# Magnetic impurities in the honeycomb Kitaev model

Kusum Dhochak[1], R. Shankar[2] and V. Tripathi[1]

[1]*Department of Theoretical Physics, Tata Institute of Fundamental Research,*
*Homi Bhabha Road, Navy Nagar, Mumbai - 400005, India\* and*
[2]*Institute of Mathematical Sciences, C. I. T. Campus, Taramani, Chennai - 600113, India*

We study the effect of coupling magnetic impurities to the honeycomb lattice spin$-1/2$ Kitaev model in its spin liquid phase. We show that a spin-$S$ impurity coupled to the Kitaev model is associated with an unusual Kondo effect with an intermediate coupling unstable fixed point $K_c \sim J/S$ separating topologically distinct sectors of the Kitaev model. We also show that the massless spinons in the spin liquid mediate an interaction of the form $S_{i\alpha}^2 S_{j\beta}^2 / R_{ij}^3$ between distant impurities unlike the usual dipolar RKKY interaction $S_{i\alpha} S_{j\alpha} / R_{ij}^3$ noted in various 2D impurity problems with a pseudogapped density of states of the spin bath. Furthermore, this long-range interaction is possible only if the impurities (a) couple to more than one neighboring spin on the host lattice and (b) the impurity spin $S \neq 1/2$.

Impurity effects are an essential part of our understanding of strongly correlated electron systems , both as a probe for the underlying electronic state as well as due to the numerous nontrivial effects they have on the properties of the system [1, 2]. Recently many studies have been made of impurity effects as a probe for the putative quantum spin liquid state in underdoped cuprate superconductors [3] and geometrically frustrated magnets [4]. The $S = 1/2$ honeycomb lattice Kitaev model [5] provides a very appealing playground in this context - it has a gapless spin liquid phase and short range spin correlations [6] making it different from many other extensively studied spin liquids [3, 4, 7]; and crucially, the model is integrable via several schemes of spin-fractionalization into fermions [5, 8]. The Kitaev model has been studied in various contexts ranging from the possibility of quantum computation with the anyons [5, 9] that the model predicts, understanding dynamics of quantum quenches in a critical region [10] to fractional charge excitations in topological insulators [11]. However no study of magnetic impurity effects in the Kitaev spin liquid has yet been made, which constitutes the subject of this paper.

We study the behavior of spin-$S$ impurities in the gapless spin liquid regime of the Kitaev model on the honeycomb lattice. The impurity coupling $K$ scales away from an unstable fixed point $K_c \sim J/S$ irrespective of the sign of impurity coupling, similar to impurity problems in pseudogapped bosonic spin liquids [12]. The Kitaev magnetic impurity problem is nevertheless qualitatively different for two important reasons. First, as we show below, the unstable fixed point separates topologically distinct sectors in the Kitaev model, with the strong coupling sector associated with non-abelian anyons. Second, the gapless spinons in the Kitaev spin liquid mediate a non-dipolar RKKY interaction proportional to $S_{i\alpha}^2 S_{j\beta}^2 / R_{ij}^3$ between distant magnetic impurities provided that (a) each impurity couples to more than one lattice site on the host and (b) the impurity spin $S \neq 1/2$. The absence of long-range interaction for $S = 1/2$ impurities opens a way for local manipulation of the Kitaev

system. A comparison of Kondo effect and RKKY interaction in graphene [13, 14], a bosonic spin bath [12] and the Kitaev model are shown in Table I.

