Topological Quantum Phase Transitions of Anisotropic Antiferromagnetic Kitaev Model Driven by Magnetic Field

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The evolution of quantum spin liquid states (QSL) of the anisotropic antiferromagnetic (AFM) Kitaev model with the [001] magnetic field by utilizing the finite-temperature Lanczos method (FTLM) is investigated. In this anisotropic Kitaev model with \( K_x = K_y \) and \( K_x + K_y + K_z = -3 \) K (\( K \) is the energy unit), due to the competition between anisotropy and magnetic field, the system emerges four exotic quantum phase transitions (QPTs) when \( K_z = -1.8 \) and \(-1.4 \) K, while only two QPTs when \( K_z = -0.6 \) K. At these magnetic-field tuning quantum phase transition points, the low-energy excitation spectrums appear level crossover, and the specific heat, magnetic susceptibility and Wilson ratio display anomalies; accordingly, the topological Chern number may also change. These results demonstrate that the anisotropic interacting Kitaev model with modulating magnetic field displays more rich phase diagrams, in comparison with the isotropic Kitaev model.

1. Introduction

The search and study of the highly entangled quantum spin liquid (QSL) state have been the current frontier of condensed matter physics, especially after Kitaev proposed an exactly solvable model on the two-dimensional (2D) honeycomb lattice. The Kitaev model exhibits the gapless or gapped QSL ground state related to the Majorana fermions resulting from spin fractionalization.\(^{11}\) In this model the three nearest-neighbor (NN) bond-depending interactions are Ising-type anisotropic terms with the remarkable frustration and fluctuations, and the gapless or gapped QSL state appears when they are all equal or asymmetric.\(^{11}\)

So far, the candidate “Kitaev materials” are mainly implemented in the “spin-orbit entangled \( j = 1/2 \) Mott insulators”, which are 4d\(^{5}\) and 5d\(^{5}\) transition-metal oxide Mott insulators in the presence of strong relativistic spin-orbit coupling and electronic correlations.\(^{2,3}\) The possible Kitaev materials are honeycomb iridium oxides Na\(_2\)IrO\(_3\)\(^{4}\) and Li\(_2\)IrO\(_3\)\(^{6}\) with Ir\(^{4+}\) (5d\(^{5}\)) valence and Ru-based material RuCl\(_3\)\(^{6}\) with Ru\(^{4+}\) (4d\(^{5}\)) valence. In these compounds, the exchange easy axis of main interactions depends on the spatial orientation of the exchange bond,\(^{7,8}\) providing prototypes of the Kitaev couplings.

The Kitaev-type exchange interactions \( K_x, K_y, \) and \( K_z \) are anisotropic in the NN \( X, Y, \) and \( Z \)-bonds in these realistic Kitaev materials. For example, the generalized spin Hamiltonian in Na\(_2\)IrO\(_3\) is anisotropic, that is, \( K_x = K_y > K_z \approx -30 \) meV. These parameters fitting from the ab initio electronic structure calculations\(^{9,11}\) are consistent with those from the inelastic neutron scattering\(^{12,13}\) and the resonant X-ray magnetic scattering\(^{14}\) experiments well. Meanwhile, applying a magnetic field may drive the isotropic Kitaev model from a gapless QSL, through a new \( U(1) \) gapless QSL, to a polarized ferromagnetic (FM) phases,\(^{15}\) or even an intermediate topological state with a high Chern number.\(^{16}\) In the present anisotropic Kitaev interactions, the external magnetic field brings about the competition with the anisotropic Kitaev coupling, which may lead to more rich quantum phases comparing the isotropic Kitaev case.

However, similar to the isotropic case, the anisotropic Kitaev model with the magnetic field is no longer exactly solvable. Up to date several theoretical approaches, such as the thermal pure quantum (TPQ) state method,\(^{15}\) the Majorana mean-field theory,\(^{17,18}\) and the variational Monte Carlo calculations,\(^{16,19}\) were proposed for the isotropic Kitaev model under external magnetic field.

