Pressure-Induced Gapless Quantum Spin Liquids on the Honeycomb Lattice

Jucai Wang\textsuperscript{1} and Zheng-Xin Liu\textsuperscript{1, 2, *}

\textsuperscript{1}Department of Physics, Renmin University of China, Beijing 100872, China
\textsuperscript{2}Tsung-Dao Lee Institute \& School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

(Dated: December 30, 2019)

Exerting high pressure is a practical way to tune the spin-spin interactions in Mott insulators and can be applied to prepare for quantum spin liquid (QSL) ground states. We illustrate this possibility by studying a realistic spin model which contains the Kitaev and $\Gamma$-interactions through extensive analytic and numerical calculations. As a consequence of the external pressure, the interaction intensities in our model are spatially anisotropic. While the anisotropic pure Kitaev model contains only two phases, the presence of non-Kitaev interactions results in a much richer phase diagram which contains several new gapless $Z_2$ QSL phases. These QSLs are characterized by a certain number of cones in the low-energy excitation spectrum, which can be reflected in the dynamic structure factors. We provide a complete classification of nodal $Z_2$ QSLs. Furthermore, a small out-of-plane magnetic field gaps out the cones in these gapless QSLs and results in Abelian or non-Abelian chiral spin liquids (CSLs), all belonging to the Kitaev’s 16-fold classification. From the dynamic structure factor and the thermal Hall conductance of the field-induced CSLs, all the QSLs can be experimentally distinguished. Our results are instructive to search for QSL phases in related materials.

\section{I. INTRODUCTION}

Quantum Spin Liquids (QSLs) are exotic phases of matter exhibiting no conventional long-range order down to the lowest temperatures. Resulting from strong quantum fluctuations, QSLs are characterized by long-range entanglement and the existence of intrinsic fractional excitations called anyons. The low energy physics of QSLs is beyond the Ginzburg-Landau-\Gamma-\textsuperscript{2,3} paradigm\textsuperscript{1} and is instead captured by topological quantum field theory or tensor category theory\textsuperscript{23}. QSL was proposed as the mother state of high-temperature superconductors since the spins in a QSL pair up with each other and form singlets\textsuperscript{3}. On the other hand, the anyons in certain gapped QSLs obey non-Abelian braiding statistics and have potential applications in topological quantum computations. However, since most spin systems in two or higher dimensions exhibit long-range magnetic order at zero temperature, it is challenging to search for a true QSL ground state. In 2006, Kitaev proposed a honeycomb lattice spin model (with discrete symmetries)\textsuperscript{3} whose ground states are exactly solvable QSLs with either gapless or gapped excitation spectra. In a suitable magnetic field, the gapless Kitaev spin liquid (KSL) is turned into a gapped CSL that supports non-Abelian anyon excitations. It was further shown that this field-induced CSL belongs to a family of chiral spin liquids (CSLs), all belonging to the Kitaev’s 16-fold classification. From the dynamic structure factor and the thermal Hall conductance of the field-induced CSLs, all the QSLs can be experimentally distinguished. Our results are instructive to search for QSL phases in related materials.

The KSL attracts lots of research interest. To realize the Kitaev model, a series of spin-orbit entangled candidate materials have been proposed and profoundly studied\textsuperscript{5,6}, such as $\alpha$-RuCl\textsubscript{3}\textsuperscript{7–11}, $\alpha$-Li\textsubscript{2}IrO\textsubscript{3}\textsuperscript{12}, Na\textsubscript{2}IrO\textsubscript{3}\textsuperscript{13–16}, Cu\textsubscript{2}IrO\textsubscript{3}\textsuperscript{17}, H\textsubscript{3}LiIr\textsubscript{2}O\textsubscript{6}\textsuperscript{18} and Na\textsubscript{2}Co\textsubscript{2}TeO\textsubscript{6}\textsuperscript{19–21}. Among these compounds, H\textsubscript{3}LiIr\textsubscript{2}O\textsubscript{6} is magnetically disordered at very low temperatures which may be caused by the dislocations of the Hydrogen atoms. However, all the other materials manifest magnetic long-range order at low temperatures, indicating the existence of non-Kitaev interactions, including the Heisenberg term, the $\Gamma$-term and the $\Gamma'$-term\textsuperscript{22}. Although the experimental realization of the Kitaev spin liquid ground state remains to be an open issue, the excitation spectra above the ordering temperature observed by inelastic neutron scattering\textsuperscript{23,24}, Raman scatterings\textsuperscript{25,26} and longitudinal thermal conductivity\textsuperscript{27} exhibit anomalous features, indicating that these materials are proximate to a quantum spin liquid phase.

Interestingly, the low-temperature magnetic order in some Kitaev materials can be suppressed under special situations. For instance, an in-plane magnetic field can lower the ordering temperature. Above a critical field strength, the materials (such as $\alpha$-RuCl\textsubscript{3}) can be driven into a disordered phase at very low temperatures. The field-induced disordered phase contains strong low-energy spin fluctuations, which behaves like a quantum spin liquid\textsuperscript{38–32}. In a slightly canted magnetic field, a half-quantized thermal Hall conductance was observed and was thought to be the smoking gun of the non-Abelian Kitaev spin liquid\textsuperscript{30}. On the other hand, external pressure can also induce a magnetically disordered phase\textsuperscript{33}. For instance, in $\alpha$-RuCl\textsubscript{3} or $\alpha$-Li\textsubscript{2}IrO\textsubscript{3}, high pressure drives the system into a dimer phase accompanied by a structural phase transition\textsuperscript{34–38}. In contrast to the strong dimer bonds, (anisotropic) pressure can also distort the lattice such that the strong bonds form zigzag-chains, as observed in Li\textsubscript{2}RhO\textsubscript{3}\textsuperscript{39}.

In the following, we illustrate that exerting high pressure is a plausible way to realize QSLs, assuming that the effect

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Intensity of interactions with and without pressure. (A) No pressure, $a$ and $b$ are lattice constants; (B) The pressure-induced dimer-type anisotropy; (C) The pressure-induced zigzag chain-type anisotropy.}
\end{figure}
of an uniaxial pressure is causing anisotropy in the intensities of spin-spin interactions and lowering the symmetry of the system.

We study a honeycomb spin model with Kitaev interactions and off-diagonal $\Gamma$-interactions [see Eq.(1)], which are suggested to be important interactions in Kitaev materials. To simplify the effect of anisotropic pressure, we assume that the strength of the interactions is dependent on bond-directions, where the strong bonds either form dimers [Fig.1(B)] or form zigzag-chains [Fig.1(C)]. From variational Monte Carlo (VMC) calculations by using Gutzwiller projected states as trial wave functions (see Appendix A), we obtain the phase diagrams as shown in Fig.2 and Fig.3. In the former case, the magnetic orders are strongly suppressed such that at intermediate anisotropy most phases are QSLs. In the latter case, the ordered phases are much more robust while two QSL phases are generated by very large anisotropy. Most of the Kitaev materials are known to have $\Gamma$-interactions. The anisotropy may be caused by, for instance, uniaxial pressure. In the following, we will discuss two different situations according to the spatial dependence.

The anisotropy is parameterized by $\delta_d$. The diagram contains three ordered phases (the FM, the IS and the Zigzag phase) and several QSLs (the KSL, the PKSL, the $Z_2$ SL, and the gSL-1–VI). The dash-dot lines represent second-order phase transitions, and the black thin lines represent first-order phase transitions. The insert is a cartoon picture of the distorted honeycomb lattice under uniaxial pressure. $\sigma_m$ symbols the mirror reflection, $C_2$ represents a two-fold rotation along $z$-bond direction, and $T_1, T_2$ are the generators of the translation group.

In the first case, we assume that the external uniaxial pressure only increases the (relative) strength of the interactions on the $z$-bonds such that the strong bonds form disconnected dimers, see Fig.1(B) for an illustration. A possible physical origin of the strong $z$-bonds is the shortening of the length of the $z$-bonds. For simplicity, we note $K_z = K$, $\Gamma_z = \Gamma$ and use only one variable $0 \leq \delta_d \leq 1$ to parameterize the degree of dimerization in the anisotropy interactions, namely, $K_x = K_y = (1 - \delta_d)K$ and $\Gamma_x = \Gamma_y = (1 - \delta_d)\Gamma$.

In the second case, we assume that the uniaxial pressure only decreases the (relative) strength of the interactions on the $z$-bonds such that the strong bonds form zigzag chains, as illustrated in Fig.1(C). A possible physical origin of the weak $z$-bond is the sharpening of angles between the spins and the intermediate atoms, which weakens the super-exchange interactions. For simplicity, we will note $K_z = K_y = K$, $\Gamma_x = \Gamma_y = \Gamma$ and use one parameter $0 \leq \delta_1 \leq 1$ to denote the degree of zigzag-chain type anisotropy such that $K_z = (1 - \delta_1)K$, $\Gamma_x = (1 - \delta_1)\Gamma$.

In both cases, for general values of $\delta_d$ or $\delta_2$, the model (1) has a $G = \mathbb{Z}_2 \times Z^2$ magnetic point group symmetry, where $Z^2 = \{E, T\}$ is the time-reversal group and $\mathbb{Z}_2 = \{E, P, C_2, \sigma_m\}$ ($P$ is the spatial inversion) is different from the usual point group $\mathbb{Z}_2$ since here $C_2$ stands for the two-fold rotation along the $z$-bonds and $\sigma_m$ is the mirror reflection whose mirror plane is perpendicular to the $C_2$ axis (see the insets of Fig.2 & Fig.3 for illustration).
constructing the mean-field Hamiltonian, we have followed the projected mean-field ground states as trial wave functions. In the model can be calculated from VMC using the Gutzwiller parameterized by strong interacting bonds form zigzag-chains and the anisotropy is pressure where the strong bonds form zigzag chains. A cartoon picture of the distorted honeycomb lattice under external (are gapless chains marked by a thick red line in one-dimension limit phase and the zigzag ordered phase are much more robust against the transition from the KSL to the gapped 2QSL, where three ordered phases, namely the ferromagnetic (FM) phase, the incommensurate spiral (IS) phase and the zigzag phase] plus two QSL phase [namely the KSL and the proximate Kitaev spin liquid (PKSL)] were found. Interestingly, the ordered phases are completely suppressed at anisotropy $\delta_d \sim 0.15$, and several new gapless QSL phases, labeled as gSL-I–VI, are generated. When the anisotropy is extremely large, the system enters a gapped dimer phase (the critical value of $\delta_d$ is greater than 0.5). Except for the gapped $Z_2$ spin liquid phase at very small $\Gamma$, all the other QSLs are gapless.

The observation of the series of gapless spin liquid phases with different numbers of cones is the central result of the present work. The phase showing up at $0.04 < \delta_d < 0.1$ above the PKSL and is labeled as gSL-I, whose spinon dispersion contains 10 Majorana cones. With the increasing $\delta_d$ (with $\Gamma < 0.6$), the system undergoes successive continuous transitions to other gapless QSLs, namely the gSL-II and gSL-III, which contain 6 Majorana cones and 2 Majorana cones respectively. At larger $\Gamma$ (with $\Gamma > 0.6$), three more gapless QSLs, namely, the gSL-IV, the gSL-V and the gSL-VI are found in sequence with the increasing of $\delta_d$ between the zigzag phase (at $\delta_d < 0.15$) and the dimer phase (at $\delta_d > 0.5$). The three QSLs contain 14, 10, 2 cones, respectively. Later we will discuss the significance of the number of Majorana cones.

