Frustrated Magnetism and Quantum Spin Liquids

TopoMag23 Crash Course

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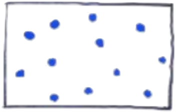
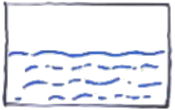
Outline

1. Order and Disorder in Matter
2. Magnetism
3. Frustrated Magnetism
4. Kitaev Quantum Spin Liquid (QSL)
5. Signature and Material

Phases Matter



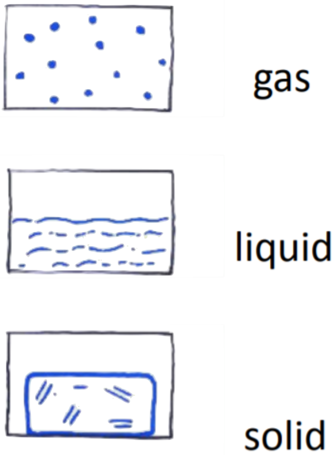
gas

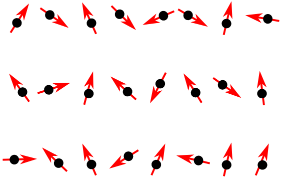


liquid

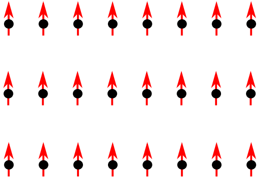
solid

Phases Matter



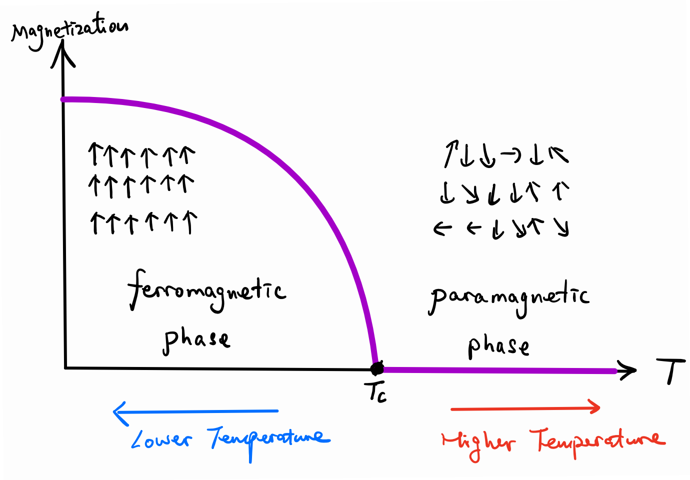


paramegnetic

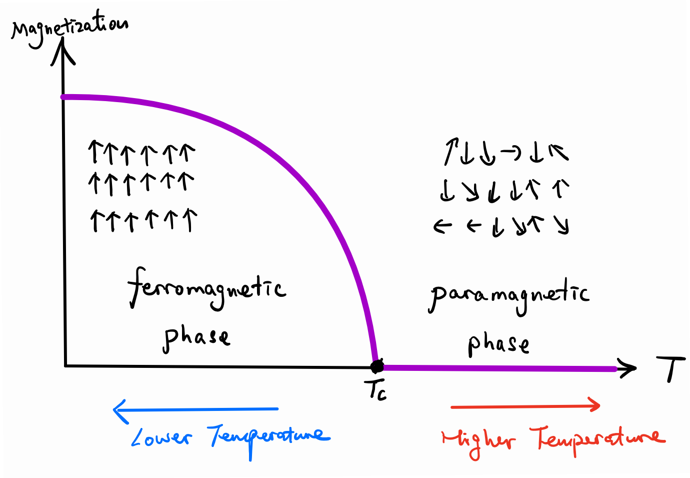


ferromegnetic

Order and Disorder



Order and Disorder



Two competing energy scales:

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

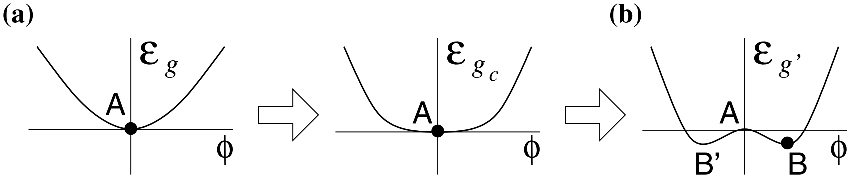
$J_{ij} \gg k_B T$: Ordered magnet
(Ferromagnet or Anti-ferromagnet)

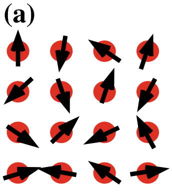
$J_{ij} \ll k_B T$: Disorderred magnet
(Paramagnet)

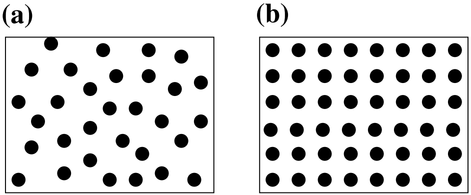
Phase transition at T_c

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 $M = N/2$:

$$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$$

Some excited states:

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

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

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

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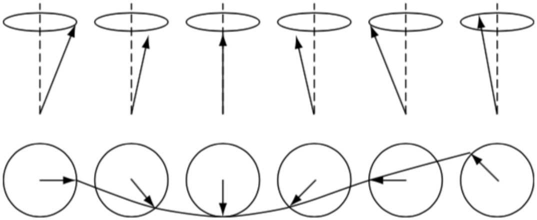
Quasi-particle (Bosons: Spin wave or Magnon)



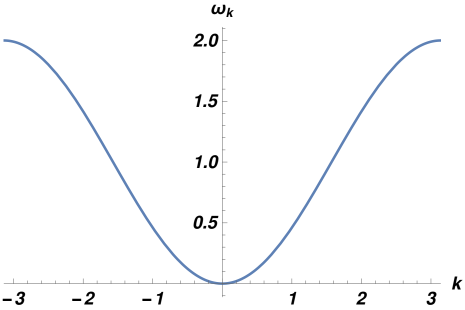
$$\mathcal{H} = \sum_k \omega_k n_k \quad \text{free magnons gas}$$

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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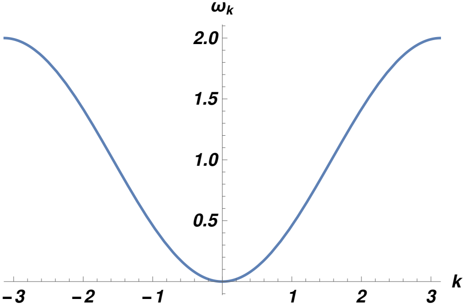

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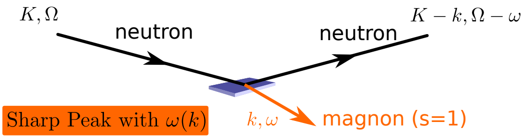
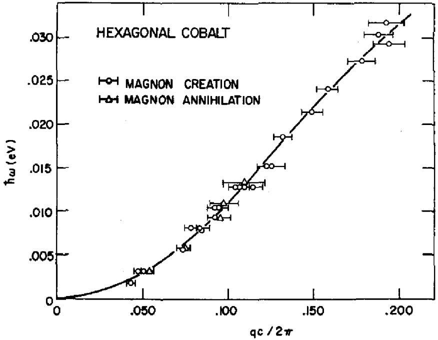


H. A. Alperin et al, J. Appl. Phys. 37, 1052 (1966)

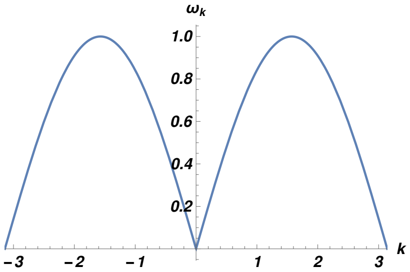


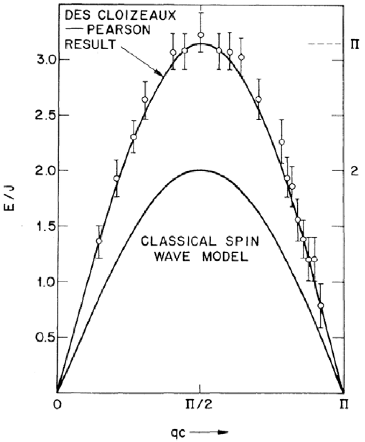
Anti-Ferromagnet

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

Dispersion of anti-ferromagnetic magnons

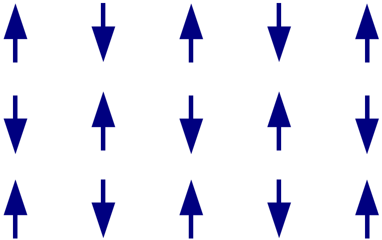
$$\omega_k \sim J|\sin(k)|$$





Geometrical Frustration

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



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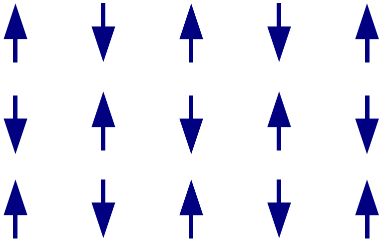
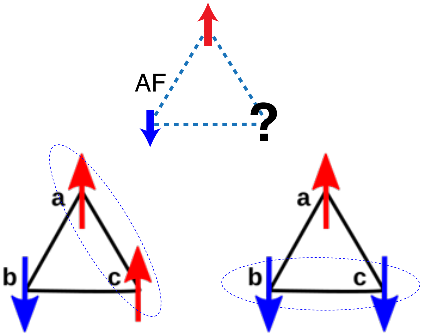
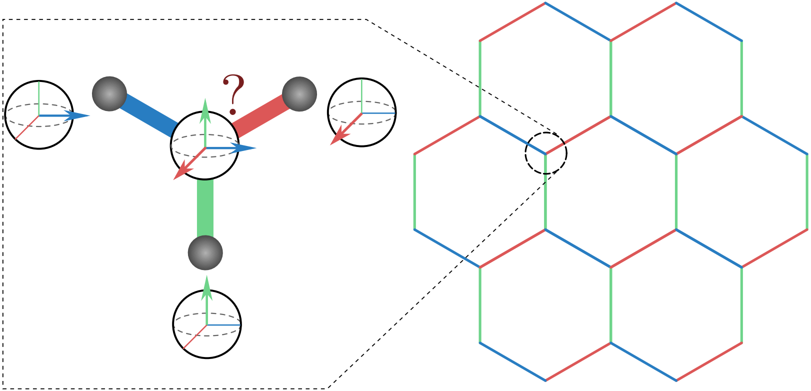


