Spin-nematic order in the spin-1/2 Kitaev-Gamma chain

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A minimal Kitaev-Gamma model has been recently investigated to understand various Kitaev systems. In the one dimensional Kitaev-Gamma chain, an emergent SU(2)1 phase and a rank-1 spin ordered phase with $O_h \rightarrow D_4$ symmetry breaking were identified using non-Abelian bosonization and numerical techniques. However, puzzles near the antiferromagnetic Kitaev region with finite Gamma interaction remained unresolved. Here we focus on this parameter region and find that there are two new phases, namely, a higher-rank spin-nematic ordered phase, and a peculiar Kitaev phase. There is no numerical signature of spin orderings nor Luttinger liquid behaviours in the Kitaev phase. The transition between the spin-nematic and the “$O_h \rightarrow D_4$” phases and the nature of the Kitaev phase are worth further studies.

I. INTRODUCTION

Low dimensional quantum magnetism is among the most active research areas in modern condensed matter physics. The interplays between quantum fluctuations, low dimensionality and frustrations lead to exotic magnetic properties including various magnetic orderings, topological orders and spin liquid behaviors. Apart from the conventional rank-1 spin orders, high rank spin tensor orders have also been intensively investigated, including the spin-nematic orders (i.e., spin-quadrupole orders and even octupole order). Another intriguing phenomenon in strongly correlated magnetic systems is the emergence of the deconfined quantum criticality. Deconfined quantum criticality is associated with continuous phase transitions between two ordered phases, which is in contrast with the conventional Landau paradigm of second order phase transitions where the system transits from a disordered phase to an ordered phase when the critical point is traversed. While most of the examples are in two-dimension (2D) and electron compounds have added to the richness of the strongly correlated magnetic behaviors. Examples of this kind include the Kitaev materials on the 2D honeycomb lattice, which are proposed to host exotic fractionalized excitations including Majorana fermions and nonabelian anyons. A generalized Kitaev model containing symmetry allowed terms in addition to the Kitaev interaction have been proposed to describe the Kitaev material. Recently, the generalized Kitaev spin-1/2 model has also been actively studied in (quasi-) 1D systems which may be realized in Ruthenium stripes in the RuCl3 material. In Ref. , the phase diagram of the 1D Kitaev-Gamma spin-1/2 chain has been studied. It is shown that about 67% of the phase diagram of the Kitaev-Gamma chain is described by an emergent SU(2)1 Wess-Zumino-Witten (WZW) model, and besides this, an ordered phase of rank-1 spin orders with $O_h \rightarrow D_4$ symmetry breaking is identified, where $O_h$ is the full octahedral group and $D_n$ represents the dihedral group of order $2n$.

In this work, we focus on the unresolved phases near the antiferromagnetic Kitaev region. To elaborate our current study, we begin with a quick review of the phase diagram of the Kitaev-Gamma chain shown in Fig. (a). Since changing the sign of the Gamma coupling leads to an equivalent Hamiltonian, it is enough to consider the upper half circle in Fig. (a) where all the phases are numbered by “I” except the “Kitaev” phase. In addition to the already established “Emergent SU(2)1” and “$O_h \rightarrow D_4$” phases, two new phases are identified, namely the “Spin-Nematic I” and “Kitaev” phases. By a combination of symmetry analysis, density matrix renormalization group (DMRG), infinite DMRG (iDMRG), and exact diagonalization (ED) numerical methods, we find that the system exhibits a spin-nematic order in the “Spin-Nematic I” phase with a four-fold ground state degeneracy. Furthermore, there is numerical evidence for both the spin-nematic and $O_h \rightarrow D_4$ order parameters to vanish at the phase transition point $\phi_c'$ as shown in Fig. (b). Therefore, $\phi_c'$ is likely a continuous phase transition point between two ordered phases. Based on this, we conjecture that $\phi_c'$ may be a deconfined quantum critical point. More numerical studies on the critical properties of $\phi_c'$ will be left for future studies. Finally, the nature of the “Kitaev” phase in Fig. (a) remains unclear with no numerical evidence of orderings nor Luttinger liquid behaviors. Whether more exotic orderings like the topological string order exist in the “Kitaev” phase is worth further studies.

II. MODEL HAMILTONIAN AND SYMMETRIES

In this section, we first give the model Hamiltonian and then briefly review the six-sublattice rotation and
the symmetries of the system.

A. Model Hamiltonian

The Hamiltonian of the spin-1/2 Kitaev-Gamma chain is defined as

$$H = \sum_{\langle ij \rangle \in \gamma \text{ bond}} \left[ KS^\alpha_i S^\gamma_j + \Gamma (S^\alpha_i S^\beta_j + S^\beta_i S^\alpha_j) \right], \quad (1)$$

in which $i, j$ are two sites of nearest neighbors; $\gamma = x, y$ is the spin direction associated with the $\gamma$ bond shown in Fig. 2 (a); $\alpha \neq \beta$ are the two remaining spin directions other than $\gamma$; $K$ and $\Gamma$ are the Kitaev and Gamma couplings, respectively. In what follows, the two couplings will be parametrized as

$$K = \cos(\phi), \quad \Gamma = \sin(\phi), \quad (2)$$

where $\phi \in [0, 2\pi]$. Under a global spin rotation around the $z$-axis by $\pi$, i.e., $R(z, \pi) : (S^x_i, S^y_i, S^z_i) \to (S^y_i, -S^x_i, S^z_i)$, the Kitaev term remains the same whereas the $\Gamma$ changes to $-\Gamma$. Therefore, we obtain the equivalence

$$(K, -\Gamma) \equiv (K, \Gamma), \quad (3)$$

or $\phi \equiv 2\pi - \phi$. Due to this equivalence, the phase diagram can be restricted to the parameter range $\phi \in (0, \pi)$, and in subsequent discussions, we will drop the numbering "$\Gamma$" in the names of the phases for simplicity.

B. The six-sublattice rotation

A useful transformation $U_6$ with a periodicity of six sites is defined as,

Sublattice 1 : $(x, y, z) \to (x', y', z')$,
Sublattice 2 : $(x, y, z) \to (-x', -z', -y')$,
Sublattice 3 : $(x, y, z) \to (y', z', x')$,
Sublattice 4 : $(x, y, z) \to (-y', -x', -z')$,
Sublattice 5 : $(x, y, z) \to (z', x', y')$,
Sublattice 6 : $(x, y, z) \to (-z', -y', -x')$,

in which "Sublattice $i$" ($1 \leq i \leq 6$) denotes the sites $i + 6n$ $(n \in \mathbb{Z})$, and $S^\alpha_i$ $(S^{\alpha n})$ is abbreviated as $\alpha (\alpha')$ for short ($\alpha = x, y, z$). After the six-sublattice rotation, the Hamiltonian $H' = U_6 H U_6^{-1}$ acquires the form

$$H' = \sum_{\langle ij \rangle \in \gamma \text{ bond}} \left[ -K S^\alpha_i S^\gamma_j - \Gamma (S^\alpha_i S^\beta_j + S^\beta_i S^\alpha_j) \right], \quad (5)$$

in which the bond $\gamma = x, y, z$ is periodic in three sites as shown in Fig. 2 (b), and the prime has been dropped in $S^\gamma_i$ for simplicity. The explicit expression of $H'$ in Eq. (5) is given in Appendix A.

We will stick to the six-sublattice rotated frame from here on in the remaining parts of this work unless otherwise stated. The Hamiltonian is simplified in the six-sublattice rotated frame in the sense that there is no cross term $S^\alpha_i S^{\alpha n} j$ where $\alpha \neq \beta$. In particular, $H'$ becomes $SU(2)$ symmetric when $K = \Gamma$. Due to the equivalence

$$\phi \equiv 2\pi - \phi.$$
established in Eq. (3), the system also has hidden SU(2) symmetry at \( K = -\hat{T} \). In the range \( \phi \in [0, \pi] \), the points \( \phi = \pi/4 \) and \( 3\pi/4 \) correspond to an ferromagnetic (FM) and antiferromagnetic (AFM) Heisenberg model, respectively.