The phase transitions from the magnetically ordered states to the QSLs are all of first order. The transition from the gSL-VI to the dimer phase is also first-order. Interestingly, the transition from gSL-III to the dimer phase is continuous at $\Gamma < 0.16$ but becomes first-order at $0.16 < \Gamma < 0.6$. The phase transitions between different QSLs are either first-order or continuous. The first-order phase transitions are characterized by discontinuous jumps of some variational parameters, and the number of Majorana cones changes suddenly. For example, the transition from the PKSL to the gSL-I and the transition from the KSL to the gSL-III are both accompanied by a sudden growth of $\phi_7$, the transition from the gSL-III to the gSL-V or to the gSL-VI is accompanied by a sudden growth of $\rho_0$, and the transition from the gSL-VII to the gSL-VIII is accompanied by the sudden growth of $\phi_7$ and $\phi_7^\ast$. The continuous transitions between QSLs, marked as red dash-dot lines in Fig. 2, are characterized by the smooth changing of the variational parameters and the merging (and pairwise disappearing) of the Majorana cones. A typical example is the transition from the KSL to the gapped $Z_2$ QSL, where the two cones merge and a gap opens. In the following continuous transitions, 4 of the cones merge in pairs and disappear simultaneously: the one from the gSL-I to the gSL-II, the one from the gSL-II to the gSL-III, and the one from the gSL-IV to the gSL-V. The transition from the gSL-V to the gSL-VI is special since 8 cones merge in pairs and disappear simultaneously at the critical point.

Now we discuss the second case (with $\delta_{zz}$ anisotropy). The phase diagram is shown in Fig. 3, which is relatively simpler. At $\Gamma = 0$, there is only one phase — the KSL. This result agrees with the exact solution. Different from the case with $\delta_{zz}$ anisotropy, the ordered phases (except for the IS phase) are much more robust against the $\delta_{zz}$ anisotropy. The FM phase locates at the vicinity of $\Gamma = 0.2$ and extends throughout the parameter region $0 \leq \delta_{zz} < 1$, its width increases with $\delta_{zz}$. At larger $\Gamma$, the PKSL phase ($0.25 < \Gamma < 0.45$) and the IS phase ($0.45 < \Gamma < 0.75$) appear in sequence at small $\delta_{zz}$.
but both are quickly suppressed at $\delta_{zz} \sim 0.05$. Above the PKSL and the IS phases, there is an overwhelming zigzag-ordered phase, which extends from $\Gamma \sim 0.25$ to the large $\Gamma$ limit below a critical $\delta_{zz}$. When the zigzag order is suppressed above $\delta_{zz} \sim 0.5$, two gapless QSLs show up in sequence, which are labeled as gSL-VII and gSL-VIII respectively and are separated by a first-order phase transition. The gSL-VII contains 16 Majorana cones in the spinon excitation spectrum while the gSL-VIII has 8. Owing to the strong $\delta_{zz}$ anisotropy, the dispersion of the spinon excitations in these two QSLs are fairly flat along the zigzag-chain direction.

In the $\delta_{zz} = 1$ limit, the system becomes decoupled zigzag chains. The system is solvable at $\Gamma = 0$, where the ground state is a gapless $Z_2$ state with extensive degeneracy and the low-energy excitations are dominated by two Majorana 'cones'. At $\Gamma > 0$, it was shown that the system has a hidden $O_h$ point group symmetry and it was shown that at $\Gamma > 0$ the ground state is a gapless state whose excitation spectrum approximately agrees with the $SU(2)$ Wess-Zumino-Witten model. We obtain a similar result (for details see Appendix F) with the difference that in our VMC calculation the (first-order) transition from the gapless $Z_2$ phase to the gapless $U(1)$ phase occurs at a small but finite $\Gamma$ (with $\Gamma/|K| \sim 0.05$) while Ref. 51 concluded that the $\Gamma = 0$ is the first-order phase transition point. Since the energy difference between the $U(1)$ state and the $Z_2$ state is very small, we infer that the phase boundary between the $U(1)$ state to the gSL-VIII phase is very close (if not equal) to $\delta_{zz} = 1$ as the zigzag chains couple with each other to form 2-dimensional lattice.

### III. PHYSICAL PROPERTIES AND DETECTIONS

#### A. Majorana cones in the QSLs

The gapless QSLs are characterized by their Majorana cones. In the following, we show that the cones in the QSLs are stable since they are symmetry-protected. Furthermore, the number of cones, which plays an important role in distinguishing different QSLs, is also determined by the symmetry group.

The mean-field descriptions of the gapless QSLs are nodal-superconductors, therefore the low-energy quantum fluctuations are described by $Z_2$ gauge fields coupling to the fermionic spinons (see Appendix A). Generally, Gutzwiller projected nodal superconductors are gapless nodal-QSLs with deconfined $Z_2$ gauge fluctuations, given that the gapless cones are robust. Indeed, the gapless cones are protected by the combination of spacial inversion $P$ and time reversal $T$, namely, $PT$. To see this, we consider a small loop in the Brillouin zone (BZ) surrounding a cone. Noticing that any momentum $k$ in the BZ is invariant under $PT$, this fully gapped 1D loop reserves $PT$ symmetry and has a $Z_2$ topological classification, which means that the cones cannot be solely gapped without breaking the $PT$ symmetry but can merge and disappear in pairs. The merging of the cones is essentially a continuous quantum phase transition. Therefore, the number of cones is not allowed to change unless the $PT$ symmetry is broken or phase transition occurs.

The symmetry group $G = \mathbb{Z}_{2h} \times Z^T_2$ imposes a constraint on the number of cones. Suppose that a cone is located at momentum $k$, then a group element $a \in G$ may transform $k$ to an inequivalent point $\alpha k$ which is also the location of a cone. The resultant momentum points form a set, called the star of wave vectors, noted as $\{\alpha k\}$. Noticing that a wavevector $k$ is invariant under its little co-group $G_k$ (a subgroup of $G$), the number of wave vectors in $\{\alpha k\}$ is equal to the number of cosets of the little co-group. If $k$ is a general momentum point, then the little co-group $G_k = \{E, PT\}$ contains 2 group elements, therefore the number of cosets, i.e. the number of wave vectors in $\{\alpha k\}$, is 4. If $k$ is on the high-symmetry line of $\sigma_m$, then the little co-group is enlarged to $G_k = \{E, PT, \sigma_m, C_2 T\}$, and correspondingly the number of vectors in $\{\alpha k\}$ reduces to 2. To reserve the symmetry $G$, the set of wave vectors of the gapless Majorana points in a QSL must be composed of several $k$ stars. Consequently, the total number of cones in a QSL is always an integer ($\nu$) + 2m where $(n, m)$ are integers (see Tab. 1).

The low-energy excitations are dominated by the excitations at the Majorana cones. Therefore the number of cones can be reflected in the low-frequency spin dynamic structure factor (DSF). In case that two QSLs have the same number of cones, the location of the cones, i.e. the values of $(n, m)$, will be important to distinguish their low energy spectra. For instance, the PKSL and the gSL-IV both contain 14 cones, but the former has $(n, m) = (2, 3)$ while the latter has $(n, m) = (3, 1)$, as shown in Fig. 4b(IV)&X; another example is the gSL-I versus the gSL-V, both of them contain 10 cones but the former has

| QSL | $(n, m)$ | # of cones | $\nu$ of CSL GSD anyon types |
|-----|---------|------------|-----------------------------|
| Z_2 SL | (0, 0)  | 0          | 0 4 $e, m, e, l$          |
| KSL  | (0, 1)  | 2          | 1 3 $\sigma, e, l$        |
| PKSL | (2, 3)  | 14         | 5 3 $\sigma, e, l$       |
| gSL-I | (1, 3)  | 10         | 1 3 $\sigma, e, l$       |
| gSL-II | (1, 1)  | 6          | 1 3 $\sigma, e, l$       |
| gSL-III | (0, 1) | 2          | -1 3 $\sigma, e, l$      |
| gSL-IV | (3, 1)  | 14         | 3 3 $\sigma, e, l$       |
| gSL-V  | (2, 2)  | 10         | 1 3 $\sigma, e, l$       |
| gSL-VI | (0, 1)  | 2          | 1 3 $\sigma, e, l$       |
| gSL-VII | (2, 4) | 16         | -2 4 $a, a, e, l$       |
| gSL-VIII | (1, 2) | 8          | 0 4 $e, m, e, l$        |

TABLE I. Information of all the QSLs appeared in Figs. 2 & 3. The middle two columns give the information of the cones, where $n$ is the number of $k$ stars locating at general positions and $m$ is the number of $k$ stars on the high symmetry line of $\sigma_m$, the total number of cones is equal to $4n + 2m$. The last three columns list the information of the field-induced CSLs, where $\nu$ is the Chern number in a weak magnetic field along $\frac{1}{\sqrt{3}}(x + y + z)$-direction. GSD abbreviates the ground-state degeneracy on a torus, and the anyon types are determined by $\nu$. $I$ denotes the vacuum and $e$ is the fermion, the two different vortices $e$ and $m$ are anti-particles of themselves, another two vortices $\sigma$ and $\tilde{e}$ are anti-particles of each other, $\sigma$ is the vortices in the non-Abelian phases when $\nu$ is odd. The self-statistics angles (also called the topological spin) of the vortices are determined by the Chern number $e^{\nu 2\pi i}$. 

VII state with

FIG. 4. Illustration of the location of the cones in the gapless QSLs. Contribution the same sign to the total Chern number then the cones in the same

(II) the 6-cone gSL-II state with negative chirality. (I) the 10-cone gSL-I state with the solid dots have positive chirality while the ones at hollow dots have

state gSL-III with

the 14-cone PKSL state with

state gSL-VI with

state gSL-III with

state gSL-I state with the 2-cone state gSL-III with (n, m) = (0, 1); (IV) the 14-cone gSL-IV state with (n, m) = (3, 1); (V) the 10-cone gSL-V state with (n, m) = (2, 1); (VI) the 2-cone state gSL-VI with (n, m) = (0, 1); (VII) the 16-cone gSL-VII state with (n, m) = (2, 4); (VIII) the 8-cone gSL-VIII state with (n, m) = (1, 2); (IX) the 2-cone state KSL with (n, m) = (0, 1); (X) the 14-cone PKSL state with (n, m) = (2, 3). The low energy DSFs of above gSLs are shown in Fig. 10.