The $S = 1/2$ Kitaev model [5] is a honeycomb lattice of spins with direction-dependent nearest neighbor exchange interactions,

$$H_0 = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z, \quad (1)$$

where the three bonds at each site (see Fig.1) are labeled as $x$, $y$ and $z$. As was shown by Kitaev, the flux operators $W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$ defined for each elementary plaquette $p$ are conserved (see Fig.1), with eigenvalues $\pm 1$, and form a set of commuting observables. Each of the Kitaev spins is represented in terms of Majorana fermions $b_i^x$, $b_i^y$, $b_i^z$, $c_i$ as $\sigma_i^\alpha = ib_i^\alpha c_i$, which span a larger Fock space, and we restrict to the physical Hilbert space of the spins by choosing the gauge [5] $D_i = ib_i^x b_i^y b_i^z c_i = 1$. On each $\alpha-$type bond, $u_{ij}^\alpha = ib_i^\alpha b_j^\alpha$ is also conserved and the ground state manifold corresponds to a vortex free state where all $W_i$ are equal. In the vortex free state, we can fix all $u_{ij} = 1$ (corresponds to $W_p = 1$) and the Hamiltonian can be written as a theory of non interacting Majorana fermions. The reduced Hamiltonian for this ground state manifold is given by $H_0 = \frac{i}{4} \sum_{jk} A_{jk} c_j c_k$, where $A_{jk} = 2J_{\alpha_{jk}}$ if $j$, $k$ are neighboring sites on an $\alpha-$bond and zero otherwise. The excited state manifolds (with finite vorticity) are separated from the ground state manifolds by a gap of order $J_\alpha$. Defining the Bravais lattice with a two point basis (Fig.1), the Hamiltonian can be diagonalized in momentum space, $H_0 = \frac{i}{4} \sum_{\mathbf{q}>0,\alpha} \epsilon_\alpha(\mathbf{q}) a_{\mathbf{q},\alpha}^\dagger a_{\mathbf{q},\alpha}$, with $\epsilon_\alpha(\mathbf{q}) = \pm|f(\mathbf{q})|$, $f(\mathbf{q}) = 2(J_x e^{ia\mathbf{q}\cdot\mathbf{n_1}} + J_y e^{ia\mathbf{q}\cdot\mathbf{n_2}} + J_z)$ and the eigenbasis, $a_{\mathbf{q},0} = \tilde{c}_{\mathbf{q},A} + \tilde{c}_{\mathbf{q},B} e^{-i\tilde{\alpha}(\mathbf{q})}$ and $a_{\mathbf{q},1} = \tilde{c}_{\mathbf{q},A} - \tilde{c}_{\mathbf{q},B} e^{-i\tilde{\alpha}(\mathbf{q})}$. Here $A/B$ is the site label for the two types of sites in Kitaev model, $a$ is the lattice constant and $\tilde{\alpha}(\mathbf{q})$ is the phase of $f(\mathbf{q})$. The sum over momenta is only over half of first Brillouin zone. $\epsilon(\mathbf{q})$ has linear dispersion around the Fermi point $\mathbf{k}_F$ (Fig.1). For

| | Graphene | $Z_2$ bosonic spin bath with pseudogap density of states $\rho(\epsilon) = C|\epsilon|$. | Kitaev, honeycomb lattice |
|---|---|---|---|
| Kondo scaling | Unstable intermediate coupling fixed pt. only for AFM coupling. Only AFM flows to strong coupling above unstable fixed pt. | Flow direction is independent of the sign of magnetic impurity coupling. Unstable intermediate coupling fixed pt. for both FM and AFM. | Scaling same as $Z_2$ bosonic spin bath case. However a topological transition is associated with the unstable fixed point. |
| RKKY | $S_{i\alpha}S_{j\alpha}/R_{ij}^3$ | $S_{i\alpha}S_{j\alpha}/R_{ij}^3$ | $S_{i\alpha}^2 S_{j\beta}^2/R_{ij}^3$ |

Table I: Comparison of Kondo effect and RKKY interaction in graphene, a $Z_2$ bosonic spin bath with a pseudogap density of states and the Kitaev model on the honeycomb lattice.
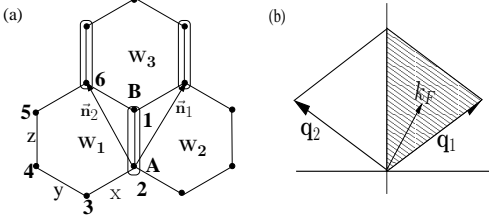