Here we give a brief summary about the phase diagram. In Ref. 58, the region \( \phi \in [\phi_c, \pi] \) is shown to be a gapless phase described by an emergent SU(2)\(_1\) WZW model, where \( \phi_c \approx 0.33\pi \). Also, a conventional rank-1 spin ordered phase with an \( O_h \to D_4 \) symmetry breaking has been identified within \( \phi \in [\phi'_c, \phi_c] \) where \( \phi'_c \approx 0.10\pi \). However, the phase below \( \phi'_c \) is not studied in Ref. 58. In this work, we identify the region \( \phi \in [\phi''_c, \phi'_c] \) to have a spin-nematic order, where \( \phi''_c \approx 0.034\pi \) determined from iDMRG calculations discussed in Sec. VI. We note that a different value of \( \phi''_c \) around 0.05\( \pi \) is obtained for finite size systems, indicating a possibly strong finite size dependence. The symmetry breaking pattern is \( O_h \to D_{3d} \) where \( D_{3d} \equiv D_3 \times Z_2 \), and the ground state degeneracy is 4. The region \( \phi \in (0, \phi''_c] \) is a new phase denoted as the “Kitaev” phase in Fig. 1 (a), the nature of which remains unclear.

C. The symmetry group

In this section, we first present a symmetry analysis to infer the absence of any rank-1 spin order in the range \( \phi \in [\phi''_c, \phi'_c] \) based on the information of the ground state degeneracy. Then all the adjacent-site spin-quadrupole order parameters are classified under the assumption that the symmetry breaking pattern is \( O_h \to D_{3d} \), where in particular, the time reversal symmetry is preserved but the spin rotational symmetries \( R(\hat{\alpha}, \pi) \) \((\alpha = x, y, z)\) are broken. Since spin-quadrupole orders are also referred as spin-nematic orders, we will use the two phrases interchangeably in this work. After that, we present extensive numerical evidence supporting the existence of the spin-nematic orders. We have also studied the spin-nematic order parameter as a function of \( \phi \) using DMRG numerics. It is shown that the order parameter decreases to zero continuously when \( \phi \) approaches \( \phi'_c \) in the “Spin-Nematic” phase, indicating a continuous phase transition.

A. Absence of rank-1 spin orders

In this section, the symmetry group of \( H' \) will be briefly reviewed which has been discussed in detail in Ref. 58.

The Hamiltonian \( H' \) in Eq. (5) is invariant under the time reversal operation \( T \), the screw operation \( R_a T_a \), the coupled operation \( R_I I \), and the global spin rotations \( R(\hat{\alpha}, \pi) \) \((\alpha = x, y, z)\), in which: \( T_a \) and \( I \) represent the spatial translation by one site and the inversion around the point \( C \) in Fig. 2 (b), respectively; \( R_a \) and \( R_I \) are given by \( R_a = R(\hat{n}_a, -2\pi/3) \) and \( R_I = R(\hat{n}_I, \pi) \), where \( R(\hat{n}, \theta) \) represents a global spin rotation around the \( \hat{n} \)-axis by an angle \( \theta \), and the rotation axes \( \hat{n}_a, \hat{n}_I \) are given by \( \hat{n}_a = \frac{1}{\sqrt{3}}(1, 1, 1)^T \), \( \hat{n}_I = \frac{1}{\sqrt{2}}(1, 0, -1)^T \). These symmetry operations generate the symmetry group \( G \) of the system:

\[
G = \langle T, R_a T_a, R_I I, R(\hat{x}, \pi), R(\hat{y}, \pi), R(\hat{z}, \pi) \rangle.
\]

Notice that the spatial translation by three sites \( T_{3a} = (R_a T_a)^3 \) is a group element of \( G \), which generates an abelian normal subgroup. It has been shown in Ref. 58 that the quotient group \( G/\langle T_{3a} \rangle \) is isomorphic to \( O_h \), where \( O_h \) is the full octahedral group. Therefore, the group structure of \( G \) can be represented as

\[
G \cong O_h \rtimes 3\mathbb{Z},
\]

where \( 3\mathbb{Z} \) is \( \langle T_{3a} \rangle \) for short, and \( \rtimes \) is the semi-direct product.

III. THE SPIN-NEMATIC ORDER PARAMETERS

In this section, we first present a symmetry analysis to infer the absence of any rank-1 spin order in the range \( \phi \in [\phi''_c, \phi'_c] \) based on the information of the ground state degeneracy. Then all the adjacent-site spin-quadrupole order parameters are classified under the assumption that the symmetry breaking pattern is \( O_h \to D_{3d} \), where in particular, the time reversal symmetry is preserved but the spin rotational symmetries \( R(\hat{\alpha}, \pi) \) \((\alpha = x, y, z)\) are broken. Since spin-quadrupole orders are also referred as spin-nematic orders, we will use the two phrases interchangeably in this work. After that, we present extensive numerical evidence supporting the existence of the spin-nematic orders. We have also studied the spin-nematic order parameter as a function of \( \phi \) using DMRG numerics. It is shown that the order parameter decreases to zero continuously when \( \phi \) approaches \( \phi'_c \) in the “Spin-Nematic” phase, indicating a continuous phase transition.

FIG. 3: Ground state degeneracy as a function of \( \phi \). The three phase transition points are \( \phi_c \approx 0.33\pi, \phi'_c \approx 0.10\pi, \phi''_c \approx 0.05\pi \), where the value of \( \phi''_c \) is different from the value determined from iDMRG numerics. It is shown that the order parameter decreases to zero continuously when \( \phi \) approaches \( \phi'_c \) in the “Spin-Nematic” phase, indicating a continuous phase transition.
\[ \phi = 0.06\pi \quad \phi = 0.07\pi \quad \phi = 0.08\pi \]

| \( E_1 \) | -3.822078 | -3.821406 | -3.822237 |
| \( E_2 - E_1 \) | 7.2 \cdot 10^{-4} | 1.0 \cdot 10^{-4} | 1.7 \cdot 10^{-4} |
| \( E_3 - E_1 \) | 7.2 \cdot 10^{-4} | 1.0 \cdot 10^{-4} | 1.7 \cdot 10^{-4} |
| \( E_4 - E_1 \) | 7.2 \cdot 10^{-4} | 1.0 \cdot 10^{-4} | 1.7 \cdot 10^{-4} |
| \( E_5 - E_1 \) | 7.7 \cdot 10^{-4} | 1.27 \cdot 10^{-3} | 1.84 \cdot 10^{-3} |
| \( E_6 - E_1 \) | 7.7 \cdot 10^{-4} | 1.27 \cdot 10^{-3} | 1.84 \cdot 10^{-3} |
| \( E_7 - E_1 \) | 8.6 \cdot 10^{-4} | 1.51 \cdot 10^{-3} | 2.09 \cdot 10^{-3} |

**TABLE I:** Energies of several lowest lying states computed with Lanczos Exact Diagonalization. The data refer to \( L = 24 \) sites. The four energies enclosed by the red squares are approximately degenerate at the corresponding \( \phi \)'s.

(a). For \( \phi \in [\phi_c', \phi_c] \), the ground states are six-fold degenerate, corresponding to the \( O_h \to D_4 \) phase which has been discussed in Ref. \[58\] and will be briefly reviewed in Sec. [IV]. In the range \( \phi''_c < \phi < \phi_c' \), numerics provide evidence for a four-fold ground state degeneracy, implying a spin ordering different from \( O_h \to D_4 \). The energies of the first seven states are displayed in Table I from which the four-fold ground state degeneracy can be observed. Indeed, the four energies enclosed by the red square at each angle \( \phi \) are approximately degenerate, and they are separated from the other states with an energy gap much larger than the splitting among them. Finally, for \( \phi < \phi''_c \), we were unable to find a definite value of the ground state degeneracy. The degeneracy has strong finite size dependences, and there is no clear energy separation between some low lying (presumably ground state) multiplet and the excited states. Therefore, no value of degeneracy is assigned to the region of \( \phi < \phi''_c \), which is denoted as the “Kitaev” phase in Fig. 3.

In this section, we will focus on the region \( \phi \in [\phi''_c, \phi'_c] \) which a has four-fold ground state degeneracy. We demonstrate that the information on the ground state degeneracy alone is enough to exclude the possibility of any conventional rank-1 spin order. The translation symmetry by three sites is assumed to be not broken, and all symmetry operations will be considered modulo \( T_{3a} \). Therefore the full symmetry group will be referred as \( O_h \) rather than \( O_h \times 3Z \).

Suppose the unbroken symmetry group to be \( D \), so that the symmetry breaking pattern is \( O_h \to D \). To obtain a four-fold degeneracy, the order of \( D \) must be 12. On the other hand, the only two subgroups of \( O_h \) that have 12 elements are the tetrahedral cubic point group \( T \) and the tetragonal point group \( D_{3d} \).