Furthermore, when the cones are gapped out by a magnetic field, the system generally obtains a Chern number \( \nu \) which can be read from their thermal Hall conductance (see Tab. I). When a cone is gapped, it contributes \( \pm \frac{1}{2} \) to the Chern number. But if the magnetic field is along a special direction, say \( \frac{1}{\sqrt{3}}(x+y+z) \), then the cones in the same \( \{*k\} \) are still symmetry-related and contribution the same sign to the total Chern number \( \nu \). The sign \( \pm \) defines the chirality of a cone which can be read from the Berry curvature. Therefore, the pattern of cones \((n, m)\) and the chirality of cones in every \( \{*k\} \) completely determine the value of \( \nu \) (see Appendix E for details).

B. Physical detections

The gapless nodal QSLs differ from the gapped ones by their low-temperature density of states, which are reflected in the temperature (T) dependence of the specific heat or the thermal conductance. The nodal ones have power-law T-dependence while the gapped ones show exponential T-dependence. The features of the cones discussed above can help us to further distinguish different nodal QSLs experimentally.

Dynamic structure factor (DSF). DSF can be measured from the neutron scattering experiment and provides useful information to distinguished different QSLs. In the following we calculate the DSF of the gapless QSLs from their mean-field dispersion with the parameters determined from VMC calculations. As mentioned above, if two QSLs have different \((n, m)\), they can be distinguished from their different DSFs. In this way, most the gapless QSLs are distinguished from the others (see Appendix D for the DSF of different QSLs).

But three of the QSLs, the KSL, the gSL-III and the gSL-VI, all have \((n, m) = (0, 1)\). It seems that they are not distinguishable. However, the KSL is special since the parameters \(\eta_1^x, \eta_1^y, \eta_2^x, \eta_2^y\) which mix the \(b^m\)-fermions \((m = x, y, z)\) and the \(c\)-fermions are zero. Consequently, the \(b^m\) fermions are gapped while the \(c\)-fermions are gapless. Therefore, the physical excitations excited by spin operators \(S^m = ib^m c\) cost finite energy. Resultantly, the low-frequency DSF is vanishing below the gap of the \(b^m\) bands. In other words, the KSL shows a gapped spin dynamics although the energy spectrum is gapless. In contrast, in the gSL-III and the gSL-VI, the \(b^m\) and \(c\) fermions are mixed at the nodal points such that the spin dynamics are gapless. But it remains a problem to distinguish the gSL-III and the gSL-VI. A solution is found in the following.

Descendent chiral spin liquids (CSLs). The cones in the gapless QSLs can be gapped out by a magnetic field via Zeeman coupling. When the Chern number \( \nu \) is nontrivial, the resultant state is a CSL given that the field is not strong. As Kitaev pointed out, the CSLs have a 16-fold classification depending on the Chern number \( \nu \) mod 16.

For a weak magnetic field\(^{56}\) with \(B_x = B_y = B_z\), the Chern numbers we obtained are \( \nu = 0, \pm 1, \pm 2, \pm 3, \pm 5 \). When \( \nu \) is odd, the CSL is non-Abelian whose ground-state degeneracy (GSD) on a torus is 3, while when \( \nu \) is even, the CSL is Abelian and the GSD is 4. Except for the \(Z_2\) SL, all the other QSLs in the phase diagram Fig. 2 give rise to non-Abelian CSLs. This is an exciting result because it indicates that anisotropic interactions are plausible to generate non-Abelian CSLs which can be applied in topological quantum computations.

Our VMC calculation of the GSD on a torus is consistent with the theoretical predictions. From the Chern number \( \nu \) we can also read the information of the elementary anyon excitations. For instance, the topological spin of the vortex in a CSL with Chern number \( \nu \) is \( e^{i\nu \pi/4} \), see Table I. The edge of a CSL is gapless and contains \( \nu \) branches of chiral Majorana excitations, each branch carries a chiral central charge \( \frac{1}{2} \). The total chiral central charge is \( c_+ = \frac{\nu}{2} \), which gives rise to a measurable physical quantity — the thermal Hall conductance which is quantized to \(k_B/4\hbar\). The mentioned gSL-III and the gSL-VI have opposite Chern
numbers and can be distinguished from their different thermal Hall conductances. Thus, combining the DSF and the thermal Hall conductance of the weak field-induced CSL, we can completely distinguish all of the QSLs appeared in the phase diagrams in Fig. 2 and Fig. 3.

The Chern number $\nu$ can be tuned by changing the magnetic field\textsuperscript{46}. For instance, $\nu$ can be turned into $-\nu$ by reversing the direction of the magnetic field. Interestingly, our phase diagram Fig. 2 provides an alternative way to change the Chern number $\nu$ without changing the magnetic field. For instance, the transition from the PKSL to the gSL-I can be achieved by increasing pressure (so as to increase $\delta_d$). In a weak magnetic field, the former has $\nu = 5$ while the latter has $\nu = 1$. Therefore, the $\nu = 5$ phase can be driven to the $\nu = 1$ phase by exerting proper pressure. Interestingly, the continuous phase transition between the gSL-II to the gSL-III indicates that the Chern number can be changed from $\nu = 1$ to $\nu = -1$ (and vice versa) with a continuous topological transition by tuning the pressure instead of reversing the direction of the magnetic field\textsuperscript{57,58}. This continuous topological phase transition with Chern number changing by 2 is protected by the $C_{2h} \times Z^2_T$ symmetry. Similarly, the phase transitions from the CSL corresponding to the gSL-V to the one corresponding to gSL-IV and to the one corresponding to gSL-VI are also topological ones where the Chern number changes by 4 and 0, respectively.

IV. DISCUSSION AND CONCLUSIONS

Complete classification of nodal Z$_2$ QSLs. Above we have shown that different gapless QSLs in Figs. 2 & 3 belong to different phases since they have distinct physical properties. However, all these QSLs share the same PSG as the KSL, namely, they have the same pattern of symmetry fractionalization in their spinon excitations. Therefore, the PSG alone is not adequate to classify all the QSLs.

As far as the $C_{2h} \times Z^2_T$ symmetry is concerned, we find that the following three ingredients together provide a complete classification of all possible nodal Z$_2$ QSLs: (1) the pattern of the cones $(n,m)$; (2) the chirality of every cone; (3) the PSGs. The indices of (1) & (2) for all the gapless QSLs in our phase diagrams are shown in Fig. 4.

Comparison to $\alpha$-RuCl$_3$ experiments. Now we try to interpret the recent high-pressure experiment in $\alpha$-RuCl$_3$\textsuperscript{34–36}, where the zigzag magnetic order is suppressed as the pressure goes above 0.8 GPa. The resultant non-magnetic phase is not likely to be a spin liquid because the low energy spin fluctuations are very weak\textsuperscript{34}. Instead, a dimerized trivial ground state is enforced by the pressure accompanied by a structural phase transition\textsuperscript{46}. To model this process, we adopt the dimer-type anisotropic $K$-$\Gamma$ interactions (with fixed $K = -1$ and $\Gamma/|K| = 1.4$) and additional antiferromagnetic Heisenberg interactions ($J$-term) which exist on the short Ru-Ru bonds only. For simplicity, we assume that $J$ changes continuously and increase linearly with the anisotropy parameter $\delta_d$, namely $J/|K| = 10\delta_d$. Our VMC simulation indeed indicates a direct first-order phase transition (at $\delta_d \sim 0.03$) from the zigzag ordered phase to a dimer phase, as shown in Fig. 5. Notice that the intermediate QSLs disappear due to the rapidly increasing Heisenberg interactions on the short bonds. This qualitatively agrees with the experimental results that a relatively low pressure can destroy the zigzag order. Our result indicates that in order to obtain QSLs from high pressure, the fast increasing Heisenberg interactions on the strong bonds should be avoided.

Conclusions. In summary, we have studied the anisotropic $K$-$\Gamma$ model using variational Monte Carlo method. We consider two types of anisotropy, one is of dimer type and the other is of zigzag-chain type. The phase diagrams are given in Fig. 2 and Fig. 3, respectively. We benchmark the calculation at $\Gamma = 0$, and our result is completely consistent with the exact solution. When $\Gamma > 0$, we observe totally eleven QSLs, including the KSL, the proximate KSL, the gapless SL-I-VIII and the gapped Z$_2$ spin liquid phase. The gapless QSLs have symmetry protected gapless nodal points, where the number and the positions of the cones are important in experimentally distinguishing different QSL phases. Most of the phase transitions between the QSLs are of first order, but continuous phase transitions are also found which are characterized by the adiabatic merging of the cones and disappearing in pairs.

We find that the PSG alone cannot completely classify the gapless QSLs. For the $C_{2h} \times Z^2_T$ symmetry we studied, a complete classification of all possible nodal Z$_2$ QSLs should also include the pattern of the cones $(n,m)$ and the chirality of every cone. Furthermore, the magnetic field can gap out the cones via Zeeman coupling and results in several different classes of CSLs. Especially, we obtained 6 classes of non-Abelian Z$_2$ CSLs with Chern number $\nu = \pm 1, \pm 3, \pm 5$, where the total number of such phases is 8 (up to edge chiral boson modes) according to Kitaev\textsuperscript{3}.

Finally, by slightly deforming our model, namely by introducing antiferromagnetic Heisenberg exchanges on the short bonds, we observe a direct first-order transition from the zigzag ordered phase to a dimerized trivial phase, which qualitatively interpret the experimental observation of $\alpha$-RuCl$_3$ under high pressure. Therefore, to prepare for QSL phases, we should avoid the direct transition from the zigzag phase to the dimerized trivial phase as happened in $\alpha$-RuCl$_3$. Namely the Heisenberg interactions on the short bonds are unwanted. It is desired to search for materials whose interactions are described by the Hamiltonian (1) in the presence of uniaxial pressure. If so, we predict that more than one QSL phases can be observed.

Furthermore, as indicated in Fig. 2 and Fig. 3, varying the intensity of the pressure will be a practical way to tune the

![Phase diagram](image-url)

FIG. 5. Phase diagram of the anisotropic $K$-$\Gamma$-$J$ model with $\Gamma/|K| = 1.4$ and $J/|K| = 10\delta_d$, where $J$ denotes the antiferromagnetic Heisenberg interactions existing on the $z$ bonds only. The direct first-order phase transition from the zigzag phase to the dimer phase qualitatively agrees with the high-pressure experiments of $\alpha$-RuCl$_3$.\textsuperscript{37,58}
phase transitions between different QSLs.

Recently, new Kitaev materials are keeping being discovered\textsuperscript{21,59–61}. Our theoretical study suggests that it deserves to experimentally study the physical properties of these new materials under uniaxial pressure, since QSL phases can be possibly generated from a magnetically ordered phase.

Acknowledgement

We thank Y. Li, J. Ma and W.-Q. Yu for informative discussions. This work was supported by the Ministry of Science and Technology of China (Grant No. 2016YFA0300504), the NSF of China (Grants No. 11574392 and No. 11974421), and the Fundamental Research Funds for the Central Universities and the Research Funds of Renmin University of China (No. 19XNLG11).