Figure 1: (a) Schematic of the Kitaev lattice showing the $A$ and $B$ sites and the $x$, $y$ and $z$ types of bonds. (b) Figure showing the reciprocal lattice vectors for the $A$ sublattice. The Dirac point for the massless Majorana fermions is denoted by $k_F$ and momentum summations are over the (shaded) half Brillouin zone.
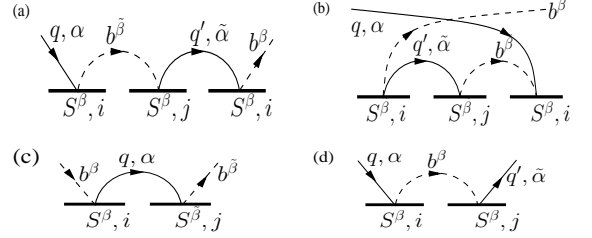


Figure 2: (a and b) Third order contributions to the $T-$matrix. Site-diagonal scattering corresponds to $i = j$ and site off-diagonal scattering, where relevant, corresponds to $i \neq j$. Thin solid lines correspond to $c-$Majoranas while dashed ones to $b-$Majoranas. Thick solid lines represent the impurity spin. (c and d) New vertices generated by off-diagonal scattering.

simplicity, and without loss of generality, we henceforth assume $J_x = J_y = J_z = J$.

**Topological Kondo effect -** Consider a spin $S$ magnetic impurity coupled to a Kitaev spin at an $A$ site ($\mathbf{r} = 0$),

$$V_K = i \sum_\alpha K^\alpha S^\alpha b^\alpha c_A(0), \qquad (2)$$

for which we perform a standard poor man's scaling analysis [15] for the Kondo coupling $K$. Consider the Lippmann-Schwinger expansion for the $T-$matrix element, $\langle b^\beta|K^\beta S^\beta b^\beta c_{a,A}|(\mathbf{q}, \alpha)\rangle$ (scattering of a $c-$Majorana with momentum $q$ and sublattice index $\alpha$ to a $b-$Majorana), $T = T^{(1)} + T^{(2)} + \cdots$, in increasing powers of $K$. The first correction to the bare $T-$matrix comes from two *third* order terms (see Fig.2): $T^{(3)} \simeq -\frac{ia^2}{\sqrt{2}} K^\beta S^\beta \frac{\rho(D)\delta D}{JD} \sum_{\tilde\beta}(K^{\tilde\beta})^2(S^{\tilde\beta})^2$. Here $\rho(\epsilon) = (1/2\pi v_F^2)|\epsilon| \equiv C|\epsilon|$ is the density of states and $D$ is the band edge energy. 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. However for $S \neq \frac{1}{2}$ with anisotropic coupling, new terms are generated and one needs to go to higher order diagrams to obtain the scaling of these new coupling terms.

Just as for the Kondo effect in graphene[13], we also need to consider the change in the density of states with bandwidth. This gives a contribution $K \rightarrow K(D'/D)^r$, $(D' = D - |\delta D|)$. For $S = 1/2$ or for symmetric impurity coupling we thus have

$$\delta K = -K\frac{\delta D}{D}\left(2K^2 a^2 CDS(S+1)/J - 1\right). \qquad (3)$$

The effective coupling $K$ has an unstable fixed point at $K_c = \sqrt{J/[2a^2\rho(D)S(S+1)]} \sim J/S$. Here we used $D \lesssim J$ and $C \sim 1/(Ja)^2$. Clearly for $K > K_c$, the coupling flows to infinity independent of the nature of coupling (ferromagnetic or antiferromagnetic), while for $K < K_c$, the coupling flows to zero.