We show that \( S^a_i \) cannot be an order parameter that has either \( T \) or \( D_{3d} \) to be the unbroken symmetry group. Otherwise, suppose \( S^a_i \) acquires a nonzero expectation value on one of the four degenerate ground states \( |\Omega\rangle \) which is assumed to be invariant under the cubic point group \( T \). Since \( R(\hat{a}, \pi) \) \((\alpha = x, y, z) \) belongs to \( T \), the sign of \( S^a_i \) can be changed using \( R(\hat{\beta}, \pi) \) where \( \beta \neq \alpha \). As a result,

\[ \langle \Omega | S^a_i | \Omega \rangle = -\langle \Omega | R^{-1}(\beta, \pi)S^a_i R(\beta, \pi) | \Omega \rangle. \]

However, since \( |\Omega\rangle \) is invariant under \( R(\hat{\beta}, \pi) \) by assumption, we conclude that \( \langle \Omega | S^a_i | \Omega \rangle = -\langle \Omega | S^a_i | \Omega \rangle \), which contradicts with \( \langle \Omega | S^a_i | \Omega \rangle \neq 0 \). Thus, \( T \) cannot be the unbroken symmetry group.

B. Symmetry classification of the spin-nematic order parameters

The analysis in Sec. [III A] excludes any conventional rank-1 spin order, therefore the only possibilities are high rank spin tensors. On the other hand, the spin-1/2 systems do not support on-site high rank spin tensors due to the relation \( S^a_i S^b_i = \frac{1}{4} \delta_{i,j} + \frac{1}{2} i e^{i\beta \gamma} S^j_i \). As a result, we have to consider spin tensors involving different lattice sites. The simplest choices are the rank-2 adjacent site spin tensors, i.e., the quadrupole orders \( S^a_i S^b_i S^c_i S^d_i \). Notice that these spin-nematic orders always preserve time reversal symmetry. Hence, the unbroken symmetry group cannot be the point group \( T \) which does not contain the time reversal operation, and the only possibility for the unbroken symmetry group is \( D_{3d} \). We are going to show that the \( D_{3d} \)-invariant spin-nematic orders do exist, and explicit expressions will be constructed.

Define a \( 9 \times 9 \) matrix \( M \) as

\[ M = \langle \Omega_e | \begin{pmatrix} S^1_i & S^2_i & S^3_i \\ \overline{S}^1_i & \overline{S}^2_i & \overline{S}^3_i \\ \overline{S}^3_i & \overline{S}^2_i & \overline{S}^1_i \end{pmatrix} | \Omega_e \rangle, \]

in which \( |\Omega_e\rangle \) is one of the four symmetry breaking ground states, and \( \overline{S}^a_i = (S^a_i, S^y_i, S^z_i)^T \) is viewed as a three-component column vector. In Eq. (9), the site indices should be understood as modulo \( 3 \) such that the expectation values are taken for adjacent sites. For example, \( S^a_i \overline{S}^a_j \) means \( S^a_{i+3n}S^a_{j+3n} \) where \( n \in \mathbb{Z} \). We note that the value of \( n \) is not essential in Eq. (9) since \( T_{3a} \) is assumed to be unbroken. Also notice that \( M \) includes all possible expectation values of adjacent-site spin-nematic order parameters.
Before proceeding on, we give the explicit expression of D_{3d}. Assuming the unbroken symmetry group to be

\[ G_1 = <T, R_a T_a, R_I T, T_{3a}>, \]

we will show that \( G_1 / <T, T_{3a}> \) is isomorphic to \( D_3 \). Hence, \( D_{3d} \) is given by

\[ D_{3d} = <T, R_a T_a, R_I T> / <T_{3a}>, \]

The isomorphism \( G_1 / <T, T_{3a}> \simeq D_3 \) can be proved using the following generator-relation representation of \( D_n \):

\[ D_n = <a, b | a^n = b^2 = (ab)^2 = e>, \]

in which \( e \) is the identity element. Define \( a = R_a T_a \), \( b = R_I T \). Then \( a^3 = T_{3a}^3 \), and \( b^2 = e \), which are both equal to the identity element modulo \( T_{3a} \). Hence \( G_1 / <T, T_{3a}> \) is a subgroup of \( D_3 \) since it is generated by \( \{R_a T_a, R_I T\} \). On the other hand, \( \{e, R_a, R_a^{-1}, R_I, R_I^{-1}, R_a R_I\} \) are all distinct operations, and are the actions of the elements of \( G_1 / <T, T_{3a}> \) restricted within the spin space. This shows that there are at least six elements in \( G_1 / <T, T_{3a}> \). But the order of \( D_3 \) is six, thus \( G_1 / <T, T_{3a}> \) is isomorphic to \( D_3 \).

Having \( D_{3d} \) at hand, the next step is to solve the most general form of \( M \) in Eq. (9) by assuming the \( D_{3d} \) invariance of \( |\Omega_c> \). Since the spin-nematic order parameters automatically maintain the time reversal symmetry, \( T \) has no restriction on the form of \( M \) and it is enough to consider \( R_a T_a \) and \( R_I T \). Using

\[
R_a T_a (S^T_1 S^T_2 S^T_3) (R_a T_a)^{-1} = (S^T_1 S^T_2 S^T_3) U_a, \\
R_I T (S^T_1 S^T_2 S^T_3) (R_I T)^{-1} = (S^T_1 S^T_2 S^T_3) U_I, \]

we obtain the constraints on \( M \) as

\[
U_a M U_a^{-1} = M, \\
U_I M U_I^{-1} = M, \]

in which

\[
U_a = \begin{pmatrix} 0 & 0 & R_a \\ R_a & 0 & 0 \\ 0 & R_a & 0 \end{pmatrix}, \\
U_I = \begin{pmatrix} 0 & 0 & R_I \\ R_I & 0 & 0 \\ 0 & R_I & 0 \end{pmatrix}, \]

where

\[
R_a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
R_I = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \]

The spin-nematic orders \( \hat{Q}_\lambda \) (\( \lambda = c,d,e,f \)) can be constructed by summing up the corresponding operators in Eq. (17,18,19,20). For example, \( \hat{Q}_c \) is given by

\[
\hat{Q}_c = \frac{1}{L} \sum_n (S^y_{1+3n} S^z_{2+3n} + S^y_{2+3n} S^z_{3+3n} + S^y_{3+3n} S^z_{1+3n}),
\]

and the other three spin-nematic orders can be obtained similarly. There are three other degenerate ground states \( |\Omega_\alpha> \) (\( \alpha = x, y, z \)) which can be obtained from \( |\Omega_c> \) by

\[
|\Omega_x> = R(\hat{x}, \pi)|\Omega_c>, \\
|\Omega_y> = R(\hat{y}, \pi)|\Omega_c>, \\
|\Omega_z> = R(\hat{z}, \pi)|\Omega_c>,
\]

where \( R(\hat{\alpha}, \pi) \) (\( \alpha = x, y, z \)) are the representative operations in the three out of four equivalent classes in \( O_h/D_{3d} \) excluding the equivalent class containing the identity element. Generically, all the four order parameters in Eq. (20) should be nonzero. We will show in the next section that this is indeed the case, though \( c, d \) are about one order of magnitudes smaller than \( e, f \).

