

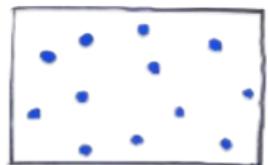
Frustrated Magnetism and Quantum Spin Liquids

TopoMag23 Crash Course

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Phases Matter



gas

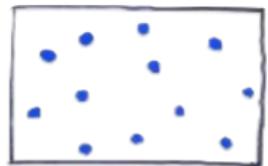


liquid



solid

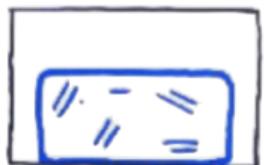
Phases Matter



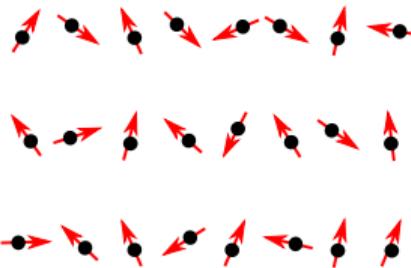
gas



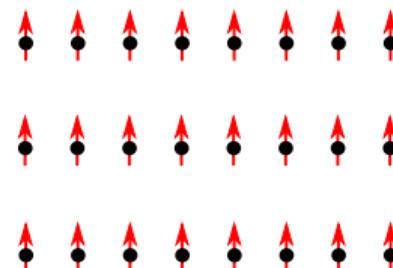
liquid



solid

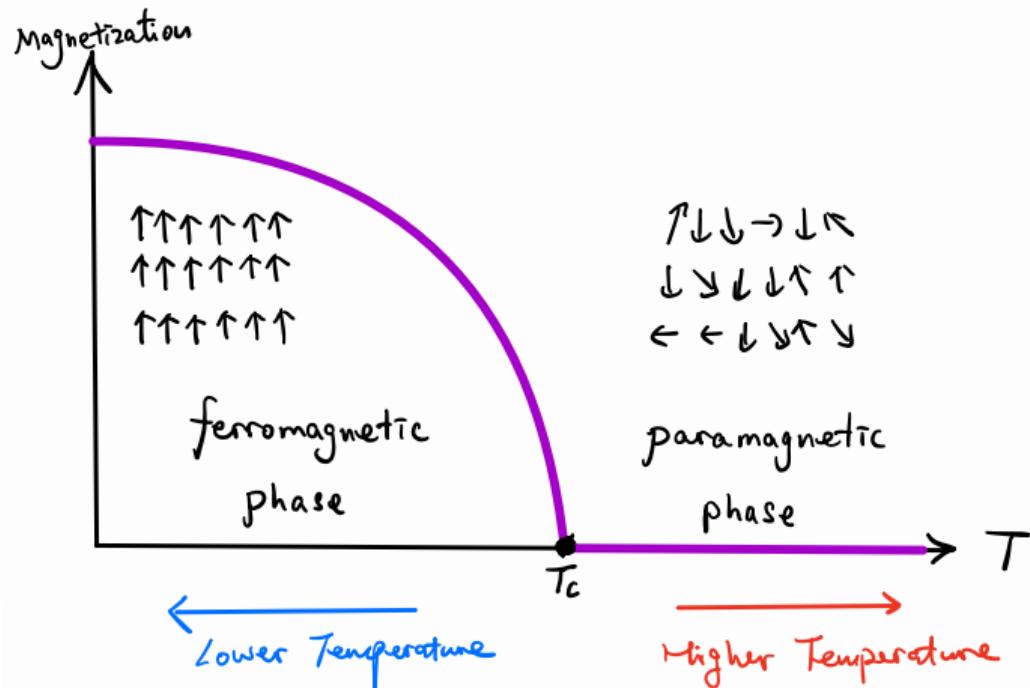


paramagnetic

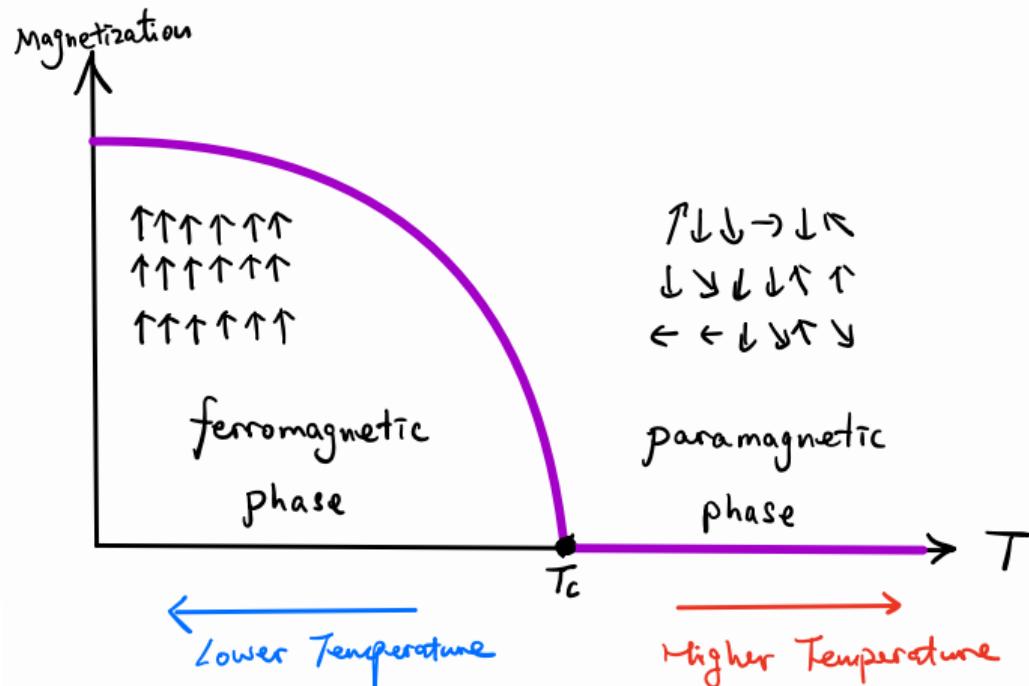


ferromagnetic

Order and Disorder



Order and Disorder



Two competing energy scales:

- ① Thermal fluctuation: $\sim k_B T$
- ② Interaction between spins J_{ij}

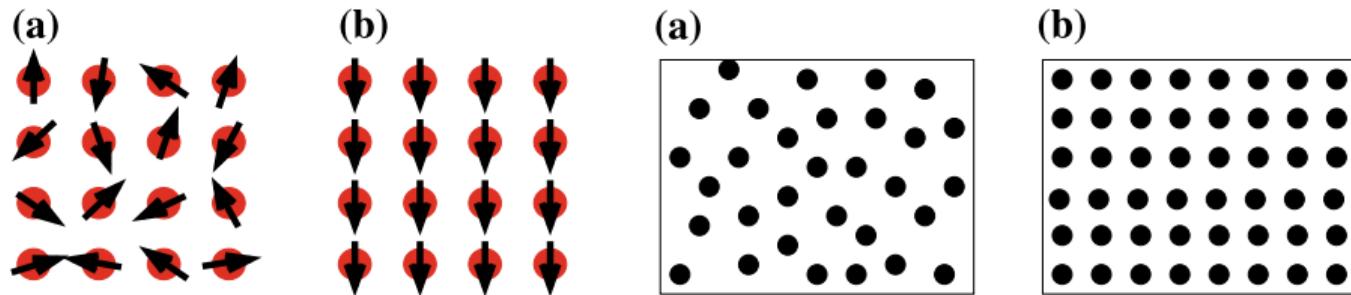
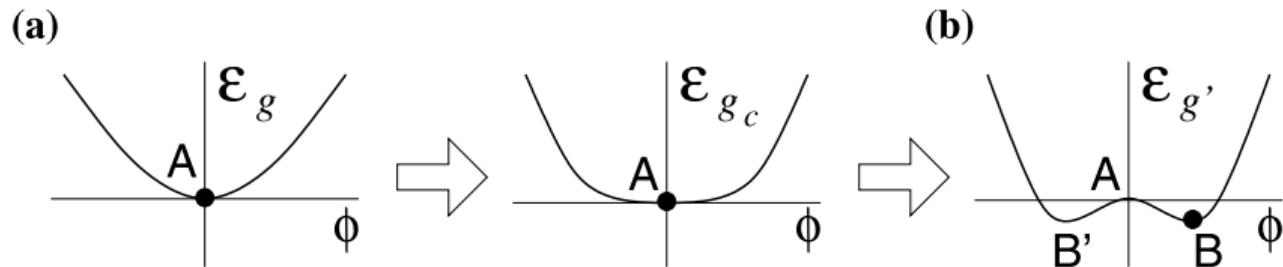
$J_{ij} \gg k_B T$: Ordered magnet
(Ferromagnet or Anti-ferromagnet)

$J_{ij} \ll k_B T$: Disordered magnet
(Paramagnet)

Phase transition at T_c

Landau's symmetry breaking theory

Ordered states spontaneously break the symmetry



Ferromagnet

$$\mathcal{H} = -J \sum_i S_i \cdot S_{i+1}$$

Lowest-energy configuration $M = N/2$:

$\uparrow \uparrow \uparrow$

Some excited states:

$\uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$

$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow$

$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \downarrow$

Ferromagnet

$$\mathcal{H} = -J \sum_i S_i \cdot S_{i+1}$$

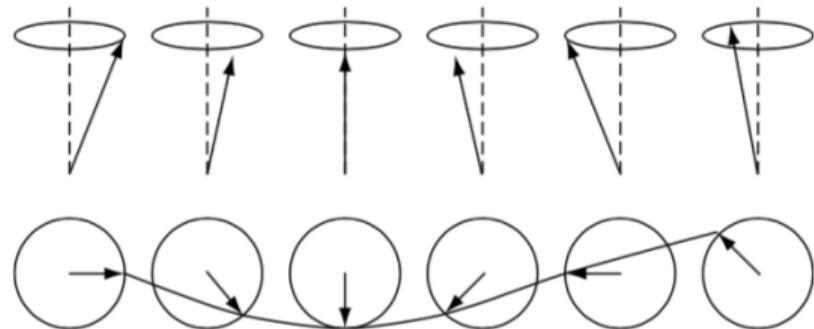
Lowest-energy configuration $M = N/2$:

$$\uparrow \uparrow \uparrow$$

Some excited states:

$$\begin{aligned} & \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \\ & \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \\ & \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \end{aligned}$$

Quasi-particle (Bosons: Spin wave or Magnon)



