Low-energy Majorana states in spin liquid transitions in a three-dimensional Kitaev model

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Abstract. A three-dimensional Kitaev model on a hyperhoneycomb lattice is investigated numerically at finite temperature. The Kitaev model is one of the solvable quantum spin models, where the ground state is given by gapped and gapless spin liquids, depending on the anisotropy of the interactions. This model can be rewritten as a free Majorana fermion system coupled with \( Z_2 \) variables. The density of states of Majorana fermions shows an excitation gap in the gapped region, while it is semimetallic in the gapless region reflecting the Dirac node. Performing the Monte Carlo simulation, we calculate the temperature dependence of the Majorana spectra. We find that the semimetallic dip is filled as temperature increases in the gapless region, but surprisingly, the spectrum develops an excitation gap in the region near the gapless-gapped boundary. Such changes of the low-energy spectrum appear sharply at the transition temperature from the spin liquid to the paramagnetic state. The results indicate that thermal fluctuations of the \( Z_2 \) fields significantly influence the low-energy state of Majorana fermions, especially in the spin liquid formation.

1. Introduction

Quantum spin liquid (QSL) is one of the fascinating subjects in condensed matter physics [1]. This is a new state of matter in magnetic insulators, which does not show long-range magnetic ordering down to zero temperature (\( T \)). Vast experimental efforts have been made to realize this exotic state, and several candidates of QSLs were proposed, for instance, in organic salts [2, 3] and transition-metal oxides [4, 5, 6]. Theoretical studies have also been performed for many models, e.g., the Heisenberg and Hubbard models on geometrically frustrated lattices [7, 8, 9]. In spite of these intensive studies, it remains controversial whether QSLs are realized or not in the theoretical models, mainly because of the difficulty in numerical simulations, such as the negative sign problem in the quantum Monte Carlo (MC) method.

The Kitaev model is a quantum spin model consisting of \( S = 1/2 \) spins [10]. This model is originally defined on a two-dimensional (2D) honeycomb lattice composed of three types of bonds. On each bond, the interaction between the nearest-neighbor spins is of Ising type but the spin component of the interaction is different among the three types of bonds. This bond-dependent interaction brings about frustration; namely, all the bond energies are not minimized simultaneously. Due to the frustration effect, a magnetic order is suppressed down to zero \( T \) and a nontrivial magnetic state emerges in the ground state. Indeed, the ground state of the
Kitaev model is exactly proved to be a QSL [11]. Depending on the anisotropy of the exchange interactions, both gapped and gapless QSLs appear in the ground state [10, 11]. Therefore, this model provides a good starting point to reveal the intrinsic properties of QSLs.

In addition, it was proposed that the Kitaev model is relevant also experimentally: the Kitaev-type interaction may be realized between \( J_{\text{eff}} = 1/2 \) spins under the strong spin-orbit coupling in iridium oxides with a layered honeycomb lattice [12]. Recently, related new iridium compounds, in which the iridium ions form a three-dimensional (3D) network were synthesized in the chemical formula \( \text{Li}_2\text{IrO}_3 \): the so-called hyperhoneycomb [13] and harmonic-honeycomb compounds [14]. In these 3D materials, the Kitaev-type interaction is also expected to be present. The discoveries have stimulated theoretical studies of the 3D Kitaev physics [15, 16, 17, 18, 19, 20, 21]. Among them, the authors and their collaborators have clarified the existence of finite-\( T \) phase transitions between the low-\( T \) QSLs and the high-\( T \) paramagnet by extensive numerical simulations [18, 19].

In this paper, we address the finite-\( T \) properties of the Kitaev model on a hyperhoneycomb lattice. This 3D Kitaev model was first introduced in Ref. [22]. One of the characteristics in the Kitaev model is that this model can be exactly solvable at zero \( T \) by rewriting it as a free Majorana fermion system coupled with \( Z_2 \) variables. We here focus on the effect of thermal fluctuations of the \( Z_2 \) variables on the Majorana fermion state. We calculate the \( T \) dependence of the density of states (DOS) of Majorana fermions, and compare the results with a free Majorana fermion system coupled with \( Z_2 \) fields above the critical temperature.

