Quantum Spin Liquids: Signatures of Fractionalization

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Roadmap

- Big picture

- 2D: Kitaev Model
  - Discovery of a new gapless QSL with a spinon Fermi surface
  - Spectrum of 1 spin flip and 2 spin flip excitations

- QSL Materials

- How do you detect a QSL?

- Going forward....
Big Picture

What is a QSL?
Why is it interesting? Important?
First Signatures of a QSL
First signatures of a QSL: large frustration parameter

\[ \chi(T) = \frac{C}{T - \theta_{cw}} \]
Spontaneously broken time reversal symmetry

\[ H = J \sum_{\langle ij \rangle} S_i^z S_j^z \]

\[ S_i = \pm \frac{1}{2} \]

\[ M = \langle S_i^z \rangle \]

\[ f = \frac{1}{T_c} \theta_{cw} \]

\[ T \rightarrow T_c \]

\[ \chi \]
First Signatures of a QSL

- Mott insulator
  (odd number of electrons in unit cell)
- Local moments
  (typically $S=1/2$ or $J_{\text{eff}}=1/2$)
- Strongly interacting moments
  $\theta_{\text{CW}} \sim 100$ K
- No magnetic ordering
  $f = \theta / T_c \sim 10^4$
First Signatures of a QSL

So why is a paramagnet interesting?

- Mott insulator
  (odd number of electrons in unit cell)
- Local moments
  (typically $S=1/2$ or $J_{\text{eff}}=1/2$)
- Strongly interacting moments
  $\theta \sim 100$ K
- No magnetic ordering
  $f = \theta / T_c \sim 10^4$
Quantum Matter

- Landau paradigm: spontaneously broken symmetry →
  local order parameter \( m \)
  bosonic excitations: magnons (for continuous spins)

- Topological Paradigm

  "IQHE"
  Topological Insulators
  Topological Superconductors
  Topological Weyl and Dirac Semimetals
  Topological magnons

"FQHE"
Quantum Spin Liquids Possess Topological Order
- Ground state degeneracy
- Long range entanglement
- Fractionalized Excitations

Review: Savary and Balents, Repts. on Progress in Physics 80, 016502 (2017)

Wen, X.-G. and Niu, Q. (1990) PRB 41, 9377
Quantum Matter

- Landau paradigm: spontaneously broken symmetry → local order parameter $m$
  - bosonic excitations: magnons (for continuous spins)

- Topological Paradigm

  - "IQHE"
    - Topological Insulators
    - Topological Superconductors
    - Topological Weyl and Dirac Semimetals
    - Topological magnons

  - "FQHE"
    - Quantum Spin Liquids
    - Possess Topological Order
      - Ground state degeneracy
      - Long range entanglement
      - Fractionalized Excitations

Important for storing information non-locally; robust against decoherence
Singlet or valence bond

\[ \frac{1}{\sqrt{2}} \left( |↑↓⟩ - |↓↑⟩ \right) \]

valence bond solid

Resonating valence bond -- candidate quantum spin liquid

Anderson 1973
Singlet or valence bond

Valence bond solid

Resonating valence bond -- candidate quantum spin liquid

Anderson 1973

Excitations of a QSL

Contrast with ordered magnet: Magnons: S=1 (bosons)

deflouned

S=1/2 spinons

Fermionic excitations
Why would a bunch of interacting spins not order at $T=0$?

1. Low spin
2. Low dimensionality
3. Frustration
   [Geometric, Interactions, …]
Fractionalization of excitations in quantum spin liquids
1d Quantum Spin Liquid

\[ |RVB\rangle = \{ |\ldots\rangle + |\ldots\rangle + \cdots \} \]

Linear superposition of all possible singlet coverings → Spin Liquid

Fractionalized \( S=1 \) magnons (bosons) into two \( S=1/2 \) neutral spinons (fermions)

Inelastic neutron scattering \( S(q,\omega) \)

\[ \omega_1(q) = \frac{\pi J}{2} |\sin qa| \]

\[ \omega_u(q) = \pi J |\sin \frac{qa}{2}| \]

Compare with \( \omega_d(q) = 2J |\sin qa| \)

KCuF\(_3\)

Broad spectrum indicates fractionalization of magnons

Lake et al Nat. Mat. 4, 329 (2005)
Black dotted: multi-spinon continuum predicted at T=0 (Muller ansatz equation)
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Kitaev Model

Honey comb lattice
Bipartite lattice; no geometric frustration

put qubit on each site

Kitaev Model: bond-dependent interactions

\[ H = K \left[ \sum_{\langle ij \rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle \in z} \sigma_i^z \sigma_j^z \right] \]
Kitaev Model: bond-dependent interactions

\[ H = K \left[ \sum_{\langle ij \rangle \in x} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle \in y} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle \in z} \sigma_i^z \sigma_j^z \right] \]
Kitaev Model: bond-dependent interactions

\[ H = K \left[ \sum_{\langle ij \rangle \in \alpha} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle \in \gamma} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle \in \zeta} \sigma_i^z \sigma_j^z \right] \]

