Phase diagram of the spin-1/2 Kitaev-Gamma chain and emergent SU(2) symmetry

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We study the phase diagram of a one-dimensional version of the Kitaev spin-1/2 model with an extra “Γ-term”, using analytical, density matrix renormalization group and exact diagonalization methods. Two intriguing phases are found. In the gapless phase, the low energy theory is described by an emergent SU(2)1 Wess-Zumino-Witten (WZW) model though the exact symmetry group is discrete. On the other hand, the relations between the local spin operators and the WZW currents and primary field contain SU(2) breaking coefficients. A modified nonabelian bosonization formula is proposed to capture such exotic emergent “partial” SU(2) symmetry. In the ordered phase, there is numerical evidence for an $O_h \rightarrow D_8$ spontaneous symmetry breaking.

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A quantum spin liquid is a phase of matter in which the constituent spins are highly entangled with each other without exhibiting any long range order [1–6]. The Kitaev spin-1/2 model on the two-dimensional (2D) honeycomb lattice is an exactly solvable spin liquid model [7], which has received considerable theoretical and experimental interest in the past decade [8–20] due to its potential in realizing quantum computers [21]. On the other hand, additional spin interactions allowed by the lattice symmetries inevitably exist in real materials. The Heisenberg term was first considered as a supplement to the Kitaev model [9]. Later it had been proposed that another off-diagonal term, dubbed the “T-term”, naturally arises in Kitaev materials [22], which dominates over the Heisenberg term in certain cases and may even be crucial to stabilize the ferromagnetic (FM) Kitaev phase [23].

In one dimension (1D), strong quantum fluctuations make 1D spin liquids even more ubiquitous [24–28]. In many circumstances, strongly interacting 1D systems are more amenable to both analytical and numerical treatments. Methods having been proven successful in 1D include conformal field theory (CFT) [27, 29–32], Bethe ansatz [36–40], and the density matrix renormalization group (DMRG) method [41–43]. Due to this reason, 1D physics is not only interesting in its own respect, but also useful in providing hints on strongly correlated physics in higher dimensions when an exact or controllable approach is lacking.

In this work, by combining the analytical, exact diagonalization (ED) and DMRG methods, we study the phase diagram of a 1D version of the Kitaev model with an extra Γ-term, termed as the spin-1/2 “Kitaev-Gamma chain”. The phase diagram is divided into a gapless phase and an ordered phase as shown in Fig. 1 (a). In the gapless phase, we find that the low energy theory is described by an emergent SU(2)1 Wess-Zumino-Witten (WZW) model, although the symmetry group $G \cong O_h \ltimes \mathbb{Z}$ of the model is discrete where $O_h$ is the full octahedral group. On the other hand, the spin-spin correlation functions exhibit SU(2) breaking prefactors as revealed by DMRG numerics, even though the exponents and the logarithmic corrections are consistent with SU(2)1 predictions. A modified nonabelian bosonization formula for the spin operators is proposed to incorporate such emergent “partial” SU(2) symmetry. Based on a renormalization group (RG) analysis, the SU(2) breaking coefficients in the “bridge” between the local spin operators and the low energy degrees of freedom is attributed to a multiplicative renormalization of the spin operators in the high energy region along the RG flow. In the ordered phase, ED and DMRG calculations show evidence of an $O_h \rightarrow D_8$ spontaneous symmetry breaking where $D_{2n}$ represents the dihedral group of order $2n$, except in a small region close to the Kitaev point which remains to be explored further. In both phases of the spin-1/2 chain, the system is either gapless or has a long range order. Hence, our study provides an interesting example beyond the Lieb-Schultz-Mattis theorem [44] since the model has no continuous spin rotational symmetry. We also discuss the relevance of our work to real materials and higher dimensional systems.

The Model

The Hamiltonian of the spin-1/2 Kitaev-
\[
H = \sum_{<ij> \in \gamma \text{ bond}} \left[ KS_i^x S_j^x + \Gamma(S_i^y S_j^y + S_i^z S_j^z) \right],
\]

\[
H' = \sum_{<ij> \in \gamma} \left[ -KS_i^x S_j^x - \Gamma(S_i^y S_j^y + S_i^z S_j^z) \right],
\]

in which the bonds \( \gamma = x, y, z \) are as depicted in Fig. 2 (b). The phase diagram is shown in Fig. 1 (a) to be a continuous and a first order phase transition point. The group structure of \( \gamma \) can be viewed as an improper element with determinant \(-1\) which also leaves the cube invariant. Indeed, these operations within the spin space generate the full octahedral group \( O_h \). On the other hand, it’s a pleasant result that \( G/\langle T_{3a} \rangle \) is isomorphic to \( O_h \) even if the spatial operations \( T_a \) and \( I \) are also included as discussed in detail in SM [49]. Thus \( G \approx O_h \times Z \) where \( Z \approx \langle T_{3a} \rangle \).

The AFM phase We first briefly review the low energy theory at the SU(2) symmetric AFM point \( \phi_{AF} = 5\pi/4 \) (equivalently \( 3\pi/4 \)). The low energy physics is described by the SU(2) WZW model [47]. The non-abelian bosonization formula [47] \( \frac{1}{\sqrt{\sigma}} \text{tr} \sigma^\alpha \) relates the local spin operators to the low energy degrees of freedom in the SU(2) WZW model, in which \( a \) is the lattice constant, \( x = na \) is the coordinate in the continuum limit, \( J_L \) and \( J_R \) are the left and right WZW currents, respectively, \( g \) is an SU(2) matrix which is also the WZW primary field, and \( \sigma^\alpha \) (\( \alpha = x, y, z \)) are the three Pauli matrices. Since the scaling dimensions of \( g \) and the currents \( J_L, J_R \) are \( 1/2 \) and \( 1 \), respectively, the zero temperature equal-time spin-spin correlation functions in the long distance limit (i.e. \( r = |i - j| \gg 1 \)) can be derived as \( \langle S_i^\alpha S_j^\beta \rangle = \delta_{\alpha\beta} \left[ -\frac{1}{4\pi^2 r^3} + (-)^r \frac{1}{2\pi^2 r^3} \ln^{1/2}(r/\alpha) \right] \), in which \( (-)^r \) is an average over the ground state, \( \alpha \) is some microscopic length scale, and the logarithmic correction arises from the marginally irrelevant term \( -\lambda J_L \cdot J_R \). Now we analyze the low energy field theory away from \( \phi_{AF} \). In the vicinity of \( \phi_{AF} \), the SU(2) breaking term \( (\Gamma - K) \sum_{<ij> \in \gamma} S_i^x S_j^x \) can be treated as a perturbation to the SU(2) WZW model. The dimension 1/2 operators \( \epsilon, N^\alpha \) and the dimension 3/2 operators \( J_{L,R}^\epsilon, J_{L,R}^N \) flip the sign under \( T_{3a} \) since \( T_a : g \rightarrow -g \). The dimension 1 operators \( J_{L,R}^\epsilon, J_{L,R}^N \) acquire a sign change under
$R(\beta, \pi)$ ($\beta \neq \alpha$). Hence they are all forbidden in the low energy theory. Among the dimension 2 operators, only the SU(2) invariant combinations $J_L \cdot J_R + J_L \cdot J_R$ and $J_L \cdot J_R$ are allowed by the $O_h$ symmetry. Higher dimensional operators are irrelevant at the CFT fixed point. Thus we conclude that there is an emergent SU(2) symmetry in a range of $\phi$ around $\phi_{AF}$. Indeed, as discussed in SM [46], the finite size spectrum calculated from ED exhibits a conformal tower structure consistent with an emergent SU(2)$_1$ symmetry.

On the other hand, when $\phi \neq \phi_{AF}$, we propose the following modified nonabelian bosonization formula with SU(2) breaking coefficients of $J_L, J_R$ and $g$:

$$\frac{1}{a} S_n^a = \left[ c_0 + c_4 \cos \left( \frac{2 \pi}{3a} x + \frac{2 \pi}{3} (\alpha - 1) \right) \right] \left( J_L^x(x) + J_R^x(x) \right)$$

$$+ \left[ c_6(-)^{i} + c_2 \cos \left( \frac{2 \pi}{3} x + \frac{2 \pi}{3} (\alpha - 1) \right) \right] \frac{1}{\sqrt{a}} \text{tr} (g(x) \sigma^a) \tag{3}$$

in which $\alpha = 1, 2, 3$ corresponding to $\alpha = x, y, z$, and $x = na$. As can be seen from Eq. (3), $(S_i^a S_{i+1}^a)$ now contains momentum $\pi/3$ and $2\pi/3$ oscillating components in addition to the uniform part $u_{\alpha}(r)$ and the staggered part $(-)^r u_{\alpha}(r)$ where both $u_{\alpha}$ and $s_{\alpha}$ are smooth. Alternatively,

$$(S_i^a S_j^b) = \delta_{a\beta} \left[ - D_{[i]}^\alpha D_{[j]}^\beta + (-)^r C_{[i]}^\alpha C_{[j]}^\beta \ln^{1/2}(r/r_0) \right] \tag{4}$$

in which $1 \leq |i| \leq 3, i \equiv [i] \mod 3, r = |i - j|, D_i^x = D_i^y = D_i^z = D_1 = c_0 + c_4, D_i^y = D_2 = D_3 = D_1 = c_0 - c_4/2$, and similar equalities hold for the $C$'s with $C_1 = C_0 + c_4$ and $C_2 = C_0 - c_4/2$. Particularly, the relations between the $D$'s (also $C$'s) are dictated by symmetries as shown in SM [46].

![Figure 3](image_url)

**FIG. 3:** $s_{\alpha}(r)$ vs. $\sin(\pi r/L)$ on a log-log scale at (a) $\phi = 1.25\pi$ and (c) $\phi = 1.15\pi$. $\sin(\pi r/L)s_{\alpha}(r)^2$ vs. $\log \sin(\pi r/L)$ at (b) $\phi = 1.25\pi$ and (d) $\phi = 1.15\pi$.

Next we proceed to numerics. Our numerics show that periodic boundary conditions (PBC) are more efficient than open boundary conditions (OBC) in demonstrating the $1/r^2$ behavior and the logarithmic corrections in Eq. (4). We stress that although DMRG simulations are more challenging with PBC, in the AFM phase a choice of $L = 144$ sites with PBC is sufficient for the purpose of demonstrating Eq. (4). To reach numerical convergence, up to $m = 1000$ DMRG states were kept and tens of finite size sweeps were performed with a truncation error of $10^{-6}$. More DMRG details are described in the SM [46].

The DMRG results for the staggered parts $s_{\alpha}(r)$ at $\phi = 1.15\pi$ are displayed in Fig. 3 (c,d), and the results for the SU(2) symmetric point are displayed in Fig. 3 (a,b) for comparison. $s_{\alpha}(\alpha = x, y, z)$ are extracted from the numerical data using a nine-point formula derived in SM [46]. In Fig. 3 (a,c), the slopes determined from a linear fit of $\log s_{\alpha}(r)$ vs. $\log(\sin(\pi r/L))$ are all close to $-1$ within 5-10%, indeed compatible with an emergent SU(2)$_1$ symmetry. To study the logarithmic corrections, $(\sin(\pi r/L)s_{\alpha}(r))^2$ vs. $\log(\sin(\pi r/L))$ is plotted in Fig. 3 (b,d) all exhibiting a good linear relation, which confirms the logarithmic factor with a power of $1/2$. In particular, the splitting of the lines in Fig. 3 (c,d) indicates an SU(2) breaking in the prefactors of $(-)^r \ln^{1/2}(r/r_0)/r$. A similar numerical study on the $\pi/3$ oscillating components is included in SM [46].

