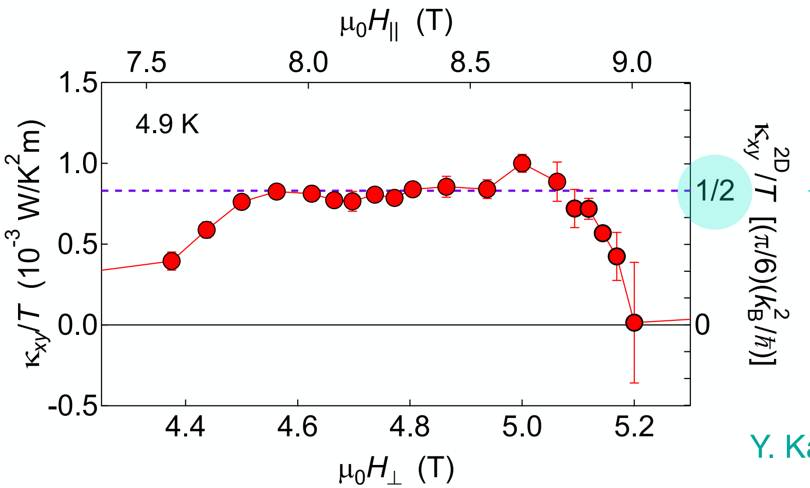
Something interesting happens for **$RuCl_3$ in a magnetic field**.



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



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



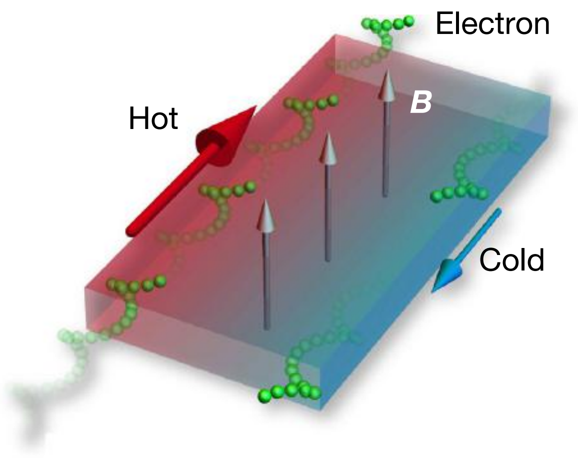
half-integer quantized
thermal Hall effect

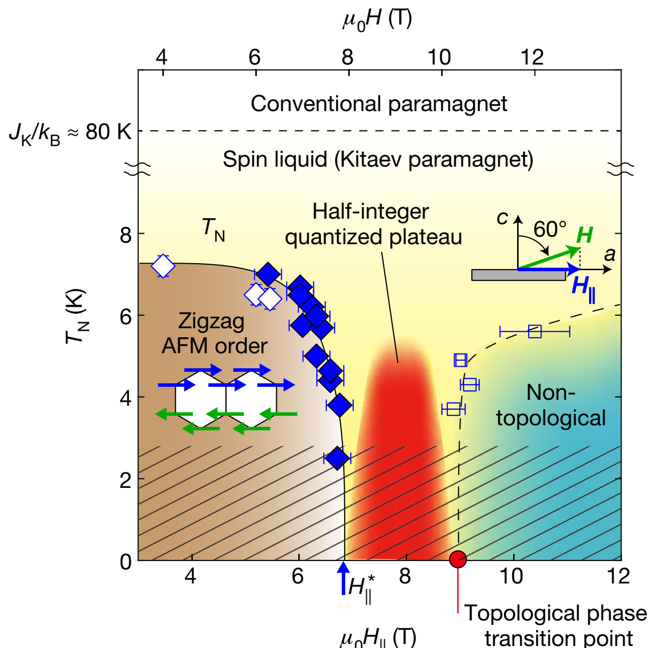
Y. Kasahara et al., Nature **559**, 227-231 (2018)