Appendix A: Variational Monte Carlo approach

Fermionic representation and variational Monte Carlo. VMC is a powerful method to study quantum magnetism, especially quantum spin liquids. It uses Gutzwiller projected mean-field states as trial wave functions. In this approach, the fermionic slave-particle representation $S^m_i = \frac{1}{2} C^m_i \sigma^m C_i$ is introduced, where $C^m_i = (c_i^{\dagger}, c_i)$, $m \equiv x, y, z$, and $\sigma^m$ are Pauli matrices. The particle-number constraint $\tilde{N}_i = n_i^+ c_i^\dagger c_i - 1$ should be imposed at every site to ensure that the size of the fermionic Hilbert space is the same as that of the original physical spin. The complex fermion operators can be seen as linear combinations of Kitaev’s Majorana fermion operators, namely, $c_\uparrow = \frac{1}{2}(b^\dagger + ic)$, $c_\downarrow = \frac{1}{2}(b^\dagger - ib)$. The spin interactions in Hamiltonian (1) are rewritten in terms of interacting fermionic operators and are decoupled into a noninteracting mean-field Hamiltonian.

The general mean-field Hamiltonian for a spin-orbit coupled spin liquid can be expressed as

$$H_{\text{mf}}^{\text{SL}} = \sum_{\langle i,j \rangle \in \alpha, \beta, \gamma} \text{Tr}[U_{ji}^{(0)} \psi_i^\dagger \psi_j] + \text{Tr}[U_{ji}^{(1)} \psi_i^\dagger \sigma^\tau \psi_j (iR_{\alpha \beta})] + \text{Tr}[U_{ji}^{(2)} \psi_i^\dagger \sigma^\gamma \psi_j (iR_{\alpha \beta})],$$

where only the nearest neighbor couplings are considered, $\psi_i = (C_i, \tilde{C}_i)$, $\tilde{C}_i = (c_i^\dagger, -c_i^\dagger)^T$, and $R_{\alpha \beta} = -\frac{1}{2} (\sigma^\alpha + \sigma^\beta)$ is a rotation matrix. The matrices $U_{ji}^{(0)}$, $U_{ji}^{(1)}$, $U_{ji}^{(2)}$, $U_{ji}^{(3)}$ can be expanded using the bases $\tau^0, \tau^x, \tau^y, \tau^z$ where $\tau^x, \tau^y, \tau^z$ are the Pauli matrices and $\tau^0$ is the identity matrix in principle. All the expanding coefficients should be treated as variational parameters. However, as will be seen later, the number of variational parameters can be reduced since they should satisfy the symmetry requirements.

To describe the magnetic order of the spin-rotation-symmetry-breaking phases, we introduce a background field $\mathbf{M}_i$, whose direction is adopted from the single-$\mathbf{Q}$ approximation\textsuperscript{43,46,49} and whose amplitude (together with a canting angle) is determined by VMC. Therefore, the full mean-field Hamiltonian for the anisotropic $K$-$\Gamma$ model on the honeycomb lattice is

$$H_{\text{mf}}^{\text{total}} = H_{\text{mf}}^{\text{SL}} - \frac{1}{2} \sum_i (\mathbf{M}_i \cdot \sigma_i C_i \chi_c + \text{h.c.}) \quad (A2)$$

The essence of the VMC approach is that the local constraint is enforced by Gutzwiller projection. The Gutzwiller projected mean-field ground states provide a series of trial wave functions $|\Psi(x)\rangle = P_G |\Psi_{\text{mf}}(x)\rangle$, where $x$ denotes the variational parameters. The energy of the trial state $E(x) = \langle \Psi(x) | H | \Psi(x) \rangle$ is computed using Monte Carlo sampling, and the variational parameters $x$ are determined by minimizing the energy $E(x)$. Our calculations are performed on a torus of $8 \times 8$ unit cells, i.e. of 128 lattice sites.

Projective symmetry groups. The number of variational parameters can be reduced if the symmetry of the mean-field Hamiltonian, namely, the projective symmetry group (PSG), is considered. The fermionic representation has a local $SU(2)$ gauge symmetry\textsuperscript{4}. In the mean-field Hamiltonian (A1), the $SU(2)$ ‘gauge symmetry’ is broken and only its subgroup $Z_2$ is still a symmetry. This $Z_2$ symmetry is called the invariant gauge group (IGG). The PSG is the central extension of the physical symmetry group by the IGG\textsuperscript{47}.

Besides $\mathcal{O}_{2h} \times Z_2^f$, the anisotropic $K$-$\Gamma$ model is also invariant under the translational group generated by $(T_x, T_y)$. After some calculations, we obtain 192 different PSGs given that the IGG is $Z_2$ (see Appendix B). The PSGs partially classify the possible spin liquid phases with the given symmetry group and IGG. A spin liquid mean-field Hamiltonian of the present model should respect one of the PSGs. For instance, the KSL phase belongs to the class (I-B)\textsuperscript{48}.

The PSG reduces the number of allowed parameters and the exact forms of $U_{ji}^{(m)}$ are given in Appendix C. We have adopt several different PSGs to construct different classes of trial SL Hamiltonians. In class (I-B) case, 9 variational parameters $(\rho^x_a, \rho^y_a, \rho^z_a, \phi^x_0, \phi^y_0, \phi^z_0, \phi^x_1, \phi^y_1, \phi^z_1)$ are adopt, with

$$U_{ji}^{(0)} = i \theta (\phi^z_a + \rho^x_a + \rho^y_a)^x$$

$$U_{ji}^{(1)} = i \theta (\phi^z_a + \rho^x_a + \rho^y_a)^y$$

$$U_{ji}^{(2)} = i \theta (\phi^z_a + \rho^x_a + \rho^y_a)^z$$

$$U_{ji}^{(3)} = i \theta (\phi^z_a + \rho^x_a + \rho^y_a)^x$$

In class (I-A) case, 9 variational parameters
The optimal parameters are determined variationally by minimizing the energy. We also use different magnetic ordered states as trial wave functions in VMC calculation. The state with lowest energy is treated as the ground state. It turns out that all the QSLs in the phase diagrams (Figs. 2 & 3) share the same PSG as the KSL.

Appendix B: Classification of PSG with lattice anisotropic

Here we present the classification of $Z_2$ projective symmetry group (PSG) on distorted honeycomb lattice with the consideration of spin-orbital coupling. The full symmetry group (SG) is the direct product of wallpaper group and time reversal, with the presentation $SG = \{T, T_1, T_2, P, \sigma_m | T^2 = 1, P^2 = 1, \sigma_{m}^2 = 1 \}$ subject to 13 definition relations. The generators of the symmetry group are illustrated in Fig. 2 or Fig. 3. The four generators of the wallpaper group act on the honeycomb lattice in the following way,

\[ T_1(x_1, x_2, A) = (x_1 + 1, x_2, A), \]
\[ T_1(x_1, x_2, B) = (x_1 + 1, x_2, B), \]
\[ T_2(x_1, x_2, A) = (x_1, x_2 + 1, A), \]
\[ T_2(x_1, x_2, B) = (x_1, x_2 + 1, B), \]
\[ P(x_1, x_2, A) = (-x_1, -x_2, A), \]
\[ P(x_1, x_2, B) = (-x_1, -x_2, B), \]
\[ \sigma_m(x_1, x_2, A) = (x_2, x_1, B), \]
\[ \sigma_m(x_1, x_2, B) = (x_2, x_1, A), \]

where each unit cell is labeled by integer coordinates $x_1$ and $x_2$ along the translation axes of $T_1$ and $T_2$. In the following, the index of sublattice $A, B$ will be omitted if an equation is independent of sublattices. Considering time reversal, the full symmetry group of the system contains 5 generators, $T, T_1, T_2, P, \sigma_m$, satisfying the following 13 definition relations:

\[ T_1 T_2 T_1^{-1} T_2^{-1} = 1 \]  
\[ T T_1 T_1^{-1} = 1 \]  
\[ T T_2 T_2^{-1} = 1 \]  
\[ P T_1 P T_1 = 1 \]  
\[ P T_2 P T_2 = 1 \]  
\[ \sigma_m T_1 \sigma_m T_2 = 1 \]  
\[ \sigma_m T_2 \sigma_m^{-1} T_1 = 1 \]  
\[ T^2 = 1 \]  
\[ P^2 = 1 \]  
\[ \sigma_m^2 = 1 \]  
\[ T P T = 1 \]  
\[ T \sigma_m P \sigma_m = 1 \]  
\[ P \sigma_m P \sigma_m = 1 \]

All the pure gauge operations that leave the mean-field ansatz invariant form a subgroup of the PSG, known as the invariant gauge group (IGG). Since spin-orbit pairing is non-vanishing in all the spin liquids obtained from our VMC, we only consider the case $IGG = Z_2$. Thus for each definition relation $g_n \ldots g_1 g_1 = 1$, there is a corresponding PSG representation

\[ G_{g_n} \ldots g_1 (i) G_{g_1}(i) G_{g_1}(i) = \eta_m, \]

where $\eta_m = \pm r^m$, $m = 1, 2, \ldots 13$ are group elements in the IGG and these parameters determine the classification of the PSG. Gauge equivalent solutions of $G_g$ are considered to belong to the same class of PSG. To reduce the gauge redundancy, we will fix part of the gauge degrees of freedom in later discussion.

Firstly, after gauge transformations, one can set $G_{T_1}(x_1, x_2) = r_1^0$, and $G_{T_2}(x_1, 0) = r_0^0$. Then Eq. (B1) can be represented as $G_{T_1}(x_1, x_2 + 1) = \eta_1 G_{T_1}(x_1, x_2)$, which yields the following solution:

\[ G_{T_1}(x_1, x_2) = \eta_1^{x_2}, \]
\[ G_{T_2}(x_1, x_2) = r_0^0. \]  

Substitute Eq. (B14) into the PSG representation of Eq. (B2) and Eq. (B3):

\[ G_T K G_T K = \eta_2 G_{T_1} \]
\[ G_T K G_T K = \eta_3 G_{T_2}, \]

we obtain

\[ G_T(x_1 + 1, x_2) K G_T(x_1, x_2) = \eta_2, \]
\[ G_T(x_1, x_2 + 1) K G_T(x_1, x_2) = \eta_3. \]

Combining Eq. (B8), namely $G_T K G_T K = \eta_8$, we obtain the solution of $G_T$

\[ G_T(x_1, x_2) = \eta_2 \eta_3 \eta_8 \eta_8^{x_1 + x_2} G_T(0, 0). \]  

From Eq. (B4)~(B7), we obtain the following equations:

\[ G_P(x_1 + 1, x_2, a) G_{T_1}(x_1, x_2, a) = \eta_4 G_{T_1}(x_1, x_2, a) G_P(x_1, x_2, a), \]
\[ G_P(x_1 + 1, x_2, a) G_{T_2}(x_1, x_2, a) = \eta_5 G_{T_2}(x_1, x_2, a) G_P(x_1, x_2, a), \]
\[ G_{\sigma_m}(x_1, x_2, a) G_{T_1}(x_1, x_2, a) = \eta_6 G_{T_1}(x_1, x_2, a) G_{\sigma_m}(x_1, x_2, a), \]
\[ G_{\sigma_m}(x_1, x_2, a) G_{T_2}(x_1, x_2, a) = \eta_7 G_{T_2}(x_1, x_2, a) G_{\sigma_m}(x_1, x_2, a), \]
where \( \alpha = A, B \) and \( \bar{\alpha} \) stands for the opposite sub-lattice of \( \alpha \).