If the impurity couples to more than one Kitaev spin in a plaquette, new contributions arise from site off-diagonal scattering ($i \neq j$ in Fig.2 a, b). Adding all these contributions, we find this also leads to a similar Kondo effect as was discussed above for the single site coupling case. There are also new terms of second order in $K$ that are generated (see Fig.2). The term corresponding to Fig. 2c is $\sim K^\beta K^{\tilde\beta} S^\beta S^{\tilde\beta} b_i^\beta b_j^{\tilde\beta}$. When projected to the vortex free ground state, it becomes $\sim (K^\beta)^2(S^\beta)^2$ generating anisotropic potential for the impurity spin. The second term, Fig.2d, is $\sim (K^\beta)^2 (S^\beta)^2 c_i c_j/J$, which, as we shall see below, contributes to the long range interaction among impurity spins.

A remarkable property of the Kondo effect in Kitaev model is that the unstable fixed point is associated with a topological transition from the zero flux state to a finite flux state. The strong coupling limit amounts to studying the Kitaev model with a missing site or cutting

the three bonds linking this site to the neighbors. Kitaev has shown [5] that such states with an odd number of cuts are associated with a finite flux, and also that these vortices are associated with unpaired Majorana fermions and have non-abelian statistics under exchange. Below we present another, perhaps more physical, way of appreciating this result.

For the Hamiltonian $H = H_0 + V_K$, the three plaquettes $W_1$, $W_2$ and $W_3$ that touch the impurity site are no longer associated with conserved flux operators, while the flux operators that do not include the origin remain conserved. The three plaquette operator $W_0 = W_1 W_2 W_3$ is still conserved and $W_0 = 1$ in the ground state of the unperturbed Kitaev model. The composite operators $\tau^x = W_2 W_3 S^x$, $\tau^y = W_3 W_1 S^y$ and $\tau^z = W_1 W_2 S^z$, where the $S^\alpha$ are Pauli spin matrices corresponding to the impurity, are also conserved. The $\tau^\alpha$'s do not mutually commute and instead obey the $SU(2)$ algebra, $[\tau^\alpha, \tau^\beta] = 2i\epsilon_{\alpha\beta\gamma}\tau^\gamma$ . This $SU(2)$ symmetry, which is exact for all couplings is realized in the spin-1/2 representation $\left( (\tau^\alpha)^2 = 1 \right)$. Thus all eigenstates, including the ground state are doubly degenerate.

Consider a strong (antiferromagnetic) coupling limit $J_K \to \infty$. The low energy states will be the ones in which the spin at the origin forms a singlet $|0\rangle$ with the impurity spin, $|\psi\rangle = |\psi K^-\rangle \otimes |0\rangle$. $|\psi K^-\rangle$ now stands for the low energy states of the Kitaev model with the spin at the origin removed. To see the action of the $SU(2)$ symmetry generators on these states, we note that they can be written as $\tau^\alpha = \tilde{W}^\alpha \otimes \sigma^\alpha \otimes S^\alpha$ and $\tilde{W}^\alpha$ do not involve the components of the spin at the origin, $\sigma^\alpha$. We then have $\tau^\alpha |\psi\rangle = -(\tilde{W}^\alpha |\psi K^-\rangle) \otimes |0\rangle$. Thus, in the strong coupling limit, the symmetry generators act nontrivially only in the Kitaev model sector. This implies that the low energy states of the Kitaev model with one spin removed are all doubly degenerate, with the double degeneracy emerging from the Kitaev sector. This implies there is a zero-energy mode in the single particle spectrum. The two degenerate states correspond to the zero mode being occupied or unoccupied. The same arguments for the double degeneracy in the Kitaev sector may be repeated for the ferromagnetic strong coupling case.