To get deep insight into the anisotropic Kitaev model under the magnetic field modulation, following the ideas of the finite-temperature Lanczos method (FTLM)\(^{20–22}\) we develop the codes of FTLM to obtain enough excited-state information at finite temperature and obtain the numerical results of the isotropic Kitaev model same to those by the TPQ method.\(^{15}\)

In this paper, we perform the FTLM to gain an insight into the evolution of the QSL states in the anisotropic antiferromagnetic
(AFM) Kitaev model with increasing magnetic field, especially focusing on the critical points of the topological quantum phase transitions (QPT).

Based on the level crossover of low-energy excitation spectrums, the anomalies of the specific heat, magnetic susceptibility, and Wilson ratio, we find extra new QPTs accompanied with the change of Chern number, in contrast with the isotropic Kitaev model, suggesting that the anisotropic Kitaev coupling competes with magnetic field to lead to new quantum phases. Combining the Majorana mean-field theory, the field-dependent Kitaev model, we find ananiewioadnewQPTsaccompaniedwiththechangeofChernnumber, in contrast with the isotropic Kitaev model. The rest of the paper is organized as follows. In Section 2, we define the anisotropic Kitaev model with an external magnetic field and outline the FTLM theory. In Sections 3 and 4, we present the main results of the numerical calculations and discuss the essence and evolution of the QSL ground states. The conclusion of this paper is given in Section 5.

2. Model Hamiltonian and Theoretical Methods

In this paper, the 2D honeycomb lattice of the Kitaev model consists of two sublattices A and B, as illustrated in Figure 1a. Here we set that the Kitaev couplings in the NN X-, Y-, and Z-bonds satisfy the conditions $K_x = K_y$ and $K_x + K_y + K_z = -3K$ for the anisotropic Kitaev model. Throughout this paper, the parameter $K$ is taken as the unity of energy, and the minus sign of $-3K$ corresponds to the AFM coupling.

We start from the following Hamiltonian with the NN Kitaev couplings $K_x$, $K_y$, and $K_z$, and the magnetic field $H_z$

$$H = -K_x \sum_{(i,j)x} S_i^x S_j^x - K_y \sum_{(i,j)y} S_i^y S_j^y - K_z \sum_{(i,j)z} S_i^z S_j^z - g \mu_B H_z \sum_{i} S_i^z$$  \hspace{1cm} \text{(1)}

where $g$ is the Landé factor, $\mu_B$ is the Bohr magneton, and $H_z$ is the external magnetic field in the [001] direction of the spin frame. $(ij)_x$, $(ij)_y$, and $(ij)_z$ limit the sum over the sites on the NN $X$, $Y$, and $Z$ directions, respectively. $S_i^a$ $(a = x, y, z)$ represents the spin component at site $i$.

We investigate this Kitaev model by employing the FTLM theory\textsuperscript{[11]} on the 18-site regular hexagon cluster with the periodic boundary condition and the full point group symmetry of the honeycomb lattice, such as the sifxod rotational symmetry ($C_6$), as illustrated in Figure 1b. FTLM algorithm is a quite effective method for finding the energy eigenvalues of the Hamiltonian matrix with fewer arithmetic operations, high accuracy, and large space size.\textsuperscript{[20,21]} First, based on the three-term recurrence relations from a randomly selected basis vector, we can derive a set of orthogonal basis vectors and construct a tridiagonal matrix in the Krylov subspace which is far smaller than the complete Hilbert space. Diagonalizing a series of similar tridiagonal matrices, we approach the low energy eigenstates of the Hamiltonian gradually and acquire the finite-temperature static expectation values, such as the total energy $E$, magnetic specific heat $C_m$, magnetic entropy $S_m$, magnetic susceptibility $\chi$, and Wilson ratio $R_w$ defined as follows

$$E = \langle H \rangle, \quad C_m = \frac{\langle (H^2) \rangle - \langle H \rangle^2}{\nu^2}, \quad \chi = \frac{\langle \tilde{S}^2 \rangle - \langle \tilde{S} \rangle^2}{t}, \quad R_w = \frac{4\pi^2}{3} \frac{\chi}{C_m} \left( \frac{1}{\nu} \right), \quad S_m = \int_0^\nu \frac{C_m}{\nu} \, dt'$$ \hspace{1cm} \text{(2)}