Parton construction:

\[ \sigma^\alpha = i b^\alpha c \]

\[ H = K \frac{i}{2} \sum_{\langle ij \rangle} \hat{U}_{ij} C_i C_j \]
Ground State:

All plaquettes have zero flux

c-majorana fermions have a Dirac dispersion
Excitations:

1. Gapped flux excitation (visons)
2. Gapless Majorana fermions

Gapless $Z_2$ Quantum Spin Liquid
Now add a magnetic field...

\[ H = H_K + \hbar \sum_{i\alpha} S_i^\alpha \]

Focus on here:
AF Kitaev interactions and field along \( \hbar || [111] \)
Non-abelian gapped Kitaev spin liquid:

- Majorana fermions get gapped
Our Main Results: Kitaev Model in a Magnetic Field

Δₚ: single spin flip energy
Δₚ: 2-spin flip energy

Results based on exact diagonalization ED and Density matrix renormalization group (DMRG)
David Ronquillo
Field-orientation-dependent spin dynamics of the Kitaev honeycomb model

Adu Vengal

Nirav Patel
Magnetic field induced intermediate gapless spin-liquid phase with a spinon Fermi surface
PNAS 201821406 (2019)

Subhasree Pradhan
Two-Magnon Bound States in the Kitaev Model in a [111]-Field
PRB 101, 180401 (2020)

Related work:
H.C. Jiang et al. arXiv 1809.08247
Y. Motome and J. Nasu, JPSJ 89, 012002 (2020)
Evidence for TWO phase transitions
Kitaev Model + Magnetic field: $h||[111]$ magnetization

$$H = H_K + h \sum_{i\alpha} S_i^\alpha$$

Density Matrix Renormalization Group calculations with 160 spins
Kitaev Model + Magnetic field: \( h \parallel [111] \)

susceptibility

\[
H = H_K + h \sum_{i\alpha} S_i^{\alpha}
\]
Evidence for gapless intermediate phase
Energy Spectra in a field

\[ \Delta E \sim |\vec{h}|/K \]
Distinct power law decay of real-space spin-spin correlations!
Evidence for QSL
Entanglement Entropy for a Gapped QSL

$$\rho_A \equiv \text{Tr}_B(\rho)$$

$$S_A = -\text{Tr}\rho_A \log \rho_A$$

"Area Law" Entanglement in a gapped system
Topological Entanglement Entropy $\gamma$

$S_A \sim \alpha L - \gamma$

with $\gamma > 0$.

Kitaev-Preskill Construction to extract $\gamma$

$$S_{\text{topo}} = S_A + S_B + S_C - S_{AB} - S_{BC} - S_{CA} + S_{ABC}$$
Energy Spectra

\[ h \parallel [111] \]

\[ \theta \sim |\vec{h}|/K \]

TEE

Ronquillo, Vengal, Trivedi, PRB 99, 140413(R) (2019)
Topological entanglement entropy:
Information resource

Topological Entanglement Entropy $H_{||[111]}$,

$S_{\text{Topo}}$

$h/K$

$- \log(2)$

Ian Osbourne
Finite $\gamma$ implies the existence of topological order

$\rightarrow$ long range entanglement structure
$\rightarrow$ Quantum dimension of excitations
Gapped Non abelian KSL

Vacuum: \( 1 \sim d_1 = 1 \)  
Fermion: \( \epsilon \sim d_\epsilon = 1 \)  
Vortex: \( \nu \sim d_\nu = \sqrt{2} > 1 \)

\[ D = \sqrt{d_1^2 + d_\epsilon^2 + d_\nu^2} = \sqrt{1 + 1 + 2} = 2 \]

\[ \gamma = \log D = \log 2 \]
Evidence for spinon Fermi surface
Kitaev Model: spin structure factor

\[
H_K = K \sum_{\langle ij \rangle} S^x_i S^x_j + S^y_i S^y_j + S^z_i S^z_j
\]

Brillouin Zone: Momenta cuts

DMRG++ Open Source:
https://web.ornl.gov/~gz1/dmrgPlusPlus/
Structure Factor $S(k)$ – Intermediate phase

\[
S_{\gamma'\gamma}(k) = \frac{1}{L^2} \sum_{i \in \gamma, j \in \gamma'} e^{-ik \cdot r_{ij}} \left[ \langle S_i \cdot S_j \rangle - \langle S_i \rangle \cdot \langle S_j \rangle \right]
\]

\[
S_{tot} = \sum_{\gamma \gamma'} S_{\gamma'\gamma}
\]

\[
S(k) = \begin{bmatrix} S_{AA} & S_{AB} \\ S_{BA} & S_{BB} \end{bmatrix}
\]
\[ S_{tot}(k) \propto \int_0^{\infty} S_{tot}(k, \omega) d\omega \]
$S(k) \rightarrow \text{spinon Fermi surface}$

DMRG Results

Conjectured
Fermi surface

$A(k, \omega = 0)$

$\omega = 0$

$\Im(k) = \sum_q A(k + q)A(q)$
Singularities at all the M points related by C3 Rotations and Translations.