It is also interesting to work out the explicit forms of the spin-nematic orders within the original frame. The spin-nematic orders in the original frame can be obtained straightforwardly by applying the inverse of the six-sublattice rotation to the expressions in Eq. (17,18,19,20). The spin-nematic orders thus obtained are summarized as follows,

\[
\hat{Q}^{(0)}_c = \frac{1}{L} \sum_j (S^z_j S^y_{j+1} + S^y_j S^z_{j+1}), \\
\hat{Q}^{(0)}_d = \frac{1}{L} \sum_n (S^z_{1+2n} S^y_{2+2n} + S^y_{1+2n} S^z_{2+2n} + S^y_{2+2n} S^z_{3+2n} + S^z_{2+2n} S^y_{3+2n}), \\
\hat{Q}^{(0)}_e = \frac{1}{L} \sum_n (S^y_{1+2n} S^z_{2+2n} + S^z_{2+2n} S^y_{3+2n}), \\
\hat{Q}^{(0)}_f = \frac{1}{L} \sum_j S^z_j S^z_{j+1},
\]

in which all the spin operators refer to the original frame.
ground state of a finite size system calculated in DMRG we note a subtlety in DMRG calculations. In general, the parameter in the six-sublattice rotated frame. Here

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
(a) & $h_z = 10^{-3}$ & No field & $h_z = -10^{-3}$ \\
\hline
$E_1$ & -3.8226887 & -3.8220786 & -3.8222885 \\
$E_2 - E_1$ & 7.99 & 10^{-4} & 6.90 & 10^{-3} & 3.51 & 10^{-3} \\
$E_3 - E_1$ & 8.55 & 10^{-4} & 6.90 & 10^{-3} & 3.52 & 10^{-3} \\
$E_4 - E_1$ & 8.55 & 10^{-4} & 6.90 & 10^{-3} & 7.68 & 10^{-4} \\
$E_5 - E_1$ & 1.14 & 10^{-3} & 7.68 & 10^{-4} & 7.68 & 10^{-4} \\
$E_6 - E_1$ & 1.14 & 10^{-3} & 7.68 & 10^{-4} & 8.31 & 10^{-4} \\
\hline
\end{tabular}
\caption{Energies of several lowest lying states computed with Lanczos Exact Diagonalization. The data refer to $L = 24$ sites, and $\phi = 0.06\pi$.}
\end{table}

C. Numerical results

Next we discuss how to numerically determine the expectation values of the order parameters. Here we make a comment about the DMRG numerics that we have performed in the calculations. In our work, the DMRG method was used on chains with length up to $L=72$ sites and periodic boundary conditions within the six-sublattice rotated frame. Even though it is known that DMRG convergence is hard for periodic boundary conditions, we checked that our results are converged using up to $m = 1000$ states with a truncation error below $10^{-6}$ as in previous investigations in Ref. [58].

The order parameter squared \((\langle D_{i}^{\alpha\beta}\rangle)^2\) can be calculated from the spin-nematic correlation functions \(\langle S_{n}^{\alpha} S_{n+1}^{\beta} \cdot S_{n+3}^{\alpha} S_{n+4}^{\beta} \rangle\) in the long distance limit (i.e., $n \gg 1$), in which $D_{i}^{\alpha\beta} = S_{i}^{\alpha} S_{i+1}^{\beta}$ is the spin-nematic order parameter in the six-sublattice rotated frame. Here we note a subtlety in DMRG calculations. In general, the ground state of a finite size system calculated in DMRG numerics may be an arbitrary linear combination of the four nearly degenerate states (becoming exactly degenerate in the thermodynamic limit) with the coefficients depending on numerical details. Thus the numerical results may not represent the true values of the correlation functions in the thermodynamic limit. In addition, when performing the finite size scaling, this may lead to a random oscillation of the correlation functions by varying the system size which does not exhibit the correct finite size scaling behavior. Fortunately, the spin-nematic correlation functions \(\langle S_{n}^{\alpha} S_{n+1}^{\beta} \cdot S_{n+3}^{\alpha} S_{n+4}^{\beta} \rangle\) acquire the same values in any of the four degenerate ground states in the thermodynamic limit, since pairs of $S_i^{\alpha}$ appear in the correlation functions which does not change sign under $R(\alpha, \pi)$ ($\alpha = x, y, z$). Therefore, the previously mentioned complexity does not exist, and the values of the order parameters can be safely extracted from the correlation functions. On the other hand, this is not the case for the \(O_h \rightarrow D_4\), where correlation functions have to be carefully recombined, which will be discussed in detail in Sec. [14].

DMRG numerics have been performed to calculate the expectation values \(\langle D_{i}^{\alpha\beta} D_{i+3}^{\alpha\beta}\rangle\) for three different system sizes. In Fig. 4(a), \(\langle D_{1}^{14} D_{1+3}^{14}\rangle\) is plotted as a function of $j$ at $\phi = 0.06\pi$ in which the black, red and green curves represent the results for the system sizes $L = 24$, 48 and 72, respectively, where $j \in 3\mathbb{Z}$. The numerical results for the correlation functions of the other five spin-nematic-c orders, i.e., \(\langle D_{i}^{1x} D_{i+3}^{1y}\rangle,\langle D_{i}^{1y} D_{i+3}^{1z}\rangle,\langle D_{i}^{2y} D_{i+3}^{2y}\rangle,\langle D_{i}^{2z} D_{i+3}^{2z}\rangle,\langle D_{i}^{3z} D_{i+3}^{3z}\rangle,\langle D_{i}^{3y} D_{i+3}^{3y}\rangle\), coincide with those for \(\langle D_{i}^{4x} D_{i+3}^{4y}\rangle\), hence not explicitly shown, which provide evidence for the relations in Eq. (19). It can be observed that the difference between the red and green curves is already very small, showing a tendency towards a convergence by increasing the system size. The asymptotic value determined by the red dashed line in Fig. 4(a) at large $n$ gives $c^2 \approx 0.00028$, where $c$ is defined in Eq. (17). Similarly, in Fig. 4(b), the numerical results for \(\langle D_{i}^{12} D_{i+3}^{13}\rangle,\langle D_{i}^{13} D_{i+3}^{12}\rangle, and \langle D_{i}^{22} D_{i+3}^{13}\rangle\) are displayed, which gives $d^2 \approx 0.00016$, $e^2 \approx 0.0199$, and $f^2 \approx 0.0082$ according to Eq. (17) [18,20], respectively. Again only one of the correlation functions in each group of Eq. (17) is displayed, and the other correlations in the same group have been numerically verified to be all equal to the chosen one.

On the other hand, the above calculations of the spin-nematic correlation functions are only able to give the magnitudes while not the signs of the order parameters. Next we numerically determine the signs. We will take the order parameter $c$ in Eq. (19) as an example, and the other three orders $d, e, f$ can be calculated in a similar way.

Define a spin-nematic-$c$ field $h_c = -\hbar_c L \hat{Q}_c$, where $\hat{Q}_c$ is given by Eq. (21). As shown in Appendix B since
FIG. 4: (a) $\langle D_{i}^{x} D_{i+1}^{x} \rangle$, (b) $\langle D_{i}^{y} D_{i+1}^{y} \rangle$, (c) $\langle D_{i}^{z} D_{i+1}^{z} \rangle$, and (d) $\langle D_{i}^{x} D_{i+1}^{x} \rangle$ as functions of $j$ ($j \in 3Z$) for three different system sizes $L = 24, 48, 72$ plotted as black, red and green curves, respectively. In (a,b,c), $D_{i}^{a} S_{i+1}^{a}$’s defined in Eq. (17,18,19,20) are the spin-nematic order parameters in the six-sublattice rotated frame, and DMRG numerics are performed at $\phi = 0.06\pi$ ($\theta = \pi/2$) with periodic boundary conditions.

$$|\Omega_{\alpha}\rangle = R(\alpha, \pi) (\alpha = x, y, z), \text{ we have}$$

$$e = \langle \Omega_{x} | S_{x}^{a} S_{y}^{a} | \Omega_{x} \rangle = -\langle \Omega_{x} | S_{x}^{a} S_{x}^{a} | \Omega_{x} \rangle = -\langle \Omega_{x} | S_{z}^{a} S_{x}^{a} | \Omega_{x} \rangle,$$

$$= -\langle \Omega_{y} | S_{x}^{a} S_{y}^{a} | \Omega_{y} \rangle = \langle \Omega_{y} | S_{y}^{a} S_{y}^{a} | \Omega_{y} \rangle = -\langle \Omega_{y} | S_{z}^{a} S_{y}^{a} | \Omega_{y} \rangle,$$

$$= -\langle \Omega_{z} | S_{z}^{a} S_{z}^{a} | \Omega_{z} \rangle -\langle \Omega_{z} | S_{x}^{a} S_{z}^{a} | \Omega_{z} \rangle = \langle \Omega_{z} | S_{z}^{a} S_{x}^{a} | \Omega_{z} \rangle.$$

$$\tag{24}$$

Next consider a small $h_e$ field which satisfies $\Delta E \ll |e|/h_e |L| < E_g$, in which $L$ is the system size, $E_g$ is the excitation gap, and $\Delta E$ is the finite size splitting of the ground state at zero field. Such choice of $h_e$ gives rise to a degenerate perturbation within the four-dimensional ground state subspace, and at the same time, no mixing between the ground states and the excited states is induced. According to Eqs. (19,24), the energies of the four ground states under $h_e$ are