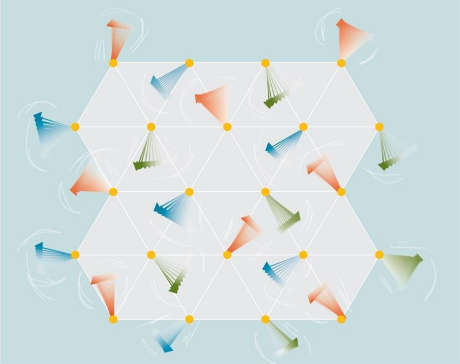
Geometrically frustrated magnet



Exchange Frustration

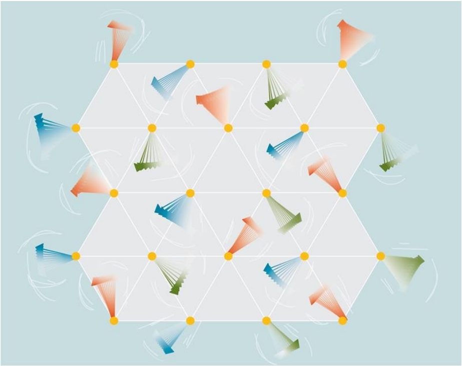


Consequences of Frustrations

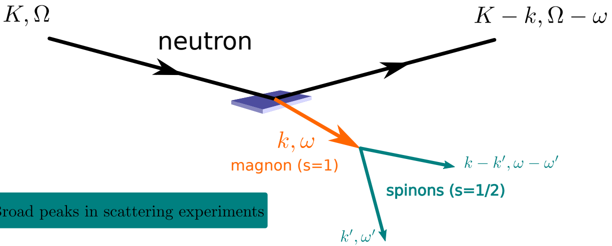


1. No order at $T \to 0$
2. No symmetry breaking
3. No $s = 1$ magnons or spin waves

Consequences of Frustrations

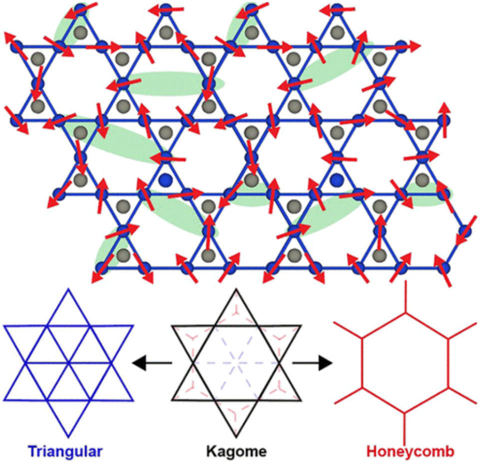


1. No order at $T \to 0$
2. No symmetry breaking
3. No $s = 1$ magnons or spin waves
4. Strong quantum fluctuation $\to$ *quantum spin liquid*
5. Elementry excitations are *Spinons* ($s = \frac{1}{2}$)
6. *Broad peaks* in neutron scattering



Broad peaks in scattering experiments

Frustrated Systems (Criteria)



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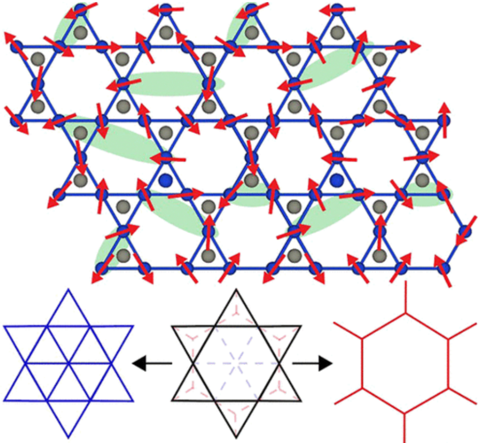

1. Localized electrons (Mott Insulator)
2. Small spins, preferably spin-$\frac{1}{2}$
3. Geometrical or exchange frustration
4. Spin-orbit coupling

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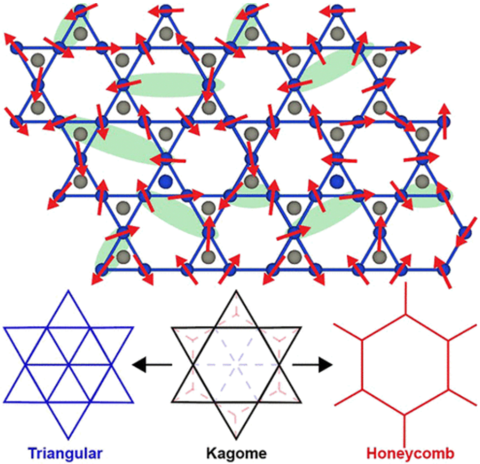