Throughout this paper, we mainly present the numerical results for the $N = 18$-site cluster, since it contains the regular hexagon boundary with full point-group symmetry without losing the generality. In this study, we set the dimension of Krylov subspace to be $2^{11}$ for the 18-site cluster with $2^{18}$ basis vectors. The dimensionless magnetic field is defined as $h_{(x,y)k} = g \mu_B H_{(x,y)k}/K$, and the dimensionless temperature is set as $t = k_B T/K$, with the energy unit $K = 1.0$.

![Figure 1](image-url)
3. Numerical Results

In probing into the physical properties and evolution of the QSL states in the anisotropic AFM Kitaev model with the [001] magnetic field, we take the range of the Kitaev couplings $K_x$ along the line marked by red, blue, and green lines with arrows shown in Figure 2. For example, the realistic materials Na$_2$IrO$_3$,[9] CrI$_3$, and CrGeTe$_3$[10] approach the cases $K_x = -1.2, -1.7$, and $-0.96$, respectively. We choose six representative points $K_x = -1.8, -1.5, -1.4, -1.2, -1.0, -0.6$, and mainly present the numerical data of three typical points with $K_x = -1.8, -1.4, -0.6$, respectively.

Along this line, in the absence of the external magnetic field, the ground state of the Kitaev model experiences a gapped QSL for $|K_x| > 1.5$, and two different gapless QSLs for $1.0 < |K_x| \leq 1.5$ and for $0.0 < |K_x| < 1.0$, as shown in the green, blue, and red segments of Figure 2; and the ground state at $|K_x| = 1.0$ is the gapless QSL with the $C_6$ rotational symmetry.[11] The three separated regions in the constraint line can represent all three different Kitaev QSLs. If one lifts this constraint, the results still fall into our present framework.

3.1. Low-Energy Excitation Spectrum

Since the level crossover of the low-energy excitation spectra could identify the QPT points,[12] we first present the magnetic field dependences of low-energy excitation spectrums $(E - E_{CS})$ in the AFM anisotropic Kitaev model for different Kitaev couplings $K_x = -1.8, -1.4, -0.6$, respectively, as shown in Figure 3a–c; here $E_{CS}$ is the energy eigenvalue of the ground state.

At $|K_x| = 1.8$ in Figure 3a, when the magnetic field increases from null, the energy degeneracy of the first and second excited states is removed at $h_{13}$, as seen in the zoom image of Figure 3a. With the further increasing field, a level crossover of the second and third excited states happens at $h_{13}$, as also shown in another zoom image of Figure 3a.

When $h_{1} > h_{13}$, we observe another two level crossover points of the first excited state and ground state at $h_{13}$ and $h_{14}$, respectively. At $h_{13}$ and $h_{14}$, one can see that the spin gaps close, similar to the behavior of the isotropic Kitaev model under magnetic field.[13] When $h_{1} > h_{14}$, the energies of excited states increase nearly linearly with the opening of a new spin gap.

When $|K_x| = 1.4$, similar to the $|K_x| = 1.8$ case, with the magnetic field increasing, the anisotropic Kitaev system also undergoes four QPT points at the critical magnetic fields $h_{11}, h_{12}, h_{13}$, and $h_{14}$, respectively, as seen in Figure 3b. Interestingly, in contrast to the system with $|K_x| = 1.8$, the phase boundaries $h_{11}$-$h_{14}$ shift to low fields with decreasing Kitaev coupling strength $|K_x|$. Moreover, when $|K_x| = 0.6$, only two level crossover points occur at $h_{13}$ and $h_{14}$, respectively, as shown in Figure 3c.