$$\delta E(|\Omega_{e}\rangle) = -eh_{e}L,$$

$$\delta E(|\Omega_{\alpha}\rangle) = \frac{1}{3}eh_{e}L,$$

$$\tag{25}$$

in which $\alpha = x, y, z$, and the energy $\delta E$ is measured with respect to the zero field case. Therefore, if $\text{sgn}(h_{e}) = \text{sgn}(e)$, $|\Omega_{e}\rangle$ is the ground state which is nondegenerate with an energy lowered by an amount $|eh_{e}|L$. On the other hand, if $\text{sgn}(h_{e}) = -\text{sgn}(e)$, the ground states are three-fold degenerate, and in fact, $|\Omega_{x}\rangle, |\Omega_{y}\rangle, |\Omega_{z}\rangle$ have the same energy which is lower than the energy at zero field by an amount $\frac{1}{3}|eh_{e}|L$. In this way, the sign of the spin-nematic order parameter can be obtained from that of the corresponding spin-nematic field by inspecting the change of the ground state degeneracy. In addition, let $\delta E_g(h)$ be the ground state energy change with a field $h$. Then according to Eq. (25), we obtain

$$\frac{\delta E_g(|h|\text{sgn}(\lambda))}{\delta E_g(|h|\text{sgn}(\lambda))} = 3.$$

in which $\lambda = c, d, e, f$.

Furthermore, we also note that with a field $h_e$ satisfying $\text{sgn}(h_e) = \text{sgn}(e)$, the state $|\Omega_{e}\rangle$ is selected as the ground state out of the initially four nearly degenerate ground states. Hence, we can directly compute the expectation value of the spin-nematic order parameters $S_{i}^{a} S_{i+3}^{a}, S_{i+1}^{a} S_{i+3}^{a}, S_{i+2}^{a} S_{i+3}^{a}, S_{i+3}^{a} S_{i+3}^{a}$ (as given by Eq. (19)) in numerics. Notice that this cannot be done at zero spin-nematic fields since the true ground state in a finite size system may be an arbitrary linear combination of the four states $|\Omega_{a}\rangle$ ($a = e, x, y, z$), which leads to a random cancellation of the expectation value due to the sign differences in Eq. (19) and Eq. (24).

In Table IV the energies of the six lowest states are displayed under different spin-nematic fields $h_{\alpha}$ ($\alpha = x, y, z, L$).
c, d, e, f) at $\phi = 0.06\pi$. The results are obtained from ED calculations on a system of $L = 24$ sites with periodic boundary conditions. As can be seen from Table I, the four states circled by the blue lines are separated from the other two states by an energy $\simeq 6.9 \times 10^{-4}$, which is one order of magnitude larger than the energy splitting among the four states which is $\simeq 0.77 \times 10^{-4}$. This provides numerical evidence for the four-fold ground state degeneracy at zero field as discussed in Fig. 3. On the other hand, as shown in Table I, the system is nondegenerate under positive spin-nematic fields for all the four $h_{\alpha}$'s where $\alpha = c, d, e, f$, but approximately three-fold degenerate when the fields are negative. According to the previous discussions, this provides numerical evidence for the spin-nematic order parameters $c, d, e, f$ to be all positive. In addition, we check if the relations in Eq. (26) for the energy changes are satisfied. According to Table I, the ratios $r = \delta E_g(|h_{\lambda}|\text{sgn}(\lambda))/\delta E_g(-|h_{\lambda}|\text{sgn}(\lambda))$ are

$$
\begin{align*}
\lambda & \quad c & \quad d & \quad e & \quad f \\
r & \quad 2.91 & \quad 2.96 & \quad 2.51 & \quad 2.70.
\end{align*}
$$

As can be seen from Eq. (27), while the ratios for $\lambda = c, d$ agree well with $3$, there are slight deviations of $r$ from $3$ for $e, f$. In fact, as will be seen from Fig. 4, while the values of $c, d, e, f$ are much larger than $c, d$. Hence, a $10^{-3}$ field is too large for $e$ and $f$ in the sense that the conditions $\Delta E \ll |\lambda||h_{\lambda}|L \ll E_g$ are spoiled when $\lambda = e, f$. In these cases, $\delta E_g$ also involves the contributions from many excited states, not just the ground state quartet. Because of this reason, the relation in Eq. (26) is not satisfied to an excellent level for $h_e, h_f \sim 10^{-3}$. A better agreement of $r$ with $3$ can be obtained for $e, f$ by choosing a much smaller value of the field $h_{\lambda}$.

Furthermore, we have also measured the expectation values of the spin-nematic orders under positive spin-nematic fields, and the results are shown in Fig. 4 It can be read from Fig. 5 that the expectation values are

$$
c \simeq 0.014, \quad d \simeq 0.012, \quad e \simeq 0.145, \quad f \simeq 0.094, \quad (28)
$$

regardless of which field $h_{\alpha}$ ($\alpha = c, d, e, f$) is applied. Here we note that as can be seen from Fig. 5 while the values of $c$ and $d$ are independent of $h_{\lambda}$ ($\lambda = c, d, e, f$), there are small variations of $e$ and $f$ under different types of spin-nematic fields. The reason is the same as before. In fact, a field of $10^{-3}$ is too large for $h_e$ and $h_f$, which mixes the ground state subspace with the excited states. As a result, in addition to the ordering in the ground state, the order parameter also acquires contributions from excited states due to a nonzero spin-nematic susceptibility. This explains why the measured values of $e$ and $f$ under $h_e, h_f$ are larger than those under $h_c, h_d$. On the other hand, by taking the square root of the extracted values from Fig. 5 we obtain

$$
c \simeq 0.017, \quad d \simeq 0.013, \quad e \simeq 0.141, \quad f \simeq 0.091. \quad (29)
$$

Comparing Eq. (28) with Eq. (29), it is clear that the values of $c, d, e, f$ obtained from the two different methods agree well.

![Figure 5: Measured spin-nematic order parameters $c$ (black), $d$ (red), $e$ (green), $f$ (blue) under small spin-nematic fields. The vertical axis is the measured order value, and the results of different fields are displayed at different horizontal coordinates. All the spin-nematic fields $h_c, h_d, h_e, h_f$ are taken positive with a magnitude equal to $10^{-3}$. In all cases, ED calculations are performed on a periodic system of $L = 24$ sites at $\phi = 0.06\pi$.](image)

![Figure 6: $O_{SN} = 4e$ as a function of $\phi$. The black, red and orange curves represent the results for finite systems of $L = 24, 48$ and 72 sites. DMRG numerics are performed with periodic boundary conditions.](image)
the region between the two dashed lines, though the black curve for the smaller system of $L = 24$ sites exhibits a large deviation from the other two curves. As can also be seen, there is a strong finite size dependence in the Kitaev phase, where the correlation function is negative for $L = 24$ and 48, but become vanishingly small for $L = 72$.

We also note that the order parameter decreases to zero continuously by passing through $\phi_c'$ from left to right, indicating a second order phase transition. Since the region $\phi > \phi_c'$ corresponds to a different ordered phase, it is likely that the phase transition point $\phi_c'$ is a deconfined quantum critical point separating two ordered phases, which will be discussed in Sec. IIIIB. Before going to that, we first discuss the “$O_h \rightarrow D_4$” phase in the next section.

**IV. THE “$O_h \rightarrow D_4$” PHASE**

In this section, we first briefly review the “$O_h \rightarrow D_4$” phase which has already been discussed in Ref. [55]. After that, we also study the evolution of the order parameters by varying $\phi$.

![FIG. 7: Spin orientations in the original frame corresponding to Eq. (30)](image)

The spin $z$-axis is taken as the chain direction.