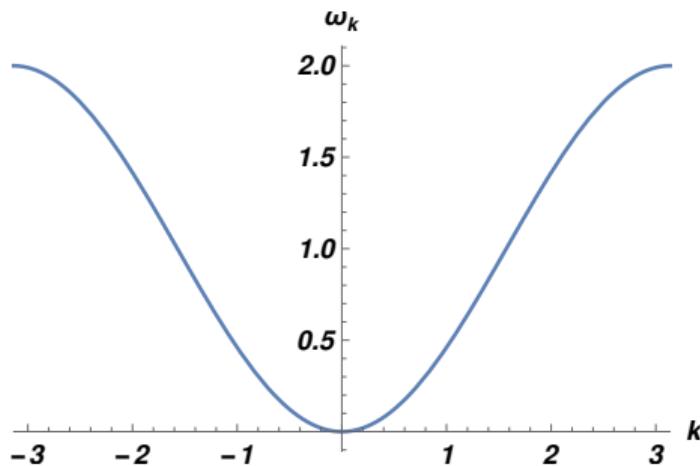
$$\mathcal{H} = \sum_k \omega_k n_k \quad \text{free magnons gas}$$

ω_k : dispersion; n_k : number of magnons

$n_k = 0$: vacuum state ($\uparrow\uparrow \cdots \uparrow$)

Dispersion of ferromagnetic magnons

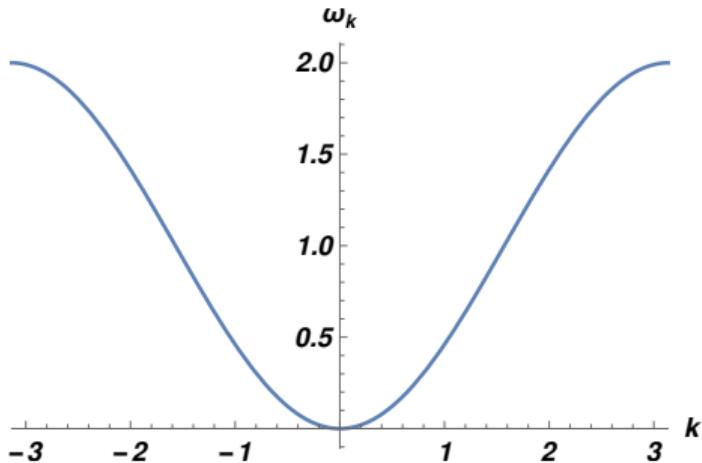
$$\omega_k \sim J[1 - \cos(k)]$$



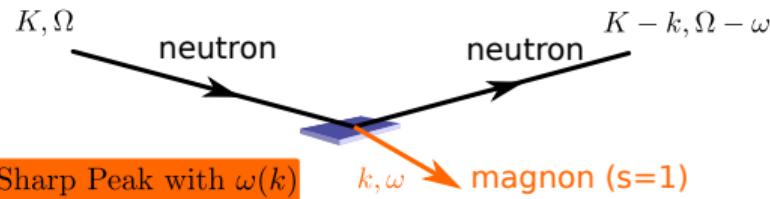
Each magnon carries $s = 1$

Dispersion of ferromagnetic magnons

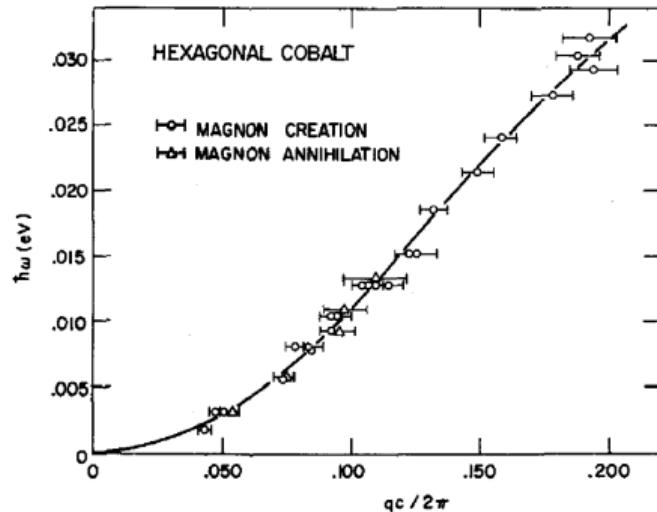
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Each magnon carries $s = 1$



H. A. Alperin et al, J. Appl. Phys. 37, 1052 (1966)

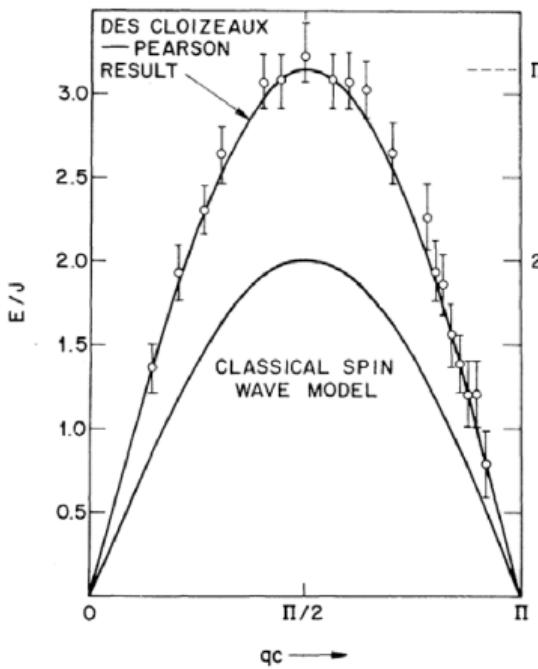
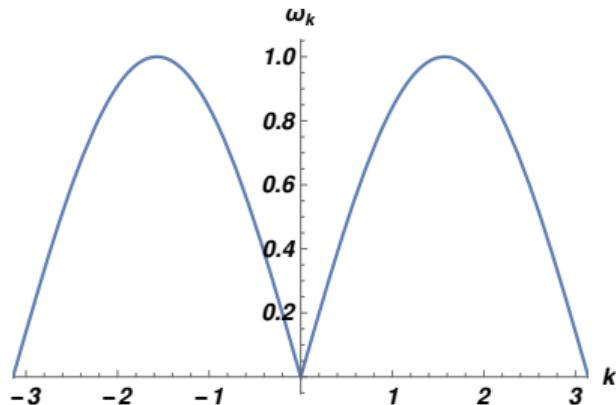


Anti-Ferromagnet

$$\mathcal{H} = J \sum_i S_i S_{i+1}, \quad \text{G.S.} = \uparrow\downarrow\uparrow\downarrow \cdots \uparrow\downarrow$$

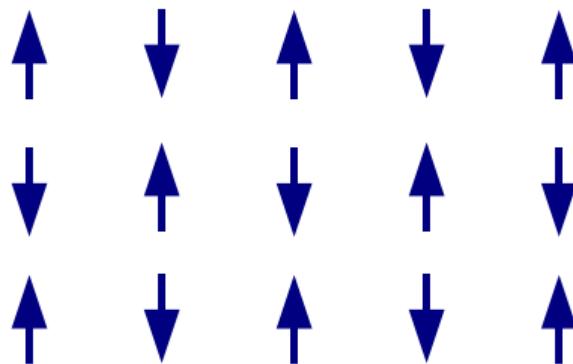
Dispersion of anti-ferromagnetic magnons