![Figure 4](image_url)

**FIG. 4:** (a) $u_{1x}(r)$ vs. $\sin(\pi r/L)$ on a log-log scale, (b) $d_{\alpha}(r)$ vs. $r$, (c) $(-)^r \sin(\pi r/L)(S_i^a S_{i+1}^a)$ vs. $r$, and (d) $C_2/C_1$ and $D_2/D_1$ as varying $\phi$. In (a,b,c), $\phi = 1.15\pi$.

We also study numerically in detail the SU(2) breaking factors in Eq. (4) at $\phi = 1.15\pi$. In Fig. 4 (c), $(-)^r \sin(\pi r/L)(S_i^a S_{i+1}^a)$ are observed to approach constant values at large $r$ (but still within a small range of $r$ such that the logarithmic differences can be neglected), which are proportional to $C_0^\alpha C_i^\beta$ according to Eq. (4). To obtain $D_1D_2, (D_1)^2, (D_2)^2$, we first pick out the data for every three sites, then the uniform component $u_{1x}(n)$ of $\{\sin(\pi(i + 3n - 1)/L)(S_i^a S_{i+3n}^a)\}_{n \in \mathbb{Z}}$...
(α = x, y, z, i = 1, 2, 3) as a function of n is extracted from a three-point formula derived in SM [60]. Fig. 1(a) shows u_{\gamma}^e(n) vs. sin(π(i + 3n - 1)/L) on a log-log scale. As is clear from Fig. 1(a), a good linear fit is obtained with a slope close to −1 within ~5%. Hence the exponent of u_{\gamma}^e(n) is determined to be indeed around 2. Fig. 1(b) displays the function f(a_0(r)) which is reconstructed from sin(πr/L)u_{\gamma}^e(n) for a fixed α but combining i = 1, 2, 3 together, and D_3^\gamma D_3^\alpha can be determined from the asymptotic value of sin(πr/L)u_{\gamma}^e(n) at large n, in which r = i + 3n − 1.

In addition, the ratios C_1/C_2 and D_1/D_2 are studied as a function of the angle φ and the results are displayed in Fig. 1(d), which provide evidence for emergent SU(2) in the entire AFM phase.

Before closing the discussions of the AFM phase, we present an RG argument to understand the origin of the SU(2) breaking coefficients. The following fermion Hamiltonian is considered

\[ H_F = -t \sum_{<ij>,\alpha} (c_{\alpha}^i c_{\alpha}^j + h.c.) - U \sum_{i} n_{\uparrow} n_{\downarrow} + \Delta \sum_{<ij> \in \gamma} S_i^\gamma S_j^\gamma \]

in which t is the hopping term, μ the chemical potential tuned to half-filling, U > 0 is a repulsive Hubbard coupling, \( \Delta = \Gamma - K \), and \( S_i^\gamma = c_{\alpha}^i \sigma_\gamma c_{\alpha}^i \). In the limit |\Delta| \ll U < t, H_F contains the same low energy physics in the spin sector as that of an SU(2) symmetric AFM Heisenberg chain perturbed by \( \Delta \sum_{<ij> \in \gamma} S_i^\gamma S_j^\gamma \). To study the renormalization of the spin operators, a term \( -\sum_{k=1} h_{\gamma}(n) S_{i+k}^{\alpha} \) can be added to H_F, in which k = 1, 2, 3 are the site indices within a unit cell, n is summed over the unit cells, and \( h_{\gamma}(n) \) are the scaling fields coupled to \( S_{i+k}^{\alpha} \) which can be separated to a uniform part \( h_{\gamma,k}^u(n) \) and a staggered part (\( -\sum_{k=1} h_{\gamma,k}^s(n) \)).

We study the flow of \( h_{\gamma,n}(\eta = u, s) \) by lowering the cutoff from \( \Lambda_0 = \pi/a \) to \( \Lambda_1 \sim \Lambda_0/b_1 \) close to the free fermion fixed point. The RG scale b_1 can be taken as ~3 where the three sites within a unit cell can no longer be clearly distinguished. Note that a linearization of the fermion dispersion is not valid at \( \Lambda_1 \), hence the SU(2) low energy description has not emerged yet. Neglecting the flow of the marginal operator D and keeping terms up to first order in \( \Delta \), the flow equations of \( h_{\gamma,n,k}(b) \) (\( \eta = u, s, k = 1, 2, 3 \)) upon decreasing \( \Lambda_0 \) to \( \Lambda_0/b \) are

\[ \frac{dh_{\gamma}^{x,n}}{d\ln b} = (1 - \nu_u \Delta) h_{\gamma,i}^x - \nu_u \Delta h_{\gamma,i}^x - \nu_d \Delta h_{\gamma,j}^x, \]

\[ \frac{dh_{\gamma}^{y,n}}{d\ln b} = h_{\gamma,j}^d, \]

in which \( i, j = 1, 2, i \neq j \), \( \lambda_u = 0.14/t, \nu_u = -0.07/t, \lambda_s = -0.04/t, \nu_s = 0.06/t \) (see SM [60]). In particular, the absence of \( \Delta \) in \( dh_{\gamma}^{\alpha,n}/d\ln b \) is due to the absence of \( S_{\alpha}^{x,3} \) in the \( \Delta \)-term of H. By solving Eq. (6), the coupling to the scaling fields at scale \( \Lambda_1 \) can be obtained by coupling all the three \( h_{\gamma,k}^x(b_1) \) to a same smeared spin operator \( S_{\gamma}^x(n) \),

\[ \sum_n b_1 [A_n(h_{\gamma,1}(n) + h_{\gamma,2}(n)) + B_n h_{\gamma,3}(n)](-\epsilon^\nu S_{\gamma}^x(n), \]

in which \( \epsilon_u = 0, 1 \). For \( \eta = u, s, A_n = (1 - (\nu_u + \lambda_u) \Delta \ln b_1), B_n = (1 - 2\nu_u \Delta \ln b_1), \) and \( h_{\gamma,k}^x(n) \) are the bare fields at the scale \( \Lambda_0 \). Hence, a difference in the coefficients develops below the scale \( \Lambda_1 \). The ratio \( D_1/D_2 (C_1/C_2) \) is equal to \( B_n/A_n = 1 + (\lambda_u - \nu_u) \Delta \) with \( n = u (\eta = s) \), which is linear in \( \phi \) for \( |\phi - \phi_{AF}| \ll 1 \) of a negative (positive) slope, indeed consistent with the numerical results shown in Fig. 1(d). Similar analysis can be applied to the y- and z-directions.

**The FM phase** We find numerical evidence of an \( O_8 \rightarrow D_8 \) spontaneous symmetry breaking in the FM phase [53] for \( \phi > 0.12\pi \), except the exact SU(2) symmetric point \( \phi_{FM} = \pi/4 \) where the symmetry breaking is \( SU(2) \rightarrow U(1) \). Since \( T_{3a} \) is unbroken in the FM phase, the spin orientations in the ground states within a unit cell and the quotient group \( G/<T_{3a}> \) will be considered in what follows. The spin polarizations in one of the symmetry breaking ground states are

\[ \langle S_1 \rangle = S_z^u, \langle S_2 \rangle = S^u z, \langle S_3 \rangle = S^u z, \]

in which \( \langle S_i \rangle \) represents the expectation value of \( S_i \) in the corresponding state, \( S^u \) and \( S^s \) are the magnitudes of the spin orders, and the little group of Eq. (117) is \( R_{\nu} T_{\nu} R(\pi, \pi) R_{\nu} T_{\nu} R(\pi, \pi) T(\pi, R_{\nu} T_{\nu})^{-1} R_{\nu} T_{\nu} R_{\nu} T_{\nu} \approx D_8 \) (see SM [46]), where the two generators of \( D_8 \) act in the spin space as \( R(\pi, \pi/2) \) and the reflection to the plane \( ACA'C' \) shown in Fig. 1(b), respectively. Hence, the symmetry breaking of Eq. (117) is \( O_h \rightarrow D_8 \), and the “center of mass” spin directions in the six distinct symmetry breaking ground states are along ±x, ±y, ±z shown as the six solid blue circles in Fig. 1(b).

Next we discuss numerics. The phase for \( 0.12\pi \lesssim \phi \neq \phi_c \) is identified. ED calculations show evidence of a six-fold ground state degeneracy at zero field, and one-fold, two-fold, three-fold degeneracies under small uniform fields \( h_z \) along \( z \), \( h_{\eta_1} \) along \( \eta_1 \), and \( h_{\eta_3} \) along \( \eta_3 \), respectively. The fields \( h_z \)’s are chosen to satisfy \( \Delta E \ll H \ll E_g \), 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 sextet at zero field. In addition, DMRG numerics show evidence of vanishing cross correlation functions \( \langle S_i^\alpha S_{i+1}^\beta \rangle (\alpha \neq \beta) \) at any field, and nonzero diagonal correlations \( \langle S_1^\alpha S_{i+1}^\alpha \rangle \) for \( \alpha = z \) with \( h_z, \alpha = x, z \) with \( h_{\eta_1}, \) and \( \alpha = y, z \) with \( h_{\eta_3} \). These are all consistent with \( O_h \rightarrow D_8 \). However, ED calculations show evidence of a four-fold ground state degeneracy at zero field in the region \( \phi \lesssim 0.12\pi \) represented by the thin
dashed line in Fig. 1 (a), which is incompatible with $O_h \rightarrow D_8$. Whether this is a finite size artifact or represents a different ordered phase remains to be explored.

Finally, we discuss the relevance of our study to real materials and higher dimensions. Since Kitaev and Gamma interactions are dominant in $\alpha$-RuCl$_3$, 1D Kitaev-Gamma chain of Ruthenium stripes can be tailored using a- or b-axis oriented superlattices made of the Mott insulator RuCl$_3$ or band insulator IrCl$_3$. Engineering of such 1D systems from superlattices out of 2D layered materials has been successful in fabricating Iridium chain systems [54]. Since Heisenberg interaction is finite in real materials, it is also worthwhile to study the effects of a small Heisenberg interaction [55]. Furthermore, our results provide a starting point for an extrapolation to higher dimensional systems. Numerical studies provide evidence for a disordered phase denoted by the “Kitaev-Gamma spin liquid” near FM Kitaev and AFM evolution of the 1D AFM phase by increasing the coupling between the chains is worth future studies which may offer further insights into possible spin liquid phases in $\alpha$-RuCl$_3$ systems.

In summary, we have studied the phase diagram of the spin-1/2 Kitaev-Gamma chain. In the gapless phase, the low energy physics is described by an emergent SU(2)$_1$ WZW model, but the prefactors in the correlation functions exhibit SU(2) breaking. A modified nonabelian bosonization formula is proposed to capture the SU(2) breaking effect. In the ordered phase, DMRG and ED numerics provide evidence for an $O_h \rightarrow D_8$ symmetry breaking except in a small region close to the Kitaev point.