Not all the parameters \( \eta_{0m} \) are independent. Some of them can be transformed into each other by certain gauge transformation \( G_g(x_1, x_2, \alpha) \rightarrow \mu(x_1, x_2, \alpha)G_g(x_1, x_2, \alpha) \), where \( \mu(x_1, x_2, \alpha) = \pm \tau^0 \). It turns out that if some \( G_g \) appears twice in an equation, the parameter \( \eta_{1m} \) in that equation is gauge invariant, otherwise that \( \eta_{1m} \) is not gauge independent and can be fixed to \( \tau^0 \) by some gauge transformation. For instance, \( G_{T_1} \) or \( G_{T_2} \) only shows up once in the equations of \( \eta_1 \) and \( \eta_7 \), so we can fix \( \eta_6 = \tau^0 \) and \( \eta_7 = \tau^0 \) by tuning the gauge of \( G_{T_1} \) and \( G_{T_2} \), respectively.

Therefore, the equations obtained from Eq. (B4)–(B7), can be further simplified into the following sublattice-independent form

\[
\begin{align*}
G_p(x_1 + 1, x_2) &= \eta_4 G_p(x_1, x_2), \\
G_p(x_1, x_2 + 1) &= \eta_5 G_p(x_1, x_2), \\
G_{\sigma_m}(x_1 + 1, x_2) &= \eta_1^{x_1} G_{\sigma_m}(x_1, x_2), \\
G_{\sigma_m}(x_1, x_2 + 1) &= \eta_1^{x_2} G_{\sigma_m}(x_1, x_2),
\end{align*}
\]

which yields the following solution

\[
\begin{align*}
G_p(x_1, x_2) &= \eta_1^{x_1} \eta_5^{x_2} G_p(0, 0), \\
G_{\sigma_m}(x_1, x_2) &= \eta_1^{x_1} \eta_5^{x_2} G_{\sigma_m}(0, 0).
\end{align*}
\]

The Eq. (B17) is consistent with Eq. (B10), \( G_{\sigma_m}(A)G_{\sigma_m}(B) = G_{\sigma_m}(B)G_{\sigma_m}(A) = \eta_1^{x_1} \eta_5^{x_2} \eta_{10} \). Furthermore, from Eq. (B11) and Eq. (B12) we find \( \eta_2 = \eta_3 \), and from Eq. (B13) we find \( \eta_4 = \eta_5 \).

Now all the \( G_g(x_1, x_2, \alpha) \) has been reduced to \( G_g(0, 0, \alpha) \) with in a single unit cell. In later discussion \( G_g(\alpha) \) will be used to denote \( G_g(0, 0, \alpha) \). The remaining task is to determine \( G_T(\alpha) \), \( G_P(\alpha) \) and \( G_{\sigma_m}(\alpha) \). Eqs.(B8)–(B13) yields the following constraints

\[
\begin{align*}
G_T(A)K G_T(A)K &= G_T(B)K G_T(B)K = \eta_8, \\
G_P(A)G_P(B) &= G_P(B)G_P(A) = \eta_9, \\
G_T(A)K G_P(A)G_T(A)K &= \eta_1 G_P(A), \\
G_T(A)K G_P(B)G_T(B)K &= \eta_1 G_P(B), \\
G_T(B)K G_{\sigma_m}(A)G_T(A)K &= \eta_2 G_{\sigma_m}(A), \\
G_T(A)K G_{\sigma_m}(B)G_T(B)K &= \eta_2 G_{\sigma_m}(B), \\
(G_P(A)G_{\sigma_m}(B))^2 &= (G_P(B)G_{\sigma_m}(A))^2 = \eta_{13}.
\end{align*}
\]

We start from the solution of \( G_T \). Suppose \( G_T = a_0 \tau^0 + ia_1 \tau_1, \ l = 1, 2, 3 \) to be the most general \( SU(2) \) matrix. From Eq. (B18), we find

\[
G_T G_T^* = (a_0^2 + a_1^2 - a_2^2 - a_3^2) \tau^0 + 2i a_2 (a_3 \tau^x + a_0 \tau^y - a_1 \tau^z)
\]

If \( \eta_8 = -\tau^0 \), the solution is \( a_0 = \pm 1, a_0 = a_1 = a_3 = 0, \ i.e. \ G_T = \mp i \tau^y \). While if \( \eta_8 = \tau^0 \), then \( a_0 = 0, a_0^2 + a_1^2 + a_3^2 = 1 \), we can chose a solution \( G_T(A) = G_T(B) = \tau^0 \). In the following we will discuss these two cases separately.

\textbf{Class (I):} \( \eta_8 = -\tau^0 \). We choose

\[
G_T(A) = i \tau^y, \quad G_T(B) = i \eta_{14} \tau^y,
\]

where \( \eta_{14} = \pm \tau^y \). Substitute into Eq. (B20)–(B23), we find \( \eta_{11} = \eta_{12} = \eta_{14} \). Without losing generality, we can fix

\[
G_{\sigma_m}(A) = \tau^0, \quad G_{\sigma_m}(B) = \eta_{10}.
\]

Plugging into Eq. (B24), we obtain \( (G_P(A))^2 = (G_P(B))^2 = \eta_{13} \). According to the sign of \( \eta_{13} \), the class (I) is divided into two subclasses. Notice that \( \eta_2 = \eta_8 = -\tau^0 \) because time reversal operation \( ((G_T K)^2 = -1) \) is independent on coordinates and sub-lattices.

\textbf{Class (I-A):} \( \eta_{13} = \tau^0 \). The solution of Eq. (B19) is

\[
G_P(A) = \tau^0, \quad G_P(B) = \eta_9.
\]

The solutions in the class (I-A) are summarized as

\[
\begin{align*}
G_{T_1}(x_1, x_2) &= \eta_1^{x_1}, \\
G_{T_2}(x_1, x_2) &= \tau^0, \\
G_T(x_1, x_2, A) &= i \tau^y, \\
G_T(x_1, x_2, B) &= i \eta_{11} \tau^y, \\
G_P(x_1, x_2, A) &= \eta_1^{x_1} \tau^0, \\
G_P(x_1, x_2, B) &= \eta_1^{x_1} \tau^0, \\
G_{\sigma_m}(x_1, x_2, A) &= \eta_1^{x_1} \tau^0, \\
G_{\sigma_m}(x_1, x_2, B) &= \eta_1^{x_1} \tau^0,
\end{align*}
\]

which are controlled by \( \eta_1, \eta_4, \eta_9, \eta_{10}, \eta_{11} \), providing \( 2^5 = 32 \) PSG’s.

\textbf{Class (I-B):} \( \eta_{13} = -\tau^0 \). Because the global gauge freedom has not been fixed, we can set

\[
G_P(A) = i \tau^y, \quad G_P(B) = -i \eta_9 \tau^y.
\]

The solutions in the class (I-B) are summarized as

\[
\begin{align*}
G_{T_1}(x_1, x_2) &= \eta_1^{x_1}, \\
G_{T_2}(x_1, x_2) &= \tau^0, \\
G_T(x_1, x_2, A) &= i \tau^y, \\
G_T(x_1, x_2, B) &= i \eta_{11} \tau^y, \\
G_P(x_1, x_2, A) &= \eta_1^{x_1} \tau^0, \\
G_P(x_1, x_2, B) &= \eta_1^{x_1} \tau^0, \\
G_{\sigma_m}(x_1, x_2, A) &= \eta_1^{x_1} \tau^0, \\
G_{\sigma_m}(x_1, x_2, B) &= \eta_1^{x_1} \tau^0,
\end{align*}
\]

which are controlled by \( \eta_1, \eta_4, \eta_9, \eta_{10}, \eta_{11} \), providing \( 2^5 = 32 \) PSG’s.

\textbf{Class (II):} \( \eta_8 = \tau^0 \). In this case

\[
G_T(A) = G_T(B) = \tau^0.
\]

Therefore Eq. (B20)–(B23) become \( KG_P(A)K = \eta_{11} G_P(A), \quad KG_P(B)K = \eta_{11} G_P(B), \quad KG_{\sigma_m}(A)K = \eta_{12} G_{\sigma_m}(A) \) and \( KG_{\sigma_m}(B)K = \eta_{12} G_{\sigma_m}(B) \). The general solution of \( KG_P K = G_g \) is \( G_g = e^{i \tau^y \theta} \), while the general solution of \( KG_{\sigma_m} K = -G_g \) is \( G_g = i \tau^z e^{i \tau^y \theta} \). According to the sign of \( \eta_{11} \) and \( \eta_{12} \), the class (II) is divided into four subclasses.
Class (II-A1): $\eta_{11} = \eta_{12} = \tau^0$. Then we can obtain the general solution of Eq. (B20)~(B23). The solutions in the class (II-A1) are summarized as

\[
\begin{align*}
G_T(x_1, x_2) &= \eta_1^{x_1}, \\
G_{T_1}(x_1, x_2) &= \tau^0, \\
G_F(x_1, x_2, A) &= \eta_2^{x_1 + x_2} \tau^0, \\
G_F(x_1, x_2, B) &= \eta_2^{x_1 + x_2} \tau^0, \\
P_p(x_1, x_2, A) &= \eta_4^{x_1 + x_2} e^{i\tau^0 \theta_1}, \\
P_p(x_1, x_2, B) &= \eta_4^{x_1 + x_2} e^{i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, A) &= \eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, B) &= \eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1},
\end{align*}
\]

which are determined by $\eta_1, \eta_2, \eta_4, \eta_0, \eta_{10}$, providing $2^5 = 32$ PSG's. Here $\theta_1$ can be any angle and $\theta_3$ is dependent on $\theta_1$ according to the sign of $\eta_{13}$. More precisely, $\theta_3 = \theta_1$ if $\eta_{13} = \tau^0$ and $\theta_3 = \theta_1 - \pi/2$ if $\eta_{13} = -\tau^0$.

Class (II-B1): $-\eta_{11} = -\eta_{12} = \tau^0$. Then we can obtain the general solution of Eq. (B20)~(B23). The solutions in the class (II-B1) are summarized as

\[
\begin{align*}
G_T(x_1, x_2) &= \eta_1^{x_2}, \\
G_{T}(x_1, x_2) &= \tau^0, \\
G_F(x_1, x_2, A) &= \eta_2^{x_1 + x_2} \tau^0, \\
G_F(x_1, x_2, B) &= \eta_2^{x_1 + x_2} \tau^0, \\
P_p(x_1, x_2, A) &= -i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
P_p(x_1, x_2, B) &= -i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, A) &= i\eta_1^{x_1 x_2} \tau^0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, B) &= i\eta_1^{x_1 x_2} \tau^0 e^{-i\tau^0 \theta_1},
\end{align*}
\]

which are determined by $\eta_1, \eta_2, \eta_4, \eta_0, \eta_{10}$, providing $2^5 = 32$ PSG's. Here $\theta_1$ and $\theta_3$ can be any angle.