$$\omega_k \sim J|\sin(k)|$$



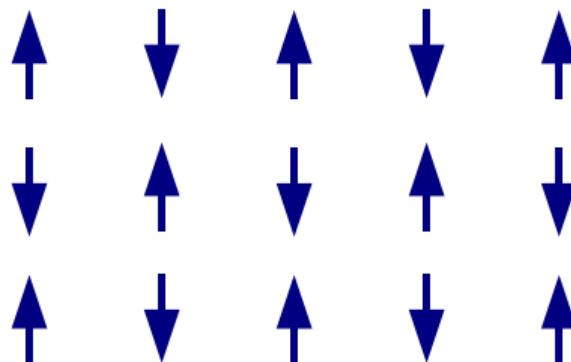
Geometrical Frustration

antiferromagnet e.g. $H = \sum S_i S_j$

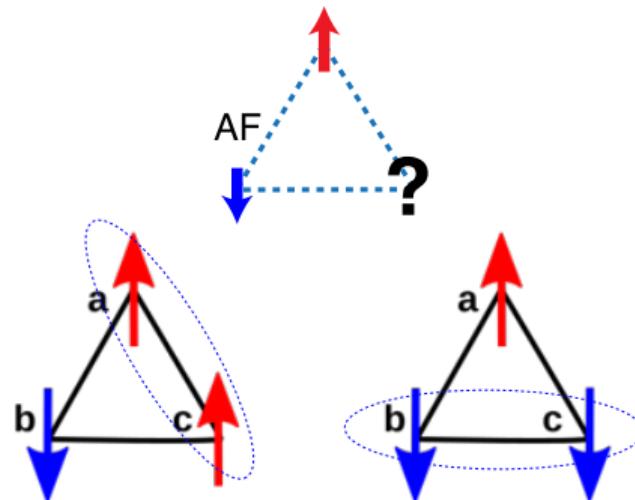


Geometrical Frustration

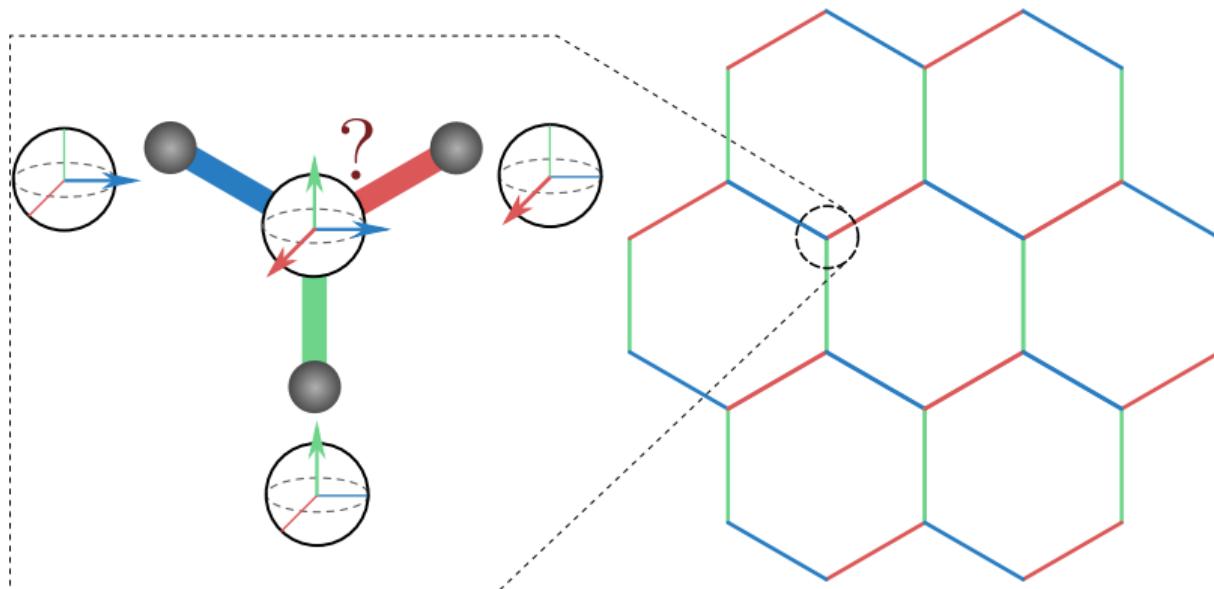
antiferromagnet e.g. $H = \sum S_i S_j$



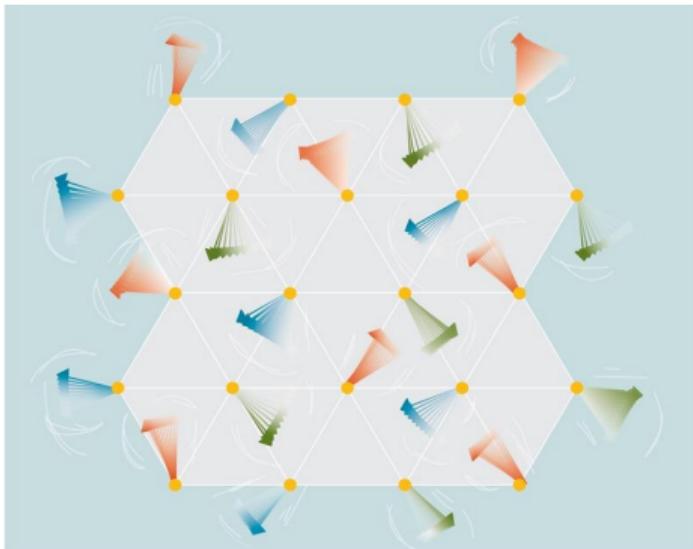
Geometrically frustrated magnet



Exchange Frustration

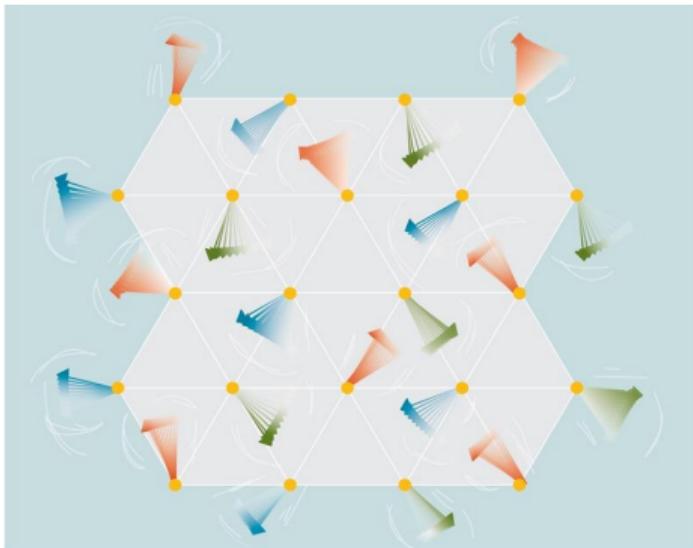


Consequences of Frustrations

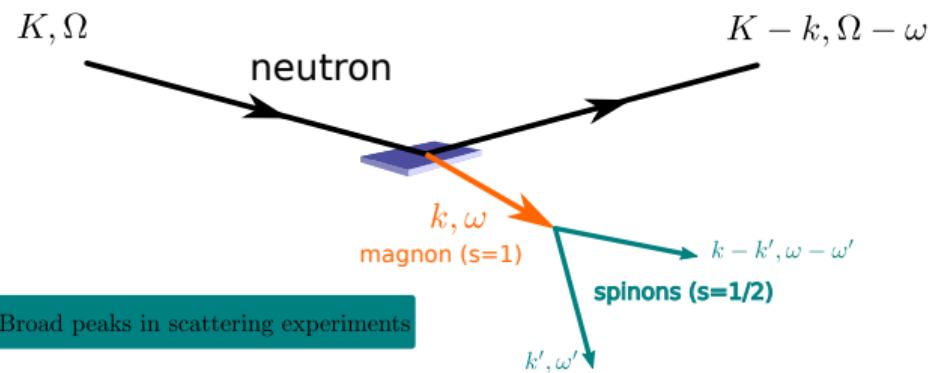


- ① No order at $T \rightarrow 0$
- ② No symmetry breaking
- ③ No $s = 1$ magnons or spin waves

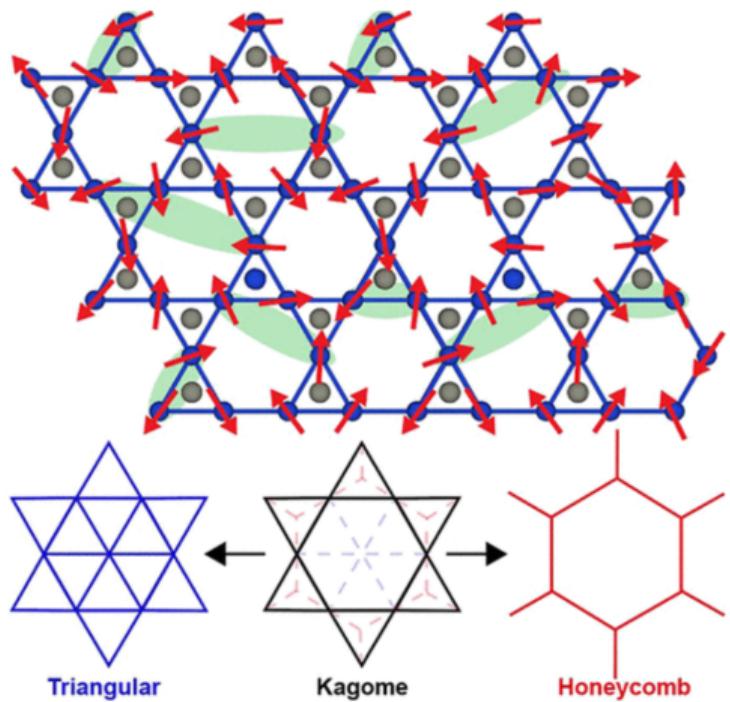
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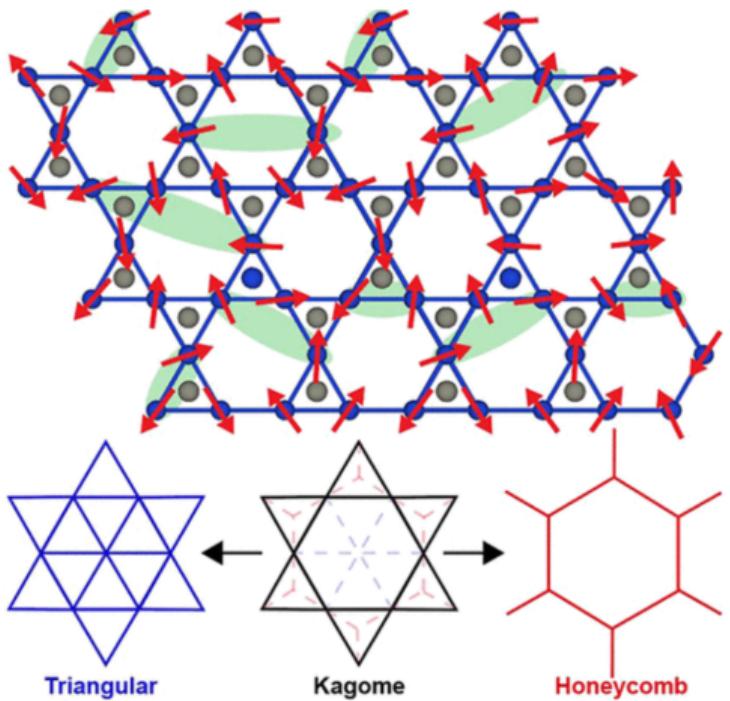
- ① No order at $T \rightarrow 0$
- ② No symmetry breaking
- ③ No $s = 1$ magnons or spin waves
- ④ Strong quantum fluctuation \rightarrow *quantum spin liquid*
- ⑤ Elementary excitations are *Spinons* ($s = \frac{1}{2}$)
- ⑥ *Broad peaks* in neutron scattering



Frustrated Systems (Criteria)

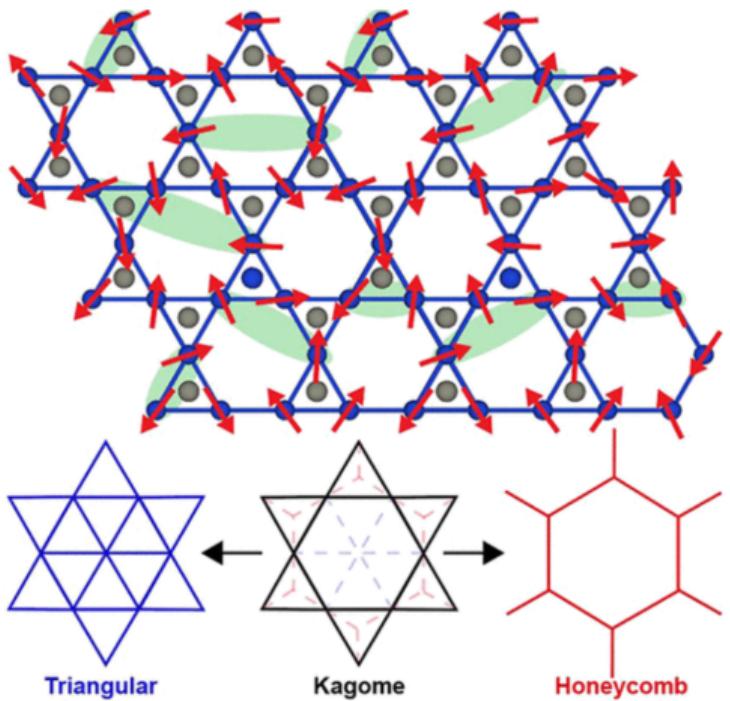


Frustrated Systems (Criteria)

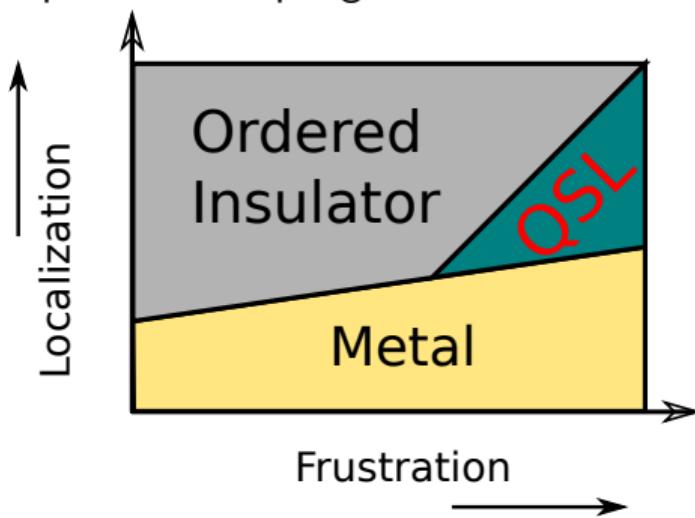


- ① Localized electrons (Mott Insulator)
- ② Small spins, preferably spin- $\frac{1}{2}$
- ③ Geometrical or exchange frustration
- ④ Spin-orbit coupling