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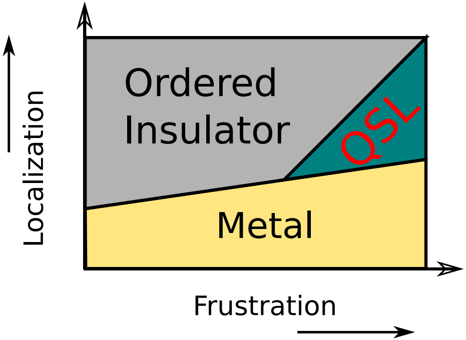
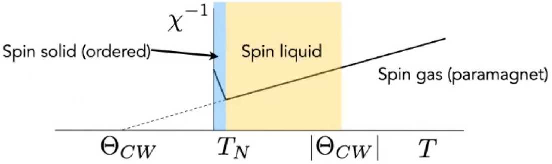


Frustration Parameter

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**:

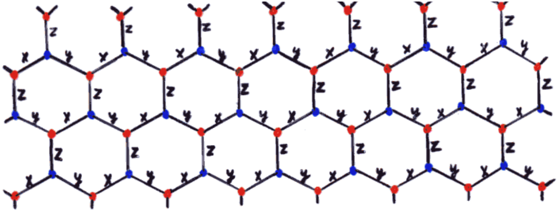
$$f = \Theta_{CW}/T_N.$$

$f \to \infty$: True QSL

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

Honeycomb model

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



Two sublattices  and 

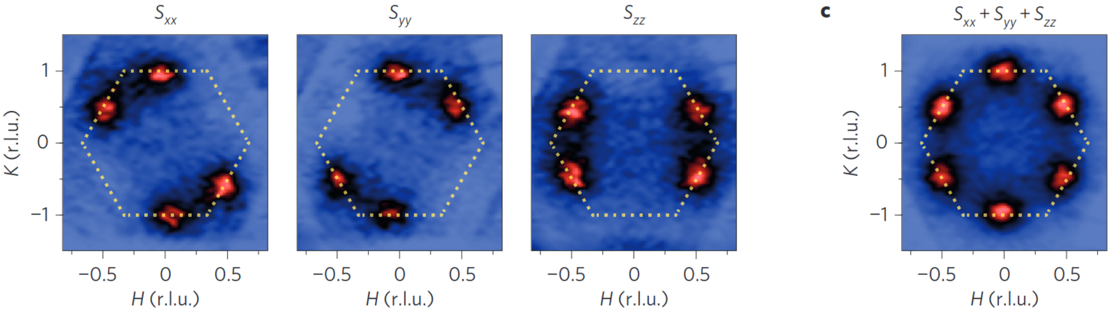
Three types of links 

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

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

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

Exchange Frustration in Materials



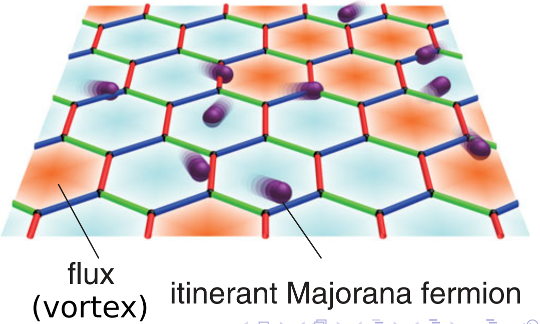
Evidence for anisotropic spin exchange from diffuse magnetic X-Ray scattering in Na_2IrO_3
Chun *et al*, Nature Physics 11, 462–466 (2015)

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)

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

??? $\downarrow$ **???**

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

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

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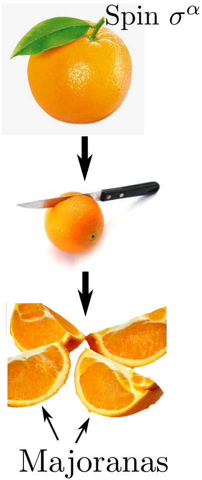

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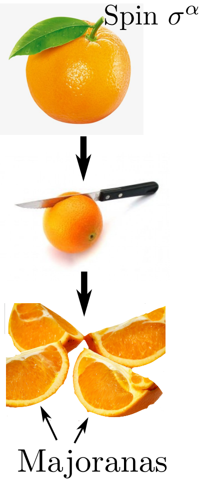


$$H = -\sum_{\alpha}\sum_{\langle jk\rangle_\alpha} f(\text{fractions of } \sigma)$$