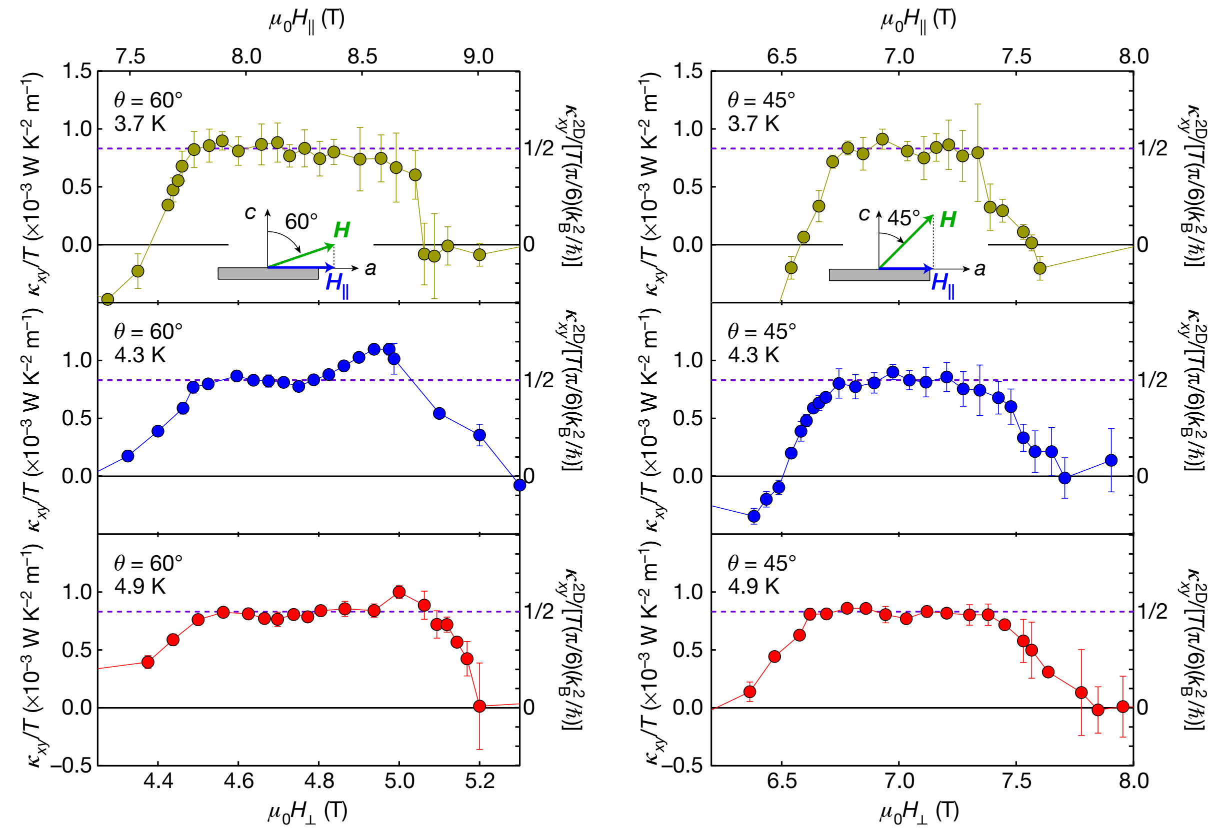
a new quantum Hall effect

S. Trebst & A. Rosch, Physik-Journal (2018)

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







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

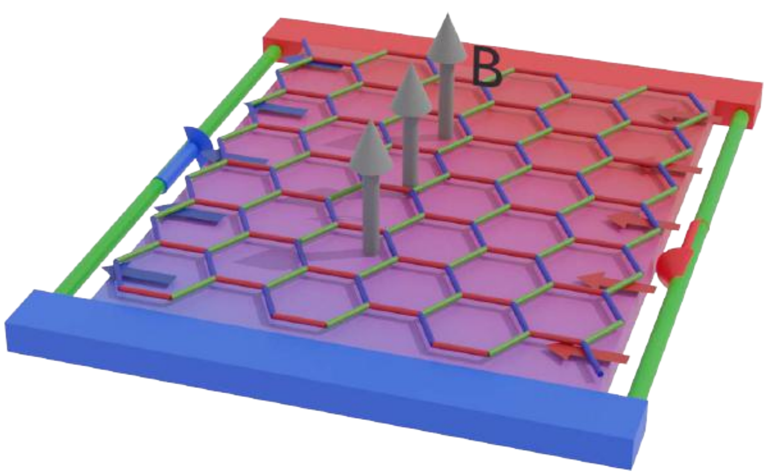
Why does this work in the presence of phonons?

Y. Vinkler-Aviv & A. Rosch, PRX **8**, 031032 (2018)
M. Ye, G. Halász, L. Savary, and L. Balents, PRL **121**, 147201 (2018)

thermal Hall effect in $RuCl_3$

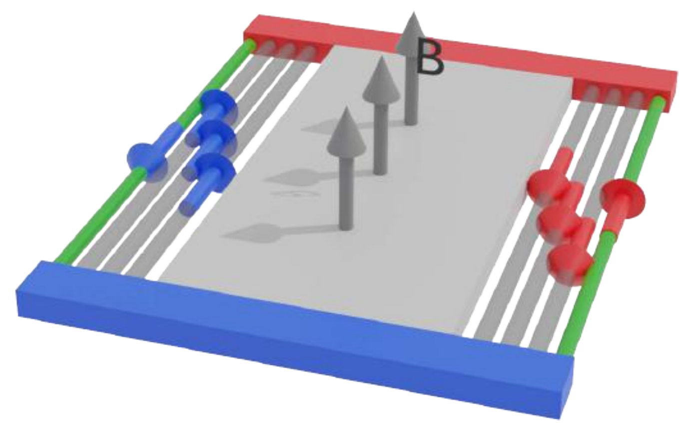
$$\kappa_{xy} = \frac{n}{2} \cdot \frac{\pi}{3} \frac{k_B^2 T}{\hbar}$$