In the “$O_h \rightarrow D_4$” phase, the spins are FM aligned. There are six degenerate ground states with all spins pointing to $\pm \hat{x}, \pm \hat{y}, \pm \hat{z}$ directions. For example, the spin polarizations in the $+\hat{z}$-state are

$$\langle \hat{S}_1 \rangle = a \hat{z}, \langle \hat{S}_2 \rangle = b \hat{z}, \langle \hat{S}_3 \rangle = b \hat{z},$$

in which $a, b$ are magnitudes of the spin orderings, and only $\{ \langle \hat{S}_i \rangle \}_{i=1,2,3}$ are shown since $T_{3a}$ is unbroken. The little group of Eq. (30) has been worked out to be [55],

$$<R_a T_a R(\hat{z}, \pi) T_1 R(\hat{z}, \pi), T(R_a T_a)^{-1} R_1 R_{1a} T_a> \cong D_4,$$

which holds modulo $T_{3a}$. Since $|O_h| = 48$ and $|D_4| = 8$, the number of degenerate ground states is $|O_h/D_4| = 6$. We also note that the spin ordering in the original frame exhibits a rather complicated pattern with a six-site periodicity as shown in Fig. 7. Since $H$ in Eq. (1) is invariant under $T_{2a}$, the translational symmetry by two sites is broken in the original frame.

To numerically compute the value of the order parameters, a small field $h_z$ is applied along $z$-direction which satisfies $\Delta E \ll h_z L \ll E_g$, where $L$ is the system size, $E_g$ is the excitation gap, and $\Delta E$ is the finite size splitting of the ground state sextet at zero field. The field $h_z$ is able to polarize the system with spin alignments given by Eq. (30). Similar to the spin-nematic case, such choice of $h_z$ ensures a degenerate perturbation within the ground state sextet while not mixing with the excited states. By applying $h_z$, the order parameters can be obtained by directly computing the expectation values $\langle \hat{S}_i \rangle$, from which the values of $a, b$ in Eq. (30) can be extracted.

Fig. [S] (a) shows $2\langle S_j^i \rangle$ as a function of the site $j$ at three representative angles $\phi = 0.06\pi, 0.13\pi$ and $0.25\pi$, in which the order parameter has been normalized to $\langle S_j^i \rangle_0 / 0.5$ since the saturation value of $S_j^i$ is 1/2. The numerical results are obtained from ED calculations on a system of $L = 24$ sites with periodic boundary conditions, and the field $h_z$ is chosen as $10^{-4}$. As can be seen from Fig. [S] (a), the order parameters are vanishingly small at $\phi = 0.06\pi$, finite at $\phi = 0.13\pi$, and saturated at $\phi = 0.25\pi$ which is the hidden SU(2) symmetric point. In addition, the pattern of $2\langle S_j^i \rangle$ at $\phi = 0.13\pi$ is fully consistent with Eq. (30).

We have numerically extracted the values of the normalized order parameters (i.e., $2a, 2b$) for $\phi \in [0, 0.4\pi]$ under a small field $h_z = 10^{-4}$. The results are displayed in Fig. [S] (b), in which the black and grey curves represent $2a$ and $2b$, respectively. Here we note that since $\Delta E$ and $E_g$ vary as $\phi$ is changed, in principle one should use a $\phi$-dependent field such that the condition $\Delta E \ll h_z L \ll E_g$ is satisfied. However, a field $h_z = 10^{-4}$ in the “$O_h \rightarrow D_4$” phase is always a good choice except in a small neighborhood of the phase transition point $\phi_c'$. In fact, since $\phi_c'$ is possibly a critical point, the ground state is nondegenerate at $\phi_c'$. For a finite size system, the critical region extends to a small finite range of $\phi$ around $\phi_c'$, within which there is no clear energy separation between the ground state manifold and the excited states. This means that the condition $\Delta E \ll h_z L \ll E_g$ cannot be satisfied in the finite size critical region. This also explains why the FM orders percolate into the “Spin-Nematic” phase (as can be seen from Fig. [S] (b)) where the ground state degeneracy is already 4 instead of 6.

To study the effects of different choices of $h_z$, the normalized order parameter $2a$ is calculated as a function of $\phi$ for $h_z = \{1, 2, 4, 7, 10\} \times 10^{-4}$, and the results are shown in Fig. [S] (c). As can be seen from Fig. [S] (c), even increasing $h_z$ by a small amount is able to lift the curve significantly in the parameter region $\phi \leq \phi_c'$. In fact, for $h_z = 10^{-3}$, the value of $2a$ is already very huge in the entire region of $\phi < \phi_c'$. This indicates that there is a large magnetic susceptibility in both the “Spin-Nematic” and the “Kitaev” phases. The origin of such a huge magnetic susceptibility remains unclear and will be left for a future study.

Finally, we also discuss the behaviors of the correlation functions in the “$O_h \rightarrow D_4$” phase in the absence of any field. Unlike the situation in the “Spin-Nematic” phase, we are facing a difficulty at this point. Generically, the finite size ground state is some arbitrary linear combination of the six nearly degenerate ground states (exactly degenerate in the thermodynamic limit). Since the correlation function $\langle S_i^\alpha S_j^\beta \rangle$ ($\alpha, \beta = x, y, z$) may take different values on the six ground states, the numerical results of
The values of \( S_i \) will have a strong finite size dependence. To resolve this difficulty, the invariant correlation functions have to be constructed which take the same values on the different ground states. In the current case, there are ten invariant correlation functions derived in Appendix C three of which are

\[ a^2 = \langle S_i^x S_i^{x+3n} + S_i^y S_i^{y+3n} + S_i^z S_i^{z+3n} \rangle, \quad (32) \]

\[ b^2 = \langle S_i^x S_i^{x+3n} + S_i^y S_i^{y+3n} + S_i^z S_i^{z+3n} \rangle, \quad (33) \]

\[ 2ab = \langle S_i^x S_i^y + S_i^x S_i^z + S_i^y S_i^x + S_i^z S_i^y + S_i^x S_i^{x+3n} + S_i^y S_i^{y+3n} + S_i^z S_i^{z+3n} \rangle, \quad (34) \]

in which the equality holds in the limit \( n \gg 1 \).

The numerical results for the three invariant correlation functions in Eqs. (32, 33, 34) are displayed in Fig. 8 (a, b, c), respectively, where three different systems sizes \( L = 24, 48, 72 \) are calculated at a representative point \( \phi = 0.157 \) \( \pi \) in the “\( O_h \rightarrow D_4 \)” phase. Periodic boundary conditions are taken in DMRG calculations with no magnetic field imposed. As can be seen from Fig. 8 (a, b, c), the lines for the three different sizes overlap, and the results have already reached good finite size convergences. The values of \( a^2, b^2, 2ab \) can be extracted from the asymptotic values of the invariant correlation functions at large \( n \). The results are \( a^2 = E_1, b^2 = E_2, 2ab = E_3 \), where \( E_1 \approx 0.177, E_2 \approx 0.209, E_3 \approx 0.3844 \). Since \( 2ab = 2\sqrt{a^2 b^2} \), we check if the relation \( E_3 = \sqrt{E_1 E_2} \) is satisfied. Indeed, \( \sqrt{E_1 E_2} \) is equal to 0.3847, which has excellently agreement with the value of \( E_3 \), thereby providing another strong evidence for the spin orientation pattern in Eq. (30).

In Fig. 9, the normalized order parameter \( O_{FM} = \sqrt{\langle S_i^x S_i^{x+3n} + S_i^y S_i^{y+3n} + S_i^z S_i^{z+3n} \rangle / n} \) \( (n \gg 1) \) is displayed as a function of \( \phi \) calculated for three system sizes \( L = 24, 48, 72 \). As can be seen from Fig. 9, \( O_{FM} \) is non-vanishing and percolates in the “Spin-Nematic” phase. This seems to suggest a coexistence of the “Spin-Nematic” and “\( O_h \rightarrow D_4 \)” orders in the range \( \phi \in [\phi_c', \phi_c] \). However, as discussed in Sec. IIIA, the fourfold ground state degeneracy is not compatible with any rank-1 spin order, which is against the possibility of a coexistence of the two orders. A probable origin of the large \( O_{FM} \) may be attributed to the large magnetic susceptibility in the “Spin-Nematic” phase as discussed in Sec. IV. Since the correlation function \( \langle S_i^a S_j^b \rangle \) is roughly speaking the response of \( S_j^b \) to a local field \( S_i^a \) at site \( i \) (to be

FIG. 8: (a) \( 2\langle S_i^x \rangle \) as a function of \( j \) at three angles \( \phi = 0.06\pi, 0.13\pi, 0.25\pi \), (b) \( 2a, 2b \) as functions of \( \phi \) with a small magnetic field \( h_z = 10^{-4} \), (c) \( 2a \) as a function of \( \phi \) at several different \( h_z \)'s. In all of (a,b,c), ED calculations are performed on a system of \( L = 24 \) sites with periodic boundary conditions.