$$\checkmark \downarrow \checkmark$$

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

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

particle

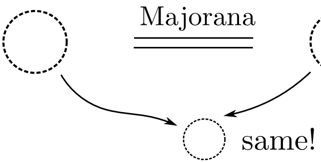
e^-

$$a^\dagger |vac\rangle = |e^-\rangle$$

anti-particle

e^+

$$a |vac\rangle = |e^+\rangle$$



Majorana's anti-particle is itself

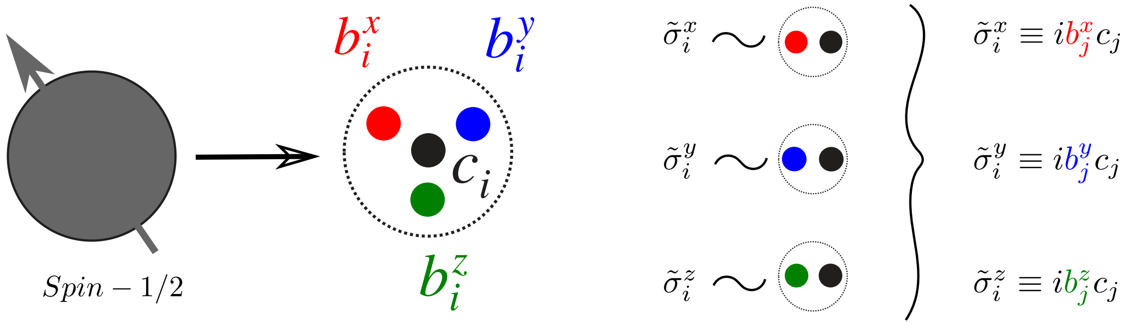
creation operator $\gamma^\dagger$

&

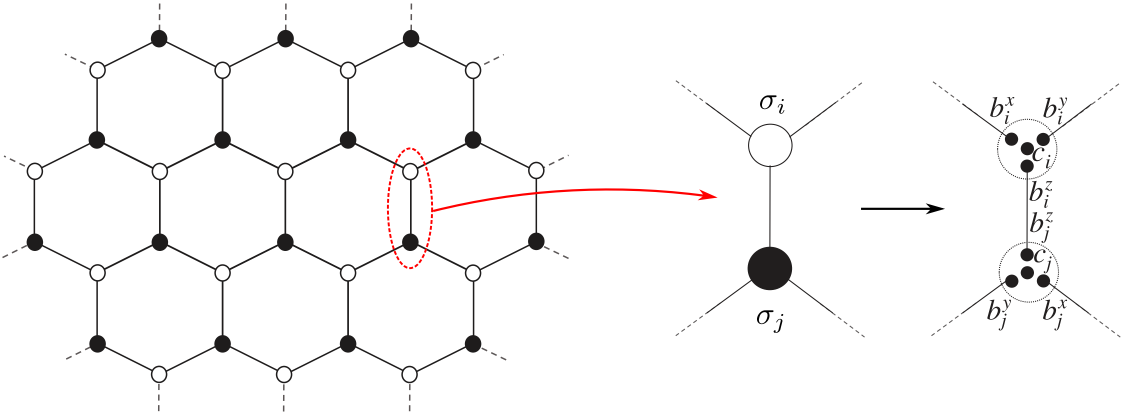
annihilation operator γ

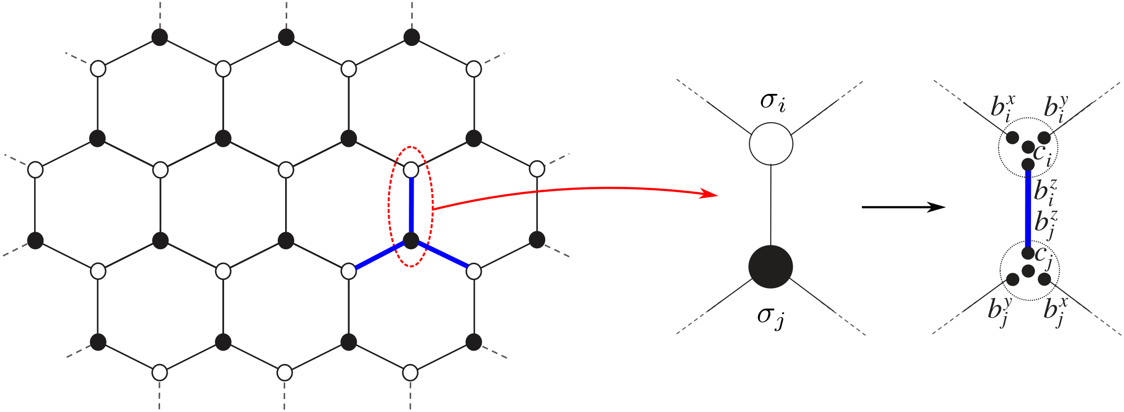
are the same

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

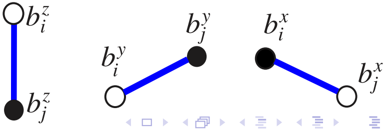


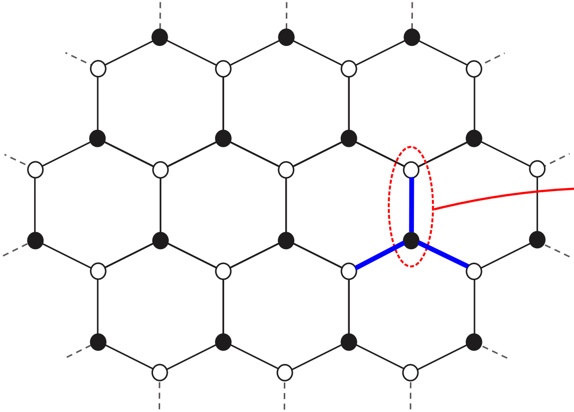
$$\tilde{\sigma}_j^\alpha = i b_j^\alpha c_j \quad \text{for } \alpha = x, y, z$$