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By performing the inverse of the six-sublattice rotation, the physical properties of $H$ can be inferred from those of $H'$. For example, interestingly, the AFM phase in the rotated frame (“Gapless I” in Fig. 1 (a)) corresponds to a phase with a noncollinear FM-like quasi-long-range order in the unrotated frame as discussed in Supplementary Materials (SM) \[46\].

A classical analysis predicts an $O_h \rightarrow D_6$ symmetry breaking which is not consistent with $O_h \rightarrow D_8$, indicating strong quantum fluctuations. The details of the classical analysis will be reported elsewhere \[55\].
Supplementary Materials

Contents

The sublattice rotations 7
- The six-sublattice rotation 7
- The three-sublattice rotation and \((K, \Gamma) \cong (K, -\Gamma)\) 8
- Noncollinear FM-like quasi-long-range order in the unrotated frame 9

Phase transitions 11
- Ground state energy as a function of \(\phi\) 11
- Numerical determination of \(\phi_c\) 11
- The central charge in the gapless region 12

The symmetry operations 13
- Proof of \(G/ <T_{3a}> \cong O_h\) 13
- Symmetry relations in the coefficients \(C^\alpha_{[i]}\)’s and in \(D^\alpha_{[i]}\)’s 16

The nine- and three-point formulas 18
- The nine-point formula 18
- The three-point formula 19

\(SU(2)_1\) conformal tower in the finite size spectrum 19

RG flows of the scaling fields 21
- Derivation of the RG flow equations 21
- Solving the flow equations 26

More on AFM phase 27
- Numerical study on the \(\pi/3\)-oscillating components of the correlation functions 27
- Finite size scaling of \(C_1/C_2\) 28

The FM phase 29
- Spin orientations with \(O_h \rightarrow D_8\) symmetry breaking 29
- ED results on the ground state degeneracies 30
- DMRG results on the correlation functions in the FM phase 31

References 32

THE SUBLATTICE ROTATIONS

The six-sublattice rotation

Denoting \(H_{ij}\) to be the term in the Hamiltonian corresponding to the bond \(<ij>\), the unrotated Hamiltonian of the Kitaev-Gamma chain is

\[
H_{12} = KS_1^x S_2^x + \Gamma(S_1^y S_2^z + S_1^z S_2^y), \\
H_{23} = KS_2^x S_3^x + \Gamma(S_2^y S_3^z + S_2^z S_3^y), \\
H_{34} = H_{12}, (3 \rightarrow 1, 4 \rightarrow 2), \text{ etc.}
\]
The six-sublattice rotation is defined as

\begin{align*}
\text{Sublattice 1} & : (x, y, z) \rightarrow (x', y', z'), \\
\text{Sublattice 2} & : (x, y, z) \rightarrow (-x', -y', -z'), \\
\text{Sublattice 3} & : (x, y, z) \rightarrow (y, z', x'), \\
\text{Sublattice 4} & : (x, y, z) \rightarrow (-y', -x', -z'), \\
\text{Sublattice 5} & : (x, y, z) \rightarrow (z', x', y'), \\
\text{Sublattice 6} & : (x, y, z) \rightarrow (-z', -y', -x'), 
\end{align*}

(10)

in which we have dropped the spin symbol $S$ for simplicity. The Hamiltonian $H'$ in the rotated basis becomes

\begin{align*}
H_{12}' & = -K S_{x1}^{s_{1x}} S_{x2}^{s_{2x}} - \Gamma (S_{y1}^{s_{1y}} S_{y2}^{s_{2y}} + S_{z1}^{s_{1z}} S_{z2}^{s_{2z}}), \\
H_{23}' & = -K S_{x2}^{s_{2x}} S_{x3}^{s_{3x}} - \Gamma (S_{y2}^{s_{2y}} S_{y3}^{s_{3y}} + S_{z2}^{s_{2z}} S_{z3}^{s_{3z}}), \\
H_{34}' & = -K S_{x3}^{s_{3x}} S_{x4}^{s_{4x}} - \Gamma (S_{y3}^{s_{3y}} S_{y4}^{s_{4y}} + S_{z3}^{s_{3z}} S_{z4}^{s_{4z}}), \\
H_{45}' & = H_{12}', (4 \rightarrow 1, 5 \rightarrow 2), \text{ etc.}
\end{align*}

(11)

The three-sublattice rotation and $(K, \Gamma) \cong (K, -\Gamma)$

In the unrotated frame, the three-sublattice rotation is defined as

\begin{align*}
\text{Sublattice 1} & : (x, y, z) \rightarrow (x'', y'', z''), \\
\text{Sublattice 2} & : (x, y, z) \rightarrow (x'', -y'', -z''), \\
\text{Sublattice 3} & : (x, y, z) \rightarrow (x'', -y'', -z''), 
\end{align*}

(12)

and the Hamiltonian $H$ is transformed into

\begin{align*}
H_{12}'' & = K S_{1x}^{s_{1x}} S_{2x}^{s_{2x}} - \Gamma (S_{1y}^{s_{1y}} S_{2y}^{s_{2y}} + S_{1z}^{s_{1z}} S_{2z}^{s_{2z}}), \\
H_{23}'' & = K S_{2y}^{s_{2y}} S_{3y}^{s_{3y}} - \Gamma (S_{2x}^{s_{2x}} S_{3x}^{s_{3x}} + S_{2z}^{s_{2z}} S_{3z}^{s_{3z}}), \\
H_{34}'' & = H_{12}'', (3 \rightarrow 1, 4 \rightarrow 2), \text{ etc.}
\end{align*}

(13)
Alternatively, by performing the following three-sublattice rotation

Sublattice 1: \((x, y, z) \rightarrow (x'''', y'''', z''')\),
Sublattice 2: \((x, y, z) \rightarrow (x''', -y'''', -z''')\),
Sublattice 3: \((x, y, z) \rightarrow (-x''', y''', -z''')\),

(14)

to the rotated Hamiltonian \(H''\), the transformed Hamiltonian \(H'''\) is

\[
\begin{align*}
H''_{12} &= -KS_1^{zz}S_2^{zz} + \Gamma(S_1^{yy}S_2^{yy} + S_1^{zz}S_2^{zz}), \\
H''_{23} &= -KS_2^{zz}S_3^{zz} + \Gamma(S_2^{yy}S_3^{yy} + S_2^{zz}S_3^{zz}), \\
H''_{34} &= -KS_3^{zz}S_4^{zz} + \Gamma(S_3^{yy}S_4^{yy} + S_3^{zz}S_4^{zz}) \\
H''_{45} &= H''_{12}^K, (4 \rightarrow 1, 5 \rightarrow 2), \text{ etc.}
\end{align*}
\]

(15)

Indeed, in either case we verify that \((K, \Gamma) \cong (K, -\Gamma)\).

**Noncollinear FM-like quasi-long-range order in the unrotated frame**

All physical properties of \(H\) in Eq. (9) can be obtained from those of \(H'\) in Eq. (11) by performing the inverse of the six-sublattice rotation in Eq. (10). In this section, we discuss the spin-spin correlation functions in the unrotated frame in the AFM phase based on the results within the rotated frame presented in the maintext. Throughout this section, \(S_i^{\alpha}\) and \(S_i^{\alpha'}\) represent a spin operator in the unrotated and rotated frames, respectively.

In the rotated frame, all the cross correlation functions vanish, i.e.,

\[
\langle \Omega\prime | S_i^{\alpha} S_j^{\beta} | \Omega \rangle = 0, \alpha \neq \beta,
\]

(16)
in which \(|\Omega\prime\rangle\) is the ground state of \(H'\). This is a consequence of the invariance of \(H'\) under \(R(\alpha', \pi)\) (\(\alpha = x, y, z\)) if the ground state does not break these symmetries (which is true in the AFM phase). For example, suppose \(R(\hat{x}', \pi)|\Omega\rangle = |\Omega\rangle\). Then

\[
\langle \Omega\prime | S_i^{\alpha} S_j^{\beta} | \Omega \rangle = \langle \Omega\prime | R^{-1}(\hat{x}', \pi)S_i^{\alpha} S_j^{\beta} R(\hat{x}', \pi)|\Omega \rangle

= \langle \Omega\prime | R^{-1}(\hat{x}', \pi)S_i^{\alpha} R(\hat{x}', \pi) \cdot R^{-1}(\hat{x}', \pi)S_j^{\beta} R(\hat{x}', \pi)|\Omega \rangle

= -\langle \Omega\prime | S_i^{\alpha} S_j^{\beta} | \Omega \rangle,
\]

(17)
in which \(R^{-1}(\hat{x}', \pi)S_i^{\alpha} R(\hat{x}', \pi) = S_i^{\alpha'}\) and \(R^{-1}(\hat{x}', \pi)S_j^{\beta} R(\hat{x}', \pi) = -S_j^{\beta'}\) are used. From Eq. (17), it is clear that \(\langle \Omega\prime | S_i^{\alpha} S_j^{\beta} | \Omega \rangle = 0\).

There is a group theoretical way to understand Eq. (16). Consider the group \(F\) generated by \(R(\alpha', \pi)\) (\(\alpha = x, y, z\)). \(F\) is isomorphic to \(D_4\) which is the dihedral group of order 4. To see this, note that the generator-relation representation of \(D_4\) is

\[
D_4 = <a, b | a^2 = b^2 = (ab)^2 = e>,
\]

(18)
in which \(a, b\) are the two generators of \(D_4\), and \(e\) is the identity element. In the group \(F\), we identify \(a = R(\hat{x}', \pi)\) and \(b = R(\hat{y}', \pi)\), and as a result, the product is \(ab = R(\hat{z}', \pi)\). Hence, all the relations in Eq. (18) are satisfied, which shows that \(F\) is a subgroup of \(D_4\). On the other hand, there are at least four elements in \(F\), i.e., 1 and \(R(\hat{\alpha}', \pi)\) (\(\alpha = x, y, z\)). Thus we conclude \(F \cong D_4\). We also note that \(D_4\) has a direct product decomposition

| \(D_4\) | \(E\) | \(C_2(z)\) | \(C_2(y)\) | \(C_2(x)\) |
|-----|-----|-----|-----|-----|
| \(A\) | 1 | 1 | 1 | 1 |
| \(B_1\) | 1 | 1 | -1 | -1 |
| \(B_2\) | 1 | -1 | 1 | -1 |
| \(B_3\) | 1 | -1 | -1 | 1 |

**Table I: Character table of \(D_4\)**


$D_4 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$, and the corresponding decomposition of $F$ is $F = \{1, R(\hat{x}, \pi)\} \times \{1, R(\hat{y}', \pi)\}$. With this preparation, we are able to interpret Eq. (18) in the language of group theory. The group $D_4$ is abelian, hence only has one-dimensional irreducible representations. The character table of $D_4$ is shown in Table I containing four irreducible representations $A, B_1, B_2, B_3$. Notice that $S_i^z, S_i^\alpha, S_i^{\hat{x}}$ are in the $B_1, B_2, B_3$ representations, respectively. Since the inner product between different irreducible representations vanishes [7], we conclude Eq. (16).