Let us examine the structure of the zero mode. Removing a Kitaev spin creates three unpaired $b-$Majoranas at the neighboring sites, say, $b_3^z$, $b_2^x$ and $b_1^y$. Note that $ib_2^x b_1^y$ is conserved and commutes with all the conserved flux operators $W_i$ but not with the two other combinations $ib_1^y b_3^z$ and $ib_3^z b_2^x$ - then one can choose a gauge where the expectation value of $ib_2^x b_1^y$ is equal to $+1$ so that these two $b$ modes drop out of the physics and we equivalently have one unpaired $b-$Majorana. The unpaired $b_3^z$ Majorana has dimension $\sqrt{2}$; so there must therefore exist an unpaired Majorana mode in the $c$ sector (again of dimension $\sqrt{2}$) so that together these two give the full (doubly
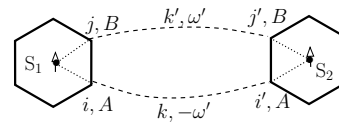


Figure 3: Schematic of a typical long-distance impurity interaction mediated by a pair of propagating $c-$Majoranas (shown by dashed lines) emanating from the ends of a Kitaev bond. Another contribution comes from crossed trajectories $(i, A \leftrightarrow j', B'$ and $j, B \leftrightarrow i', A')$.

degenerate) zero energy mode. We note that while the $b_3^z$ mode is sharply localized, the wave function of the $c$ mode can be spread out in the lattice.

That the ground state energy corresponding to a finite flux state (pinned to the defect) is lower than the zero flux case in the Kitaev model with a missing site has also been recently shown numerically[16].

**RKKY Interactions -** In the absence of impurities, in the ground state manifold (vortex free state), we have only nearest neighbor Kitaev spin correlations. This is because each Kitaev spin is a bilinear of a massless $c$ Majorana and a massive $b$ Majorana, and the $b$ Majoranas have only short range correlations. Suppose we now add impurities which may each be locally coupled to more than one Kitaev spin. Distant impurities can interact only if they are coupled via the massless Majoranas. By contracting $b$ Majoranas locally by second order perturbation in the Kondo coupling, we generate vertices of the type $(K^\alpha S^\alpha)^2 c_i c_j / J$, where $i$ and $j$ are not farther than nearest neighbor. Note that since $c_i^2 = 1$, these vertices will contain massless Majoranas only when $i$ and $j$ belong to *different* sites. This effectively means that two distant impurities coupled to a single Kitaev site each *cannot* interact. However when the impurities interact with more than one neighboring Kitaev spin, we shall see that a long range interaction of the spins is possible. As an example, we analyze the interaction when the two impurities are at the centers of distant hexagons. The interaction term is $V_K = i \sum_{j \in \text{hex}1, \alpha} K^\alpha S_1^\alpha b_j^\alpha c_j + i \sum_{j \in \text{hex}2, \alpha} K^\alpha S_2^\alpha b_j^\alpha c_j$. The effective interaction generated involving $c-$type Majorana fermions at two neighboring sites ($i \in A$, $j \in B$) is given by (see Fig.2c,d) $V_{\text{eff}} = \frac{2}{J} \sum_{a, <ij>_\alpha} (K^{\alpha_{ij}})^2 (S_a^{\alpha_{ij}})^2 c_i c_j$. Here $\alpha_{ij}$ refers to the $z-$component when neighboring sites $i$ and $j$ are along a $z-$bond, etc. Now the interaction between the two impurity spins is given by the second order term in $V_{\text{eff}}$ (or, equivalently, fourth order in $K$). These terms are of the type $\frac{1}{J^2} \langle (K^{\alpha_{ij}})^2 (S_1^{\alpha_{ij}})^2 (K^{\beta_{i'j'}})^2 (S_2^{\beta_{i'j'}})^2 c_i c_j c_{i'} c_{j'} \rangle$. Performing the fermionic averaging, the contribution (see Fig. 3) to the long range interaction from the pair of

bonds $ij$ and $i'j'$ is

$$J_{12}^{ij,i'j'} \sim -(K^{\alpha_{ij}})^2 (S_1^{\alpha_{ij}})^2 (K^{\beta_{i'j'}})^2 (S_2^{\beta_{i'j'}})^2$$
$$\times \frac{a^4}{4v_F J^2 \pi^3} \frac{1 + \cos(2\tilde{\alpha}(\mathbf{k}_F)) - 2\cos(2\mathbf{k}_F \cdot \mathbf{R}_{12})}{R_{12}^3}. \quad (4)$$

Note that for spin-1/2 impurities, $(S^\alpha)^2 = 1/4$ and for isotropic coupling where $\sum_{\text{bond pairs}} (S_1^{\alpha_{ij}})^2 (S_2^{\beta_{i'j'}})^2 = $ const., no long-ranged interaction is generated.