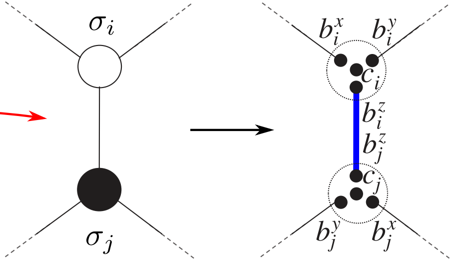

σ_i
σ_j
b_i^x b_i^y
c_i
b_i^z
b_j^z
c_j
b_j^y b_j^x



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







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

↓

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

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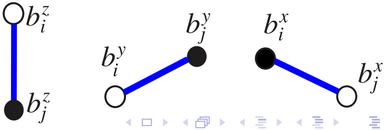
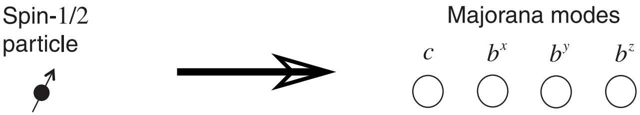


Recap

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

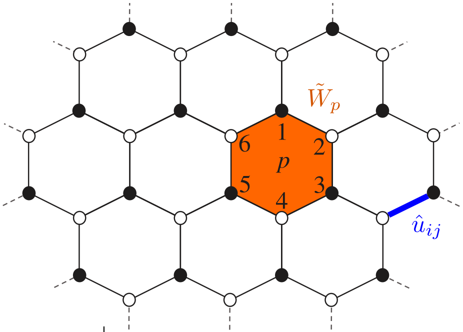


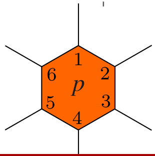
- It is a faithful representation because
  - (i) These Majoranas give the correct Hilbert space
  - (ii) These Majoranas reproduce spin-1/2's SU(2) algebra.
- The spin Hamiltonian into Majorana Hamiltonian by **Links**:

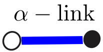
$$H = i \sum_{\alpha} \sum_{\langle ij \rangle} K_\alpha \hat{u}_{ij} c_i c_j$$

Conserved Quantities

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







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

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

$$\downarrow$$

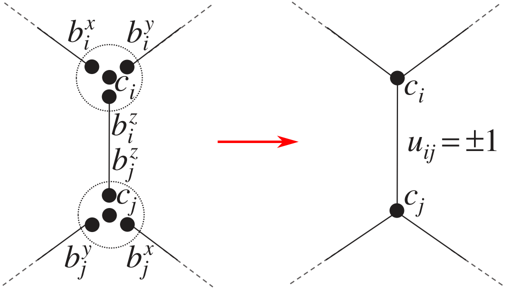
Extensive # of conserved quantites

$\{W_p\}$ and $\{u_{ij}\}$

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

The Hamiltonian using Majorana fermions:

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

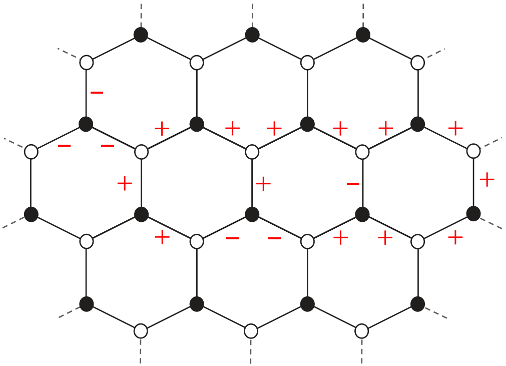


link operator: $\hat{u}_{ij} = i b_i^\alpha b_j^\alpha$

- $\hat{u}_{ij}$ 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:

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



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 $\iff \{w_p = +1\}$.

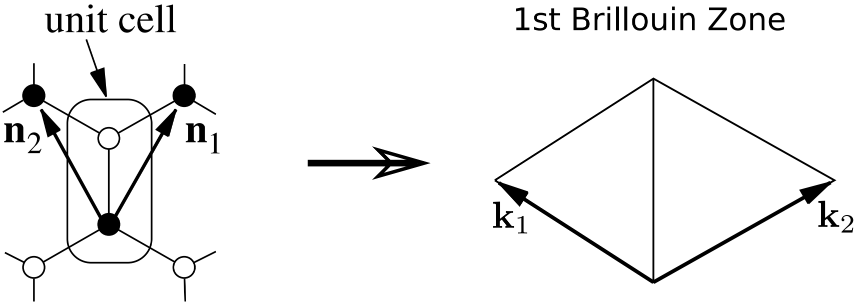
Therefore we can choose the simplist configuration $\{u_{jk} = +1\}$:

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

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

Go to momentum space by Fourier transformation:

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

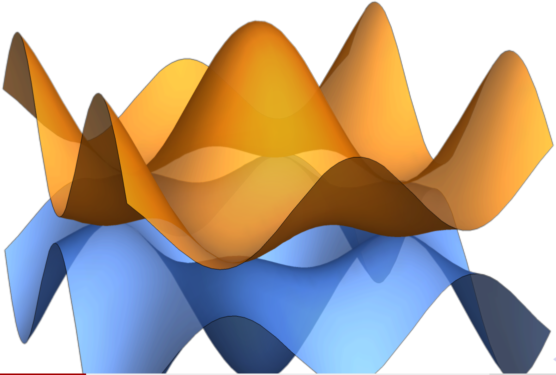


Single particle spectrum

Majorana Bands:

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

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



ARPES & $S(k, \omega)$

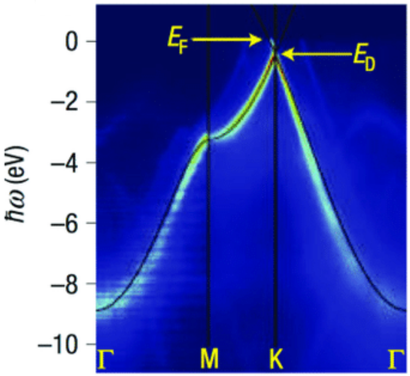


Figure: ARPES of Graphene

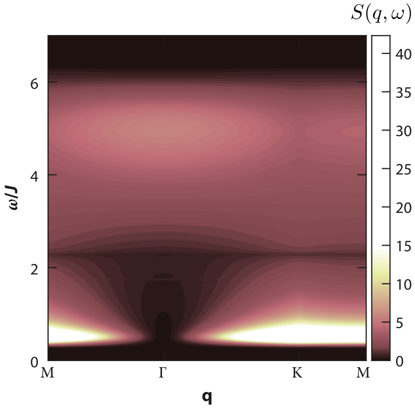
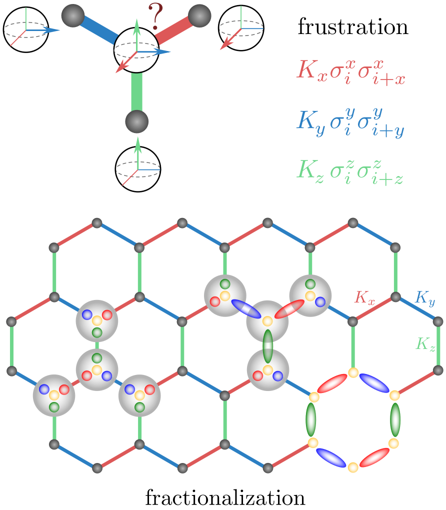
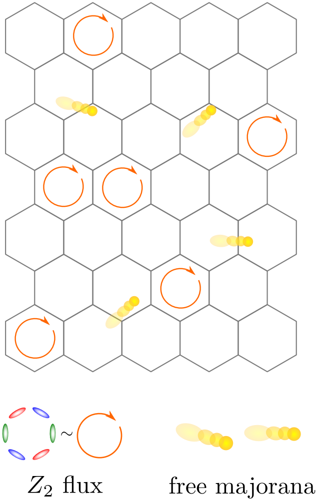


Figure: Dynamical structure factor of Kitaev model. Hermanns et al, Annu. Rev. Condens. Matter Phys. 9:17–33 (2018)

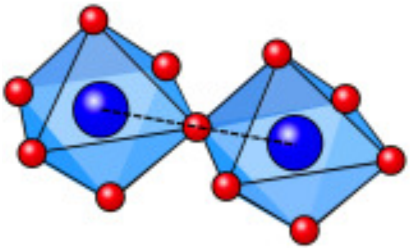
Summary of Kitaev Spin Liquid

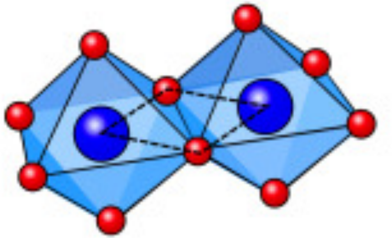




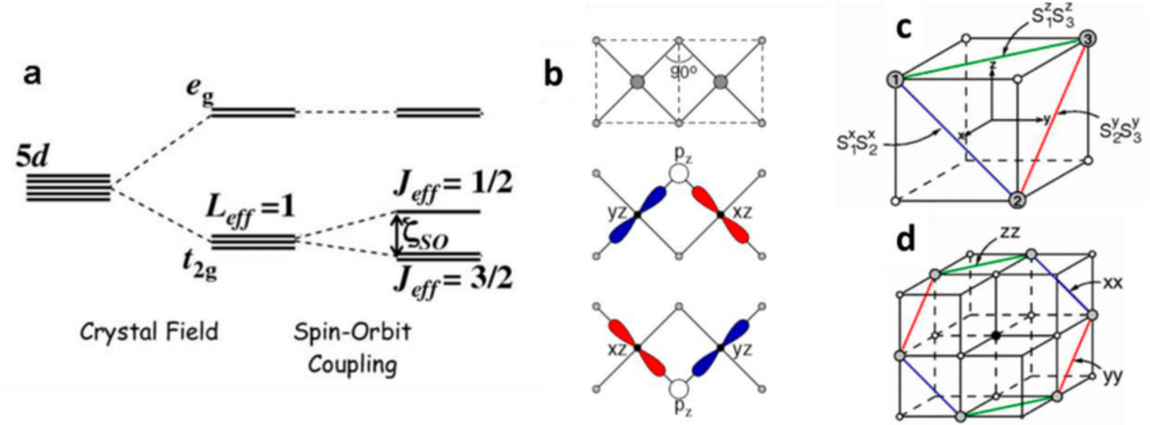
Where to look?