In the unrotated frame, Eq. (16) imposes constraints on the correlation functions by virtue of the six-sublattice rotation in Eq. (10). However, unlike Eq. (16), in the present case some of the cross correlations will be nonvanishing, while some of the diagonal correlations (i.e., $(S_i^z S_j^z)$) are zero. Consider $\langle \Omega | S_i^\alpha S_j^\alpha | \Omega' \rangle$ as an example, in which $| \Omega \rangle$ is the ground state of $H$ in the unrotated frame, $1 \leq j \leq 6$, and $n \in \mathbb{Z}$. Denote $U_6$ as the six-sublattice rotation, so that $U_6 H U_6^{-1} = H'$, and $| \Omega' \rangle = U_6 | \Omega \rangle$. Then

$\langle \Omega | S_i^\alpha S_j^\alpha | \Omega' \rangle = \langle \Omega' | U_6 S_i^\alpha S_j^\alpha U_6^{-1} | \Omega' \rangle = \langle \Omega' | U_6 S_i^\alpha U_6^{-1} \cdot U_6 S_j^\alpha U_6^{-1} | \Omega' \rangle$. (19)

Using Eqs. (10,16), we see that only the following correlations are nonzero,

$\langle \Omega | S_i^\alpha S_j^\alpha | \Omega \rangle = \langle \Omega' | S_i^\alpha S_j^\alpha | \Omega' \rangle$,

$\langle \Omega | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha | \Omega \rangle = \langle \Omega' | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha | \Omega' \rangle$,

$\langle \Omega | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha S_m^\alpha S_n^\alpha | \Omega \rangle = \langle \Omega' | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha S_m^\alpha S_n^\alpha | \Omega' \rangle$,

and all other correlations vanish. In the long distance limit $n \gg 1$, all the six correlations in Eq. (20) are positive due to the staggered nature of the correlation functions in the rotated frame. Due to the ln$^{1/2}(r)/r$ power law decay behavior, Eq. (20) exhibits a noncollinear FM-like quasi-long-range order. Similar analysis can be performed on $\langle \Omega | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha S_m^\alpha | \Omega \rangle$ and $\langle \Omega | S_i^\alpha S_j^\alpha S_k^\alpha S_l^\alpha S_m^\alpha S_n^\alpha S_l^\alpha S_m^\alpha | \Omega \rangle$.

Before closing this section, we further note that all the above analysis in the unrotated frame can alternatively be performed using the $D_4$ group in the unrotated frame, which is given by $\{1, U_6^{-1} R(\hat{x}, \pi) U_6, U_6^{-1} R(\hat{y}', \pi) U_6, U_6^{-1} R(\hat{z}', \pi) U_6\}$. It is straightforward to work out the actions of $U_6^{-1} R(\hat{\alpha}', \pi) U_6$:

$U_6^{-1} R(\hat{x}, \pi) U_6$:

Sublattice 1. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, -y, -z)$

Sublattice 2. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, y, -z)$

Sublattice 3. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, -y, z)$

Sublattice 4. $R(\hat{y}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 5. $R(\hat{y}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 3. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, y, z)$

$U_6^{-1} R(\hat{y}', \pi) U_6$:

Sublattice 1. $R(\hat{y}', \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 2. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 3. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, y, z)$

Sublattice 4. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, y, z)$

Sublattice 5. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 3. $R(\hat{y}, \pi): (x, y, z) \rightarrow (-x, y, z)$

$U_6^{-1} R(\hat{\alpha}', \pi) U_6$:

Sublattice 1. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 2. $R(\hat{y}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 3. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, y, z)$

Sublattice 4. $R(\hat{x}, \pi): (x, y, z) \rightarrow (x, y, z)$

Sublattice 5. $R(\hat{z}, \pi): (x, y, z) \rightarrow (-x, y, z)$

Sublattice 3. $R(\hat{y}, \pi): (x, y, z) \rightarrow (-x, y, z)$

in which “sublattice i” means all the lattice sites $i = 6n$ where $n \in \mathbb{Z}$, and $S_i^\alpha$ is denoted as $\alpha$ under “sublattice i” for short. Notice that the transformations acquire rather complicated forms in the unrotated frame. However, the group structure is still $D_4$, and equations like Eq. (20) are direct consequence of the symmetry operations in Eqs. (21,22,23).
PHASE TRANSITIONS

Ground state energy as a function of $\phi$

The ground-state energy density, defined as $\epsilon_0 = E_0/L$, is a thermodynamic quantity that serves as an indicator of phase transitions. The order of the transition is given by the first discontinuous derivative of $\epsilon_0$. The ground-state energy per site and its derivatives are depicted in Fig. 6. As is clear from Fig. 6, there are signatures of discontinuous first order derivative $\partial \epsilon_0 / \partial \phi$ (and hence diverging $\partial^2 \epsilon_0 / \partial \phi^2$) at $\phi = \phi_c, \pi, \bar{\phi_c}$. On the other hand, there is no evidence of discontinuity up to $\partial^2 \epsilon_0 / \partial \phi^2$ at $\phi = 0$. Thus, we conclude that there are numerical evidence for $\phi_c, -K$, and $\bar{\phi_c}$ to be first order transition points, while the transition at $K$ is possibly continuous.

![Figure 6: Ground-state energy per site and its derivatives as a function $\phi$, determined numerically for a periodic system with $L = 24$ sites.](image)

Numerical determination of $\phi_c$

We determine $\phi_c$ as the phase transition point separating the gapless and ordered phases with the following procedure. Fig. 7(a) shows the gap $\Delta = E_1 - E_0$ in the finite size spectrum for a system size of $L = 28$ sites calculated using DMRG with open boundary conditions (OBC), where $E_0$ is the energy of the ground state and $E_1$ the energy of the first excited state. When chains with OBC are considered, $m = 600$ DMRG states and up to 10 finite size sweeps were performed, with a final truncation error smaller than $10^{-9}$. The rounded dome structure appearing for $\phi > 0.33\pi$ corresponds to the finite size gap in the gapless AFM phase. To determine the value of $\phi_c$ more accurately, we zoomed in the interval $0.3 < \phi < 0.4$ (Fig. 7(b)). Here, several system sizes from $L = 24$ up to $L = 144$ are considered with periodic boundary conditions (PBC). The convergence of DMRG results was checked using up to $m = 1000$ DMRG states and performing several tens of finite size sweeps, with a final truncation error smaller than $10^{-6}$. We emphasize that the use of chains with periodic boundaries is not necessary for the determination of the value of $\phi_c$. In fact, Fig. 7(a) and Fig. 7(b) provide evidence that the numerical results do not depend on the choice of boundary conditions.

In the gapless phase the finite size gap shows a perfect linear behavior as $\Delta = A\phi + B$. Fig. 7(c) shows the extrapolated values of $\phi_c = -B/A$ as a function of the inverse system size $1/L$. Finally the value $\phi_c \simeq 0.3351\pi$ is obtained by extrapolating to the thermodynamic limit as shown by the red dashed line in Fig. 7(c).
FIG. 7: (a) $\Delta = E_1 - E_0$ as a function of $\phi$ where $E_0$ is the energy of the ground state and $E_1$ the energy of the first excited state, (b) $\Delta$ vs. $\phi$ in the range $\phi \in [0.3\pi, 0.4\pi]$ close to the phase transition point for several different system sizes $L$, and (c) the extrapolated value of $\phi_c$ as a function of $1/L$. In (a), $\Delta$ is calculated using DMRG on a system of $L = 28$ sites with open boundary conditions ($m = 600$ DMRG states were kept and up to 10 finite size sweeps were performed to reach convergence). In (b), $\Delta$ is computed on a chain with periodic boundary conditions. In this case, to reach numerical convergence, up to $m = 1000$ DMRG states were kept and tens of finite size sweeps were performed with a final truncation error of $10^{-6}$. In (c), $\phi_c = -B/A$ is determined by extrapolating the fitted red linear dashed line in (b) to $\Delta = 0$ at the corresponding $L$. The eventual value of $\phi_c \approx 0.3351\pi$ in (c) is obtained by a linear extrapolation of the finite size $\phi_c$ to $L \to \infty$.

FIG. 8: Entanglement entropy $S_L(x)$ of a subregion $x$, with rest of the system, in a periodic chain of length $L = 30$. This data has been obtained for the choice $\phi = 0.85\pi$. By fitting against the conformal distance on the horizontal axis, we obtain $c = 1$, which is consistent with the analytical analysis in the maintext.

The central charge in the gapless region

To extract the central charge of the critical phase, we study periodic systems of length $L$ and compute the entanglement entropy $S_L(x)$ of a subregion $x$. The entanglement, for a CFT with central charge $c$, is expected to scale as

$$S_L(x) = \frac{c}{3} \ln \left[ \frac{L}{\pi} \sin \left( \frac{\pi x}{L} \right) \right] + \cdots.$$  \hspace{1cm} (24)

A typical numerical fit for central charge, which we verified for multiple points in the gapless phase, is shown in Fig. 8. We find the $c = 1$ to very good accuracy, thereby further corroborating the phase diagram.
THE SYMMETRY OPERATIONS

Proof of $G/<T_{3a}\cong O_h$

The full octahedral group $O_h$ is the symmetry group of a cube as shown in Fig. 9 and is the largest among the five cubic point groups in three dimensional space. $O_h$ contains 48 group elements. In $O_h$, there are 24 rotations which can be classified into five conjugacy classes \{E, 3C_2, 6C_4, 6C'_4, 8C_3\} where $E$ represents the identity element. The actions of these 24 rotations on the x-, y- and z-axes and their geometrical meanings as symmetry operations of a cube are summarized in Table II. The other 24 elements of $O_h$ are improper transformations with determinant $-1$ which can be obtained by multiplying the 24 rotations with the spatial inversion operation $i$. Correspondingly, the improper elements can also be classified into five conjugacy classes, i.e., \{i, 3\sigma_h, 6\sigma_d, 6\sigma_r, 8\sigma_{6}\}.

There is a generator-relation representation for the $O_h$ group \cite{3}:

\[ O_h = \langle r, s, t \mid r^2 = s^2 = t^2 = (rs)^3 = (st)^4 = (rt)^2 = e \rangle, \] (25)

in which $e$ is the identity element, and the geometrical meanings of the generators $r, s, t$ as symmetry operations of a cube are three reflections. We are going to construct $r, s, t$ out of $T, R, a_T, R_{I, I}, R_{I'}$. Then we will show that on the one hand they indeed satisfy the above relations modulo $T_{3a}$, and on the other hand, the group generated by the constructed $r, s, t$ contains at least 48 elements. Since $|O_h| = 48$, this proves that $G/<T_{3a}>$ is isomorphic to $O_h$.