FIG. 9: Invariant correlation functions in the “\( O_h \rightarrow D_4 \)” phase for (a) Eq. (32), (b) Eq. (33) and (c) Eq. (34), in which \( j = 3n \). In (a,b,c), DMRG numerics are performed on periodic systems at \( \phi = 0.15\pi \) where three different system sizes \( L = 24, 48, 72 \) are calculated shown by the black, red, green curves, respectively.
more precise, it corresponds to the frequency-dependent susceptibility integrated over all frequencies), it is possible that $\langle S_i^x S_j^x \rangle$ can acquire a large expectation value if the system size is not large enough. Unfortunately, there is no available estimation about the crossover system size $L_c$ above which the correlation function $\langle S_i^x S_j^x \rangle$ becomes vanishingly small, since a theory about the spin-nematic phase is not developed at the moment. A better clarification for this issue in a future study will be desirable.

We note that there is another argument which is against the coexistence of a rank-1 spin order with the spin-nematic order. Suppose $O_{FM}$ in Fig. 10 represents a true rank-1 order in the “Spin-Nematic” phase. As can be read from Fig. 10, $O_{FM} \sim 0.4$ at $\phi = 0.08\pi$, corresponding to $a \sim 0.2$. Then a field $h_z = 2 \times 10^{-4}$ is able to lower the energy of the +z state by $ah_z L \sim 10^{-4}$ for $L = 24$, which is already much larger than the finite size splitting $\Delta E \sim 1.7 \times 10^{-4}$ of the ground state quartet as can be read from Table 2. Therefore, the field $h_z = 2 \times 10^{-4}$ should be able to fully polarize the system. However, as can be seen from Fig. 8, $O_{FM}$ is much smaller than 0.4 at $\phi = 0.08\pi$, contradicting the picture of the coexistence of a rank-1 spin order at $\phi = 0.08\pi$.

V. EVIDENCE FOR THE DECONFINED QUANTUM CRITICAL POINT

In this section, we combine the previous results and show evidence for $\phi'_c$ to be a continuous phase transition point separating two ordered phases.

Fig. 10 (b) displays the normalized order parameters of the “Spin-Nematic” and “$O_h \rightarrow D_4$” phases when $\phi$ is varied. The orange and black curves show $O_{SN} = 4e$ and $O_{FM} = 2a$ as functions of $\phi$, where $e$ and $a$ are the defined in Eq. (19) and Eq. (30), respectively. As can be seen from Fig. 10 (b), there is evidence for both $O_{SN}$ and $O_{FM}$ to vanish at $\phi'_c$. Hence $\phi'_c$ is likely a deconfined quantum critical point which corresponds to a continuous phase transition separating two ordered phases. The percolation of $O_{FM}$ into the “Spin-Nematic” phase is possibly due to a large magnetic susceptibility as discussed in Sec. IV.

In Fig. 11 (a), $\chi^c = -\partial^2 e_0 / \partial \phi^2$ is shown as a function of $\phi$, calculated by using iDMRG and for several different systems sizes $L = 18, 24, 26, 30$ using ED, where $e_0 = E / L$ is the ground state energy per site. As can be seen from Fig. 11 (a), all the finite size ED results show no singular behavior around $\phi'_c \sim 0.1\pi$, indicating a continuous phase transition, though the iDMRG results exhibit some irregularities around 0.101$\pi$. To further elucidate the nature of the phase transition at $\phi'_c$, we have studied $\lambda_1$ as a function of $\phi$ shown in Fig. 11 (b), where $\lambda_1$ is the largest eigenvalue of the reduced density matrix of a subsystem of the first $L / 2 - 1$ sites. As can be observed from Fig. 11 (b), there is a dip at $\phi''_c \sim 0.101\pi$ where the derivative of $\lambda_1$ with respect to $\phi$ is not continuous. This provides evidence for a phase transition to occur at $\phi'_c$.

Finally, we mention that the nature of the phase transition point $\phi'_c$ remains unclear at the moment. The critical properties of $\phi'_c$ and the corresponding conformal field theory or deconfined quantum critical theory describing the low energy physics at $\phi'_c$ will be left for future studies.

VI. THE “KITAEV” PHASE

In this section, we briefly discuss the “Kitaev” phase in the range $\phi \in [-\phi''_c, \phi'_c]$, where the physics remains unclear. As shown in Fig. 12, the study of the ground state energy shows no signature of singularity at the AFM Kitaev point $\phi = 0$, therefore the intervals $[-\phi''_c, 0]$ and $[0, \phi'_c]$ are likely in the same phase. As can be seen from Fig. 11 (a), the ED results of $\chi^c$ show big peaks for $L = 18, 24, 26, 30$ sites around $\phi = 0.05\pi$, except $L = 24$ where the peak is small. However, it can be observed that the peak position shifts to smaller value of $\phi$ by increasing the system size. Indeed, the iDMRG results of $\chi^c$ in Fig. 11 (a) predicts $\phi''_c$ to be 0.034$\pi$, which is consistent with the sudden jump of $\lambda_1$ in Fig. 11 (b) at the same value of $\phi$. Based on this, we conjecture that there may be a strong finite size dependence of $\phi''_c$, and the thermodynamic value of $\phi''_c$ is possibly 0.034$\pi$ as given by the iDMRG results in Fig. 11 (a,b).

The study of the ground state degeneracy in the Kitaev phase shows a strong finite size dependence and no reliable value can be extracted. Fig. 1 (b) indicates that there is no spin-nematic nor rank-1 spin orders in the Kitaev phase. The AFM Kitaev point ($K > 0, \Gamma = J = 0$) is exactly solvable through Jordan-Wigner transformation, and it is known that the ground state is 2$^d$-1-fold
FIG. 11: (a) $\chi_\phi = -\partial^2 e_0 / \partial \phi^2$ vs $\phi$ calculated from ED for $L = 18, 24, 26, 30$ sites and iDMRG, (b) $\lambda_1$ vs $\phi$ calculated from iDMRG, where $e_0 = E/L$ is the ground state energy per site, and $\lambda_1$ is the largest eigenvalue of the reduced density matrix of a subsystem of $L/2 - 1$ sites.

FIG. 12: (a) $E/L$, (b) $\partial(E/L)/\partial \phi$, and (c) $\partial^2(E/L)/\partial \phi^2$ as functions of $\phi$. DMRG calculations are performed on $L = 24$ sites with periodic boundary conditions.

degenerate for a system of finite size $L^{[60]}$. In the thermodynamic limit, this becomes an exponentially large infinite degeneracy. Therefore, it is expected that there are huge quantum fluctuations in the Kitaev phase. The irregular behaviors in the Kitaev phase in the iDMRG results in Fig. 11 (a,b) possibly arise from convergence problems due to the large number of nearly degenerate states (exactly degenerate at $\phi = 0$). Whether there exists a topological string order in the Kitaev phase remains to be explored further.

VII. CONCLUSION

In summary, we have studied the phase diagram of the spin-1/2 Kitaev-Gamma chain with an AFM Kitaev coupling. In addition to the emergent SU(2)$_1$ and the $O_h \rightarrow D_4$ phases established in Ref. $[8]$ two new phases are identified, i.e., a phase of spin-nematic orders and a "Kitaev" phase. Numerics provide evidence for the phase transition between the $O_h \rightarrow D_4$ and the spin-nematic phases to be a continuous phase transition, which likely corresponds to a deconfined quantum critical point. More detailed studies on the critical properties of this phase transition will be left for future considerations. The nature of the “Kitaev” phase remains unclear, in which no evidence of any spin ordering nor Luttinger liquid behavior is found. Whether there exists any topological string order $[51]$ is worth further studies.

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Appendix A: Explicit expressions of the Hamiltonian

In this appendix, we spell out the terms in the Hamiltonians in different frames. In general, we write the Hamiltonian \( H \) as \( H = \sum_{j=1}^{L} H_{j,j+1} \) where \( H_{j,j+1} \) is the term on the bond between the sites \( j \) and \( j+1 \). The forms of \( H_{j,j+1} \) will be written explicitly.