Frustrated Systems (Criteria)



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Frustration Parameter

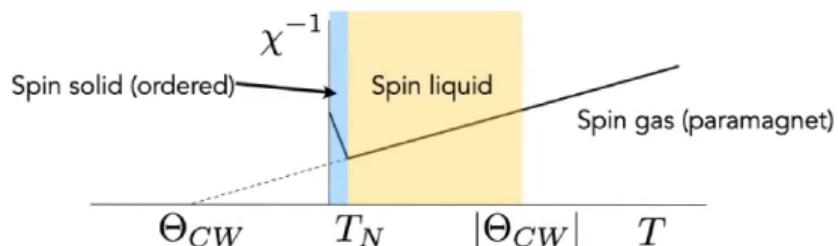
Two temperature scales:

- T_N at which magnetic order develops
 - Curie–Weiss temperature Θ_{CW}

$$\chi \sim \frac{C}{T - \Theta_{CW}}$$

The **frustration** parameter:

$$f = \Theta_{CW}/T_N.$$

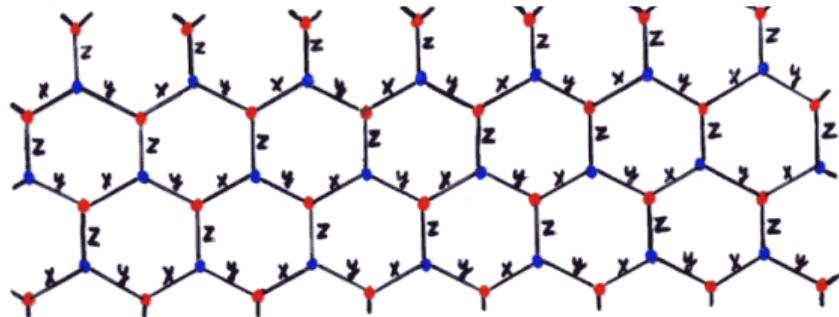


$f \rightarrow \infty$: True QSL

$f > 100$ is a good indication of possible QSL.

Honeycomb model

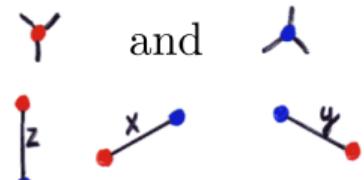
We follow the description in (Kitaev, 2006; Pachos, 2007)



Spin $\frac{1}{2}$ on each site, coupled to nearest neighbor by anisotropic spin-spin interaction.

Two sublattices

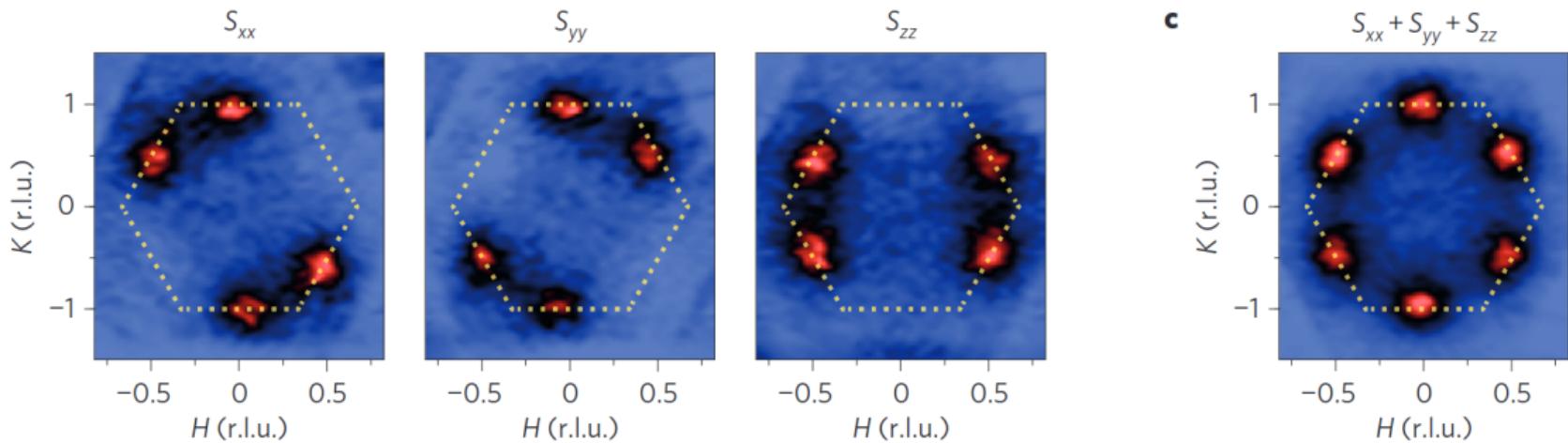
Three types of links



$$H = -K_x \sum_{\langle jk \rangle_x} \sigma_j^x \sigma_k^x - K_y \sum_{\langle jk \rangle_y} \sigma_j^y \sigma_k^y - K_z \sum_{\langle jk \rangle_z} \sigma_j^z \sigma_k^z$$

$$H = - \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} K_{\alpha} \sigma_j^{\alpha} \sigma_k^{\alpha}$$

Exchange Frustration in Materials



Evidence for anisotropic spin exchange from diffuse magnetic X-Ray scattering in Na_2IrO_3
Chun *et al*, Nature Physics 11, 462–466 (2015)

Exact Solution of Kitaev QSL (A. Kitaev, 2006)

$$H = - \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} K_{\alpha} \sigma_j^{\alpha} \sigma_k^{\alpha}$$

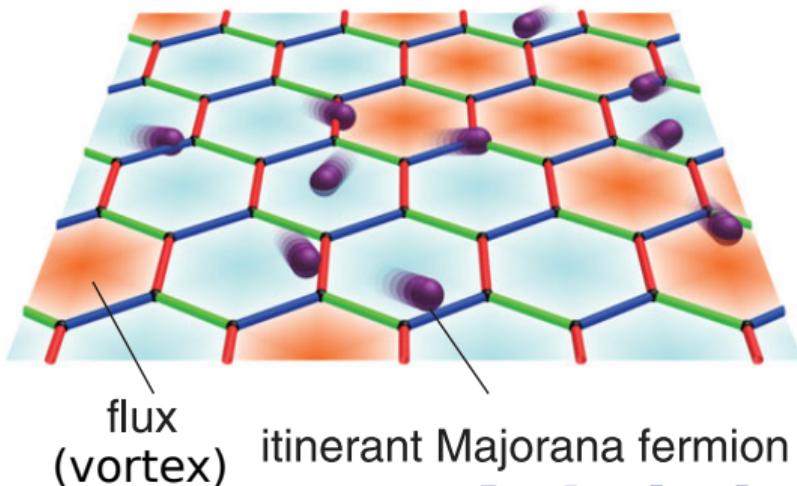
It has exact QSL ground state at $T = 0$ Note: spin σ is localized (Mott Insulator)

① 2 types of *fractionalized* excitations:

- Vortex (Z_2 flux) W_p
- Itinerant Majorana fermion c

② Hamiltonian \sim Free c gas

③ Gapless Majorana bands



Fractionalization (The Exact Solution)

$$H = - \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} K_{\alpha} \sigma_j^{\alpha} \sigma_k^{\alpha}$$

??? ↓ ???

$$H = \sum_k \epsilon(k) \hat{n}_k$$

- ① What is the elementary excitation counted by \hat{n}_k
- ② What is the band structure $\epsilon(k)$

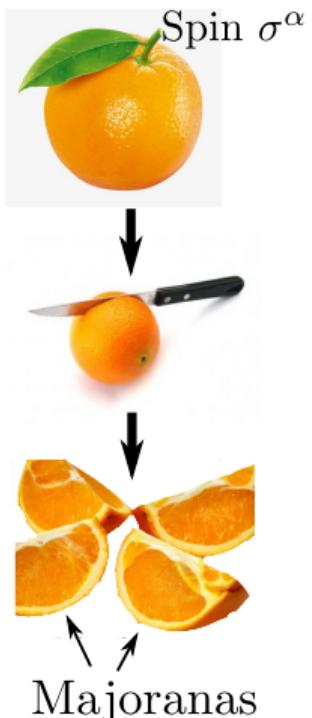
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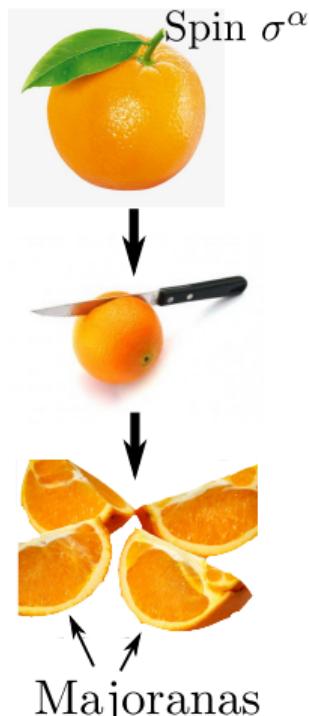
Fractionalization (The Exact Solution)

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- ① What is the elementary excitation counted by \hat{n}_k
- ② What is the band structure $\epsilon(k)$



$$H = - \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} f(\text{fractions of } \sigma)$$

✓ ↓ ✓

$$H = \sum_k \epsilon(k) \hat{n}_k$$

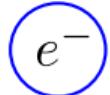
- ① fractions are Majoranas
- ② \hat{n}_k counts # Majorana modes
- ③ $\omega(k)$ gives Majorana bands

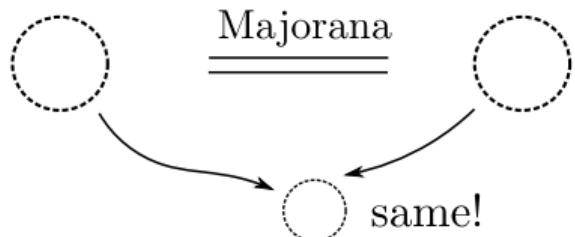
... and how to cut



- More degrees of freedom to manipulate (cut 1 into 4)
- It must preserve the number of distinguishable states (as a faithful representation)
- It must preserve the SU(2) algebra of spins $[\sigma^\alpha, \sigma^\beta] = 2i\epsilon_{\alpha\beta\gamma}\sigma^\gamma$

Majorana: no anti-particle

<p>particle</p> 	<p>anti-particle</p> 
$a^\dagger vac\rangle = e^-\rangle$	$a vac\rangle = e^+\rangle$