Before proceeding on, we fix some notations. Let $R$ be a rotation in spin space defined as $(R(S^x), R(S^y), R(S^z)) = (S^x, S^y, S^z)R$, in which $R$ is a $3 \times 3$ orthogonal matrix corresponding to $R$. Let $R'$ be another rotation with $R'$ the corresponding matrix. Then the composition $RR'$ is given by

\[ RR' : (S^x, S^y, S^z) \rightarrow (S'^x, S'^y, S'^z)RR'. \] (26)

For later convenience, recall that $R_a = R(\hat{n}_a, -2\pi/3)$ and $R_I = R(\hat{n}_I, \pi)$ satisfy

\[ R_a : (S^x_i, S^y_i, S^z_i) \rightarrow (S^x_i, S^y_i, S^z_i), \]
\[ R_I : (S^x_i, S^y_i, S^z_i) \rightarrow (-S^x_i, -S^y_i, -S^z_i), \] (27)

in which $\hat{n}_a = \frac{1}{\sqrt{3}}(1, 1, 1)^T$ is parallel to the line of $OA$ in Fig. 9 and $\hat{n}_I = \frac{1}{\sqrt{2}}(1, 0, -1)^T$ is parallel to the line passing through the point that bisects the edge $CD'$ and the point that bisects $C'D$ in Fig. 9. Hereafter within this section, the site index $i$ will be dropped in subsequent discussions for simplifications of notations.
TABLE II: List of 24 the group elements of the point group $O$. In accordance with the notations in Fig. [9] $OM$ represents the vector pointing from the center of the cube (i.e. the point $O$) to the vertex or the direction $M$, where $M$ is one of $A, A', B, B', C, C', D, D'$ when it is a vertex of the cube, and is one of $X, Y, Z, X', Y', Z'$ when it represents a direction. $X, Y, Z$ represent the positive directions of the three axes $x, y, z$, and $X', Y', Z'$ represent the negative directions of the three axes. The symbol $[MN]$ represents the line passing through the point that bisects the edge $M'N$, where $M, N, M', N'$ are all vertices of the cube. The caption and the first four columns of the table are taken from W. Yang, T. Xiang, and C. Wu, Phys. Rev. B 96, 144514 (2017).

| $E$ | $(x, y, z)$ | $I$ | $e$ |
|-----|-----------|-----|-----|
| 3C2 | $(x, -y, -z)$ | $R(OX, \pi)$ | $r(ts)^2r$ |
|     | $(-x, y, z)$ | $R(OY, \pi)$ | $rs(st)^2rs$ |
|     | $(-x, -y, z)$ | $R(OZ, \pi)$ | $(st)^2$ |
| 6C4 | $(x, z, -y)$ | $R(OX, \pi)$ | $trsr$ |
|     | $(x, -z, y)$ | $R(OY, \pi)$ | $rsts$ |
|     | $(-z, y, x)$ | $R(OY, \pi)$ | $ssts$ |
|     | $(y, -x, z)$ | $R(OZ, \pi)$ | $stsr$ |
|     | $(-y, x, z)$ | $R(OZ')$, $\pi$ | $ts$ |
| 6C4 | $(y, x, -z)$ | $R([AC]$, $\pi$) | $rsts$ |
|     | $(-y, -x, -z)$ | $R([BD]$, $\pi$) | $(rs)^2rst$ |
|     | $(z, -y, x)$ | $R([AB]$, $\pi$) | $rt$ |
|     | $(-z, y, -x)$ | $R([CD]$, $\pi$) | $(st)^2rst$ |
|     | $(-x, -y, z)$ | $R([AD]$, $\pi$) | $strs$ |
|     | $(-x, z, -y)$ | $R([BC]$, $\pi$) | $tsrst$ |
| 8C5 | $(y, z, x)$ | $R(OA, \pi)$ | $rs$ |
|     | $(z, x, y)$ | $R(OA', \pi)$ | $sr$ |
|     | $(-y, -z, x)$ | $R(OB, \pi)$ | $trst$ |
|     | $(z, -x, y)$ | $R(OB', \pi)$ | $tsrt$ |
|     | $(y, -z, x)$ | $R(OC, \pi)$ | $ststs$ |
|     | $(-z, x, y)$ | $R(OC', \pi)$ | $tsrst$ |
|     | $(-y, z, -x)$ | $R(OD, \pi)$ | $(st)^2rs$ |
|     | $(-z, -x, y)$ | $R(OD', \pi)$ | $(st)^2sr$ |

The constructions of $r, s, t$ are as follows,

| Generator | Expression | Spin space | Geometrical |
|-----------|------------|------------|-------------|
| $r$       | $T \cdot R_I I$ | $(x, y, z) \rightarrow (z, y, x)$ | Reflection to $ABA'B'$-plane |
| $s$       | $T \cdot (R_a T_a)^{-1} \cdot R_I I \cdot R_a T_a$ | $(x, y, z) \rightarrow (y, x, z)$ | Reflection to $ACA'C''$-plane |
| $t$       | $T \cdot R(\hat{y}, \pi)$ | $(x, y, z) \rightarrow (x, -y, z)$ | Reflection to $xz$-plane |

in which the second, the third and the fourth columns give the expressions of $r, s, t$ in terms of the symmetry operations $T, R_a T_a, R_I I, R(\hat{x}, \pi), R(\hat{y}, \pi), R(\hat{z}, \pi)$ of the model, the actions in the spin space where $S^*a$ is denoted as $a$ for short, and the geometrical meanings as symmetries of a cube in Fig. [9] respectively. Now we verify the relations $r^2 = s^2 = t^2 = e$. First,

$$r^2 = T^2 \cdot I^2 \cdot (R_I)^2 = 1,$$

since $T^2 = 1, I^2 = 1$ and $(R_I)^2 = [R(\hat{n}_I, \pi)]^2 = R(\hat{n}_I, 2\pi) = 1$. Secondly,

$$s^2 = T^2 \cdot (T_a^{-1} I T_a)^2 \cdot (R_a^{-1} R_I R_a)^2 = T_{-a} I T_a \cdot T_{-a} I T_a \cdot [R(R_a^{-1} \hat{n}_I, \pi)]^2 = T_{-a} I^2 T_a \cdot R(R_a^{-1} \hat{n}_I, 2\pi) = 1,$$

in which $T_a^{-1} = T_{-a}$, and $R_a R(\hat{n}, \theta) R_0^{-1} = R(R_0 \hat{n}, \theta)$ is used. Finally for $t$, we obtain

$$t^2 = T^2 \cdot [R(\hat{y}, \pi)]^2 = 1.$$
Using the expressions of \(r, s, t, \) it is straightforward to work out the expressions of \(rs, st, rt, \) as

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Operation} & \text{Expression} & \text{Spin space} & \text{Geometrical} \\
\hline
rs & (R_aT_a)^{-1} & (x, y, z) \rightarrow (y, z, x) & R(OA, \frac{2\pi}{\alpha}) \\
st & R_aT_a \cdot R(\hat{z}, \pi) \cdot R_I I \cdot R(\hat{z}, \pi) & (x, y, z) \rightarrow (y, -x, z) & R(\hat{z}, \frac{\pi}{2}) \\
rt & R(\hat{z}, \pi) \cdot R_I I \cdot R(\hat{z}, \pi) & (x, y, z) \rightarrow (z, -y, x) & R([AB], \pi) \\
\hline
\end{array}
\]  

(32)

in which \([AB] \) represents the line passing through the point that bisects the edge \(AB'\) and the point that bisects \(A' B\) in Fig. 9. Next we verify the relations \((rs)^3 = (st)^4 = (rt)^2 = e\). Firstly,

\[
(rs)^3 = (R_a)^{-3} \cdot (T_a)^{-3} \\
= [R(\hat{n}_a, -2\pi/3)]^{-3} \cdot T_{-3a} \\
= R(\hat{n}_a, 2\pi) \cdot T_{-3a} \\
= T_{-3a},
\]

(33)
in which \(R_a = R(\hat{n}_a, -2\pi/3)\) is used, and clearly \((rs)^3 = e\) modulo \(T_{3a}\). Secondly,

\[
(st)^4 = (T_a I)^4 \cdot [R_a R(\hat{z}, \pi) R_I R(\hat{z}, \pi)]^4 \\
= T_a (IT_a I) T_a (IT_a I) \cdot [R(\hat{z}, \pi/2)]^4 \\
= T_a T_{-a} T_a T_{-a} \cdot R(\hat{z}, 2\pi) \\
= 1,
\]

(34)
in which \(IT_a I = T_{-a}\) and \(R_a R(\hat{z}, \pi) R_I R(\hat{z}, \pi) = R(\hat{z}, \pi/2)\) are used. Finally,

\[
(rt)^2 = I^2 \cdot [R(\hat{z}, \pi) R_I R(\hat{z}, \pi)]^2 \\
= [R(R(\hat{z}, \pi) \hat{n}_I, \pi)]^2 \\
= 1.
\]

(35)

This proves that all the relations in Eq. 25 are satisfied. Hence \(G/<T_{3a}>\) is isomorphic to a subgroup of \(O_h\).

We note that the time reversal operation acquires a rather complicated form in terms of the generators. In fact, we have

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Operation} & \text{Expression} & \text{Spin space} & \text{Geometrical} \\
\hline
sr(st)^2r(st) & T & (x, y, z) \rightarrow (-x, -y, -z) & \text{Inversion of the cube} \\
\hline
\end{array}
\]  

(36)

To verify the expression of \(T\), using Eq. 28 32, one obtains

\[
T = (rs)^{-1}(st)^2r(st) \\
= (T_{-a})^{-1}(T_a I)^2 I(T_a I) \cdot R_a [R(\hat{z}, \pi/2)]^2 (TR_I) R(\hat{z}, \pi/2) \\
= (T_a T_a) I(T_a I(T_a I) T_a) I \cdot R_a R(\hat{z}, \pi) R_I R(\hat{z}, \pi/2) \cdot T.
\]

(37)

The spatial part of Eq. 37 is \(T_{2a} IT_{2a} I = T_{2a} T_{-2a} = 1\). Using Eq. 27, \(R(\hat{z}, \pi) : (x, y, z) \rightarrow (-x, -y, z), R(\hat{z}, \pi/2) : (x, y, z) \rightarrow (y, -x, z)\), and the composition rule Eq. 26, it is a straightforward calculation to verify that \(R_a R(\hat{z}, \pi) R_I R(\hat{z}, \pi/2) : (x, y, z) \rightarrow (x, y, z)\). Thus \(sr(st)^2r(st)\) is equal to \(T\).