One may question the stability of these QPT critical points when extending to infinite systems. Based on the low-energy spectrums, we display the finite-size extrapolation of the critical magnetic fields $h_{11}, h_{12}, h_{13}$, and $h_{14}$ of the anisotropic Kitaev model for different Kitaev couplings $K_x = -1.8$ and $-1.4$, respectively, with the 8-, 12-, 16-, 18-, and 24-site clusters. The numerical results are shown in Figure 4. One can see that the four QPT critical fields $h_{11}, h_{12}, h_{13}$, and $h_{14}$ approach finite values when the system-size $N$ becomes large enough, suggesting the robustness of these QPT critical points at $h_{11} - h_{14}$ and the finite-size effect does not qualitatively change our conclusion. Thus, the numerical results we present here for the 18-site cluster with the regular hexagon boundary and full point-group symmetry are quantitative reliability.

3.2. Magnetic Specific Heat

In order to investigate the evolution of the anisotropic Kitaev QSL state with magnetic field thoroughly, the temperature versus magnetic-field phase diagrams based on the magnetic specific heats $C_m$ for different Kitaev couplings $K_x = -1.8, -1.4, -0.6$ have illustrated in Figure 5a–c, respectively.

At $|K_x| = 1.8$ shown in Figure 5a, we find that with the magnetic field increasing, four feature points are observed at low temperature, which correspond to the critical magnetic fields $h_{13} - h_{14}$ obtained in last subsection and in Figure 3a.

One notices that at the critical magnetic fields $h_{13}, h_{13}$, and $h_{14}$, the magnetic specific heats display three peaks when $h_i$ increases, respectively, demonstrating the features of the QPTs. These critical fields are robust with the temperature increasing when $t < 0.01$. Whereas, at the critical magnetic field $h_{13}$, the magnetic specific heats display a dip, showing that $h_{13}$ has features different from another three critical fields.

Same to the critical fields of the spin excitation spectrums, when $|K_x| = 1.4$, with the magnetic field increasing, the anisotropic Kitaev system also goes through four QPT points at the critical magnetic fields $h_{11}, h_{12}, h_{13}$, and $h_{14}$, respectively, as seen in Figure 5b. As expected, the phase boundaries $h_{11} - h_{14}$ move toward low fields with the decreasing Kitaev coupling strength $|K_x|$. When $|K_x| = 0.6$, there are only two
Figure 3. The low-energy excitation spectra ($E - E_{GS}$) of anisotropic Kitaev model as functions of dimensionless magnetic field $h_z$ for different Kitaev couplings $K_Z = -1.8$ (a), $-1.4$ (b), and $-0.6$ (c), respectively. The energy unit is $K, N = 18$.

Figure 4. Finite-size scaling results of the critical magnetic fields $h_{c1}$, $h_{c2}$, $h_{c3}$, and $h_{c4}$ of the anisotropic AFM Kitaev model under the [001] magnetic field for different Kitaev couplings $K_Z = -1.8$ (a), $-1.4$ (b), respectively, with the 8-, 12-, 16-, 18-, and 24-site clusters.

phase transition points at $h_{c3}$ and $h_{c4}$, respectively, as shown in Figure 5c.

Moreover, we also plot the magnetic specific heats as functions of the temperature for several typical quantum phases in the different regions separated by the critical magnetic fields, as shown in Figure 6a–c. When $|K_Z| = 1.8$, as seen in Figure 6a, we plot the $t$-dependent specific heat curves at five typical fields $h_z = 0, 0.64, 0.76, 0.84, and 1.0$, which could represent five different quantum phases among $0 < h_z < 1$. At $h_z = 0$, $C_m$ displays two peaks, that is, low-temperature (low-$T$) and high-temperature (high-$T$) peaks at the critical temperatures $t_{c1}$ and $t_{c2}$, associated with the local and itinerant Majorana fermion modes,[11] and the spectral weight of the high-$T$ peak is greater than that of the low-$T$ peak. When $h_z = 0.64$, the spectral weight of the low-$T$ peak in magnetic specific heat is significantly greater than the high-$T$ one, which reveals a different quantum phase from the one at $h_z = 0$. Then, at $h_z = 0.76$, an intermediate peak appears at a feature temperature $t_{c3}$ between the low-$T$ and high-$T$ peaks, and it only exists in the present anisotropic Kitaev model, which may result from the interaction between the local and itinerant Majorana fermion modes in magnetic field; thus it implies a new quantum phase. When $h_z = 0.84$, in contrast to the case $h_z = 0.76$, the spectral weights of the low-$T$ and high-$T$ peaks transfer to the intermediate peak, thus the intermediate peak raises. Finally, at $h_z = 1.0$, the low-$T$ peak merges into the intermediate peak, and the high-$T$ peak tends to merge to them with the disappearance of the local and itinerant Majorana fermion modes.

