Majorana excitations in the anisotropic Kitaev model with an ordered-flux structure

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Abstract. We investigate the anisotropic $S = 1/2$ Kitaev model on the honeycomb lattice with the ordered-flux structure. By diagonalizing the Majorana Hamiltonian for the flux configuration, we find two distinct gapped quantum spin liquids. One of them is the gapped state realized in the large anisotropic case, where low energy properties are described by the toric code. On the other hand, when the system has small anisotropy, the other gapped quantum spin liquid is stabilized by the ordered-flux configuration. Since these two gapped quantum spin liquids are separated by the gapless region, these are not adiabatically connected to each other.

1. Introduction
Quantum spin liquids in the Kitaev model [1, 2] have been studied intensively in recent years because of their potential applications in topological quantum computation and spintronics. It is known that in the Kitaev model, spin degrees of freedom are split into itinerant Majorana fermions and localized fluxes due to the spin fractionalization. The ground state belongs to the flux-free state and low energy properties are described by itinerant Majorana fermions. In fact, the Majorana edge current has been observed in the half-quantized plateau in the thermal quantum Hall effect [3, 4]. Furthermore, the Majorana-mediated spin transport has been theoretically suggested [5], which should stimulate further investigation to realize quantum devices using Majorana fermions.

In our previous study [6], we have found that the gapped quantum spin liquid is realized in a certain flux configuration. This indicates that the flux configuration is a key role in controlling Majorana excitation. On the other hand, it is known that the large anisotropy in the exchange couplings stabilizes the gapped quantum spin liquid, which should be described by the toric code [7]. Then a question arises. Are the above gapful states with distinct origins are adiabatically connected to each other? To answer this question, we focus on a flux configuration to investigate how the anisotropy in the exchange couplings affects the Majorana excitations.

2. Model and Hamiltonian
We consider the Kitaev model on the honeycomb lattice, which is given by

$$H = -J_x \sum_{\langle i,j \rangle_x} S_i^x S_j^x - J_y \sum_{\langle i,j \rangle_y} S_i^y S_j^y - J_z \sum_{\langle i,j \rangle_z} S_i^z S_j^z,$$

where $\langle i,j \rangle_\alpha$ shows the nearest-neighborhood pair on the $\alpha (= x, y, z)$-bonds. $S_i^\alpha (= \frac{1}{2} \sigma_i^\alpha)$ is the $\alpha$-component of the $S = 1/2$ spin at the $i$th site and $\sigma_i^\alpha$ is the $\alpha$-component of the Pauli matrix.
J_α(>0) is the exchange coupling on the α-bonds. The model Hamiltonian is schematically shown in Fig. 1(a). There is a local conserved quantity on each hexagonal plaquette in the honeycomb lattice. The operator $W_p$ is defined on a plaquette $p$ as

$$W_p = \sigma^x_{p1} \sigma^y_{p2} \sigma^z_{p3} \sigma^x_{p4} \sigma^y_{p5} \sigma^z_{p6},$$

where $p_i (i = 1, 2, \cdots, 6)$ is the site on the plaquette $p$ [see Fig. 1(b)]. This satisfies $[W_p, W_p'] = 0, [W_p, H] = 0$, and $W_p^2 = 1$. The corresponding eigenvalue $w_p$ takes ±1. The eigenstate of the Hamiltonian can be specified by the set of the eigenvalues $w_p$. It is known that the ground state is realized with $w_p = +1$ for all plaquettes. Therefore, a plaquette with $w_p = -1$ can be regarded as an excited nux.

In the study, we discuss Majorana excitations in the Kitaev system with certain nux-configurations. To this end, we first use the Jordan-Wigner transformation, $S^z_i = \prod_{i'}^{i-1} (1 - 2n_{i'}) c_{i'}$, $S^+_i = \prod_{i'}^{i-1} (1 - 2n_{i'}) c_{i}$, where $c_{i}$ and $c_{i'}$ are the creation and annihilation operators of the fermion at the $i$th site. The Hamiltonian is rewritten into

$$H = -\frac{J_x}{4} \sum_{\langle rb, r'w \rangle_x} (c_{rb} + c_{rb}^\dagger) (c_{r'w} - c_{r'w}^\dagger) - \frac{J_y}{4} \sum_{\langle rb, r'w \rangle_y} (c_{rb} + c_{rb}^\dagger) (c_{r'w} - c_{r'w}^\dagger)$$

$$- i\frac{J_z}{4} \sum_r (2n_{rb} - 1) (2n_{rw} - 1),$$

where $c_{rb}$ is an annihilation operator of the fermion at the black (white) site on the $r$th $z$-bond. $\langle rb, r'w \rangle_\alpha$ indicates the nearest-neighbor pair connected by the $\alpha$-bond. Here, we define Majorana fermion operators $\gamma, \bar{\gamma}$ [8, 9, 10] as