Next we show that the quotient group \(G/<T_{3a}>\) contains at least 48 elements. One can verify that by restricting the actions to the spin space, the 24 operations in the last column of Table 11 are exactly given by the third column of Table 11 where \(\alpha\) is \(S^\alpha\) for short \((\alpha = x, y, z)\). This exhausts the 24 proper elements of the \(O_h\) group as a symmetry group of a cube in the spin space. Furthermore, by multiplying the 24 operations in the last column of Table 11 with \(T = (rs)^{-1}(st)^2r(st)\), and again restricting to the spin space, we obtain the other 24 improper elements of the \(O_h\) group acting in the spin space. Then let’s recover the spatial components of these 48 operations generated by \(r, s, t, \) and view them as elements in \(G/<T_{3a}>\). Since these 48 operations already act differently in the spin space from each other, they must be distinct elements in \(G/<T_{3a}>\). This shows that \(G/<T_{3a}>\) has at least 48 group elements. Combining with the previously established fact that \(G/<T_{3a}>\) is isomorphic to a subgroup of \(O_h\), we conclude that \(G/<T_{3a}>\) is actually isomorphic to \(O_h\). We also note that the Hilbert space of the spin-1/2 Kitaev-Gamma chain is a projective representation of \(O_h\), since a rotation by \(2\pi\) is \(-1\) for half-odd-integer spins.
We make a further comment on the group structure. Note that \( O_h = O \times \{1, i\} \) where “\( i \)” is the inversion. The cubic point group \( O \) has 24 elements and is isomorphic to \( S_4 \), the permutation group of four elements. \( S_4 \) has a generator-relation representation as follows \([3]\),

\[
S_4 = \langle a, b, c | a^2 = b^3 = c^4 = abc = e \rangle, \tag{38}
\]

or alternatively, it can also be generated by two generators,

\[
O = \langle R, S | R^3 = S^4 = (RS)^2 = E \rangle. \tag{39}
\]

We note that in our case, we can take

\[
a = rt, b = rs, c = st, \tag{40}
\]

and

\[
R = rs, S = st. \tag{41}
\]

**Symmetry relations in the coefficients \( C_{[i]}^\alpha \)'s and in \( D_{[i]}^\alpha \)'s**

Suppose the spin operators \( S_i^\alpha \) at low energies can be written in terms of \( J_L^\alpha, J_R^\alpha, g \) as,

\[
\frac{1}{a} S_i^\alpha = D_{[i]}^\alpha J_L^\alpha + D_{[i]}^\alpha J_R^\alpha + C_{[i]}^\alpha \frac{1}{\sqrt{a}} (-)^{x/a} N^\alpha, \tag{42}
\]

in which \( N^\alpha = \text{itr}(g\sigma^\alpha) \). We’ll analyze what constraints the \( O_h \) symmetry will put on the coefficients.

First, consider the time reversal symmetry \( T \). The transformations of \( S_i^\alpha, J_L^\alpha, J_R^\alpha \) and \( N^\alpha \) under \( T \) are

\[
T : \quad S_i^\alpha \rightarrow -S_i^\alpha \]
\[
J_L^\alpha(x) \rightarrow -J_R^\alpha(x) \]
\[
J_R^\alpha(x) \rightarrow -J_L^\alpha(x) \]
\[
N^\alpha(x) \rightarrow -N^\alpha(x). \tag{43}
\]

Performing time reversal transformation on both sides of Eq. (42), we obtain,

\[
-\frac{1}{a} S_i^\alpha = -D_{[i]}^\alpha J_R^\alpha - D_{[i]}^\alpha J_L^\alpha - C_{[i]}^\alpha \frac{1}{\sqrt{a}} (-)^{x/a} N^\alpha. \tag{44}
\]

On the other hand, from Eq. (42),

\[
-\frac{1}{a} S_i^\alpha = -D_{[i]}^\alpha J_R^\alpha - D_{[i]}^\alpha J_L^\alpha - C_{[i]}^\alpha \frac{1}{\sqrt{a}} (-)^{x/a} N^\alpha. \tag{45}
\]

Comparing Eq. (44) and Eq. (45), it is clear that

\[
D_{[i]}^\alpha = D_{[i]}^\alpha. \tag{46}
\]

Next consider the symmetry operation \( R_a T_a \). The transformations of \( S_i^\alpha, J_L^\alpha, J_R^\alpha \) and \( N^\alpha = \text{trg}(\sigma^\alpha) \) under \( R_a T_a \) are

\[
R_a T_a : \quad S_i^\alpha \rightarrow (R_a)_{\alpha\beta} S_{i+1}^\beta \]
\[
J_L^\alpha(x) \rightarrow (R_a)_{\alpha\beta} J_L^\beta(x) \]
\[
J_R^\alpha(x) \rightarrow (R_a)_{\alpha\beta} J_R^\beta(x) \]
\[
N^\alpha(x) \rightarrow - (R_a)_{\alpha\beta} N^\beta(x), \tag{47}
\]

in which \( (R_a)_{\alpha\beta} \) is the matrix element of the vector representation of the rotation \( R_a \), and the minus sign in the transformation of \( N^\alpha(x) \) is because \( T_a : g \rightarrow -g \). Applying \( R_a T_a \) to \( S_i^\alpha \), under the same logic as the time reversal case, we obtain

\[
D_{2}^T(J_L^\alpha + J_R^\alpha) + C_{2}^T \frac{1}{\sqrt{a}} (-)^{x/a+1} N^z = D_{1}^T(J_L^\alpha + J_R^\alpha) + C_{1}^T \frac{1}{\sqrt{a}} (-)^{x/a} (-)N^z, \tag{48}
\]
from which

\[ D_1^x = D_2^y, \quad C_1^x = C_2^y. \]  

(49)

Similar analysis on other spin operators gives

\[
\begin{align*}
C_1^x &= C_2^x = C_3^x, \quad D_1^x = D_2^x = D_3^x, \\
C_1^y &= C_2^y = C_3^y, \quad D_1^y = D_2^y = D_3^y, \\
C_1^z &= C_2^z = C_3^z, \quad D_1^z = D_2^z = D_3^z.
\end{align*}
\]  

(50)

There is another symmetry \( R_I \) in the \( O_h \) group. The transformations of \( S_i^\alpha, J_i^\alpha, J_R^\alpha \) and \( N^\alpha = \text{trg}(\sigma^\alpha) \) under \( R_I \) are

\[
R_I : \quad S_i^\alpha \rightarrow (R_I)^\alpha_{\beta} S_{-\beta}^\alpha, \]

\[
J_i^\alpha(x) \rightarrow (R_I)^\alpha_{\beta} J_{-\beta}^\alpha(x), \]

\[
J_R^\alpha(x) \rightarrow (R_I)^\alpha_{\beta} J_{-\beta}^R(x), \]

\[
N^\alpha(x) \rightarrow (R_I)^\alpha_{\beta} N_{-\beta}(x). \]

(51)

Applying \( R_I \) to \( S_1^x \), we obtain

\[
-D_3^x(\overline{J}_t^x(-x) + J_R^x(-x)) - C_3^x \frac{1}{\sqrt{a}} (-x/a)^{-3/2} N^z(-x) = -D_1^x(\overline{J}_t^x(-x) + J_R^x(-x)) - C_1^x \frac{1}{\sqrt{a}} (-x/a)^{3/2} N^z(-x),
\]

which gives

\[ D_1^x = D_2^y, \quad C_1^x = C_2^y. \]  

(53)

In summary, by using the \( O_h \) symmetry, we are able to show the following relations

\[
\begin{align*}
D_1^x &= D_2^y = D_3^z (= D_1), \\
D_1^y &= D_2^x = D_3^y = D_2^y = D_2^z (= D_2),
\end{align*}
\]  

(54)

and

\[
\begin{align*}
C_1^x &= C_2^x = C_3^x (= C_1), \\
C_1^y &= C_2^y = C_3^y = C_1^y = C_2^y = C_3^y (= C_2).
\end{align*}
\]  

(55)

Note that the difference in \( D_1, D_2 \) and in \( C_1, C_2 \) will introduce a \( 4k_f \) and a \( 2k_f \) oscillating component in the nonabelian bosonization formula, respectively, where \( k_f = \pi/6a \). We now separate the components with different momenta in \( D^x_{[i]} \) by performing a Fourier transformation. Other directions and the \( C^\alpha_{[i]} \)'s can be treated in a similar manner. Let

\[ D^x_{[i]} = A \cos\left(\frac{2\pi}{3}j + \psi\right) + B. \]  

(56)

Then

\[
A \cos\left(\frac{2\pi}{3} + \psi\right) + B = D_2
\]

\[
A \cos\left(\frac{4\pi}{3} + \psi\right) + B = D_2
\]

\[
A \cos(\psi) + B = D_1,
\]

(57)

which solves

\[
A = \frac{2(D_1 - D_2)}{3},
\]

\[
B = \frac{2(D_2 + D_1)}{3},
\]

\[
\psi = 0.
\]

(58)
In a compact form, we have
\[
D_{[j]}^\alpha = \frac{2(D_1 - D_2)}{3} \cos\left(\frac{2\pi}{3} j + \frac{2\pi}{3} (\alpha - 1)\right) + \frac{2D_2 + D_1}{3}, \\
C_{[j]}^\alpha = \frac{2(C_1 - C_2)}{3} \cos\left(\frac{2\pi}{3} j + \frac{2\pi}{3} (\alpha - 1)\right) + \frac{2C_2 + C_1}{3},
\] (59)
in which \(\alpha = 1, 2, 3\) corresponding to \(x, y, z\).

Now we are able to write the nonabelian bosonization formula with different momenta separated, i.e.
\[
\frac{1}{a} S_i^\alpha = [c_0 + c_4 \cos(\frac{2\pi}{3} x + \frac{2\pi}{3} (\alpha - 1))] (J_L^\alpha(x) + J_R^\alpha(x)) [c_6(-)^e + c_2 \cos(\frac{\pi}{3} x + \frac{2\pi}{3} (\alpha - 1))] \frac{1}{\sqrt{a}} \text{tr}(g(x)\sigma^\alpha),
\] (60)
in which
\[
c_0 = \frac{2D_2 + D_1}{3}, \quad c_2 = \frac{2(C_1 - C_2)}{3}, \quad c_4 = \frac{2(D_1 - D_2)}{3}, \quad c_6 = \frac{2C_2 + C_1}{3}.
\] (61)

**THE NINE- AND THREE-POINT FORMULAS**

**The nine-point formula**

At large distances, the uniform and the \(2\pi/3\)-oscillating components decay much faster than the staggered and the \(\pi/3\)-oscillating components. Due to this reason, we will derive a nine-point formula to extract the staggered and the \(\pi/3\)-oscillating components of the spin-spin correlation functions, assuming no uniform and the \(2\pi/3\)-oscillating components.

