Magnetic impurities in the honeycomb Kitaev model

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Outline

- Introduction, Motivation
- Brief overview of the honeycomb Kitaev Model
- Kondo Effect in the Kitaev model
- Topological nature of the Kondo transition and non abelian anyon
- Inter-impurity coupling
Introduction

- Kitaev model: spin-1/2 model on honeycomb lattice
  - Interesting properties: exactly solvable, gapless Majorana fermionic excitations.
  - Spin liquid ground state with very short range correlations.
  - Anyonic excitations, relevant to quantum computation.
- Magnetic/non-magnetic impurities effects
  - probe of electronic state of the host system (gapless/gapped, nature of quasiparticle excitations etc).
  - gives rise to interesting effects: unusual Kondo effect in gapless bosonic spin liquids (Florens et al. PRL 2006), renormalized Curie susceptibility (Sachdev et al. PRB 2006), creation and manipulation of non-abelian anyons.
Introduction

Magnetic impurity effects in the Kitaev model

- Probe the quantum spin liquid state.
- Interesting Kondo effect due to Majorana fermion nature of the quasiparticles.
  - Unstable fixed point in the Kondo coupling scaling.
  - Change of flux sector/topology of the ground state.
  - Localized fluxes with zero energy Majorana fermion at its core: non-abelian anyonic statistics.
- Inter-impurity interactions mediated by dispersing Majorana modes: long range interaction present despite very short range correlations in ground state.
  - Non-zero only if the impurities couples to more that one neighbouring Kitaev spins.
  - Very different from the RKKY interaction mediated by electrons.
Kitaev Model: brief description

A honeycomb lattice of spin-1/2 with nearest neighbour direction dependent interactions.

\[ H_0 = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z, \]

Conserved flux operators on each plaquett:

\[ W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z, \quad \text{eigenvalues } \pm 1 \]
Kitaev Model: brief description

The Hamiltonian can be solved exactly by representing spins in terms of Majorana fermions $\sigma_i^\alpha = i b_i^\alpha c_i$
The ground state manifold corresponds to a vortex free state where all $W_i$ are equal.
Gauge condition: $D_i = i b_i^x b_i^y b_i^z c_i = 1$.

$$u_{ij}^\alpha = i b_i^\alpha b_j^\alpha, \quad [u_{ij}, H] = 0, \quad [u_{ij}, u_{kl}] = 0$$

$$W_p = \prod_{\langle ij \rangle, i \in A, j \in B} u_{ij}; \quad \text{In the vortex free state, fix } u_{ij} = 1$$

$$H_0 = \frac{i}{4} \sum_{jk} A_{jk} c_j c_k,$$

$A_{jk} = 2J_{\alpha_{jk}}$ if $j, k$ are neighboring sites on an $\alpha-$bond and zero otherwise.
Kitaev Model: brief description

- Model of free majorana fermions on honeycomb lattice.
- Excitation spectrum: \( \epsilon_\alpha(q) = \pm 2|J_x e^{i q \cdot n_1} + J_y e^{i q \cdot n_2} + J_z| \)
- \( q \) varies over only half of the BZ
- Gapless phase when \( J \)'s satisfy triangle inequality
  \[ |J_z| \leq |J_x| + |J_y| \] etc.
- Linear dispersion near the Fermi point.
Kondo coupling to external magnetic spin

- Kondo effect in metals:

\[ H = \sum_{k,\alpha} \epsilon_k c_{k,\alpha}^{\dagger} c_{k,\alpha} + \frac{K}{2} \sum_{i,\alpha,\beta} \tilde{S}_i \cdot \sigma \ c_{i,\alpha}^{\dagger} c_{i,\beta} \]

\[ \frac{d \ln K}{d \ln D} \propto -K \rho(\epsilon_F) \]

Flows to infinity for antiferromagnetic K and to 0 for ferromagnetic.

- Possibility of a new type of Kondo effect in Kitaev model due to Majorana nature of excitations
Kondo coupling to external magnetic spin

- Kondo coupling term in the Hamiltonian:

\[
V_K = \sum_{\alpha} K^\alpha S^\alpha \sigma^\alpha (0) = i \sum_{q \in HBZ, \alpha} \frac{K^\alpha}{\sqrt{2N}} S^\alpha b^\alpha (\tilde{c}_q + \tilde{c}_q^\dagger)
\]
Kondo coupling to external magnetic spin

Poor man’s scaling for $K$.