A **half-quantized thermal Hall response** is direct evidence for gapless **Majorana modes**.



Kitaev material $RuCl_3$

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



ν=5/2 FQH state in a 2DEG

M. Banerjee et al., Nature **559**, 205–210 (2018)

thermal Hall effect in $RuCl_3$

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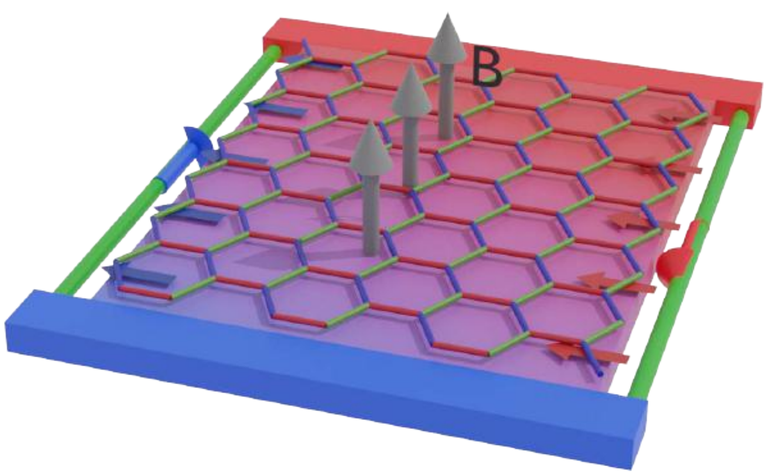
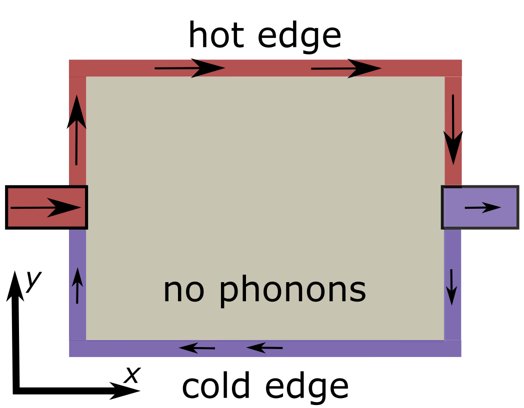
Y. Vinkler-Aviv & A. Rosch, PRX **8**, 031032 (2018)
M. Ye, G. Halász, L. Savary, and L. Balents, PRL **121**, 147201 (2018)