Class (II-A2): $-\eta_{11} = -\eta_{12} = \tau^0$. Then we can obtain the general solution of Eq. (B20)~(B23). The solutions in the class (II-A2) are summarized as

\[
\begin{align*}
G_T(x_1, x_2) &= \eta_1^{x_2}, \\
G_{T}(x_1, x_2) &= \tau^0, \\
G_F(x_1, x_2, A) &= \eta_2^{x_1 + x_2} \tau^0, \\
G_F(x_1, x_2, B) &= \eta_2^{x_1 + x_2} \tau^0, \\
P_p(x_1, x_2, A) &= i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
P_p(x_1, x_2, B) &= i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, A) &= \eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, B) &= -i\eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1},
\end{align*}
\]

which are determined by $\eta_1, \eta_2, \eta_4, \eta_0, \eta_{10}$, providing $2^5 = 32$ PSG's. Here $\theta_1$ can be any angle while $\theta_3$ is dependent on $\theta_1$ according to the sign of $\eta_{13}$. More precisely, $\theta_3 = \theta_1$ if $\eta_{13} = -\tau^0$ and $\theta_3 = \theta_1 - \pi/2$ if $\eta_{13} = \tau^0$.

Class (II-B2): $-\eta_{11} = \eta_{12} = \tau^0$. Then we can obtain the general solution of Eq. (B20)~(B23). The solutions in the class (II-B2) are summarized as

\[
\begin{align*}
G_T(x_1, x_2) &= \eta_1^{x_2}, \\
G_{T}(x_1, x_2) &= \tau^0, \\
G_F(x_1, x_2, A) &= \eta_2^{x_1 + x_2} \tau^0, \\
G_F(x_1, x_2, B) &= \eta_2^{x_1 + x_2} \tau^0, \\
P_p(x_1, x_2, A) &= i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
P_p(x_1, x_2, B) &= i\eta_4^{x_1 + x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, A) &= i\eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1}, \\
G_{\sigma_m}(x_1, x_2, B) &= -i\eta_1^{x_1 x_2} \eta_0 e^{-i\tau^0 \theta_1},
\end{align*}
\]

which are determined by $\eta_1, \eta_2, \eta_4, \eta_0, \eta_{10}$, providing $2^5 = 32$ PSG's. Here $\theta_1$ and $\theta_3$ can be any angle.

Finally, the number of algebraic PSG's in our classification is 192.

The PSG of Kitaev’s exact spin liquid solution (we will call it Kitaev PSG in later discussion) is belonging to one of the above 192 classifications. Noticing that the $c$-fermions in Kitaev’s solution is never mixed with other flavors, i.e. $(b_1, b_2, b_3)$, the corresponding PSG should keep c-fermion invariant. Under this condition, it is easy to figure out the gauge operations $G_g$:

\[
\begin{align*}
G_T &= G_T = 1, \quad (B41) \\
G_P(A) &= -G_P(B) = -\tau^0, \quad (B42) \\
G_{\sigma_m}(A) &= -G_{\sigma_m}(B) = e^{-i\frac{\pi}{2} g^2 (r^x + r^y)}, \quad (B43) \\
G_T(A) &= -G_T(B) = i\tau^z. \quad (B44)
\end{align*}
\]

It turns out that the PSG of Kitaev spin liquid can be identified with one of the PSG in class (I-B), with invariants $\eta_1 = \eta_4 = \tau^0$ and $\eta_0 = \eta_{10} = \tau^0$ upon $SU(2)$ gauge transformations on $G_P, G_{\sigma_m}$ in Eq. (B37)~(B40). The gauge transformations are $W_A = i e^{i\frac{\pi}{2} r^z} \tau^x$ on A-sublattice and $W_B = e^{i\frac{\pi}{2} r^z} \tau^x$ on B-sublattice.

**Appendix C: Spin-liquid states based on PSG**

Although we obtain 192 algebraic PSGs, it’s impractical to study all the spin liquid ansatz respecting all the different PSGs. In our VMC calculations, we only consider several PSGs which are close to the Kitaev’s PSG class.

If only nearest neighbor coupling terms are considered, the most general mean-field ansatz takes the following form

\[
H_{mf} = \sum_{\langle i,j \rangle} Tr[U_{ji}^{(0)} \psi_i^\dagger \psi_j] + Tr[U_{ji}^{(1)} \psi_i^\dagger \sigma^z (R_{ij}) \psi_j] + Tr[U_{ji}^{(2)} \psi_i^\dagger \sigma^y \psi_j] + Tr[U_{ji}^{(3)} \psi_i^\dagger \sigma^y R_{ij} \psi_j]. \quad (C1)
\]

If above ansatz describes a quantum spin liquid state it should preserve certain PSG. On the other hand, the PSG restricts
the number of parameters in the mean-field ansatz $U_{ji}^{(m)\nu}$. In the following we will firstly give the explicit form of spin liquid ansatz for several special PSGs. And we will perform Gutzwiller projection to these ansatz and pick up the one with the lowest energy as the ground state.

1. Spin-liquid mean field ansatz

We first consider a special solution in class (I-B), namely the Kitaev class with invariants $\eta_1 = \eta_4 = \tau^0$ and $\eta_9 = \eta_{10} = \eta_{11} = -\tau^0$.

To preserve the mirror symmetry (B43) and time reversal symmetry (B44), it requires that $U_{ji}^{(m)\nu}$, $m = 0, 1, 2, 3$ take the following form: on the z-bonds

$$U_{ji}^{(0)z} = i \phi_j^x + \phi_j^z (\tau^x - \tau^y),$$  \hspace{1cm} (C2)

$$U_{ji}^{(1)z} = i \phi_j^x (\tau^x + \tau^y) + i \phi_j^z \tau^z, \hspace{1cm} (C3)

$$U_{ji}^{(2)z} = i \phi_j^x (\tau^x + \tau^y) + i \phi_j^z \tau^z, \hspace{1cm} (C4)

$$U_{ji}^{(3)z} = \phi_j^x + i \phi_j^z (\tau^x - \tau^y); \hspace{1cm} (C5)

and on the x-bonds and y-bonds

$$U_{ji}^{(0)x} = i \phi_j^x + \phi_j^y \tau^x - \phi_j^y \tau^y + \phi_j^z \tau^z, \hspace{1cm} (C6)

$$U_{ji}^{(1)x} = i \phi_j^x \tau^x + i \phi_j^y \tau^y + i \phi_j^z \tau^z, \hspace{1cm} (C7)

$$U_{ji}^{(2)x} = i \phi_j^x \tau^x + i \phi_j^y \tau^y + i \phi_j^z \tau^z, \hspace{1cm} (C8)

$$U_{ji}^{(3)x} = \phi_j^x + i \phi_j^y \tau^x + i \phi_j^z \tau^y + i \phi_j^z \tau^z, \hspace{1cm} (C9)

$$U_{ji}^{(0)y} = i \phi_j^x + \phi_j^y \tau^x - \phi_j^y \tau^y - \phi_j^z \tau^z, \hspace{1cm} (C10)

$$U_{ji}^{(1)y} = i \phi_j^x \tau^x + i \phi_j^y \tau^y + i \phi_j^z \tau^z, \hspace{1cm} (C11)

$$U_{ji}^{(2)y} = i \phi_j^x \tau^x + i \phi_j^y \tau^y + i \phi_j^z \tau^z, \hspace{1cm} (C12)

$$U_{ji}^{(3)y} = \phi_j^x - i \phi_j^y \tau^x - i \phi_j^y \tau^y - i \phi_j^z \tau^z. \hspace{1cm} (C13)

The inversion symmetry (B42) further requires that the parameters $\phi_j^x, \phi_j^y, \phi_j^z$ and $\phi_j^x, \phi_j^y$ must be vanishing. If the full symmetry group $G = \mathcal{L}_{2h} \times Z_2^T$ is considered, then the allowed parameters include $\phi_j^x, \phi_j^z, \phi_j^x, \phi_j^x, \phi_j^z, \phi_j^z, \phi_j^z, \phi_j^x, \phi_j^y, \phi_j^x, \phi_j^y, \phi_j^x, \phi_j^y, \phi_j^y$. Besides the Kitaev decoupling further contribute a few parameters, namely

$$H_{\text{mf}} = \sum_{(ij) \in \mathcal{E}} \left[ i \rho_j^x c_i c_j + i \rho_j^y b^\dagger_i b^\dagger_j + i \rho_j^y (b_i^\dagger b^\dagger_j + b^\dagger_i b^\dagger_j) \right].$$

These parameters can be transformed into matrix as

$$\tilde{U}_{ji}^{(0)\nu} = i (\rho_j^x + \rho_j^y), \hspace{1cm} (C14)

$$\tilde{U}_{ji}^{(1)\nu} = i (\rho_j^y - \rho_j^x) (\tau^x + \tau^y), \hspace{1cm} (C15)

$$\tilde{U}_{ji}^{(2)\nu} = i (\rho_j^y + \rho_j^x) \tau^y, \hspace{1cm} (C16)

$$\tilde{U}_{ji}^{(3)\nu} = i (\rho_j^y - \rho_j^x) (\tau^x - \tau^y). \hspace{1cm} (C17)

In principle, all these parameters are used as independent variational parameters in the VMC calculation. For simplicity, we let $\phi_1^x = \phi_2^x = \phi_3^x, \phi_1^z = \phi_2^z = \phi_3^z, \phi_1^y = \phi_2^y = \phi_3^y, \rho_1^x = \rho_2^x = \rho_3^x, \rho_1^y = \rho_2^y = \rho_3^y$ and $\theta = \phi_1^y = \phi_2^y = \phi_3^y = \phi_1^x = \phi_2^x = \phi_3^x = \phi_1^z = \phi_2^z = \phi_3^z$. It is reasonable since the values of these parameters are small and have small contribution to the energy. Therefore, in our VMC calculation we adopt the following parameters: $\rho_1^x, \rho_1^y, \rho_1^z, \phi_1^x, \phi_1^y, \phi_1^z, \phi_2^x, \phi_2^y, \phi_2^z, \phi_3^x, \phi_3^y, \phi_3^z$ and $\rho_{\nu}^x$. As another example in class (I-B), we give the ansatz with uniform $\pi$-flux. The invariants are slightly different from the above: $\eta_1 = \tau^0$ and $\eta_9 = \eta_{10} = \eta_{11} = -\tau^0$. The general form preserving the mirror symmetry and time reversal symmetry reads $\tilde{U}_{ji} = (-\tau^0)^\nu (U_{ji}^{(m)\nu} + U_{ji}^{(m)\nu'})$, where $U_{ji}^{(m)\nu}$ are given in Eq. (C2)–(C13) and $U_{ji}^{(m)\nu'}$ are given by Eq. (C14)–(C17). We use $(-\tau^0)^\nu$ to note the sign pattern of the uniform $\pi$-flux in each hexagon with doubled unit cell. Therefore, the $\pi$-flux state also contains 9 variational parameters: $\rho_1^x, \rho_1^z, \rho_2^x, \phi_1^x, \phi_1^z, \phi_2^x, \phi_2^y, \phi_2^z, \phi_3^x$ and $\theta$. The $\pi$-flux state is generally gapped.