2. Model

We study the Kitaev model on a hyperhoneycomb lattice, whose Hamiltonian is given by

\[
\mathcal{H} = -J_x \sum_{\langle ij \rangle_x} \sigma^x_i \sigma^x_j - J_y \sum_{\langle ij \rangle_y} \sigma^y_i \sigma^y_j - J_z \sum_{\langle ij \rangle_z} \sigma^z_i \sigma^z_j,
\]

where \( \sigma^x_i, \sigma^y_i, \) and \( \sigma^z_i \) are Pauli matrices describing a spin-1/2 state at a site \( i \); \( J_x, J_y, \) and \( J_z \) are exchange constants [10]. The model is defined on the hyperhoneycomb lattice shown in Fig. 1(a) [22]; the interactions \( J_x, J_y, \) and \( J_z \) are defined on three different types of the nearest neighbor bonds, \( x \) (blue), \( y \) (green), and \( z \) bonds (red), respectively. The ground state of this model is obtained exactly, similarly in the 2D Kitaev model on a honeycomb lattice [10]. The phase diagram is completely the same as that of the 2D model, and consists of gapped and gapped QSL phases, as shown in Fig. 1(b) [10]: the QSL with gapless excitation is stabilized in the center triangle including the isotropic case \( J_x = J_y = J_z \), while the QSL with an excitation gap appears in the outer three triangles with anisotropic interactions.

3. Method

We study thermodynamic properties of the model in Eq. (1) by an unbiased MC method. The method is based on the Majorana fermion representation of the model, described below. First, the Jordan-Wigner transformation is applied by regarding the 3D hyperhoneycomb lattice as a set of one-dimensional chains composed of \( x \) and \( y \) bonds. These chains are connected by the \( z \) bonds with each other. A site \( i \) on the hyperhoneycomb lattice can be represented by a pair of integers \( (m,n) \), where \( m \) identifies a chain and \( n \) is the site index on the \( m \)-th chain. Then, the spin operators are written by spinless fermion operators \( (a_i, \ a_i^\dagger) \) as \( S^+_i = (S^-_i)^\dagger = \frac{1}{2} (\sigma^x_i + i \sigma^y_i) = \prod_{n=1}^{n_i} (1 - 2n_{m,n'}) a_{m,n} a_i^\dagger a_i \) and \( \sigma^z_i = 2n_{m,n} - 1 \), where \( n_i \) is the number operator defined by \( n_i = a_i^\dagger a_i \). The Ising-type interactions in Eq. (1) are written as
In the second line of Eq. (2), we introduced Majorana fermion operators, $c$ and $\tilde{c}$, from the spinless fermion operators, $a$ and $a^\dagger$, as $c_w = (a_w - a_{w}^\dagger)/i$, $\tilde{c}_w = (a_w + a_{w}^\dagger)$, $c_b = (a_b + a_{b}^\dagger)/i$, and $\tilde{c}_b = (a_b - a_{b}^\dagger)/i$. In addition, we introduced $Z_2$ operators as $\eta_r = i\tilde{c}_b\tilde{c}_w$ on each $z$ bond $r$ [24]. Since all the $Z_2$ operators commute with the Hamiltonian given by Eq. (2), the eigenstates of the system are characterized by the set of eigenvalues $\eta_r = \pm 1$. It is worth noting that this Majorana representation is faithful, in contrast to that used to obtain the exact solution in the original Kitaev’s paper: the latter has a redundancy in the Hilbert space, which requires a projection onto the original physical space to compute physical quantities [10]. Therefore, the present formulation is useful for the calculations not only in the ground state but also for the excited states. In the Jordan-Wigner transformation, however, the boundary hopping term acquires a string factor composed of multiple products of fermion operators, if the periodic boundary condition is imposed. To avoid this boundary problem, we take open boundary conditions along the chains.

The Hamiltonian in Eq. (2) is a free Majorana fermion system coupled with the $Z_2$ variables $\{\eta_r\}$ on the $z$ bonds. The partition function of the system described by the Hamiltonian in Eq. (2) is given by $Z = \text{Tr}_{\{\eta_r\}} \text{Tr}_{\{c_i\}} e^{-\beta H} = \text{Tr}_{\{\eta_r\}} e^{-\beta F_f(\{\eta_r\})}$ (we set the Boltzmann constant $k_B=1$), and $F_f(\{\eta_r\})$ is the free energy of the Majorana fermion system for a given configuration of $\{\eta_r\}$: $F_f(\{\eta_r\}) = -T \ln \text{Tr}_{\{c_i\}} e^{-\beta H(\{\eta_r\})}$. Since the Hamiltonian $H(\{\eta_r\})$ is given in a quadratic
Figure 2. (a)-(d) The DOS of Majorana fermions for the 3D Kitaev model on the hyperhoneycomb lattice in the gapless region in Fig. 1(b): (a) $\alpha = 0.75$, (b) $\alpha = 0.8$, (c) $\alpha = 0.9$, and (d) $\alpha = 1.0$. Except for the results at $T = 0$ and $T = \infty$, the DOS are calculated by the MC simulation in $L = 6$ clusters, where the smearing factor $\delta$ defined in Eq. (4) is chosen to be 0.02. The temperatures are taken in the vicinity of $T_c$ (see also Fig. 3). (e) and (f) The DOS of Majorana fermions for the 2D Kitaev model on a honeycomb lattice: (e) $\alpha = 0.8$ and (f) $\alpha = 0.9$. Except for the results at $T = 0$ and $T = \infty$, the DOS are calculated by the MC simulation in $L = 12$ clusters with $\delta = 0.02$.