Let \(f(j) \ (j \in \mathbb{Z})\) be
\[
f(j) = (-)^j s(j) + \cos\left(\frac{\pi}{3} j\right) p(j) + \sin\left(\frac{\pi}{3} j\right) q(j).
\] (62)

Write \(f(i)\) in terms of \(i - j\), we have
\[
f(i) = (-)^{i-j} s'(i-j) + \cos\left(\frac{\pi}{3} (i-j)\right) p'(i-j) + \sin\left(\frac{\pi}{3} (i-j)\right) q'(i-j),
\] (63)
in which
\[
s'(i-j) = (-)^j s(i), \\
p'(i-j) = \cos\left(\frac{\pi}{3} j\right) p(i) + \sin\left(\frac{\pi}{3} j\right) q(i), \\
q'(i-j) = -\sin\left(\frac{\pi}{3} j\right) p(i) + \cos\left(\frac{\pi}{3} j\right) q(i).
\] (64)

Expanding \(s', p', q'\) as
\[
s'(k) = s_2 k^2 + s_1 k + s_0 \\
p'(k) = p_2 k^2 + p_1 k + p_0 \\
q'(k) = q_2 k^2 + q_1 k + q_0,
\] (65)
the constants \(s_0, p_0, q_0\) can be determined as
\[
s_0 = -\frac{1}{27} f(-4 + j) + \frac{2}{27} f(-2 + j) - \frac{8}{27} f(-1 + j) + \frac{1}{3} f(j) - \frac{8}{27} f(1 + j) + \frac{2}{27} f(2 + j) - \frac{1}{27} f(4 + j),
\]
\[
p_0 = \frac{1}{27} f(-4 + j) - \frac{2}{27} f(-2 + j) + \frac{8}{27} f(-1 + j) + \frac{2}{3} f(j) + \frac{8}{27} f(1 + j) - \frac{2}{27} f(2 + j) + \frac{1}{27} f(4 + j),
\]
\[
q_0 = -\frac{1}{9\sqrt{3}} f(-4 + j) - \frac{2}{9\sqrt{3}} f(-2 + j) - \frac{8}{9\sqrt{3}} f(-1 + j) + \frac{8}{9\sqrt{3}} f(1 + j) + \frac{2}{9\sqrt{3}} f(2 + j) + \frac{1}{9\sqrt{3}} f(4 + j).
\] (66)
Then $s(j), p(j), q(j)$ can be expressed as

\begin{align*}
  s(j) &= (-)^j s_0 \\
p(j) &= \cos(\frac{\pi}{3} j) p_0 - \sin(\frac{\pi}{3} j) q_0 \\
  q(j) &= \sin(\frac{\pi}{3} j) p_0 + \cos(\frac{\pi}{3} j) q_0.
\end{align*}

(67)

The three-point formula

Let $f(j)$ ($j \in \mathbb{Z}$)

\begin{align*}
  f(j) &= u(j) + (-)^j s(j). \\
\end{align*}

(68)

The three-point formula can be used to extract the uniform part $u(j)$ and the stagger part $s(j)$, as

\begin{align*}
  u(j) &= \frac{1}{4} f(j - 1) + \frac{1}{2} f(j) + \frac{1}{4} f(j + 1), \\
  s(j) &= (-)^j \left[ -\frac{1}{4} f(j - 1) + \frac{1}{2} f(j) - \frac{1}{4} f(j + 1) \right].
\end{align*}

(69)

SU(2), CONFORMAL TOWER IN THE FINITE SIZE SPECTRUM

In this section, we study numerically the finite size spectrum of an AFM Kitaev-Gamma chain, and verify that the spectrum exhibits a conformal tower structure consistent with the emergent SU(2)$_1$ symmetry.

We first briefly review the SU(2) symmetric AFM Heisenberg point, i.e., $\phi = 5\pi/4$, following the treatment in Ref. [4]. Due to the existence of the marginally irrelevant term $-u\vec{J}_L \cdot \vec{J}_R$ which breaks the chiral SU(2) symmetry, the SU(2)$_1$ symmetry emerges only logarithmically along the RG flow. In particular, there is a finite size correction to the energy spectrum only suppressed by $1/\ln L$ [3]. At small system size, the effects of such logarithmic correction are notable which obscures the emergent SU(2)$_1$ structure. However, as shown in Refs. [4, 5], there is a clever trick to get around such problem. One adds to the nearest neighbor Heisenberg Hamiltonian a next nearest neighbor term, so that the Hamiltonian now becomes

\begin{align*}
  H'_{AFM} &= J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + J_2 \sum_n \vec{S}_n \cdot \vec{S}_{n+2}.
\end{align*}

(70)

At certain value $J_{2c}$, the bare marginal operator is killed, i.e., $u' = 0$ within $-u'\vec{J}_L \cdot \vec{J}_R$. In fact, $J_{2c}$ is the phase transition point between the gapless spin liquid phase and an ordered dimerized phase [4]. According to Ref. [4], when $J_2$ is tuned to $J_{2c} = 0.2401 J$, the finite size spectra are arranged to a nearly perfect conformal tower structure fully consistent with the SU(2)$_1$ predictions without any logarithmic corrections. Using exact diagonalization, we have reproduced the results in Ref. [4] as shown in Fig. 10(a), with the eigenenergies computed on a finite system with $L = 30$ sites under periodic boundary conditions. The energies are rescaled in unit of $\pi v/L$ where $v = 1.1745 J$. As can be seen from Fig. 10(a), the eigenenergies are grouped into equally spacing plateaus at $n \pi v/L$ with $n \in \mathbb{Z}$. For several lowest $n$‘s, the degeneracies are: 4 for $n = 1$, 6 for $n = 2$, 8 for $n = 3$, all consistent with the emergent SU(2)$_1$ symmetry.

To confirm the absence of the marginal operator $-u\vec{J}_L \cdot \vec{J}_R$ at $J_{2c}$, we further calculate the spin-spin correlation function $\langle S_1^\alpha S_{r+1}^\alpha \rangle$ ($\alpha = x$) using DMRG on a system of a size $L = 144$ with a periodic boundary condition. We stress that, although it is well known that DMRG simulations are more challenging in the presence of periodic boundary conditions, these were only used to demonstrate evidence for the logarithmic corrections predicted by the bosonization expression in the main text. Our analysis indeed shows that system sizes of the order of ~150 sites are sufficient for this purpose. To reach numerical convergence in the presence of PBC, up to $m = 1000$ DMRG states were kept and tens of finite size sweeps were performed with a final truncation error of $10^{-6}$. Since the momentum $\pi$ and $\pm \pi/3$ components decay as $1/r$ at long distances which dominates over the momentum 0 and $\pm \pi/3$ components which decay as $1/r^2$, we will assume that $\langle S_1^\alpha S_{r+1}^\alpha \rangle$ only contains the $\pi$ and $\pm \pi/3$ oscillating components. Then the nine-point formula can be applied and the staggered part $s_{\alpha \alpha}(r)$ can be extracted which should behave as $\sim 1/\sin(\pi r/L)$ with no logarithmic factor. Indeed, as shown by the red points in Fig. 10(c), $(s_{\alpha \alpha}(r) \sin(\pi r/L))^2 \text{ vs. } \log(\sin(\pi r/L))$
is nearly a flat line consistent with an absence of the logarithmic factor. On the other hand, the black dots show the results of $\left( s_{\alpha\alpha}(r) \sin(\pi r/L) \right)^2$ vs. $\log \left( \sin(\pi r/L) \right)$ when $J_2 = 0$. The linear relation of the black dots indicates a behavior of $s_{\alpha\alpha}(r)$ as $\sim \ln^{1/2} \left( \sin(\pi r/L) \right)/\sin(\pi r/L)$. Hence, this provides evidence for the role of $J_{2\text{c}}$ in killing the marginal operator.

Next we apply the same methods to a representative point $\phi = 1.15\pi$ away from the SU(2) symmetric point. Again by adding a $J_2$ term, the Hamiltonian now is

$$H_{K\Gamma}' = -J \sum_{<i,j>_{\gamma}} \left[ \cos(\phi)S_i^\gamma S_j^\gamma + \sin(\phi)(S_i^\alpha S_j^\alpha + S_i^\beta S_j^\beta) \right] + J_2 \sum_n \vec{S}_n \cdot \vec{S}_{n+2}. \quad (71)$$

In Fig. 10(d), $\left( s_{\alpha\alpha}(r) \sin(\pi r/L) \right)^2$ vs. $\log \left( \sin(\pi r/L) \right)$ at $J_2 = 0$ are plotted with black dots showing a linear relation with a nonzero slope. On the other hand, the slope is zero when $J_2 = 0.135J$ as can be seen from the red dots. Thus, this time the critical $J_{2\text{c}}$ is $0.135J$ which is able to remove the marginal operator $-uJ_L \cdot \vec{J}_R$ in the low energy theory. In Fig. 10(b), the energies of the first 20 states are plotted for $L = 18, 24, 30$ in units of $\pi v'/L$. Here $v' = 0.6479J$ is determined by an extrapolation of $E_1(L) - E_0(L)$ as a function of $1/L$ to $1/L \to 0$, in which $E_0(L)$ and $E_1(L)$ are the energies of the ground state and the first excited state, respectively. As can be seen from Fig. 10(b), the SU(2)$_1$ conformal tower structure in the finite size spectrum is improved by increasing $L$. And in fact, a good agreement with the SU(2) symmetric case in Fig. 10(a) is already obtained when $L = 30$. This provides strong evidence for the emergent SU(2)$_1$ symmetry at low energies even away from $\phi = 1.25\pi$. 

FIG. 10: Energies of the first 20 eigenstates with appropriately chosen $J_{2\text{c}}$ for (a) $\phi = 1.25\pi$, and (b) $\phi = 1.15\pi$; and $(s_{\alpha\alpha}(r) \sin(\pi r/L))^2$ (\(\alpha = x\)) vs. $\log \sin(\pi r/L)$ with and without $J_2$ shown by black and red dots, respectively, for (c) $\phi = 1.25\pi$ and (d) $\phi = 1.15\pi$. In (a,b), the spectra are calculated using ED with a periodic boundary condition for both values of $\phi$. The system size is taken as $L = 30$ for $\phi = 1.25\pi$ in (a), and $L = 18, 24, 30$ for $\phi = 1.15\pi$ in (b). In (c,d), the correlation functions are computed using DMRG on a system of $L = 144$ sites with periodic boundary conditions. $s_{\alpha\alpha}$ is then extracted from a nine-point formula in the same way as discussed in the main text.
RG FLOWS OF THE SCALING FIELDS

Derivation of the RG flow equations

Conceptually, the RG flow of the theory described by the following Hamiltonian (i.e., $H_F$ in the maintext)

$$H_F = -t \sum_{\langle ij \rangle, \alpha} (c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.}) - \mu \sum_{\alpha} c_{i\alpha}^\dagger c_{i\alpha} + U \sum_i n^+_i n^-_i + \Delta \sum_{\langle ij \rangle \in \gamma} S_i^z S_j^z - \sum_{kn\alpha} h_k^n(n) S_{k+3n}$$

(72)

can be separated into three steps,

$$\Lambda_0 \to \Lambda_1 \to \Lambda_2 \to E(\gg \frac{1}{L}),$$

(73)

where $\Lambda_0 = \pi/a$ is the bare cutoff, $\Lambda_1$ is the energy scale at which the three sites within a unit cell get smeared, $\Lambda_2$ is the energy scale at which a linearization of the free fermion dispersion applies, and $1/E$ is the length scale of the correlation functions. Below the energy scale $\Lambda_2$, the fermion becomes a Dirac fermion and can be written alternatively in terms of a charge boson and an SU(2) WZW boson using nonabelian bosonization. However, now we study the flow in the energy region $\Lambda_0 \to \Lambda_1$.

We first give a heuristic argument to the RG flow equations based on the operator product expansion (OPE) in real space. The origin of the multiplicative renormalizations of the scaling fields is clear in this approach. However, the OPE approach is not rigorous since it only applies to the continuum limit, and now the flow is within the high energy region. Later we will derive the RG flow in a more rigorous manner in the framework of Wilsonian momentum shell RG.