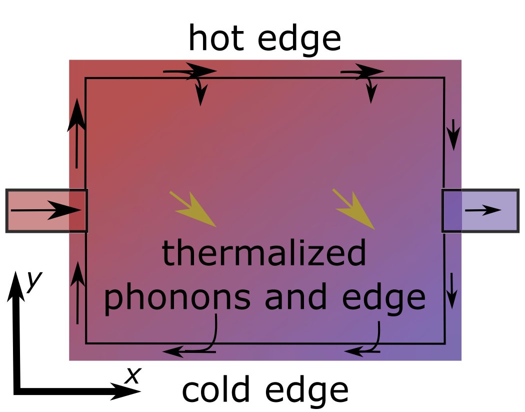


Kitaev material $RuCl_3$

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

But why is it quantized in the first place?
Why is there no leakage into the bulk,
via gapless acoustic phonons?





thermal Hall effect in $RuCl_3$

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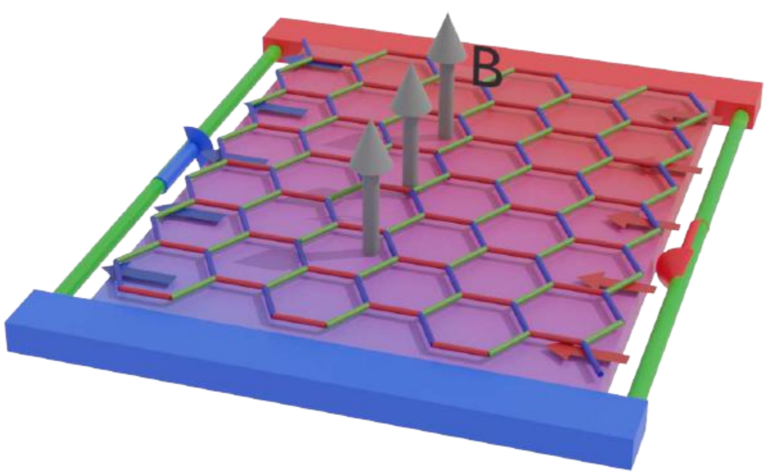
Y. Vinkler-Aviv & A. Rosch, PRX **8**, 031032 (2018)
M. Ye, G. Halász, L. Savary, and L. Balents, PRL **121**, 147201 (2018)