- perturbation expansion $T = T^{(1)} + T^{(2)} + \cdots$ in increasing powers of $K$, for the $T$–matrix element: $\langle b^\beta | iK^\beta S^\beta b^\beta c_{a,A} | (q, \alpha) \rangle$.

- follow its variation as a function of the decrease of the bandwidth $(-D, D)$.

- Diagrams that contribute to 3rd order term:

\[\begin{align*}
\text{(a)} & \quad b^\beta \quad q', \tilde{\alpha} \\
& \quad S^\beta, i
\end{align*}\]

\[\begin{align*}
\text{(b)} & \quad q, \alpha \\
& \quad b^\beta \\
& \quad S^\beta, i
\end{align*}\]
Kondo coupling to external magnetic spin

- Adding the two contributions (taking $E \simeq 0$),

$$T^{(3)} \sim -\frac{iK^\beta S^\beta}{\sqrt{2}} \frac{\rho(D)\delta D}{JD} \sum_{\tilde{\beta}} (K^{\tilde{\beta}})^2 (S^{\tilde{\beta}})^2.$$ 

- If either the impurity is a $S = \frac{1}{2}$ spin, or the Kondo interaction is rotationally symmetric, the above contribution renormalizes the Kondo coupling constant.

- For $S \neq \frac{1}{2}$ with anisotropic coupling, new terms are generated, need to go to higher order diagrams to obtain the scaling of these new coupling terms.
Kondo coupling to external magnetic spin

- Linear dispersion gives further contribution to the scaling of $K$ (D. Withoff and E. Fradkin, PRL 64, 1835 (1990)).
- For $\rho(\epsilon) = (1/2\pi v_F^2)|\epsilon| \equiv C|\epsilon|^{r}$, $r = 1$
  \[ K \to K(D'/D)^r, \quad (D' = D - |\delta D|). \]
- $\delta K = -K \frac{\delta D}{D} \left(2K^2a^2CDS(S + 1)/J - 1\right)$.
- The effective coupling $K$ has an unstable fixed point at $K_c = \sqrt{J/[2a^2\rho(D)S(S + 1)]} \sim \sqrt{J/S^2a^2CD} \sim J/S$.
- For $K > K_c$, coupling flows to infinity independent of its sign (ferromagnetic or antiferromagnetic).
- Same scaling observed for bosonic Z2 bosonic spin-liquid with pseudogap DOS (Florens et al).
Localized Majorana, finite flux and change of topology

- In the strong coupling limit, the impurity spin forms a bound state with the Kitaev spin (say at the origin).
- Majorana fermions associated with the Kitaev spin at the origin no longer available for pairing with the Majoranas at the three neighboring sites.
- We can equivalently study the Kitaev model with the site at origin removed.
Localized Majorana, finite flux and change of topology

- \(W_1, W_2\) and \(W_3\) do not commute with \(H = H_0 + V_K\).
- \(W_0 = W_1 W_2 W_3\) is still conserved, \(W_0 = 1\) in the ground state of unperturbed Kitaev model.

Define composite operators \(\tau^x = W_2 W_3 S^x\), \(\tau^y = W_3 W_1 S^y\) and \(\tau^z = W_1 W_2 S^z\),

- \(\tau^\alpha\)'s obey the SU(2) algebra, \([\tau^\alpha, \tau^\beta] = 2i \epsilon_{\alpha\beta\gamma} \tau^\gamma\).
- The SU(2) symmetry is exact for all couplings, is realized in the spin-1/2 representation \((\tau^\alpha)^2 = 1\).
Localized Majorana, finite flux and change of topology

- All eigenstates, including the ground state are doubly degenerate ($\tau^z = \pm 1$).
- In strong coupling limit, double degeneracy arises from the Kitaev model with one spin removed.
- For strong (antiferromagnetic) coupling limit $J_K \rightarrow \infty$, the spin at the origin forms a singlet $|0\rangle$ with the impurity spin,

$$|\psi\rangle = |\psi K^-\rangle \otimes |0\rangle.$$

- Action of the $SU(2)$ symmetry generators on these states:

$$\tau^\alpha = \tilde{W}^\alpha \otimes \sigma_0^\alpha \otimes S^\alpha.$$

$$\tau^\alpha |\psi\rangle = - (\tilde{W}^\alpha |\psi K^-\rangle) \otimes |0\rangle.$$

Double degeneracy coming from $\tilde{W}^\alpha |\psi K^-\rangle$. 
Localized Majorana, finite flux and change of topology

- Three unpaired $b$–Majorana Fermions: $b^z_3$, $b^x_2$ and $b^y_1$

- $ib^x_2 b^y_1$: Conserved; Commutes with all the conserved $W_i$'s.