form in terms of the Majorana fermion operators, it is easily diagonalized in the form of

$$\mathcal{H}(\{\eta_r\}) = \sum_{\lambda=1}^{N/2} \varepsilon_{\lambda}(\{\eta_r\}) \left( f_\lambda f_\lambda^\dagger - \frac{1}{2} \right),$$

where $f_\lambda (f_\lambda^\dagger)$ is the annihilation (creation) operator of a spinless fermion and $N$ is the number of lattice sites. We perform the Markov-chain MC simulation for the classical local variables $\eta_r = \pm 1$ so as to reproduce the Boltzmann distribution of $e^{-\beta F_f(\{\eta_r\})}$.

We performed the replica exchange MC simulations for avoiding the freezing of MC sampling at low $T$, on the $L = 4$, 5, and 6 clusters where $N = 4L^3$ [26]. We impose open boundary conditions for the $a$ and $b$ directions as mentioned above, and a periodic boundary condition for the $c$ direction [see Fig. 1(a)]. We prepared 16 replicas and performed the single-flip update in the simulation for each replica. We spent 40,000 (16,000) MC steps for measurement and 10,000 (1,000) MC steps for thermalization in the $L = 4$ and 5 clusters ($L = 6$ cluster).
4. Results

Before going into the MC results at finite \( T \), let us first discuss the behavior of the DOS of Majorana fermions at zero \( T \) and in the high-\( T \) limit. The DOS is defined by

\[
D(\omega, \{ \eta_r \}) = \frac{2}{N} \sum_{\lambda} \delta (\omega - \varepsilon_{\lambda}(\{ \eta_r \})) = -\frac{2}{\pi N} \sum_{\lambda} \text{Im} \frac{1}{\omega - \varepsilon_{\lambda}(\{ \eta_r \}) + i\delta} \bigg|_{\delta \to +0} .
\]

The results at \( T = 0 \) are easily obtained by performing the Fourier transformation for the Majorana fermions to diagonalize the Hamiltonian given in Eq. (2), as the ground state is given by a uniform configuration of the \( Z_2 \) variables with all \( \eta_r = +1 \). On the other hand, the high-\( T \) limit is given by random configurations of \( \eta_r \): the DOS at \( T = \infty \) is obtained by a simple average of Eq. (4) over random configurations of \( \{ \eta_r \} \). The calculations at \( T = 0 \) are performed by replacing the integrals by the sum over grid points of 300 \( \times \) 300 in the Brillouin zone, while the \( T = \infty \) results are calculated for \( L = 12 \) clusters with taking 2,400 random configurations.

The results at \( T = 0 \) and \( T = \infty \) are shown in Figs. 2(a)-2(d) while changing the anisotropy parameter \( \alpha \). The parameter \( \alpha \) is defined so as to satisfy \( J_x = J_y = \alpha/3 \) and \( J_z = 1 - 2\alpha/3 \) [see Fig. 1(b)]: hence, the results in Figs. 2(a)-2(d) are in the region where the ground state is gapless (\( \alpha = 0.75 \) is critical). Indeed, at \( T = 0 \), the low-energy DOS is proportional to the excitation energy \( \omega \) as shown in Figs. 2(a)-2(d), reflecting the Dirac-type semimetallic band structure. On
the other hand, the DOS at $T = \infty$ shows contrasting behavior depending on the values of $\alpha$: an excitation gap opens for $\alpha \lesssim 0.8$, whereas the DOS becomes metallic with nonzero values at $\omega = 0$ for $\alpha \gtrsim 0.9$. There is a boundary at $0.8 < \alpha_c(T = \infty) < 0.9$ between the gapped and gapless behavior in the high-$T$ limit. This critical value of $\alpha$ is clearly larger than that at $T = 0$, $\alpha_c(T = 0) = 0.75$. These results indicate that the Majorana fermion gap opens with increasing $T$ in the region of $\alpha_c(T = 0) < \alpha < \alpha_c(T = \infty)$.