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

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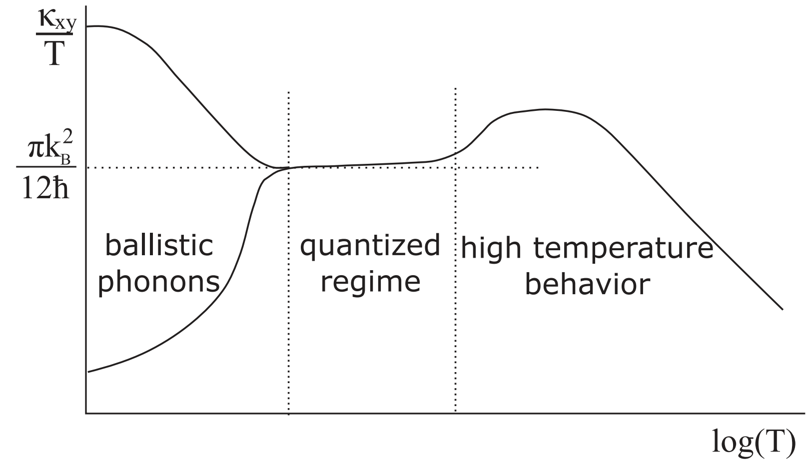
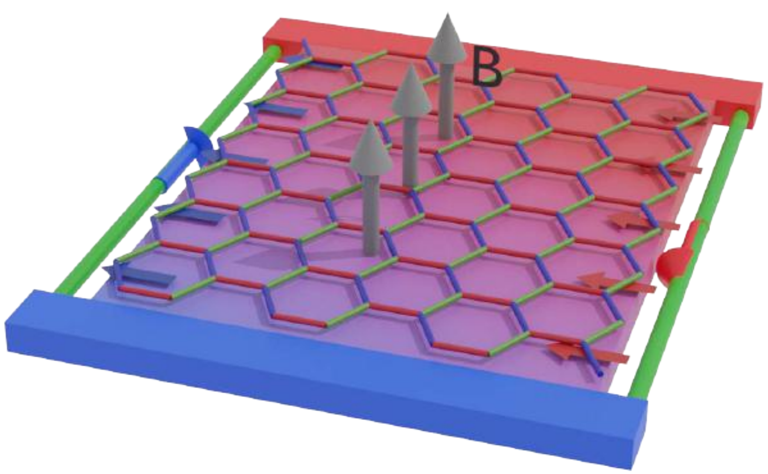


thermal Hall effect in $RuCl_3$

A **half-quantized thermal Hall response**
is direct evidence for gapless **Majorana modes**.

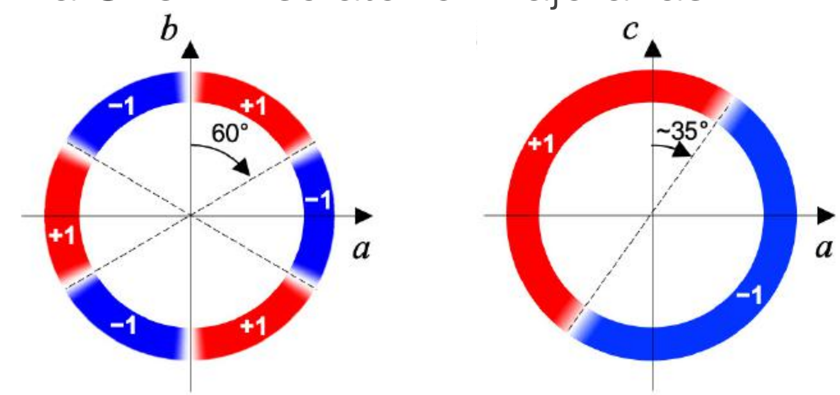
How can we distinguish whether the quantized thermal Hall effect arises from the formation of **Landau levels** or a non-trivial **Chern insulator**?