$$\begin{cases} i\gamma_{rb} = c_{rb} + c_{rb}^\dagger, \\ i\bar{\gamma}_{rb} = c_{rb} + c_{rb}^\dagger, \\ i\gamma_{rw} = c_{rw} + c_{rw}^\dagger, \\ i\bar{\gamma}_{rw} = c_{rw} + c_{rw}^\dagger, \end{cases}$$

where Majorana operators satisfy $\gamma_{i}^\dagger = \gamma_i, \bar{\gamma}_{i}^\dagger = \bar{\gamma}_i, \{\gamma_i, \bar{\gamma}_j \} = \{\bar{\gamma}_i, \gamma_j \} = 2\delta_{ij}$. The Hamiltonian is given as

$$H = -i\frac{J_x}{4} \sum_{\langle rb, r'w \rangle_x} \gamma_{rb}\gamma_{r'w} - i\frac{J_y}{4} \sum_{\langle rb, r'w \rangle_y} \gamma_{rb}\gamma_{r'w} - i\frac{J_z}{4} \sum_r \eta_r \gamma_{rb}\gamma_{rw},$$
where $\eta_r = i \gamma_1 \gamma_2 \gamma_3 \gamma_4 \gamma_5$. Since $\eta_r$ satisfies $[H, \eta_r] = 0$, $[\eta_r, \eta_r'] = 0$, and $\eta_r^2 = 1$, $\eta_r$ is a local conserved quantity and the corresponding eigenvalue takes $\pm 1$. The local operator $W_p$ is represented as $W_p = \eta_{pl} \eta_{pr}$, where $\eta_{pl}$ and $\eta_{pr}$ are defined on the left and right $z$-bonds on the plaquette $p$ [see Fig. 1(b)].

**Figure 2.** Flux configuration in the Kitaev model studied here. Each plaquette with orange shade shows $w_p = -1$ and that without shade shows $w_p = +1$. Each rectangle including 6 $z$-bonds represents the unit cell, which is marked with thin yellow shade.

In the present study, we focus on an ordered-flux structure shown in Fig. 2 as a simple example. This flux-configuration is represented by the set $\{\eta_{r_1}, \eta_{r_2}, \ldots, \eta_{r_6}\} = \{1, 1, 1, -1, -1, -1\}$ and its periodic arrangements. From the previous study [6], it is known that in the isotropic case with $J_x = J_y = J_z$, the excitation gap appears in the Majorana excitations. Here, we consider the Majorana excitations in the anisotropic Kitaev model under the conditions $J_x + J_y + J_z = 3$, and $J_x = J_y$.

### 3. Result

By diagonalizing the Hamiltonian of the Kitaev model with the flux configuration, we obtain the Majorana excitations. The results for the Majorana gap are shown in Fig. 3. When $J_z = 0$,

**Figure 3.** Gap magnitude $\Delta$ as a function of the coupling $J_z$. The purple solid (green dashed) line represents the ordered-flux configuration (the ground state). Inset shows magnified image around $J_z = 1.285$. The isotropic case corresponds to $J_z = 1$. 
the system is reduced to the quantum spin chain composed of $x$- and $y$-bonds. In this limit, the flux configuration never affects the Majorana excitation, and $\Delta = 0$. This gapless state is stable against the introduction of the exchange $J_z$, as shown in Fig. 3. Beyond $(J_z)_{c1} \approx 0.7129$, the Majorana gap appears, takes a maximum at $J_z = 1$, and finally closes at $(J_z)_{c2} \approx 1.2834$. Thus, we can conclude that the gapped quantum spin liquid is stabilized by the flux-configuration since the Kitaev system in the flux-free state is gapless in this parameter regime, as shown in Fig. 3. When $(J_z)_{c2} < J_z < (J_z)_{c3} \approx 1.2889$, the gapless quantum spin liquid state is realized, although the region is very narrow, as shown in the inset of Fig. 3. For $J_z > (J_z)_{c3}$, another gapped quantum spin liquid state emerges with $\Delta \approx J_z$. In this case, the flux configuration plays no essential role and the ground state should be described by the toric code. Therefore, our results suggest that origins for these two gapful quantum spin liquids are distinct from each other.

4. Summary
We have studied the anisotropic $S = 1/2$ Kitaev model on the honeycomb lattice with the ordered-flux structure. In this flux configuration, two distinct gapped quantum spin liquids appear when $J_z$ varies. With large anisotropy, the system is well described by the toric code. On the other hand, when the system has small anisotropy, another gapped quantum spin liquid is realized. These two gapped quantum spin liquids are separated by the gapless region. Therefore, these are not adiabatically connected to each other and thus we conclude that they have different origins. In the sense, one can potentially control the motion of the Majorana excitations using both the flux configuration and anisotropy in the exchanges [11]. The systematic study for other ordered-flux structures are left for future work.

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