In the unrotated frame, the form of \( H_{j,j+1} \) has a two-site periodicity. We have

\[
H_{2n+1,2n+2} = K S_{2n+1}^y S_{2n+2}^y + \Gamma (S_{2n+1}^y S_{2n+2}^z + S_{2n+1}^z S_{2n+2}^y), \\
H_{2n+2,2n+3} = K S_{2n+2}^x S_{2n+3}^y + \Gamma (S_{2n+2}^x S_{2n+3}^z + S_{2n+2}^z S_{2n+3}^x). 
\]  
(A1)

In the six-sublattice rotated frame, the form of \( H_{j,j+1} \) has a three-site periodicity. We have

\[
H'_{3n+1,3n+2} = -K S_{3n+1}^x S_{3n+2}^x - \Gamma (S_{3n+1}^y S_{3n+2}^y + S_{3n+1}^z S_{3n+2}^z), \\
H'_{3n+2,3n+3} = -K S_{3n+2}^y S_{3n+3}^y - \Gamma (S_{3n+2}^x S_{3n+3}^x + S_{3n+2}^z S_{3n+3}^y), \\
H'_{3n+3,3n+4} = -K S_{3n+3}^z S_{3n+4}^z - \Gamma (S_{3n+3}^y S_{3n+4}^y + S_{3n+3}^x S_{3n+4}^x). 
\]  
(A2)

Appendix B: The spin-nematic order parameters

Recall from Sec. III that the order parameter matrix \( M \) satisfies

\[
U_a M U_a^{-1} = M, \quad (B1)
\]

and

\[
U_I M U_I^{-1} = M,. \quad (B2)
\]

The requirement Eq. (B1) leads to

\[
M = \begin{pmatrix}
A & C^T \\
C & R_a^{-1} C R_a^{-1}
\end{pmatrix}, \quad (B3)
\]

in which \( A \) is a symmetric matrix. Eq. (B2) put further constraints on \( A \) and \( C \) as

\[
(R_a R_I) A (R_a R_I)^{-1} = A, \\
(R_a R_I) C (R_a R_I)^{-1} = C^T. \quad (B4)
\]

Next we solve all possible forms of \( A \) and \( C \) satisfying Eq. (B4). Using \( R_a \) and \( R_I \) given in Eq. (16), we are able to obtain

\[
A = \begin{pmatrix} 
\lambda & \nu & \sigma \\
\nu & \lambda & \sigma \\
\sigma & \sigma & \mu
\end{pmatrix}, \quad C = \begin{pmatrix} 
a & c & d \\
d & b & f \\
c & e & b
\end{pmatrix}. \quad (B5)
\]

As a result, there are ten linear independent solutions of \( M \), summarized as follows,

\[
\lambda = \langle S_{1}^{x} S_{1}^{x} \rangle = \langle S_{1}^{y} S_{1}^{y} \rangle = \langle S_{1}^{z} S_{1}^{z} \rangle = \langle S_{1}^{y} S_{1}^{x} \rangle = \langle S_{1}^{x} S_{1}^{y} \rangle \]
\[
\mu = \langle S_{1}^{x} S_{1}^{x} \rangle = \langle S_{1}^{y} S_{1}^{y} \rangle = \langle S_{1}^{z} S_{1}^{z} \rangle \]
\[
\nu = \langle S_{1}^{x} S_{1}^{x} \rangle = \langle S_{1}^{y} S_{1}^{y} \rangle = \langle S_{1}^{z} S_{1}^{z} \rangle = \langle S_{1}^{y} S_{1}^{x} \rangle = \langle S_{1}^{x} S_{1}^{y} \rangle \]
\[
\sigma = \langle S_{1}^{x} S_{1}^{x} \rangle = \langle S_{1}^{y} S_{1}^{y} \rangle = \langle S_{1}^{z} S_{1}^{z} \rangle = \langle S_{1}^{y} S_{1}^{x} \rangle \]
\[
\sigma = \langle S_{2}^{z} S_{2}^{z} \rangle = \langle S_{2}^{y} S_{2}^{y} \rangle = \langle S_{2}^{x} S_{2}^{x} \rangle \]
\[
\sigma = \langle S_{3}^{z} S_{3}^{z} \rangle = \langle S_{3}^{y} S_{3}^{y} \rangle = \langle S_{3}^{x} S_{3}^{x} \rangle = \langle S_{3}^{y} S_{3}^{x} \rangle = \langle S_{3}^{x} S_{3}^{y} \rangle. \quad (B6)
\]
We note that the spin-nematic fields

There are six equivalent classes in the quotient

| matrix Φ. and Φ is a 9

For

In this appendix, we construct the invariant correlation functions in the "O₇ → D₄" phase. Before proceeding to the constructions of the invariant correlation functions, we first make some comments on the symmetry breaking pattern. There are six equivalent classes in the quotient O₇/D₄, which is not a group since D₄ is not a normal group of O₇. The six representative elements in the equivalent classes can be chosen as the group elements in D₃ = <R₉,T₀,R₁I>, mod T₃₀. Notice that this is intuitively correct since R₉ and R₁ is able to rotate the +ẑ-direction to the other five directions within ±ξ (α = x, y, z).

Next consider the correlation function ⟨SαₓSβᵧ⟩. In what follows, we will write i, j to be modulo 3, but always bear in mind that |i − j| → ∞. All the two point correlation functions are encoded in the following operators ˆΦ,

\[ ˆΦ = ˆS^T Φ ˆS, \]  

in which

\[ ˆS = (S_x \ S_y \ S_z \ S_y \ S_z \ S_y \ S_z \ S_x \ S_z)^T, \]  

and Φ is a 9 × 9 numerical matrix. The 81 independent correlation functions correspond to the 81 choices of the matrix Φ.
Let $\mathcal{U} \in D_3$, and $\hat{U}$ be the corresponding operator in the Hilbert space. Let $U$ be a $9 \times 9$ orthogonal matrix defined as

$$\hat{U}^{-1}\hat{S}\hat{U} = US. \quad \text{(C3)}$$

Let $|\Omega_z\rangle$ be the ground state with all spins pointing to the $+\hat{z}$-direction. Then the other degenerate ground states can be obtained from $\mathcal{U}|\Omega_z\rangle$. Then the invariance of the correlation function requires

$$\langle \Omega_z|\hat{U}^\dagger\hat{\Phi}\hat{U}|\Omega_z\rangle = \langle \Omega_z|\hat{\Phi}|\Omega_z\rangle. \quad \text{(C4)}$$

Using Eq. (C1) and Eq. (C3), we obtain

$$\langle \Omega_z|\hat{S}^T U^T \Phi US|\Omega_z\rangle = \langle \Omega_z|\hat{S}^T \Phi S|\Omega_z\rangle, \quad \text{(C5)}$$

which is satisfied if

$$U^T \Phi = \Phi. \quad \text{(C6)}$$

Since $\mathcal{U} \in D_3$, it is enough to choose the two generators $R_x T_a$ and $R_1 I$ of $D_3$. As long as for these two generators satisfy Eq. (C6), do the other group elements in $D_3$. The corresponding matrix $U_a, U_I$ of these two generators have already been given in Eq. (15). Therefore, we see that Eq. (C6) is exactly the same as Eq. (B1) for $R_x T_a$ and as Eq. (B2) for $R_1 I$. Thus the solutions of $\Phi$ are just the same as those of $M$ in Appendix B.

In summary, the ten invariant correlation functions are

$$a^2 + 2b^2 = \tilde{S}_1 \cdot \tilde{S}_1 + \tilde{S}_2 \cdot \tilde{S}_2 + \tilde{S}_3 \cdot \tilde{S}_3,$$

$$a^2 = S_1^z S_1^z + S_2^z S_2^z + S_3^z S_3^z,$$

$$0 = (S_1^x S_1^x + S_2^x S_2^x + S_3^x S_3^x),$$

$$0 = (S_1^y S_1^y + S_2^y S_2^y + S_3^y S_3^y),$$

$$b^2 = S_1^z S_2^z + S_1^z S_3^z + S_2^z S_3^z,$$

$$2ab = (S_1^x S_2^x + S_1^x S_3^x) + (S_2^x S_3^x + S_1^y S_3^y) + (S_2^x S_3^x + S_1^z S_3^z),$$

$$0 = (S_1^z S_2^z + S_1^z S_3^z),$$

$$0 = (S_2^z S_3^z + S_3^z S_3^z),$$

$$0 = S_1^y S_3^y + S_1^y S_3^y,$$

$$0 = S_2^y S_3^y + S_2^y S_3^y,$$

$$0 = S_3^y S_3^y,$$

in which the symbols $\langle \cdot \cdot \cdot \rangle$ are omitted on the right hand sides of the equations.