"Fermi Surface" of spinons in a Mott insulator!

Test using VMC on projected wave function.
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1-spin flip spectral functions
1-spin flip and 2 spin-flip spectral functions

\[ S(\omega) = \frac{-1}{N\pi} \text{Im} \left[ \sum_{m \neq 0,i} \frac{\left| \langle 0 | S_i^\alpha | m \rangle \right|^2}{\omega + E_0 - E_m + i\eta} \right] \]

\[ P^{\gamma}(\omega) = \frac{-1}{N\pi} \text{Im} \left[ \sum_{m \neq 0,i} \frac{\left| \langle 0 | S_i^\alpha S_i^\alpha_{i+\gamma} | m \rangle \right|^2}{\omega + E_0 - E_m + i\eta} \right] \]
$H/K = 0.00$
Gapless $Z_2$ KSL

$H/K = 0.20$
$Z_2$ Gapped KSL

$H/K = 0.30$
$U(1)$ Gapless QSL

$H/K = 0.35$

$H/K = 0.42$

$H/K = 0.60$

$H/K = 0.80$

$H/K = 1.00$

$(b) (I) (II) (III)$

$\Delta_p$

$\Delta_e$

$\Delta_{\phi}$

$\Delta_{\phi}^*$

$0.2$

$0.35$
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Main ingredients for Kitaev materials
Spin-Orbit coupled Mott Insulators

$$|\uparrow\rangle_{eff} \sim i |zx, \downarrow\rangle + |yz, \downarrow\rangle + |xy, \uparrow\rangle$$

$$|\downarrow\rangle_{eff} \sim -i |zx, \uparrow\rangle + |yz, \uparrow\rangle - |xy, \downarrow\rangle$$
Destructive interference between the two pathways generates bond-dependent interactions
G. Jackeli and G. Khaliullin,
PRL 102, 017205 (2009)

\[ | J_z = + \frac{1}{2} \rangle = \frac{1}{\sqrt{3}} \left[ | d_{xy} \uparrow \rangle + | d_{yz} \downarrow \rangle + i | d_{xz} \downarrow \rangle \right] \]

hopping via $p_z$ orbital on ligand changes $d_{yz} \rightarrow d_{xz}$

$d_{xz} \rightarrow d_{yz}$
Crystal structure of $\alpha$-RuCl$_3$ → candidate Kitaev material
$\alpha$-RuCl$_3$
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Thermal Hall Conductivity

\[ \nabla_y T \rightarrow J^Q_y \rightarrow J^Q_x \]

\[ \nabla_x T \]

\[ J^Q_y = 0 \quad \text{(impose condition)} \]

\[ J^Q_x = \mathbf{K} (-\nabla T) \]

\[ \mathbf{K} = \begin{pmatrix} K_{xx} & K_{xy} \\ -K_{xy} & K_{xx} \end{pmatrix} \]
Material: $\alpha$-RuCl$_3$ \approx$ Kitaev Magnet

$J_k \approx 80 \text{ K}$

For $S = \frac{1}{2}$

$1 \text{ Tesla} \approx 1 \text{ K}$

$K_{xy} = \left( \frac{1}{2} \right) K_Q$

$K_Q = \frac{\pi^2}{3} \frac{k_B^2}{\hbar}$
Signatures of a QSL: **quantized** thermal Hall conductance

\[ \kappa_{xy}^{2D} = \left[ \frac{1}{2} \right] \pi \frac{k_B^2}{6 \hbar} T \]

\[ \kappa_{xy}^{2D} = \kappa_{xy} d \]

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Predictions for Kitaev magnets

Frustration from bond-dependent interactions

Fermi surface of neutral, gapless spinons in an insulator!

Chiral spinon edge mode \( \rightarrow \) Quantized thermal Hall conductance

Kitaev (2006)
Jackeli, Khaliullin (2009)

Ronquillo, Vengal, Trivedi, PRB 99, 140413 (2019)
Patel & Trivedi, PNAS 116, 12199 (2019)
Pradhan, Patel, Trivedi, PRB 101, 180401 (2020)
Going forward.....

1. Predictions for Raman scattering to observe magnon bound states

2. Spin and heat transport

3. Observation of neutral spinon Fermi surfaces

4. Doped QSLs → ??