Kitaev material $RuCl_3$

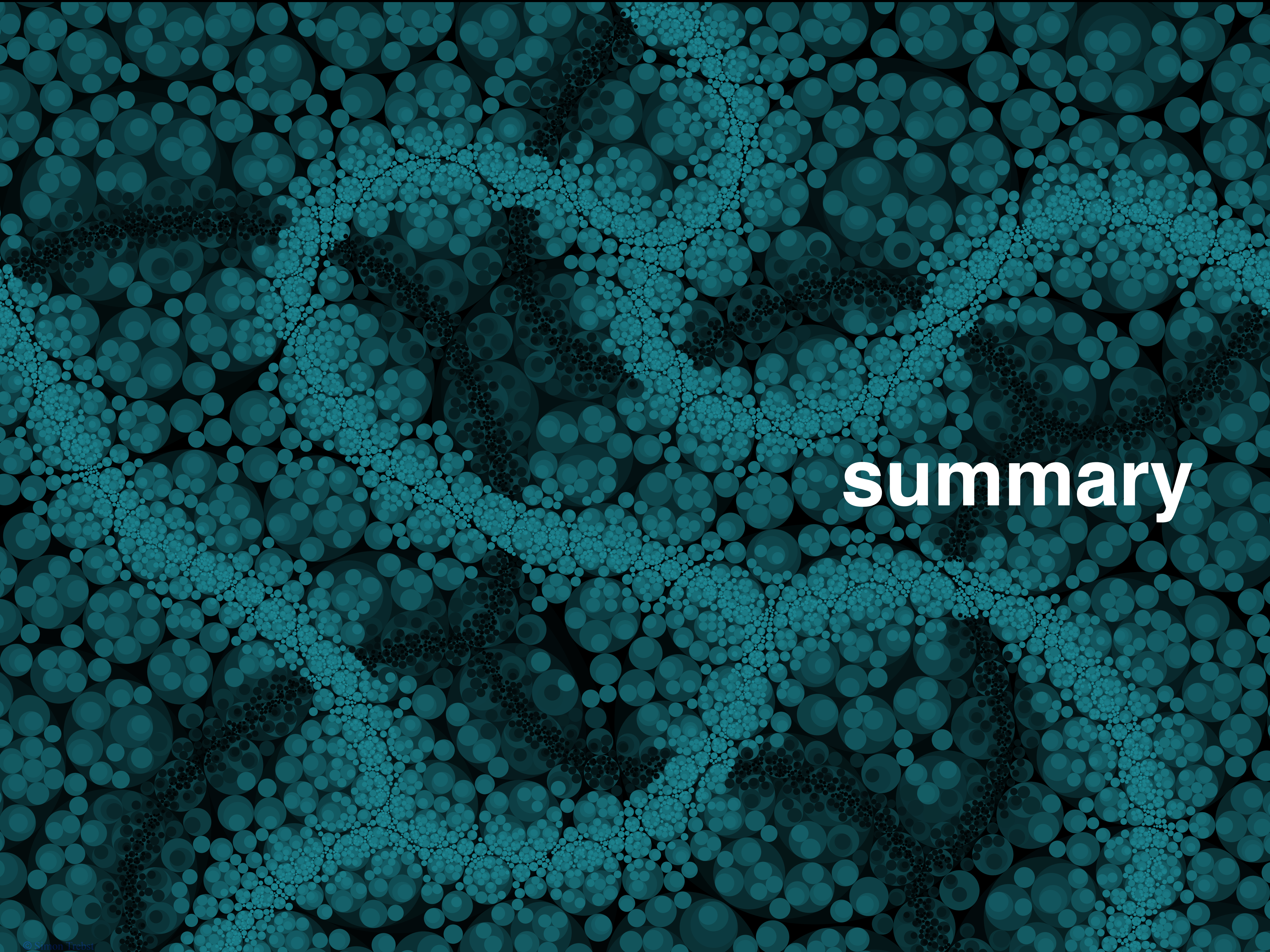
Y. Kasahara et al., Nature **559**, 227-231 (2018)

The Kitaev spin liquid is a **chiral spin liquid**,
a Chern insulator of Majoranas.



Its Hall quantization is **angle-dependent** and occurs even for an in-plane field (**anomalous thermal Hall effect**).

T. Yokoi et al., Science (2021)



summary

Summary

lecture notes
arXiv:1701.07056

chapter 12

Kitaev materials

- a family of spin-orbit assisted j=1/2 Mott insulators
- bond-directional exchange induces frustration
- unconventional forms of magnetism

Bond-directional exchange

- (proximate) spin liquids
- signatures of Majorana fermions and Z_2 gauge field
- spin textures

Family of lattice geometries

- honeycomb – Na_2IrO_3, α-Li_2IrO_3, $(H_{3/4}Li_{1/4})_2IrO_3$, $RuCl_3$
- triangular – $Ba_3IrTi_2O_9$, $Ba_3Ir_2TiO_9$, $Ba_3Ir_2InO_9$
- 3D – β-Li_2IrO_3, γ-Li_2IrO_3, metal-organic compounds

Thanks!