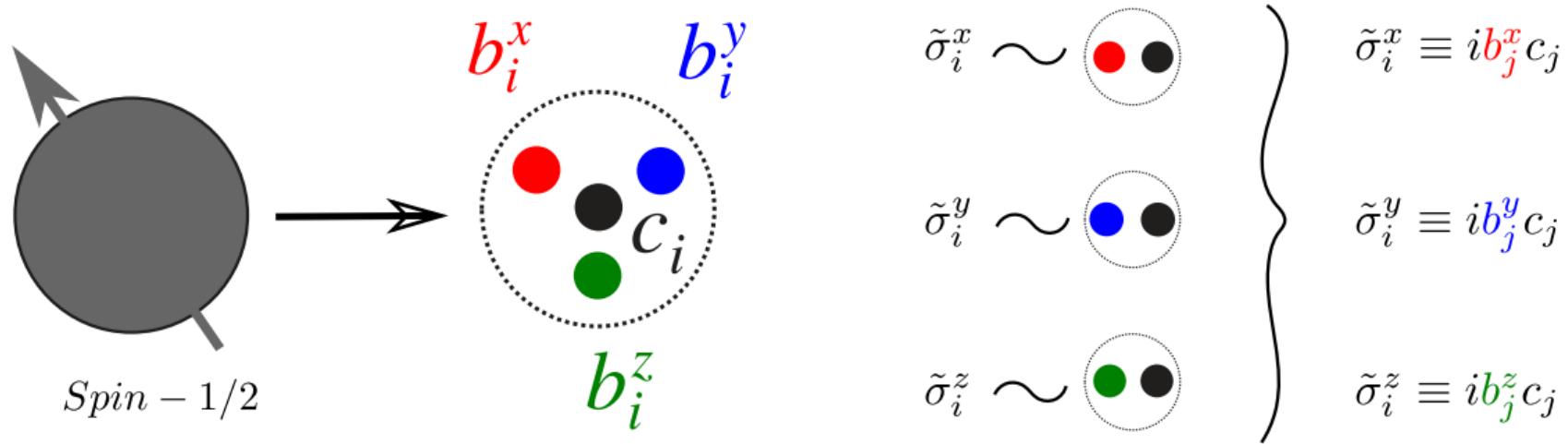
Majorana's anti-particle is itself

creation operator γ^\dagger
&

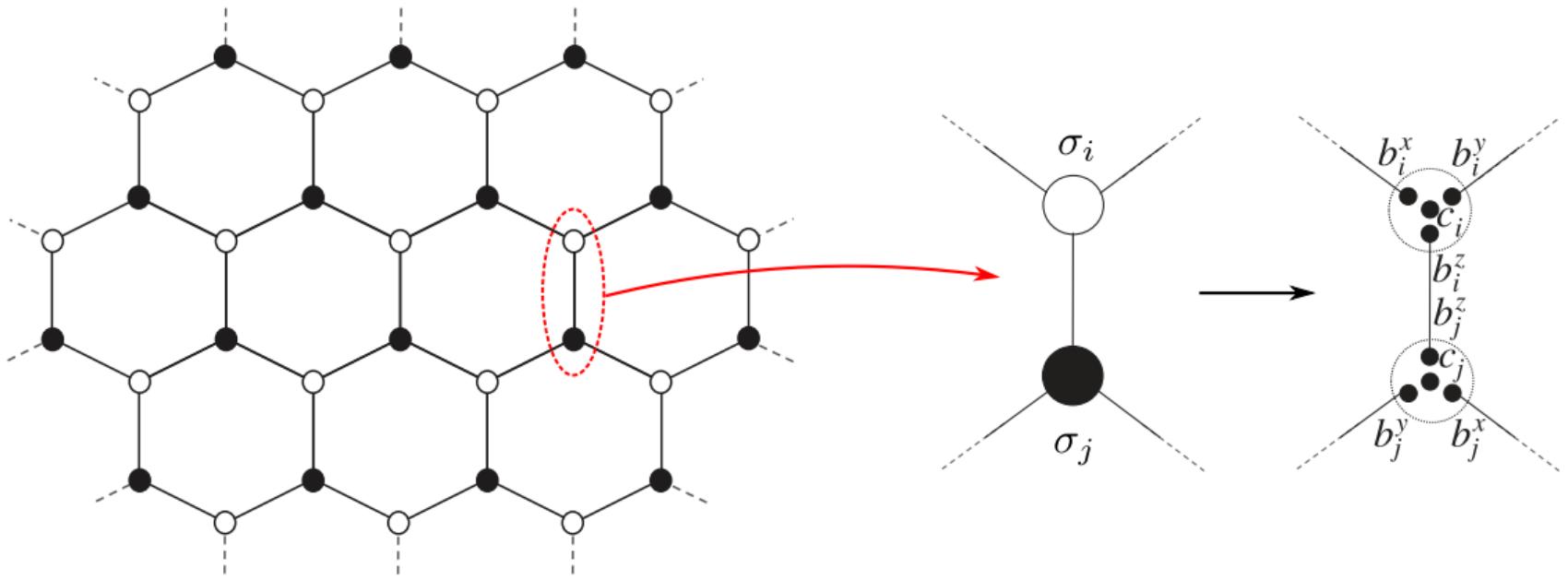
annihilation operator γ

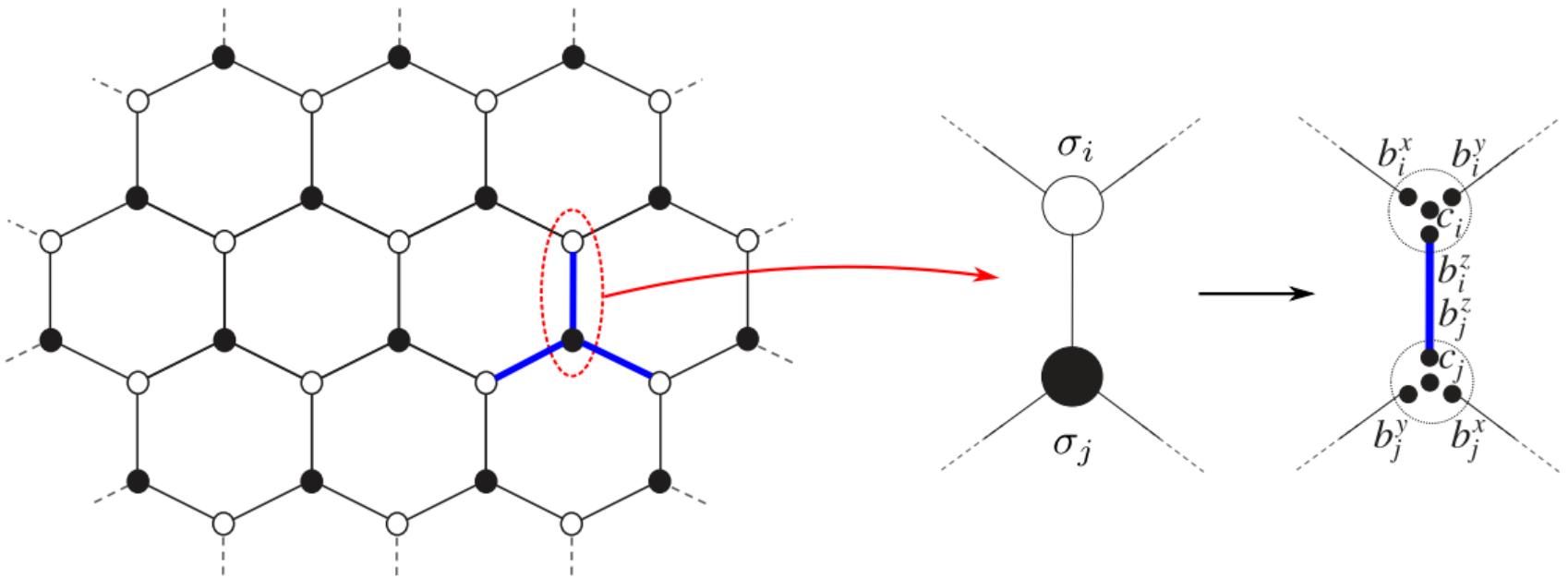
are the same

$$\boxed{\gamma = \gamma^\dagger}$$

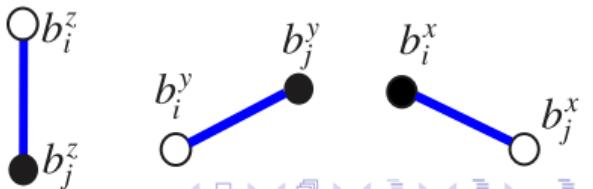


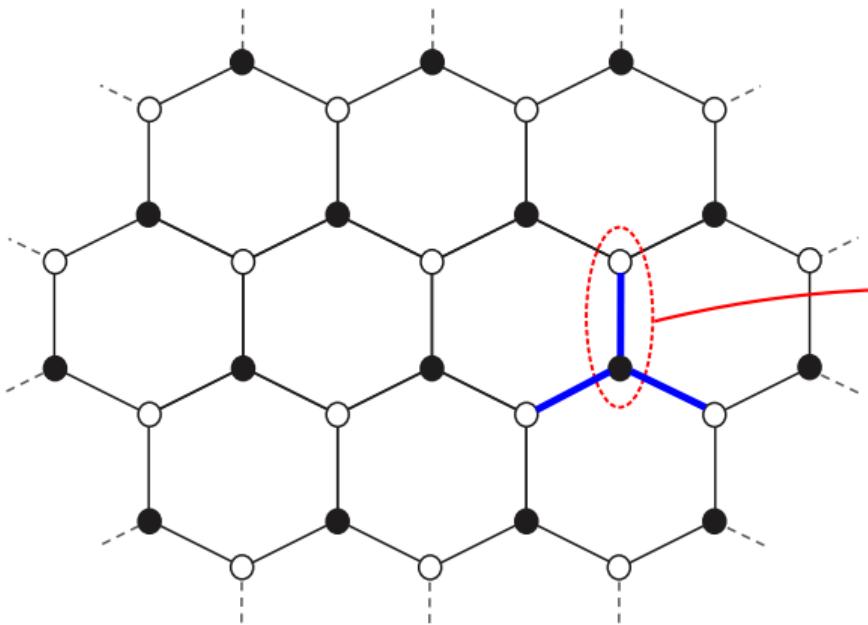
$$\boxed{\tilde{\sigma}_j^\alpha = i b_j^\alpha c_j \quad \text{for } \alpha = x, y, z}$$