When $|K_Z| = 1.4$, as seen in Figure 6b, we also plot $C_m - t$ curves at five typical fields $h_z = 0, 0.36, 0.5, 0.62, and 1.0$. The behavior of the magnetic specific heat of each quantum phase as the function of temperature is similar to the case of $|K_Z| = 1.8$. When $|K_Z| = 0.6$, we choose three typical fields $h_z = 0, 0.3, and 1.0$ in the three regions separated by $h_{c3}$ and $h_{c4}$ to plot the $C_m - t$ curves, as seen in Figure 6c. Accordingly, from the behaviors of the magnetic specific heat we give rise to two QPT critical points at $h_{c3}$ and $h_{c4}$ and three quantum phases.

These results demonstrate that in the anisotropic Kitaev QSL, the thermodynamic behaviors of these quantum phases defined by the critical magnetic fields $h_{c3}$ and $h_{c4}$ for all $|K_Z|$, as well as $h_{c3}$ and $h_{c4}$ for $|K_Z| = 1.4 and 1.8$, are different, showing that these quantum phases are essentially different. As we show later, the four QPTs undergo successively from the gapped QSL to gapless
Figure 5. The phase diagrams of the anisotropic Kitaev systems based on the magnetic specific heats $C_m$ with the dimensionless magnetic field $h_z$ and temperature $t$ for different Kitaev couplings $K_Z = -1.8$ (a), $-1.4$ (b), and $-0.6$ (c), respectively.

The QSL-to-another gapless QSL, to the $U(1)$ gapless QSL, and to the polarized FM phases for $|K_Z| = 1.4$ and 1.8; or from the gapless QSL to the $U(1)$ gapless QSL, and to the polarized FM phases for $|K_Z| = 0.6$, similar to the isotropic case.

3.3. Spin Susceptibility

To further confirm the evolution of ground states of the anisotropic AFM Kitaev model, the temperature versus magnetic-field phase diagrams based on the products of the magnetic susceptibilities and temperature $\chi \cdot t$ for different Kitaev couplings $K_Z = -1.8$, $-1.4$, and $-0.6$ have been described in Figure 7a–c.

When $|K_Z| = 1.8$ and $t < 0.01$, with the magnetic field increasing, the critical magnetic fields $h_{c1}$, $h_{c3}$, and $h_{c4}$ indicated in the $t - h_z$ phase diagram of $\chi \cdot t$ shown in Figure 7a are definite, as discussed above. In contrast, when $|K_Z| = 1.4$, three QPT points at the critical magnetic fields $h_{c1}$, $h_{c3}$, and $h_{c4}$ in the anisotropic Kitaev system are also clear, as seen in Figure 7b. When $|K_Z| = 0.6$, the two phase transition points at $h_{c3}$ and $h_{c4}$ are definite, as shown in Figure 7c.

To further investigate the features of different quantum phases, we also plot the temperature dependences of the magnetic susceptibilities for the typical quantum phases as mentioned in the last subsection. Figure 8 shows the variations of magnetic susceptibility times temperature, $\chi \cdot t$, on increasing $t$; these curves display almost constants when $t < t_{c1}$ and converge to constants when $t \gg t_{c2}$. From Figure 8a–c, we can see that these $\chi \cdot t$ curves of different quantum phases exhibit significantly different trends in the intermediate temperature range between $t_{c1}$ and $t_{c2}$, demonstrating the advantage of our FTLM for distinguishing the finite-temperature properties of different QSL phases. In the temperature range between $t_{c1}$ and $t_{c2}$, when $|K_Z| = 1.8$, as seen in Figure 8a, the $\chi \cdot t$ curves show the kinks, twists, or dips, depending on $h_z = 0, 0.64, 0.76$, and 0.84 in different QSL phases; when $h_z = 1.0$, $\chi \cdot t$ exhibits a remarkable dip around $t_{c3}$, implying the presence of magnons in the polarized FM phase. When $|K_Z| = 1.4$ and 0.6, as shown in Figure 8b,c, the $\chi \cdot t$ curves of the different quantum phases separated by $h_{c1} - h_{c4}$ are also distinguishable, similar to the counterparts at $|K_Z| = 1.8$.