Corner sharing vs edge-sharing



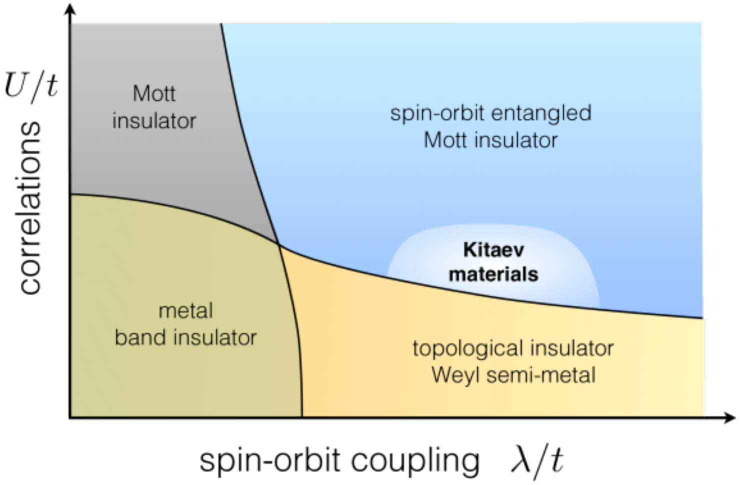


Anisotropy from Spin-orbital coupling

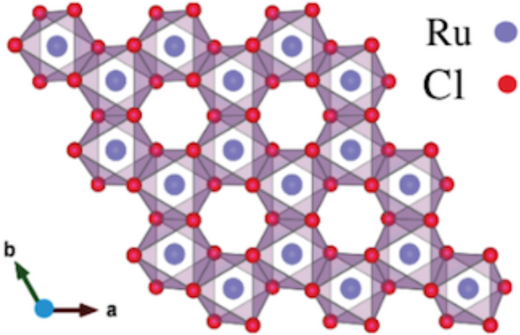


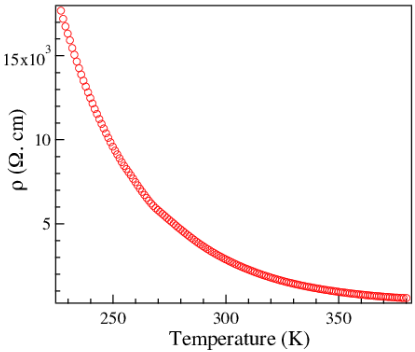
Jackeli and Khaliullin, Phys. Rev. Lett., 102 017205 (2009)

Where to look?

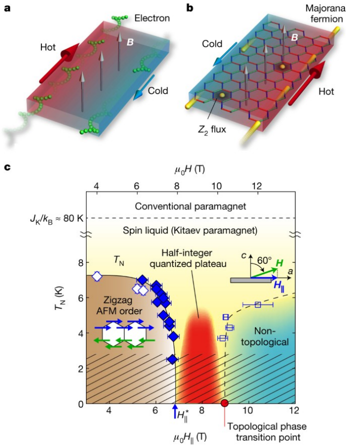


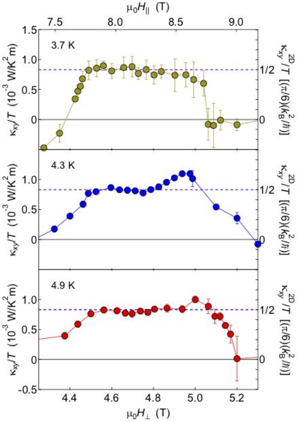
α-$RuCl_3$





α-$RuCl_3$



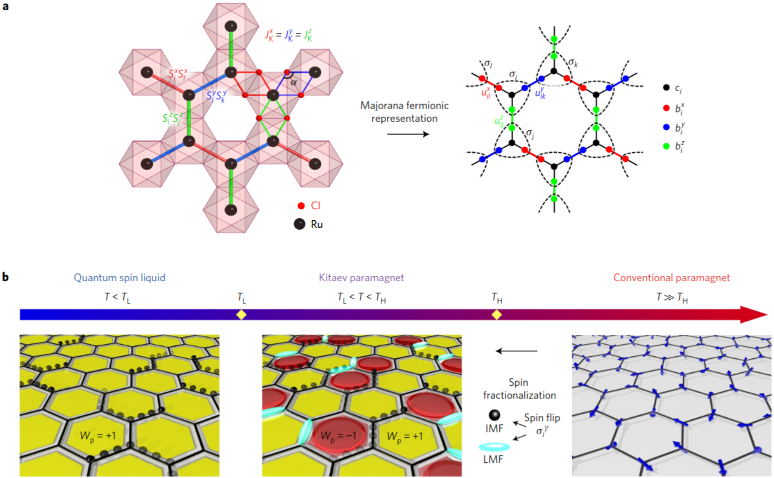


Matsuda Group. Nature 559, 227-231 (2018)

Half-quantized thermal conductivity:

Indicating Majorana fermions in QSL

Conclusion


a
Cl
Ru
Majorana fermionic representation
b
Quantum spin liquid
Kitaev paramagnet
Conventional paramagnet
Spin fractionalization
Spin flip
IMF
LMF

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