In order to clarify how the DOS evolves and the gap opens as $T$ increases, we calculate the thermal average of the DOS in Eq. (4) by the MC simulation introduced in Sec. 3. The results are shown in Figs. 2(a)-2(d) together with those at $T = 0$ and $T = \infty$. We here show the data in the vicinity of the critical temperatures $T_c$, which are estimated by the peak temperatures of the specific heat shown in Fig. 3 [19]. We note that $T_c$ is much lower than the energy scale of the bare exchange constants. This result is attributed to the frustration effect originating from the bond-dependent interaction intrinsic in the Kitaev model. As shown in Figs. 2(a)-2(d), the low-energy part of the DOS changes rapidly near $T_c$, and develops a gap (fills a semimetallic dip) for $\alpha \lesssim (\gtrsim) \alpha_c(T = \infty)$.

For comparison, we also performed the calculations for the 2D Kitaev model where the ground state phase diagram is the same as that in the 3D case. In the 2D case, there are two peaks in the specific heat (not shown) but the low-$T$ peak does not grow with increasing the system size, which indicates the absence of phase transition [19]. The DOS of Majorana fermions in the 2D case at $\alpha = 0.8$ and $\alpha = 0.9$ are shown in Figs. 2(e) and 2(f), respectively; the MC results are shown for the temperatures in the vicinity of the low-$T$ peak of the specific heat together with those at $T = 0$ and $T = \infty$. As shown in these figures, the low-energy behavior of the DOS is similar to that in the 3D Kitaev model: the boundary between gapless and gapped regions exists at $0.8 < \alpha_c(T = \infty) < 0.9$ in the high-$T$ limit also in the 2D case.

To quantify the $T$ dependence of the low-energy DOS, we introduce the integral $I_\Omega$ of the low-energy part of the DOS defined by $I_\Omega = \int_{\Omega} \langle D(\omega, \{ \eta_r \}) \rangle d\omega$ (the bracket denotes the thermal average). Figure 3 summarizes the values of $I_{\Omega=0.1}$, along with the specific heat $C_v$. The results clearly show that the DOS rapidly changes near $T_c$, where $C_v$ exhibits a sharp peak at $T_c$. As shown in Figs. 3(a) and 3(c), the low-energy weight of the DOS, $I_{\Omega=0.1}$, rapidly decreases near $T_c$ as $T$ increases, reflecting the opening of the gap in the spectra for $\alpha \lesssim \alpha_c(T = \infty)$ at higher $T$. On the other hand, in the case of $\alpha > \alpha_c(T = \infty)$, $I_{\Omega=0.1}$ rapidly increases in the vicinity of $T_c$, corresponding to the filling of the semimetallic dip, as shown in Figs. 3(e) and 3(g). Thus, the low-energy Majorana fermion states are significantly modified by the phase transition from the low-$T$ QSL to high-$T$ paramagnet. As shown in our previous study [19], the $Z_2$ fields $\eta_r$ are rapidly disordered near $T_c$, which is monitored by a rapid decrease of the average density of the local conserved quantity $W_p$ given by the product of $\eta_r$ on the shortest ten-site loop of the hyperhoneycomb lattice. Hence, our results indicate that the thermal fluctuations affect the low-energy Majorana states through the $Z_2$ variables. Interestingly, the effect appears in a contrasting way below and above the boundary $\alpha_c(T = \infty)$, which is different from the quantum critical point $\alpha_c(T = 0) = 0.75$.

5. Summary
In summary, we have investigated the temperature variation of the Majorana fermion state in the 3D Kitaev model on the hyperhoneycomb lattice by using the Monte Carlo simulation. We found that the density of states of Majorana fermions evolves in a characteristic way in the gapless quantum spin liquid region. There is a clear boundary for the finite-temperature behavior: the semimetallic Majorana fermion state develops an excitation gap in the region closer to the ground state phase boundary to the gapped region, whereas it is filled to be metallic in the other region. We showed that the evolution appears in the vicinity of the critical temperature for the spin liquid formation. Our results indicate that the low-energy spectra of Majorana fermions...
are significantly affected by thermal fluctuations in the $Z_2$ variables.

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