The inverses of the magnetic susceptibilities are also shown in the insets in Figure 8a–c. In the high-$T$ region, all of the susceptibilities display a linear relationship $1/\chi = (T + \Theta_W)/C_A$ approximately, where $\Theta_W$ is the Curie-Weiss temperature and $C_A$ is a constant, following the Curie-Weiss law of the AFM magnets.

Figure 6. Temperature dependences of the magnetic specific heats $C_m$ with the dimensionless magnetic fields $h_z = 0.0 - 1.0$ for $K_Z = -1.8$ (a), $-1.4$ (b), and $-0.6$ (c), respectively.
very well. Interestingly, all of the Curie–Weiss temperatures are approximately equal to 0.25 for $|K_Z| = -1.8$, -1.4, and -0.6, seeming to stem from the constant condition $K_X + K_Y + K_Z = -3.0$. In the low-$T$ region with $t < 0.3$, all the curves of inverses of magnetic susceptibilities bend anomalously and pass through the zero point, which violates the Curie–Weiss law and exhibits the features of the gapped or gapless QSL. On the whole, the field-driven QPT features in the spinsusceptibility are not so definite in comparison with that in magnetic specific heat.

3.4. Wilson Ratio

In order to further identify the QPT critical points of the anisotropic AFM Kitaev model, we also plot the temperature versus magnetic-field phase diagrams based on the dimensionless Wilson ratios $R_W$. $R_W$ can quantify the spin correlations and fluctuations. For different Kitaev couplings $K_Z = -1.8$, -1.4, and -0.6, the phase diagrams are shown in Figure 9a–c, respectively. From these phase diagrams, we can see that all the Wilson ratios are larger than one, that is, $R_W > 1$, indicating the strongly correlated features of the QSL ground states with the enhanced spin fluctuations.

When $|K_Z| = 1.8$, with the increase of magnetic field, three remarkable feature points at $h_{11}$, $h_{13}$, and $h_{14}$ are marked in Figure 9a. These three critical magnetic fields lie in the low-$R_W$ regions since the low-$T$ specific heats reach the maximum values. As a contrast, $h_{12}$ falls in the high-$R_W$ region. A similar situation also occurs when $|K_Z| = 1.4$, with the increase of the magnetic field, and the four QPT points at the critical magnetic fields $h_{11}$, $h_{13}$, and $h_{14}$ are shown in Figure 9b. When $|K_Z| = 0.6$, the two phase transition points at $h_{3}$ and $h_{4}$ are displayed in Figure 9c. From Equation (2), we know that the Wilson ratio is proportional to spin susceptibility times temperature $\chi \cdot t$ over specific heat $C_m$. From Figure 9, most of the QPT features of the critical points are clear in the phase diagrams. Due to the large $\chi \cdot t$, that is, spin fluctuations $\langle \vec{S}^2 \rangle - \langle \vec{S} \rangle^2$ from the boundary effect of the finite-size systems, the Wilson ratio is large.

3.5. Magnetic Moment Under the Magnetic Field

We also present the magnetic moments of sublattices $m = \langle S_z \rangle$ and their derivatives with respect to the magnetic field, $dm/dh_z$, as functions of magnetic field $h_z$ at zero temperature, which are illustrated in Figure 10a,b. The magnetic moments have been

Figure 7. The phase diagrams of the anisotropic Kitaev systems based on the magnetic susceptibilities times temperature $\chi \cdot t$ with the dimensionless magnetic field $h_z$ and temperature $t$ for different Kitaev couplings $K_Z = -1.8$ (a), -1.4 (b), and -0.6 (c), respectively.