Link Operator: $\hat{u}_{ij} = i b_i^\alpha b_j^\alpha$

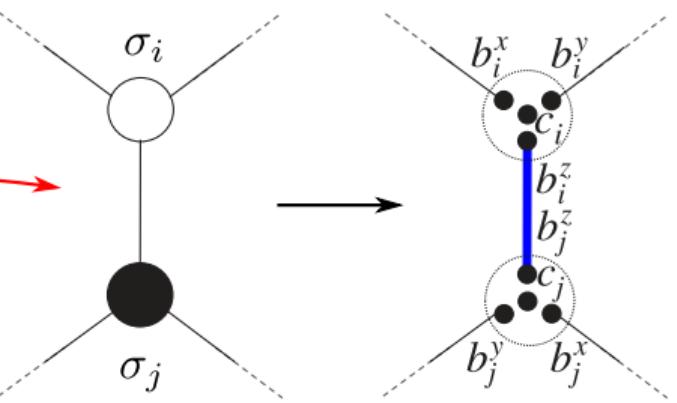




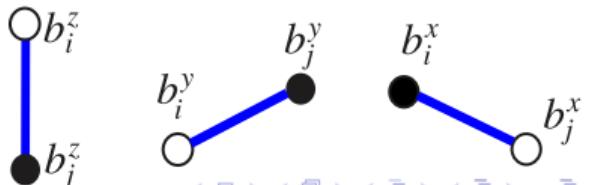
$$H = - \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} K_{\alpha} \sigma_j^{\alpha} \sigma_k^{\alpha}$$



$$\tilde{H} = i \sum_{\alpha} \sum_{\langle ij \rangle_{\alpha}} K_{\alpha} \hat{u}_{ij} c_i c_j$$



Link Operator: $\hat{u}_{ij} = i b_i^{\alpha} b_j^{\alpha}$



Recap

- We have mapped a single spin-1/2 particle into 2 fermionic modes, then to 4 Majorana modes:

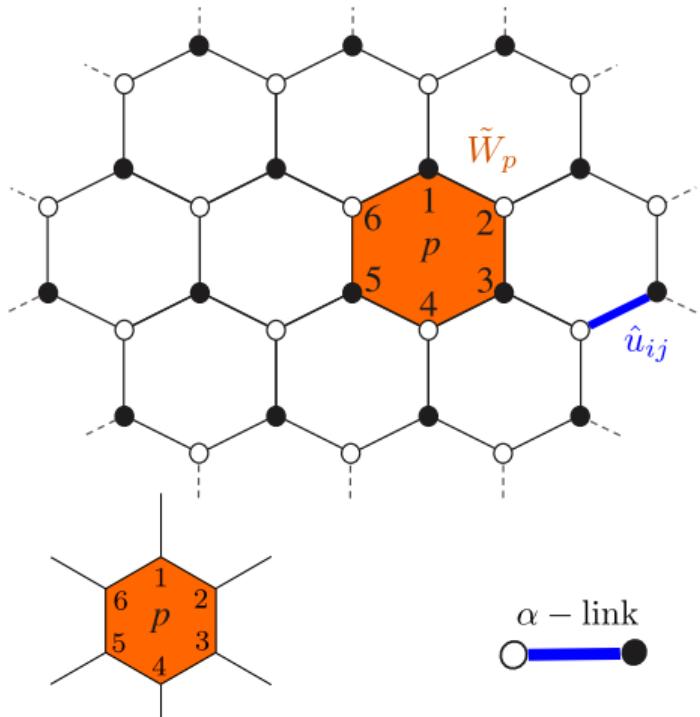


- It is a faithful representation because
 - (i) These Majoranas give the correct Hilbert space
 - (ii) These Majoranas reproduce spin-1/2's SU(2) algebra.
- The spin Hamiltonian into Majorana Hamiltonian by **Links**:

$$H = i \sum_{\alpha} \sum_{\langle ij \rangle} K_{\alpha} \hat{u}_{ij} c_i c_j$$

Conserved Quantities

Link Operators (vector potential) and **Plaquette operators** (flux)



$$[\hat{u}_{ij}, H] = 0$$

$$[\tilde{W}_p, H] = 0$$

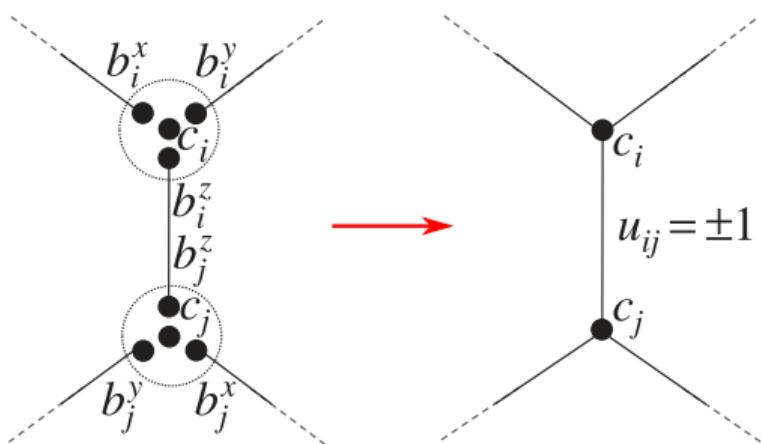
↓

Extensive # of conserved quantities
 $\{\tilde{W}_p\}$ and $\{\hat{u}_{ij}\}$

Link is Conserved: $u_{ij} = \pm 1$

The Hamiltonian using Majorana fermions:

$$\tilde{H} = - \sum_{\langle ij \rangle_\alpha} K_\alpha \tilde{\sigma}_i^\alpha \tilde{\sigma}_j^\alpha = i \sum_{\langle ij \rangle_\alpha} [K_\alpha (ib_i^\alpha b_j^\alpha)] c_i c_j \equiv i \sum_{\langle ij \rangle_\alpha} K_\alpha \hat{u}_{ij} c_i c_j.$$

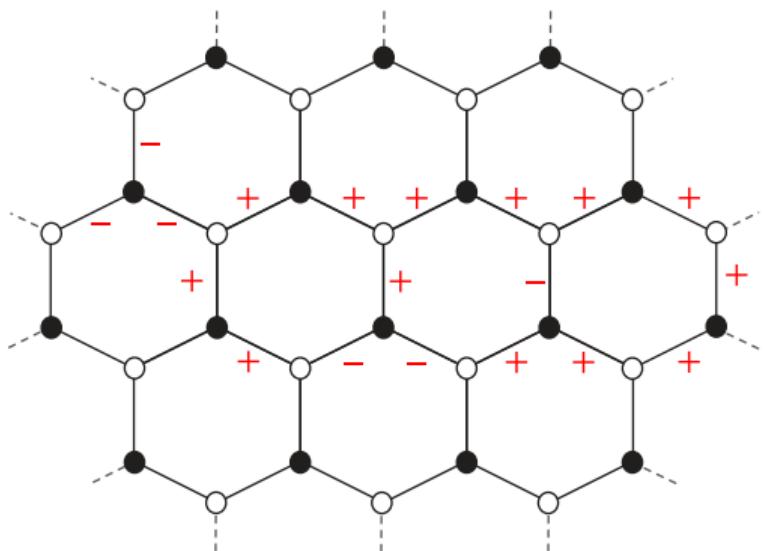


link operator: $\hat{u}_{ij} = ib_i^\alpha b_j^\alpha$

- \hat{u}_{ij} is conserved: $[\hat{u}_{jk}, H] = 0$.
- $\hat{u}_{jk}^2 = 1$, hence its eigen values are ± 1 .

With u_{ij} being static numbers, the Hamiltonian becomes quadratic of c_i Majoranas:

$$H = \sum_{\langle ij \rangle_\alpha} (iK_\alpha \hat{u}_{ij}) c_i c_j \Rightarrow H = \sum_{\langle ij \rangle_\alpha} (iK_\alpha u_{ij}) c_i c_j$$



What to assign to $\{u_{ij}\}$ for low energy state?

Diagonalize the Ground State Hamiltonian

Recall that we wanted to diagonalize H represented by sectors of $\{u_{jk}\}$ in $\tilde{\mathcal{L}}$:

$$H = \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} (iK_{\alpha} u_{jk}) c_i c_j.$$

Now the redundant dofs can be projected out by simply fixing a $\{w_p\}$ sector.

Theorem

Lieb (1994): Ground state has no vortices $\iff \{w_p = +1\}$.

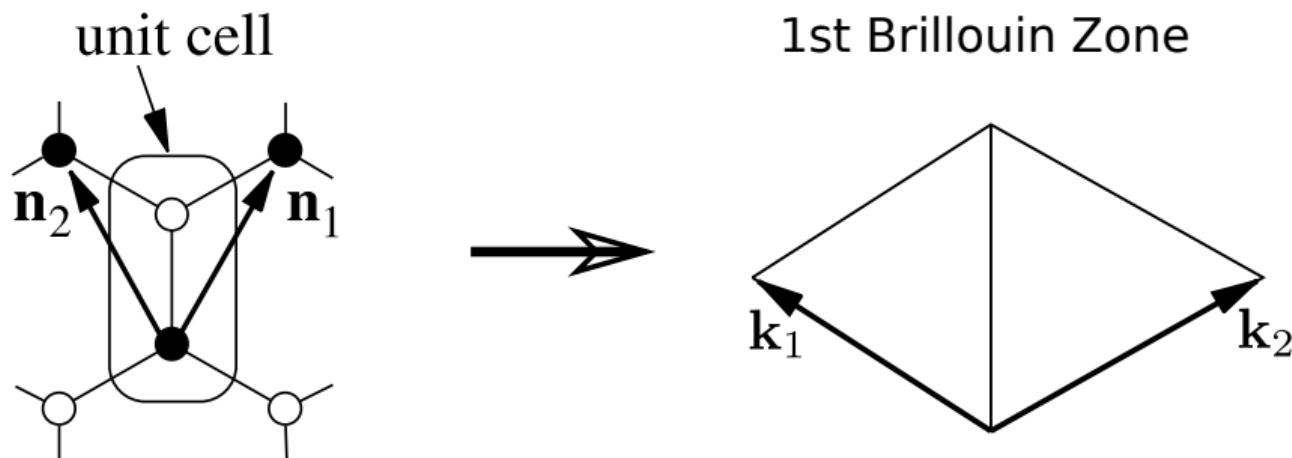
Therefore we can choose the simplest configuration $\{u_{jk} = +1\}$:

$$\{u_{jk} = +1\} \Rightarrow H = \boxed{\sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} iK_{\alpha} c_j c_k}$$

$$H = \sum_{\alpha} \sum_{\langle jk \rangle_{\alpha}} iK_{\alpha} c_j c_k \Rightarrow \text{Quadratic Hamiltonian of itinerant Majoranas}$$

Go to momentum space by Fourier transformation:

$$c_j = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_j} a_{\vec{k}}, \quad c_k = \frac{1}{\sqrt{N/2}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_k} b_{\vec{k}}.$$