To summarize, we studied the effect of impurity quantum spins coupled to the ground state manifold of the Kitaev model in the gapless spin-liquid state. We found an unusual Kondo effect with an unstable fixed point demarcating a topological transition between zero flux and finite flux sectors. Where more than one impurity is present, we showed that under certain circumstances, the massless spinons in the Kitaev model mediate a higher order (non-dipolar) RKKY interaction between distant impurity spins. The topological transition and the non-dipolar impurity interaction make the Kitaev Kondo effect qualitatively different from the Kondo effect in some bosonic spin liquids that also have an unstable fixed point. We expect a similar scaling for the Kondo coupling and RKKY interaction for other spin models [17] with a similar Majorana structure and phase diagram.

In the strong Kondo coupling limit we showed that a non-abelian anyon is created consisting of an unpaired $b-$Majorana localized in its vicinity and its delocalized $c-$counterpart. The localized $b-$Majorana at the finite flux defect is very reminiscent of the localized Majoranas in the cores of half vortices in $p-$wave superconductors [18]. One difference, as pointed out by Kitaev, is that in $p-$wave superconductors, the currents associated with the fluxes are charged (and thus interact with impurity potentials). Besides, the individual charges acquire abelian phases of their own. Another difference is that in the Kitaev model, the full (doubly degenerate) zero mode is made of a $b$ and a $c$ Majorana while in the superconductor, two vortex core Majoranas make a zero mode [23]. $p-$wave paired ground states in the Kitaev model and its vortex excitations have also been studied in Ref. [19].

We note that if we could adiabatically move the impurity spin (say by making it on a STM tip), then we could move the anyons and thus perform the braiding operations as is required for quantum computation. This method is more practical than perturbing an entire plaquette with terms like $\mu W_i$ that involve at least six Kitaev spins.

The temperature dependent impurity susceptibility can be measured by NMR Knight shift experiments [20]. For weak Kondo coupling, the magnetic susceptibility of the impurity is Curie-like with logarithmic corrections, which flow to zero regardless of the sign of Kondo coupling. In the strong coupling limit, we consider antiferromagnetic coupling for $S = 1/2$ impuri-

ties, where the anyons are vacancies in the Kitaev lattice. The magnetic susceptibility has been shown [16] to have the form $\chi(T) \sim \frac{1}{T \ln(D/T)}$ for a pair of nearby vacancies on the same sublattice while for a single vortex, $\chi(T) \sim \ln(D/T)$. In the absence of vacancies, the low temperature magnetic susceptibility is small because of the spin gap in the Kitaev ground state. The nuclear relaxation rate $T_1^{-1}$ may also be used as an impurity probe [21]. Using $\chi(T, \omega) \approx (\chi^{-1}(T, 0) - i\omega)^{-1}$ and $T_1^{-1} \propto A^2 I(I+1)T[\text{Im}\chi(T, \omega)/\omega]_{\omega \to 0}$, where $A$ is the hyperfine coupling of spin$-I$ nuclei with the defect, one gets $T_1^{-1} \sim T[\ln(D/T)]^2$ for the single vortex and $T_1^{-1} \sim 1/T[\ln(D/T)]^2$ for the two nearby defects case, both of which qualitatively differ from the Korringa law $T_1^{-1} \sim T$ for the usual Kondo effect at low temperatures. There are already numerous proposals in the literature how a Kitaev model could be realized [22], and we are hopeful that eventually these novel impurity effects may also be experimentally studied.

* Electronic address: vtripathi@theory.tifr.res.in
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