Secondly, we provide another example in class (I-A), with invariants $\eta_1 = \eta_4 = \eta_9 = \tau^0$, and $\eta_{10} = \eta_{11} = -\tau^0$.

The general form of $U_{ji}^{(m)\nu}$ that preserves the mirror symmetry (B31)–(B32) is similar to the form in the Kitaev PSG. The inversion symmetry (B29)–(B30) further requires that the parameters $\phi_1^x, \phi_1^y, \phi_1^z, \phi_2^x, \phi_2^y, \phi_2^z, \phi_3^x, \phi_3^y, \phi_3^z$ must be vanishing. To reduce the number of variational parameters, we let $\phi_1^x = \phi_1^y, \phi_1^z = -\phi_2^z, \phi_2^y = -\phi_2^x, \phi_2^z = -\phi_2^y$ and $\theta = \phi_1^y = \phi_2^y = \phi_3^y = \phi_1^x = \phi_2^x = \phi_3^x$. Therefore, in our VMC calculation we adopt the following parameters for the given PSG in class (I-A): $\phi_1^x, \phi_1^y, \phi_2^z, \phi_3^y, \phi_2^x, \phi_3^x, \phi_2^y, \phi_3^x$ and $\theta$.

2. Gutzwiller projection and the VMC-chosen ground states

In this section, we only consider the parameter interval where magnetically ordered states are not favored in energy. We perform Gutzwiller projection to the ansatz given in Appendix C1 to calculate the energy and further determine the ground state using VMC. In the following discussion the Gutzwiller projected $Z_2$ gapless ansatz’s will be noted as $\check{g}$SLs, especially the spin liquid belonging to PSG class (I-A) is noted as SL-A. In addition to these $Z_2$ spin liquids, we also consider competing $U(1)$ spin liquid ansatz’s.

Our VMC calculation is performed in a lattice with 8 × 8 unit cells (i.e.128 sites). It turns out that all the spin liquid states appeared in phase diagrams Fig. 2 and Fig. 3 belong to the same PSG class — the Kitaev’s PSG class. It should be noted that, as illustrated in Ref.46, quantum spin liquid states preserving the same PSG can fall into different phases. Here we only compare the projected states from different PSGs and will leave the discussion of distinguishing different quantum phases (with the same PSG) to Appendix D and Appendix E.

We first consider the case with dimer-anisotropy. The data with $\Gamma/|K| = 0.1$ and $\Gamma/|K| = 0.3$ are shown in Fig. 6 and Fig. 7, respectively. It can be seen that the $g$SLs are always...
the lowest in energy comparing to all the other ansatz’s. We have confirmed that these gSLs are all $Z_2$ deconfined. The $Z_2$ deconfinement can be reflected in the ground state degeneracy (on a torus) of the resultant gapped state in a magnetic field, as listed in Tab. III in Appendix E.

The VMC calculations seem to indicate that at big $\Gamma$ there is a phase transition from the gSLs to a $\pi$-flux state (belonging to another PSG in class (I-B)) before the system enters the trivial dimer phase. The data with $\Gamma/|K|=1$ are shown in Fig. 8. The $\pi$-flux state is very competing but still a little bit higher in energy comparing with the gSL-VI or gSL-VIII. To verify the $Z_2$ deconfinement of the projected states, we put the gSL-VII and gSL-VIII into a small magnetic field along $\frac{1}{\sqrt{3}}(x + y + z)$-direction. For both cases, the resultant gapped states are ‘almost’ 4-fold degenerate on a torus (for details see Appendix E).

**Appendix D: Dynamic structure factor of QSL phases**

The spin dynamic structure factor (DSF) reflects the low-energy excitations in a spin system and can be measured by neutron scattering experiments. In this section, the DSFs of QSL phases are calculated at the mean-field level.

The data for the gapless QSLs (PKSL, gSL-I∼VIII) are in Fig. 10 in sequence. We find that the DSFs are nonzero at very low frequency, indicating that these QSLs all have the gapless spin response, in contrast to the Kitaev spin liquid. Generally, the states with different numbers of cones have qualitatively different DSFs and are easily distinguished.

Furthermore, the DSF is sensitive to the locations of gapless points. Especially, if two gapless spin liquids contain the same number of Majorana cones but the cones are located at different positions in the BZ, then their DSFs will be different. For example, gSL-IV and PKSL both have 14 cones, their DSFs shown in Figs. 10(IV)&(IX) are distinguishable.

The gSL-III and gSL-VI both have two cones and the cones are located at similar positions in the BZ. So it is no wondering that their DSFs are qualitatively the same, as shown in Figs. 10(III)&(VI). These two phases can be distinguished by other methods, see Appendix E.
the resultant gapped chiral spin liquid. The remaining symmetry also constrains the Chern number in a weak field along a given direction. In the following, we will illustrate that in an applied magnetic field the symmetry of the system reduces from $G = \mathbb{Z}_2^6 \times \mathbb{Z}_2^T$ to $G_c = \{E, C_2T, P, \sigma_m T\}$. Noticing that one of the wave vectors in the same $\{k\}$ contains at most 4 wave vectors, the wave vectors in the same $\{k\}$ can be transformed into each other by the group elements in $G_c$.

Since the Chern number comes from the cones (each cone contribute a Chern number $\frac{1}{2}$ or $-\frac{1}{2}$ when it opens a gap), in the following we show that the cones in the same $\{k\}$ contribute the same Chern number (all equal to $\frac{1}{2}$ or all equal to $-\frac{1}{2}$). For example, if a state contains 6 cones with $n = 1$ and $m = 1$, then the total Chern number in a weak field $B$ $\frac{1}{\sqrt{3}}(x+y+z)$ can only be one of the following: $3 = 2 + 1$, $1 = 2 - 1$, $-1 = -2 + 1$, $-3 = -2 - 1$. The results listed in Tab. I are consistent with the symmetry constraint.

We firstly consider the inversion symmetry $P$. The symmetry operator on the fermions in the following way,

$$PB_k P^{-1} = M_P B_{-k},$$

(E1)

where $B_k = (c_{k1A}, c_{k2A}, c_{k1B}, c_{k2B}, c_{k1}^\dagger A, c_{k2}^\dagger A, c_{k1}^\dagger B, c_{k2}^\dagger B)^T$, and $M_P = I \otimes (-i\sigma_y) \otimes I$ (I is the 2 by 2 identity matrix) is determined by the Kitaev PSG (B42).

Since the total mean-field Hamiltonian $H = \sum_k B_k^\dagger H_k B_k$ is invariant under inversion operator (B42), therefore

$$H_{-k} = M_P H_k M_P^\dagger,$$

(E2)

We have shown that the gapless points in the gapless QSL phases (namely, the PKSL and the gSL-I–VIII, see Fig. 4) are a set of several $\{k\}$. The points in the same $\{k\}$ are related by $P$ or $C_2$ symmetry operation and are marked by the same color. This relation restricts the number of cones to be $4n + 2m$. In the following, we will illustrate that in an applied magnetic field the remaining symmetry also constrains the Chern number in the resultant gapped chiral spin liquid.

Chern number in a field with $B \parallel \frac{1}{\sqrt{3}}(x+y+z)$. When a magnetic field is added along $B \parallel \frac{1}{\sqrt{3}}(x+y+z)$-direction, the time-reversal symmetry is violated, and the symmetry group reduces from $G = \mathbb{Z}_2^6 \times \mathbb{Z}_2^T$ to $G_c = \{E, C_2T, P, \sigma_m T\}$. Noticing that one of the wave vectors in the same $\{k\}$ contains at most 4 wave vectors, the wave vectors in the same $\{k\}$ can be transformed into each other by the group elements in $G_c$.

Since the Chern number comes from the cones (each cone contribute a Chern number $\frac{1}{2}$ or $-\frac{1}{2}$ when it opens a gap), in the following we show that the cones in the same $\{k\}$ contribute the same Chern number (all equal to $\frac{1}{2}$ or all equal to $-\frac{1}{2}$). For example, if a state contains 6 cones with $n = 1$ and $m = 1$, then the total Chern number in a weak field $B \parallel \frac{1}{\sqrt{3}}(x+y+z)$ can only be one of the following: $3 = 2 + 1$, $1 = 2 - 1$, $-1 = -2 + 1$, $-3 = -2 - 1$. The results listed in Tab. I are consistent with the symmetry constraint.

We firstly consider the inversion symmetry $P$. The symmetry operator on the fermions in the following way,

$$PB_k P^{-1} = M_P B_{-k},$$

(E1)

where $B_k = (c_{k1A}, c_{k2A}, c_{k1B}, c_{k2B}, c_{k1}^\dagger A, c_{k2}^\dagger A, c_{k1}^\dagger B, c_{k2}^\dagger B)^T$, and $M_P = I \otimes (-i\sigma_y) \otimes I$ (I is the 2 by 2 identity matrix) is determined by the Kitaev PSG (B42).

Since the total mean-field Hamiltonian $H = \sum_k B_k^\dagger H_k B_k$ is invariant under inversion operator (B42), therefore

$$H_{-k} = M_P H_k M_P^\dagger,$$

(E2)
If $|\phi_k\rangle$ is the eigenvector of $H_k$ with eigenvalue $\epsilon_k$, $H_k|\phi_k\rangle = \epsilon_k|\phi_k\rangle$, then $H_\pm M_\pm|\phi_k\rangle = \epsilon_k M_\pm|\phi_k\rangle$, namely, $M_\pm|\phi_k\rangle = |\phi_{\pm k}\rangle$ is the eigenvector of $H_\pm$ with eigenvalue $\epsilon_k$. The Berry connections at $-\mathbf{k}$ and $\mathbf{k}$ in the same energy band are related as the following.

$$A_k = \langle \phi_k | \partial_k | \phi_k \rangle = \langle \phi_k | (| \phi_{k+\delta k} \rangle - | \phi_{k-\delta k} \rangle) / \delta k$$

$$= \langle \phi_k | M_\rho (M_\rho | \phi_{k+\delta k} \rangle - M_\rho | \phi_{k-\delta k} \rangle) / \delta k$$

$$= \langle \phi_{-\mathbf{k}} | (| \phi_{-\mathbf{k}+\delta k} \rangle - | \phi_{-\mathbf{k}-\delta k} \rangle) / \delta k$$

$$= -A_{-\mathbf{k}}.$$  

It can be further shown that the Berry curvature $F_{xy} = \partial_y A_x - \partial_x A_y$, in the first BZ is symmetric under inversion, $F_{xy}(-\mathbf{k}) = F_{xy}(\mathbf{k})$ for every band. This result is verified numerically, as shown in Fig. 11. We note that the Berry curvatures of each band are also symmetric under inversion operation. Therefore, the cones related by inversion symmetry have the same contribution to the Chern number. The proof of the other symmetry, $\sigma_m T$, is very similar and will not be repeated here.

Chern number in a generic Magnetic field. We claim that the spin liquid states with different number of Majorana cones belong to different phases. This conclusion is partially confirmed by the fact that in a weak magnetic field $B \parallel \frac{1}{\sqrt{3}}(x+y+z)$ the resultant Chern numbers for states with different number of cones are generally different. However, there are exceptions. Notice that the gSL-I, gSL-II, gSL-V and gSL-VI contain 10,6,10,2 cones, respectively, but their Chern numbers are all equal to 1.