- Does not commute with $ib^y_1 b^z_3$ and $ib^z_3 b^x_2$

- Choose a gauge s.t. $i\langle b^x_2 b^y_1 \rangle = 1$

- One unpaired $b$–Majorana with dimension $\sqrt{2}$; $\implies$ unpaired Majorana mode in the $c$ sector (together give the full doubly degenerate zero energy mode).
The $b^2_3$ mode is sharply localized, the wave function of the $c$ mode can be spread out in the lattice.

An unpaired zero energy Majorana Fermion is associated with finite flux (Kitaev 06).

Also shown by Willans et al that in presence of a vacancy, the state with finite flux pinned to vacancy has lower ground state energy.

Unit flux with a localized zero energy b-Majorana fermion at its core: Non-abelian statistics (similar to quantum half vortices in p-wave superconductors).
Interaction between external spins

- In bare Kitaev model ground state, spin correlations very short ranged (only nearest neighbour) due to $b$–Majoranas being localized.

- Possibility of interaction between distant spins mediated by dispersing $c$–Majorana Fermions.

- Two distant impurities coupled to a single Kitaev site each do not interact via dispersing Majoranas.

- Impurities can interact only if they are coupled more than one neighbouring Kitaev spins: bonds.
Interaction between external spins

- The Kondo coupling term is

\[ V_K = i \sum_{j \in \text{hex1,} \alpha} K^\alpha S_1^\alpha b_j^\alpha c_j + i \sum_{j \in \text{hex2,} \alpha} K^\alpha S_2^\alpha b_j^\alpha c_j. \]

- Effective interaction generated involving \(c\)--type Majorana fermions at two neighboring sites \((i \in A, j \in B)\):

\[ V_{\text{eff}} = \sum_{\nu} \langle \Omega_b | V | \nu \rangle \frac{1}{E_0 - E_\nu} \langle \nu | V | \Omega_b \rangle \approx \frac{2}{J} \sum_{\alpha, \langle ij \rangle} (K^{\alpha ij})^2 (S_a^{\alpha ij})^2 c_i c_j, \]

\(|\Omega_b\rangle\) refers to the ground state configuration of \(b\)--Majoranas \(i.e.\) all \(u_{ij} = ib_i b_j = 1.\)
Interaction between external spins

- Interaction between the two impurity spins is given by the second order term in $V_{\text{eff}}$

\[ \frac{1}{J^2} \langle (K_{ij}^\alpha)^2 (S_{ij}^\alpha)^2 (K_{i'j'}^{\beta})^2 (S_{i'j'}^\beta)^2 c_ic_jc_{i'}c_{j'} \rangle. \]

- Performing the fermionic averaging,

\[ J_{ij,i'j'}^{\alpha} \sim -(K_{ij}^\alpha)^2 (S_{ij}^\alpha)^2 (K_{i'j'}^{\beta})^2 (S_{i'j'}^\beta)^2 \times \frac{a^4}{4v_F J^2 \pi^3} \frac{1 + \cos(2\tilde{\alpha}(k_F)) - 2 \cos(2k_F \cdot R_{12})}{R_{12}^3}. \]

- For spin-1/2 impurities, $(S^\alpha)^2 = 1/4$ and for isotropic coupling where $\sum_{\text{bond pairs}} (S_{ij}^\alpha)^2 (S_{i'j'}^\beta)^2 = \text{const.}$, no long-ranged interaction is generated.

- Non-dipolar interaction unlike dipolar $S_i \cdot S_j$ interaction in metals.
▶ Kondo effect in Kitaev model associated with an unstable fixed point separating sectors of different topology.
▶ Strong coupling limit corresponds to non-Abelian anyon with a zero energy unpaired Majorana fermion.
▶ RKKY interaction is non-dipolar due to Majorana fermionic excitations.
▶ Change of topology and nondipolar interaction make the Kitaev Kondo effect different from earlier studied Kondo effects in spin-liquids.
Thank You