Figure 8. Temperature dependences of the products of the magnetic susceptibilities and temperature $\chi \cdot t$ and the inverse $1/\chi$ (Inset) at different magnetic fields for $K_Z = -1.8$ (a), -1.4 (b), and -0.6 (c), respectively.
rising up all the way with the increasing magnetic field because of magnetic polarization, among which we can find a few of turning points in these \( m - h_z \) curves in Figure 10a. Particularly it displays a small discontinuity at \( h_{c4} \), seeming to be a first-order QPT. More information could be found in the peaks of the zero-temperature susceptibility \( \frac{d m}{d h_z} - h_z \) curves in Figure 10b. The positions of these peaks almost one-to-one correspond to three distinct critical magnetic fields \( h_{c1} \), \( h_{c3} \), and \( h_{c4} \) for \( |K_Z| = 1.8 \) and 1.4, and to two critical fields \( h_{c3} \) and \( h_{c4} \) for \( |K_Z| = 0.6 \), respectively. Also, one finds a small shoulder for \( |K_Z| = 1.8 \) and a small peak for \( |K_Z| = 1.4 \) at \( h_{c2} \), which may arise that it comes from the high-order level crossover in the low-energy excitations.

Note that the zero-temperature magnetic susceptibility \( \frac{d m}{d h_z} \) should be quantitatively consistent with that obtained from the fluctuation-dissipation theorem in Equation (2) in zero field limit in infinite system. Whereas, in the present finite-size clusters, due to the boundary effect, these two definitions display slight difference quantitatively in the positions of these QPT critical points. When \( h_z > h_{c4} \), we still observe an extra peak in \( \frac{d m}{d h_z} \) for \( |K_Z| = 1.4 \) or \( |K_Z| = 0.6 \). But in this case, the system has already entered the spin-polarized FM phase, this extra peak beyond \( h_{c4} \) might come from the finite-size effect.

We also plot the dependences of the critical magnetic fields \( h_{c1}, h_{c2}, h_{c3}, \) and \( h_{c4} \) on the Kitaev coupling strength \( |K_Z| \), as shown in Figure 10c. All these critical magnetic fields go up with the Kitaev coupling increasing. This arises from the fact that the total spin gap increases with the lift of \( |K_Z| \).

4. Chern Numbers and Discussions

The competition of anisotropic Kitaev coupling and applied magnetic field resulting in at most five quantum phases could also seen in the Majorana fermion mean-field theory.\textsuperscript{[17,18]} For example, within the Majorana mean-field approximation, we find that for \( K_Z = -1.8 \), there are four QPT critical points at \( h_{c1,2,3,4} = 0.51, 0.73, 0.87, \) and 0.96, respectively, as shown in Figure 11. From which one finds that the spectral features of these five phases are distinctly different, further confirming the presence of four QPT critical points. The spinon energy dispersions in other parameter cases could be found in the Supporting Information.\textsuperscript{[28]}

Since the Kitaev model possesses topological transitions, we further explore the evolution of the topological properties of the anisotropic Kitaev model with magnetic field, especially the topological QPTs. With the help of the Majorana mean-field method, we could discuss the topological order with the
Figure 11. The zero-temperature spinon spectrums of the anisotropic Kitaev systems as functions of the magnetic field $h_z$ for five typical phases at $h_z=0$, $0.58$, $0.82$, $1.2$, and $h_z=0.73$, respectively.

Figure 12. The Chern numbers $C_n$ of the anisotropic Kitaev systems as functions of the magnetic field $h_z$ at $t=0$ for different Kitaev couplings $K_Z=−1.8$ (a), $−1.4$ (b), and $−0.6$ (c), respectively. Here the phase boundaries are determined through the spinon dispersions by the Majorana fermion mean-field method.

Continuous energy dispersions over the whole first Brillouin zone, and thus calculate the topological Chern numbers with the Wilson loop. We display the magnetic field dependences of the Chern numbers $C_n$ at zero temperature, as shown in Figure 12a–c.