This issue is solved by changing field orientation. With applied field $B \parallel x$ and $B \parallel \frac{1}{\sqrt{3}}(x+y-z)$, the resultant Chern numbers are shown in Tab. II. It can be seen that the states containing different numbers of cones indeed behave differently.

| Field orientation | gSL-I | gSL-II | gSL-V | gSL-VI |
|-------------------|-------|--------|-------|--------|
| $B \parallel x$   | $\nu = -3$ | $\nu = -1$ | $\nu = 1$ | $\nu = 1$ |
| $B \parallel \frac{1}{\sqrt{3}}(x+y-z)$ | $\nu = 1$ | $\nu = 1$ | $\nu = 3$ | $\nu = -1$ |

TABLE II. Chern numbers in differently oriented magnetic fields.

Ground state degeneracy. To see if the Gutzwiller projected wave functions are indeed nontrivial, namely, to check if the $Z_2$ gauge fields are deconfined after projection, we calculate the ground state degeneracy (GSD) on a torus. To this end, we change the boundary conditions and calculate the overlap matrix between the Gutzwiller-projected states, namely, $\rho_{\alpha\beta} = \langle P G \phi_\alpha | P G \phi_\beta \rangle = \rho_{\alpha\beta}$, where $\alpha, \beta \in \{+,+,+,-,-,-\}$ are the boundary conditions (+ stands for periodic boundary condition and − stands for anti-periodic boundary condition) along $x, y$-direction, respectively. If the Chern number of the mean-field ground state is odd, then the state $|\phi_{+,+}\rangle$ vanishes after Gutzwiller projection, therefore there are at most 3-fold degenerate ground states on a torus and the $\rho$ matrix is 3 by 3. Otherwise, if the Chern number is even, then there are at most 4-fold degenerate ground states and the $\rho$ matrix is 4 by 4.

If the matrix $\rho$ has only one significant eigenvalue and all the others are vanishingly small, then the GSD is 1 which means that the $Z_2$ gauge field is confined. On the other hand, if $\rho_{\alpha\beta}$ has more than one (nearly degenerate) nonzero eigenvalues, then the GSD is nontrivial and hence the $Z_2$ gauge fluctuations are deconfined. The data for the eigenvalues of $\rho$ for projected mean-field states carrying different Chern numbers are summarized in Tab. III.

The first eigenvalue of gSL-VIII $1.3 \times 10^{-7}$ is very small, which seems to indicate that the GSD is not 4. However, the situation is quite similar in the $Z_2$ spin liquid state in the pure Kitaev model, where the smallest eigenvalue is $1.4 \times 10^{-3}$ and is much smaller than other eigenvalues. Recalling that the Kitaev model is exactly solvable, where the gapped states belongs to the toric code phase and is $Z_2$ deconfined. Therefore, we also believe that the gSL-VIII is also $Z_2$ deconfined and nontrivial.

Particularly, we calculate the GSD of the $\pi$-flux state discussed in Appendix C.2. For a torus with $12 \times 12$ unit cells, the eigenvalues of the overlap matrix $\rho$ are given by $2.5 \times 10^{-5}, 2.9 \times 10^{-5}, 6.4 \times 10^{-5}, 3.99988$. The last eigenvalue is by far larger than the remaining three ones, therefore the GSD is 1 and therefore the projected $\pi$-flux state is trivial. Actually, we have performed a finite-size scaling calculation (not shown), which indeed indicates that the GSD of this state is 1 in the large-size limit.

Appendix F: $K$-I Chain

In the $\delta_{zz} = 1$ limit, the system becomes decoupled spin chains. A single chain is shown to exhibit a hidden $O_3$ symmetry and supports a gapless phase described by an emergent $SU(2) \times SU(2)$ Wess-Zumino-Witten model. Under a six-sublattice rotation, the spin chain can be mapped into a model with three sublattices.
where $\gamma = x, y, z$. Furthermore, it was shown that a three-sublattice rotation can map $(K, \Gamma)$ to $(K, -\Gamma)$.$^{31}$

For the parameters $K < 0$ and $\Gamma > 0$ that we are studying, the transformed model (F1) can be further transformed into a fully anti-ferromagnetic one by a three-sublattice transformation:

$$H^{1D} = \sum_{(i,j) \in \alpha \beta \gamma} \langle K | S_i^\gamma S_j^\gamma + | \Gamma | (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) . \tag{F2}$$

We adopt two different types of ansatz’s. In the first one, we treat the original $K-\Gamma$ interaction and the mean-field Hamiltonian of the chain is descending from the two-dimensional ansatz (C1), which contains spinon pairing terms and gives rise to a $Z_2$ spin liquid state. In the second one, we start from the transformed three-sublattice model (F2) since it is equivalent to the $K-\Gamma$ chain up to unitary transformations. Noticing that $|K|S_i^\gamma S_j^\gamma + |\Gamma|(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) = |\Gamma|S_i^\alpha S_j^\beta + (|K| - |\Gamma|)S_i^\gamma S_j^\gamma$, we can introduce the following $U(1)$ ansatz,

$$H_{U(1)} = \sum_{(i,j) \in \gamma} \chi(c_{i,\gamma}^\dagger c_{j,\gamma} + c_{i,\gamma}^\dagger c_{j,\gamma}^\dagger) + \chi^2 C_i^\dagger \sigma^\gamma C_j + h.c.$$  

where $C_i^\dagger = (c_{i,\gamma}^\dagger, c_{i,\gamma}^\dagger)$ and 4 variational parameters, namely $\chi, \chi^2, \chi^\gamma, \chi^z$ appear in above equation. Finally, a $U(1)$ spin liquid state for the original $K-\Gamma$ model can be obtained from above $U(1)$ ansatz by performing the inverse of the three-sublattice and six-sublattice transformations.

We have also considered magnetically ordered states but find that disordered states are favored in energy. Our VMC calculation indicates that there exists a finite $Z_2$ phase at small $|\Gamma|$ which is separated from the $U(1)$ state by a first-order phase transition at $|\Gamma|/|K| \approx 0.05$, see Fig. 12.

Our result is qualitatively consistent with previous results$^{31}$, except that our $Z_2$ phase shrinks to a single first-order phase transition point at $\Gamma = 0$ in Ref.$^{51}$

\footnotesize

* liuxzphys@ruci.edu.cn

1. L. Balents, Nature (London) 464, 199 (2010).
2. M. Levin, X.-G. Wen, Phys. Rev. B 71, 045110 (2005).
3. A. Kitaev, Ann. Phys. 321, 2 (2006).
4. I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, Phys. Rev. B 38, 745 (1988).
5. G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009).
6. J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev. Lett. 105, 027204 (2010).
7. J. M. Fletcher, W. E. Gardner, A. C. Fox, and G. Topping, J. Chem. Soc. A 1038 (1967).
8. K. W. Plumb, J. P. Clancy, L. J. Sandilands, V. V. Shankar, Y. F. Hu, K. S. Burch, H.-Y. Kee, and Y.-J. Kim, Phys. Rev. B 90, 041112(R) (2014).
9. J. A. Sears, M. Songvilay, K. W. Plumb, J. P. Clancy, Y. Qiu, Y. Zhao, D. Parshall, and Y.-J. Kim, Phys. Rev. B 91, 144420 (2015).
10. R. D. Johnson, S. C. Williams, A. A. Haghighirad, J. Singleton, V. Zapf, P. Manuel, I. I. Mazin, Y. Li, H. O. Jeschke, R. Valenti, and R. Coldea, Phys. Rev. B 92, 235119 (2015).
11. H.-B. Cao, A. Banerjee, J.-Q. Yan, C. A. Bridges, M. D. Lumsden, D. G. Mandrus, D. A. Tennant, B. C. Chakoumakos, and S. E. Nagler, Phys. Rev. B 93, 134423 (2016).
12. S. C. Williams, R. D. Johnson, F. Freund, S. Choi, A. Jesche, I. Kimchi, S. Manni, A. Bombardi, P. Manuel, P. Gegenwart, and R. Coldea, Phys. Rev. B 93, 195158 (2016).
13. Y. Singh and P. Gegenwart, Phys. Rev. B 82, 064412 (2010).
14. X. Liu, T. Berlijn, W.-G. Yin, W. Ku, A. Tsvelik, Y.-J. Kim, H. Gretarsson, Y. Singh, P. Gegenwart, and J. P. Hill, Phys. Rev. B 83, 220403(R) (2011).
15. F. Ye, S.-X. Chi, H.-B. Cao, B. C. Chakoumakos, J. A. Fernandez-Baca, R. Custelcean, T.-F. Qi, O. B. Korneta, and G. Cao, Phys. Rev. B 85, 180403(R) (2012).
16. S. K. Choi, R. Coldea, A. N. Kolmogorov, T. Lancaster, I. I. Mazin, S. J. Blundell, P. G. Radaelli, Y. Singh, P. Gegenwart, K. R. Choi, S.-W. Cheong, P. J. Baker, C. Stock, and J. Taylor, Phys. Rev. Lett. 108, 127204 (2012).
17. M. Abramchuk, C. Oszosz-Keskinbora, J. W. Krizan, K. R. Metz, D. C. Bell, and F. Tafti, J. Am. Chem. Soc. 139, 15371 (2017).
18. K. Kitagawa, T. Takayama, Y. Matsumoto, A. Kato, R. Takano, Y. Kishimoto, S. Bette, R. Dinneben, G. Jackeli, and H. Takagi, Nature (London) 554, 341 (2018).
19. E. Lefrancçois, M. Songvilay, J. Robert, G. Nataf, E. Jordan, L. Chaix, C. V. Colin, P. Lejay, A. Hadji-Azzem, R. Ballou, and V. Simonet, Phys. Rev. B 94, 214416 (2016).
20. A. K. Bera, S. M. Yusuf, A. Kumar, and C. Ritter, Phys. Rev. B 95, 094424 (2017).
21. W. Yao, Y. Li, arXiv:1908.09427.
22. L. Janssen, E. C. Andrade, and M. Vojta, Phys. Rev. B 96, 064430 (2017).
23. S.-H. Do, S.-Y. Park, J. Yoshitake, J. Nasu, Y. Motome, Y. S. Kwon, D. T. Adroja, D. J. Voneshen, K. Kim, T.-H. Jang, J.-H. Park, K.-Y. Choi and S. Ji, Nat Phys 13, 1079 (2017).
24. A. Banerjee, P. Lampen-Kelley, J. Knolle, C. Balz, A. A. Aczel, B. Winn, Y. Liu, D. Pajerowski, J.-Q. Yan, C. A. Bridges, A. T. Savici, B. C. Chakoumakos, M. D. Lumsden, D. A. Tennant, R. Moessner, D. G. Mandrus, and S. E. Nagler, npj Quantum Materials 3, 8 (2018).
25. L. J. Sandilands, Y. Tian, K. W. Plumb, Y.-J. Kim, and K. S.