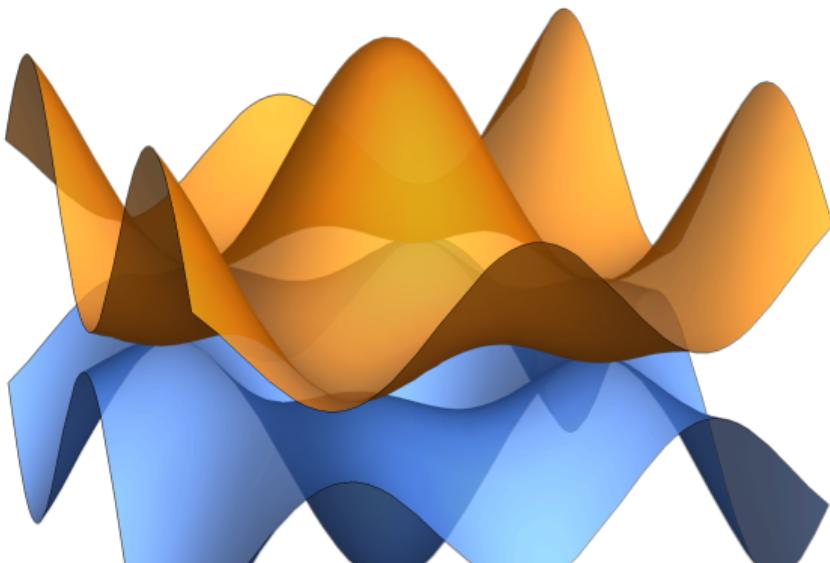


Single particle spectrum

Majorana Bands:

$$\epsilon(\vec{k}) = \pm \frac{1}{2} |f(\vec{k})|$$

For $K_\alpha = C$ it's identical to TB Graphene:



ARPES & $S(k, \omega)$

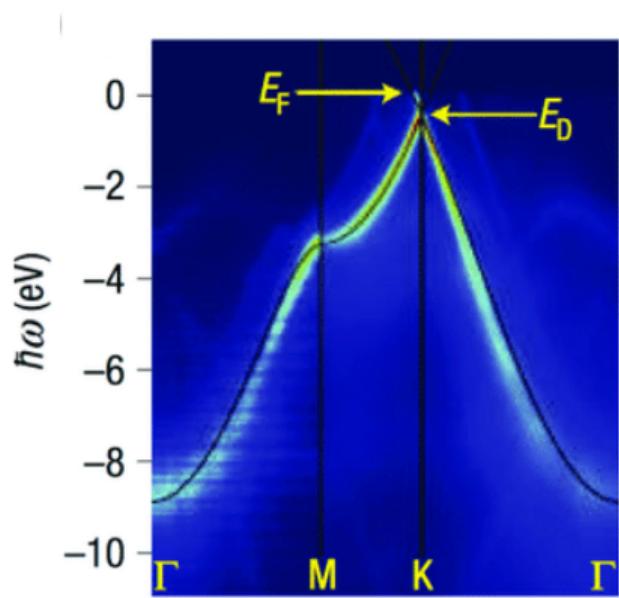


Figure: ARPES of Graphene

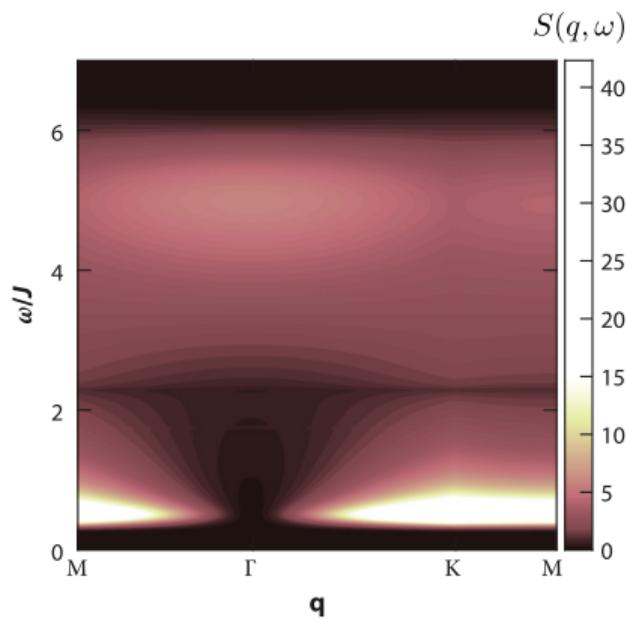
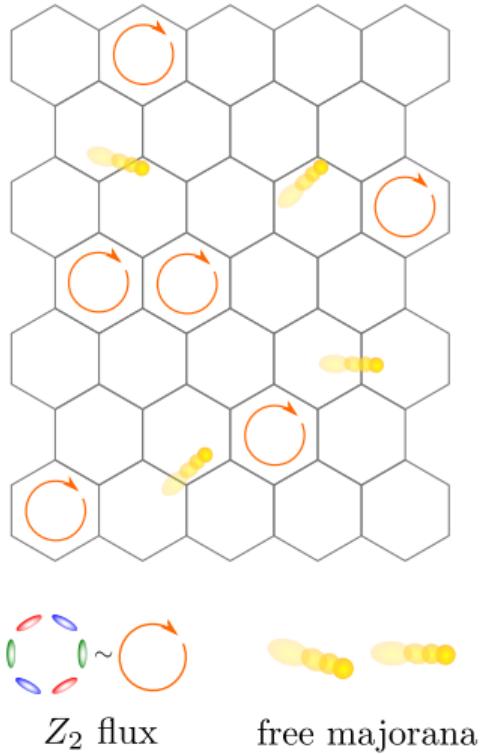
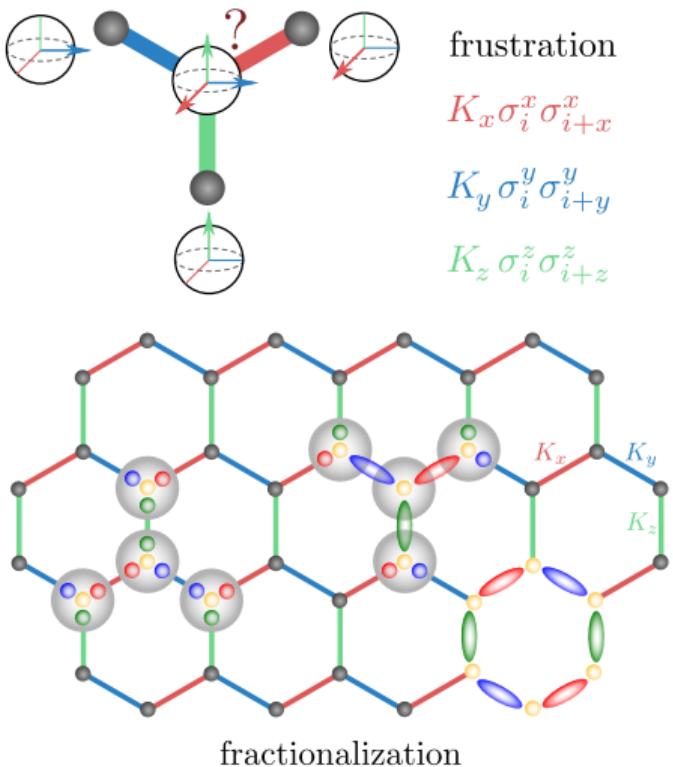


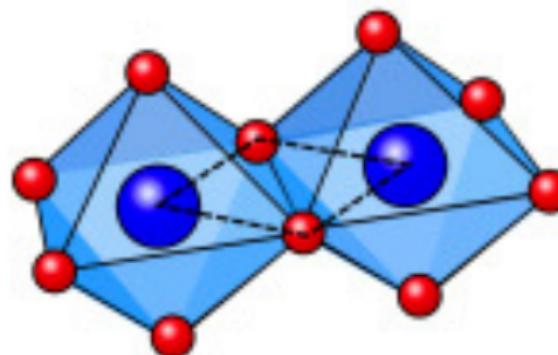
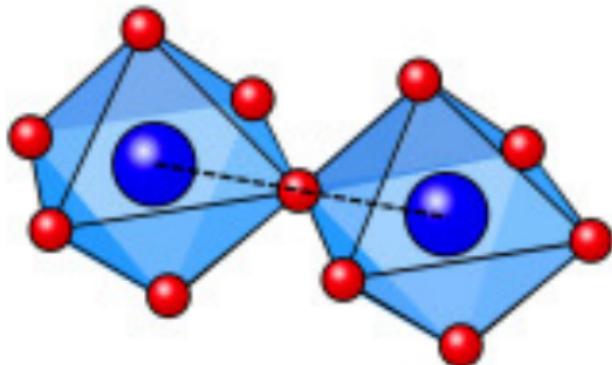
Figure: Dynamical structure factor of Kitaev model. Hermanns et al, Annu. Rev. Condens. Matter Phys. 9:17–33 (2018)

Summary of Kitaev Spin Liquid

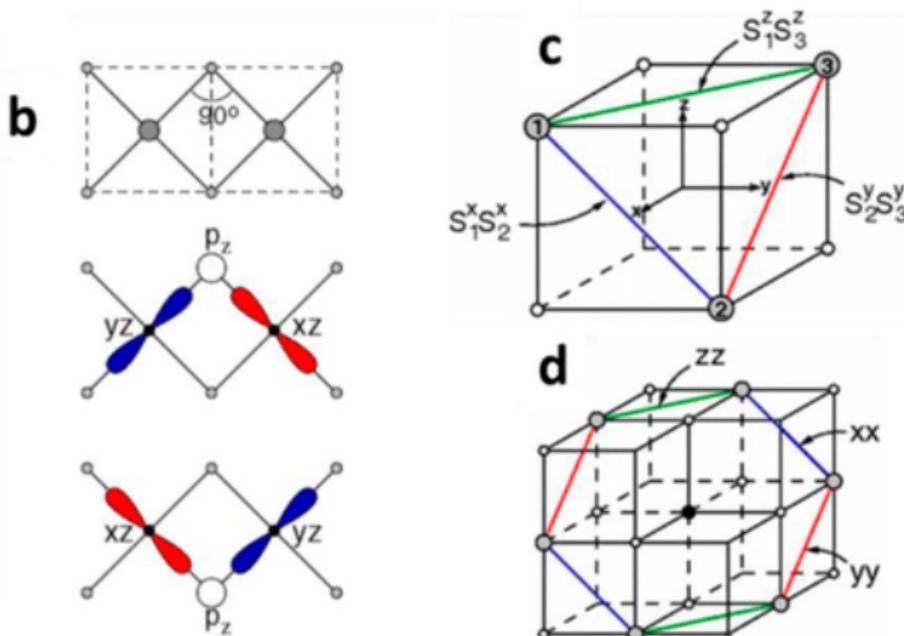
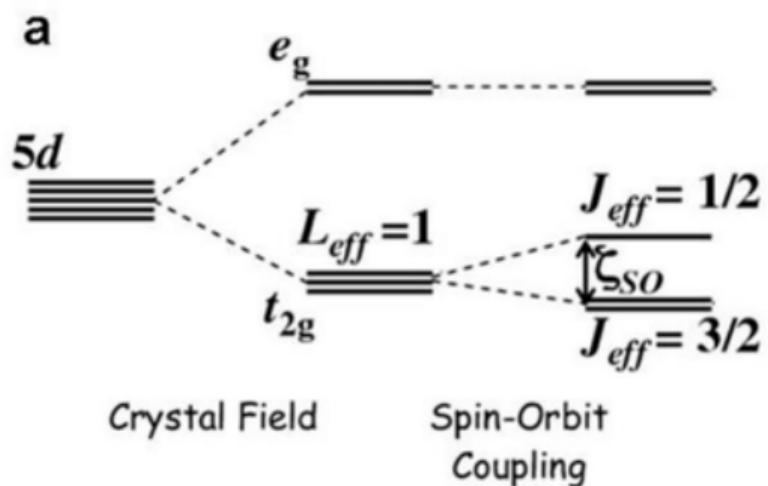


Where to look?