When $|K_Z|=1.8$, from Figure 12a, we can discover that the turning points of the Chern number correspond to the three critical magnetic fields one to one, which confirm the topological QPTs at $h_{c1}$, $h_{c2}$, and $h_{c3}$. Specifically, at $h_{c1}$, the Chern number goes from 0 to 1 with the transition from the original gapped QSL to a gapless QSL. At $h_{c3}$, it changes from 1 to $−1$ with the transition from another gapless QSL to a new $U(1)$ gapless QSL.\(^{[15]}\) At $h_{c2}$, it turns from $−1$ to 0 with the transition from the $U(1)$ gapless QSL to the polarized FM phase. However, when $h_z$ passes through $h_{c1}$, the Chern number keeps 1 with the transition from the gapless QSL to another gapless QSL, and at $h_{c2}$, the system enters into a gapless QSL with six Weyl points at $K$ and $K'$, similar to the isotropic case. These indicate that at $h_{c2}$ the topological order does not change, implying that $h_{c2}$ is not a topological QPT point, but a trivial one.

When $|K_Z|=1.4$, as seen in Figure 12b, we observe that the Chern number turns from 1 to $−1$, and finally to 0; the two
topological QPT points occur at $h_3$ and $h_4$, respectively, and the QPTs at $h_3$ and $h_4$ are topologically trivial. From the spinon spectrums obtained by the mean-field method for $|K_z| = 1.4$, we find that through the critical magnetic fields $h_2$, $h_3$, and $h_4$, the system transits from the original gapless QSL to another gapless QSL, to the $U(1)$ gapless QSL, and finally to the polarized FM phase. And at $h_3$, the system also goes into a gapless QSL with six Weyl points at $K$ and $K'$. Meanwhile, we do not observe the gap opening again in the spinon spectrum at $h_3$ for $|K_z| = 1.4$ in the Majorana mean-field approximation, different from the $|K_z| = 1.8$ case. When $|K_z| = 0.6$, the two QPT points at $h_3$ and $h_4$ are also topological with the variations of the Chern number, from 1 to $-1$, and finally to 0, as seen in Figure 12c. Accordingly, the system transits from the original gapless QSL to the new $U(1)$ gapless QSL, and to the polarized FM phase. Hence, most of the field-driven phase transitions in the present anisotropic Kitaev model are topological QPTs.

From the preceding study, one can see that different from the isotropic Kitaev model under magnetic field,[17,18] the anisotropic Kitaev coupling competing with applied magnetic field results in more rich quantum phases and QPTs. Notice that the positions of the QPT critical points obtained from the level crossovers in the present FTLM approach are slightly different from those obtained from the Majorana mean-field approach, partially arising from the finite-size effect in the former, also partially from the underestimate of the spin fluctuations in the latter. Nevertheless, these critical fields lift up monotonically with the increasing Kitaev coupling $|K_z|$, which originates from the fact that the energy gap of the system increases with the anisotropy.

5. Conclusion

In summary, by employing the FTLM and combining the Majorana mean-field method, we study the nature and evolution of the QSL ground states in the anisotropic AFM Kitaev model with the [001] magnetic field. In this Kitaev model with $K_x = K_y$, $K_y + K_x + K_z = -3$ K, compared with the isotropic Kitaev model, one finds that magnetic field may drive the appearance of new quantum phases, partially with the variation of the topological Chern number. Because of the competition between anisotropic term $K_x$ and magnetic field $h_z$, the system exhibits three topological and one trivial QPTs when $K_z = -1.8$ K, and two topological and two trivial QPTs when $K_z = -1.4$ K; whereas the system with $K_z = -0.6$ K displays only two topological QPTs, similar to the isotropic case.

Our results have shown that the anisotropic Kitaev coupling competing with magnetic field leads to an intriguing rich phase diagram, and applied magnetic field could modulate and regulate the topologically different gapless and gapped QSL states, paving a way for the realization of quantum computations in realistic Kitaev materials.[1,25,30] These results demonstrate that anisotropic Kitaev models may exhibit more interesting physics, and the nature of these new QSL phases deserves further investigation.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

anisotropic antiferromagnetic Kitaev model, magnetic field effects, quantum spin liquids, topological quantum phase transitions

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