Corner sharing vs edge-sharing

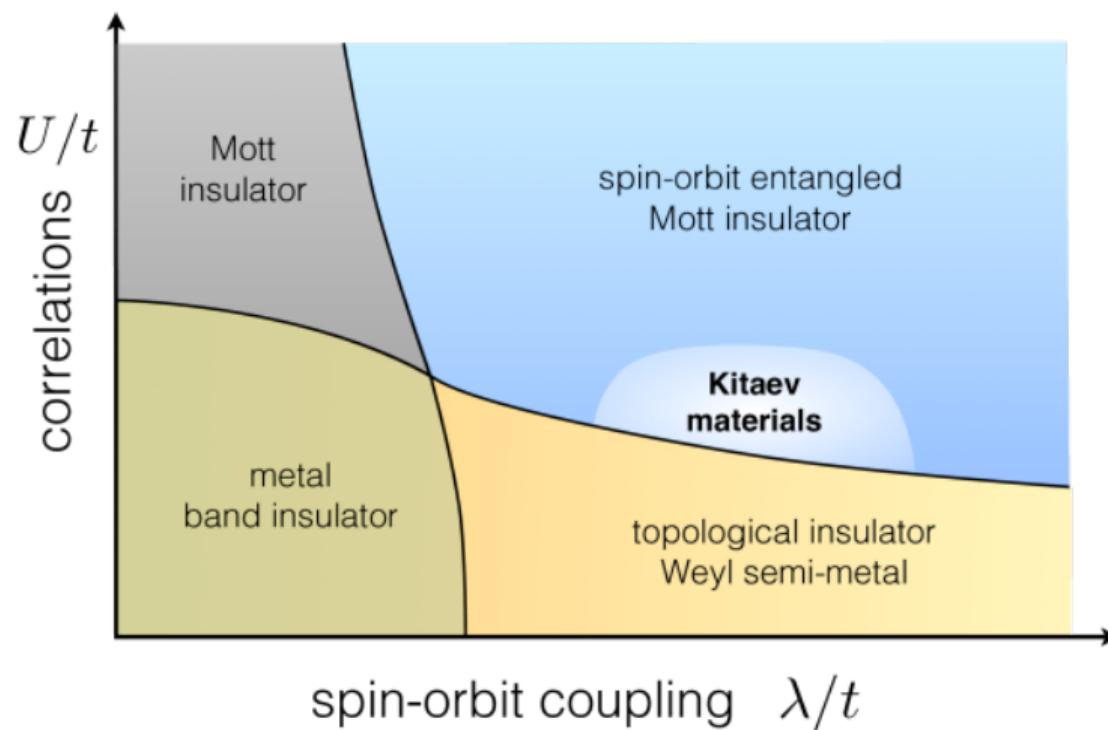


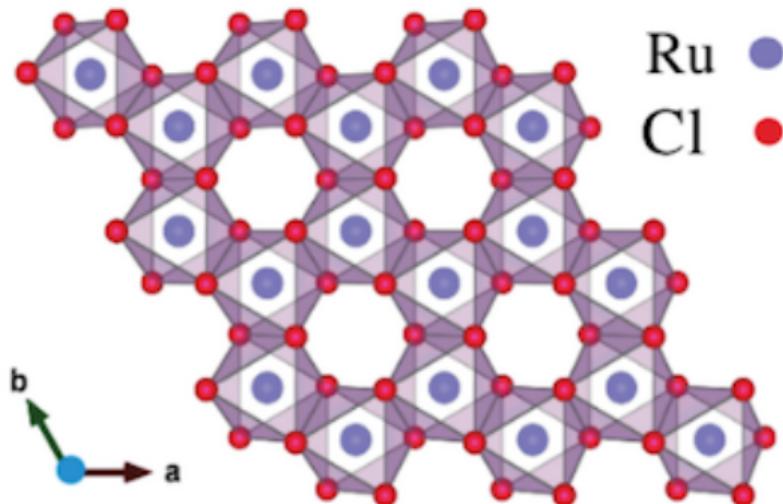
Anisotropy from Spin-orbital coupling



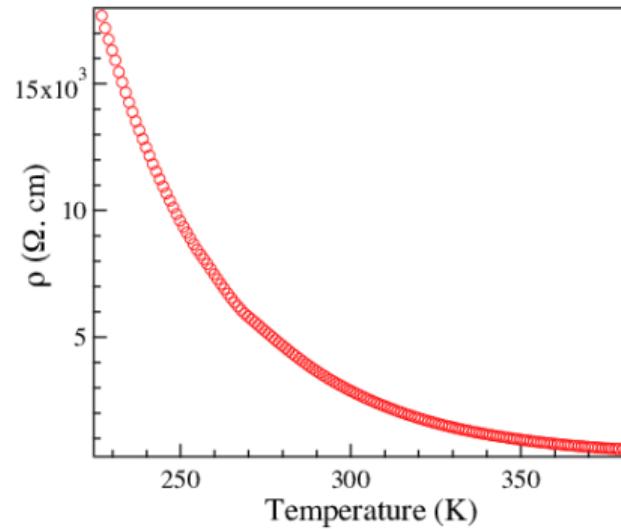
Jackeli and Khaliullin, Phys. Rev. Lett., 102 017205 (2009)

Where to look?

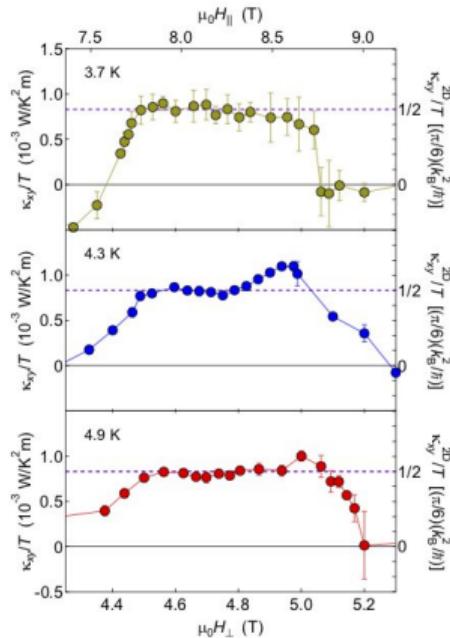
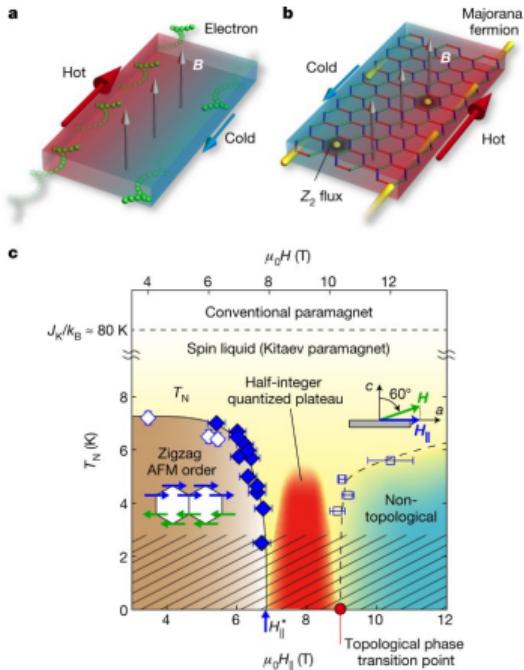


$\alpha\text{-RuCl}_3$ 

Ru Cl



α -RuCl₃

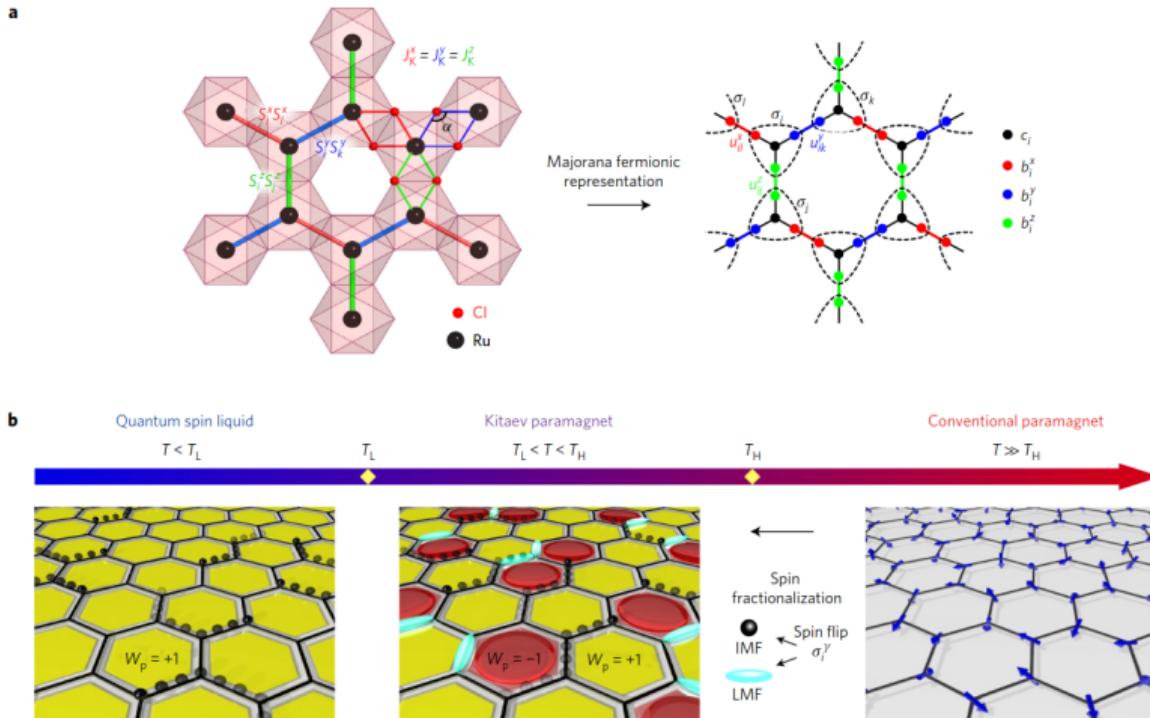


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Half-quantized thermal conductivity:

Indicating Majorana fermions in QSL

Conclusion



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