First recall how the RG flow can be obtained from the OPE between operators $[6]$. Let $\sum g_i \hat{O}_i$ be in the Hamiltonian, in which $\hat{O}_i$ is an operator with scaling dimension $x_i$. If the OPEs between $\hat{O}_i$'s are given by

$$\hat{O}_i(x) \hat{O}_j(y) \sim \frac{c_{ij}}{|x-y|^d + x_i} \hat{O}_k\left(\frac{x+y}{2}\right),$$

(74)

then the flow for the coupling $g_k$ up to one-loop level is

$$\frac{dg_k}{d\ln b} = (d - x_i)g_k - \frac{1}{2} S_d c_{ijk} g_i g_j,$$

(75)

in which $x$, $y$ are spacetime coordinates, $d$ is the spacetime dimension, and $S_d = (2\pi)^{d/2}/\Gamma(d/2)$ is the solid angle of the $(d-1)$-dimensional unit sphere. In our case, take $h_{u,1}^x$ as an example. Heuristically, if we take the discrete unit cell index $n$ as a continuous variable, and combine $n$ with $\tau$ into $x = (\tau, n)$, then we obtain the following OPE ($j = 1, 2, 3$),

$$S_i^x(x)S_j^x(x) \sim \langle S_i^x(x)S_j^x(y)\rangle S_1^x(x).$$

(76)

Hence $h_{u,j}^x$ ($j = 1, 2, 3$) all contribute to the renormalization of $h_{u,1}^x$. The RG flow equation is then

$$\frac{dh_{u,1}^x}{d\ln b} = (1 - \lambda_2 \Delta) h_{u,1}^x - \lambda_2 \Delta h_{u,2}^x - \lambda_3 \Delta h_{u,3}^x,$$

(77)

in which $\lambda_2$ is determined by the contraction $\langle S_i^x(x)S_j^x(y)\rangle$. Furthermore, $\lambda_2 = \lambda_3$ due to the inversion symmetry of the free fermion band structure. In addition, from a simple argument we expect that $\lambda_2 > \lambda_3 = \lambda_2$. This is because at short distances the $j = 2$ contraction in Eq. (76) contains less oscillation than the $j = 1, 3$ cases, since at $x = y$, the $j = 2$ contraction is on-site while the $j = 1, 3$ terms are off-site. Thus we are able to obtain the form of the RG equations presented in the main text in a simple manner, and even the relation $\lambda > 0 > \nu$ is expected. For the staggered part $h_{u,1}^x$, roughly speaking, one needs to change $\Delta$ to $-\Delta$ since the spin operators on two adjacent sites differ by a sign. Thus the slope of $C_2/C_1$ and $D_2/D_1$ around $\phi = \phi_{AF}$ should be opposite in sign.

In what follows, the flows of $h_{u,1}^x$ and $h_{u,1}^y$ will be considered in a momentum shell RG approach. The signs and the magnitudes of the coefficients $\lambda_i$'s will be determined. We will neglect the flows of $U$ and $\Delta$ since they are marginal near the free fermion fixed point, and the RG stopping scale $b_1 \sim 3$ is not very large. We also ignore the contribution from $U$ to the flows of the scaling fields, since this contribution is SU(2) symmetric.

Now we proceed to a momentum shell RG treatment. Let's first write the terms within the action in the frequency-momentum space. The $\Delta$-term is represented as the diagram in Fig. 11 in which $i, j = 1, 2, 3$, and $<ij> = x, z, y$.
for the bonds $<12>, <23>, <31>$. In the frequency-momentum space, the expression corresponding to Fig. 11 is (denoting $<ij>$ as $\gamma$ for short)

$$
\Delta \int d\tau \sum_n S_i^\gamma(\tau,n)S_j^\gamma(\tau,n)
$$

$$
= \Delta \int d\tau \sum_n S^\gamma(\tau,i+3n)S^\gamma(\tau,j+3n)
$$

$$
= \frac{\Delta}{N\beta} \int d\tau \sum_n \sum_{k_1,k_2,k_3,k_4} c^\dagger(k_1)\frac{1}{2}\sigma^\gamma c(k_2) \cdot c^\dagger(k_3)\frac{1}{2}\sigma^\gamma c(k_4)c^i(\omega_1-\omega_2+\omega_3-\omega_4) e^{i(k_1-\bar{k}_2)(i+3n)a\hat{x}} e^{i(k_3-\bar{k}_4)(j+3n)a\hat{x}},
$$

in which $k = (i\omega, \tilde{k})$, $a$ is the lattice spacing, $N$ is the total number of sites, $\beta$ is the inverse of temperature, $n$ is summed over the unit cells, and $\hat{x}$ is the unit vector in the spatial direction. By integrating over $\tau$ and summing over $n$, and using

$$
\frac{1}{N} \sum_n e^{i(k_1-\bar{k}_2+k_3-\bar{k}_4)3na\hat{x}} = \frac{1}{3} \sum_{m=1}^3 \delta_{k_1-\bar{k}_2+k_3-\bar{k}_4+\frac{2\pi}{3a}m}\hat{x},
$$

Eq. (78) is equal to

$$
\frac{\Delta}{N\beta} \frac{1}{3} \sum_{m_1,m_2,m_3} c^i(\tilde{k}_1) e^{-\frac{\pi}{3a}m_1} c^i(\tilde{k}_2) e^{-\frac{\pi}{3a}m_2} c^i(\tilde{k}_3) e^{-\frac{\pi}{3a}m_3} c^i(\tilde{k}_4) \frac{1}{2}\sigma^\gamma c(k_2) \cdot c^\dagger(k_3)\frac{1}{2}\sigma^\gamma c(k_4).
$$

Hence we obtain

$$
\Delta \int d\tau \sum_n S_i^\gamma(\tau,n)S_j^\gamma(\tau,n) = \Delta \frac{1}{3N\beta} \sum_m e^{-\frac{\pi}{3a}m_j} \sum_{k,p,q} e^{i\tilde{q}(p-q)\frac{\pi}{3a}} c^i(k+q)\frac{1}{2}\sigma^\gamma c(k) \cdot c^\dagger(p-q)\frac{1}{2}\sigma^\gamma c(p+\frac{2\pi}{3a}m\hat{x}).
$$
The magnetic field term is represented as the diagram in Fig. 12. The expression in the frequency-momentum space is

$$\int d\tau \sum_n h_\alpha^n(\tau, n)S_\alpha^n(\tau, n)$$

$$= \int d\tau \sum_n h_\alpha^n(\tau, n)S_\alpha^n(\tau, l + 3n)$$

$$= \int d\tau \sum_n \frac{1}{N\beta} \sum_q h_\alpha^n(-q)e^{-i\omega\tau}e^{-i\vec{q}\cdot3na\hat{x}} \sum_{q'} S_\alpha^n(q')e^{i\omega\tau}e^{i\vec{q}'\cdot(l+3n)a\hat{x}}$$

$$= \frac{1}{3} \sum_q \sum_m e^{i\vec{q}\cdot l a\hat{x}} e^{i\frac{2\pi}{m}ml} h_\alpha^n(-q)S_\alpha^n(q + \frac{2\pi}{3a}m\hat{x}).$$  \hspace{1cm} (82)

In terms of the fermion operators, we have

$$\int d\tau \sum_n h_\alpha^n(\tau, n)S_\alpha^n(\tau, n) = \frac{1}{3} \sum_{kq} \sum_m e^{i\vec{q}\cdot l a\hat{x}} e^{i\frac{2\pi}{m}ml} h_\alpha^n(-q)c^1(k + \frac{2\pi}{3a}m\hat{x})\frac{1}{2}\sigma^\alpha c(k - q),$$  \hspace{1cm} (83)

in which $c^1(k) = (c^1_r(k), c^1_i(k))$. In what follows, we focus on the uniform part $h_\alpha^n(\tau, n)$. Then the momentum transfer $\vec{q}$ is $|q| \sim 0$. If we want to consider the staggered part $h^n_{s,i}$, we should write $\vec{q} \rightarrow \vec{q} + \pi/3$, with $|\vec{q}| \sim 0$.

![Diagram](image)

FIG. 13: Diagram of the renormalization of the scaling fields due to the SU(2) breaking $\Delta$-term.

Next we consider the renormalization of $h_\alpha^n_{u,i}$ due to the effect of the $\Delta$-term. In what follows, we will drop the subscript “u” for simplicity. The diagram is shown in Fig. 13 in which the momentum integrated within the loop corresponds to the fast mode (represented as > in the figure) in the treatment of a momentum shell RG. Take the renormalization of $h_\alpha^i$ as an example. Notice that the term $\Delta \int d\tau \sum_{l} S_{\alpha + 3n}^n(\tau)\bar{S}_{\alpha + 3n}(\tau)$ contributes to the renormalization of $h_\alpha^i$ by contracting $S_{\alpha + 3n}^n(\tau)$ with $S_{\alpha + 3n}(\tau)$ ($l = 1, 2, 3$). Thus in Fig. 13 we should make the substitution $i \rightarrow 1, j \rightarrow 2, l \rightarrow l$.

The analytic expression corresponding to Fig. 13 is

$$\Delta \frac{1}{3N\beta} \sum_m e^{-i\frac{2\pi}{m}mj} \sum_{kq} e^{i\vec{q}\cdot(\gamma-j)\vec{a}\hat{x}} c^1(k + q)\frac{1}{2}\sigma^\gamma c(k)\cdot \frac{1}{3} \sum_{k'q'm'} e^{i\vec{q'}\cdot l a\hat{x}} e^{i\frac{2\pi}{m}ml} h_\alpha^n(-q')$$

$$\times \langle c^1(p - q)\frac{1}{2}\sigma^\gamma c(p + \frac{2\pi}{3a}m\hat{x})c^1(k' + \frac{2\pi}{3a}m'\hat{x})\frac{1}{2}\sigma^\alpha c(k' - q') \rangle_f,$$  \hspace{1cm} (84)

in which $\langle \rangle_f$ represents averaging over fast modes. The averaging leads to the following momentum constraints,

$$p + \frac{2\pi}{3a}m = k' + \frac{2\pi}{3a}m',$$

$$p - q = k' - q',$$

which gives

$$m' = m + \bar{m},$$

$$p = k' + \frac{2\pi}{3a}\bar{m},$$

$$q = q' + \frac{2\pi}{3a}\bar{m},$$  \hspace{1cm} (86)
in which $\bar{m} = 1, 2, 3$. Then Eq. (84) becomes

$$\Delta \frac{1}{9N\beta} \sum_{m,m,k,k'/q'} e^{-i\frac{2\pi}{a} m j} e^{i\theta'(i-j)a\hat{x}} e^{i\frac{3\pi}{a}(m+m)l} h^\alpha_i\langle -q' \rangle c^\dagger (k + q' + \frac{2\pi}{3a}\bar{m}\hat{x}) \frac{1}{2} \sigma^\gamma c(k)$$

$$\times \langle c^\dagger (k' - q') \frac{1}{2} \sigma^\gamma c(k' + \frac{2\pi}{3a}(m + \bar{m})\hat{x}) \frac{1}{2} \sigma^\alpha c(k' - q') \rangle t.$$  \hspace{6.2cm} (87)

To further simplify the expression, $e^{-i\frac{2\pi}{a} m j}$ and $e^{-i\frac{2\pi}{a}\bar{m} j}$ are first collected together, then combined with $e^{i\frac{3\pi}{a}(m+\bar{m})l}$. The combined factor is then put together with the $\langle \rangle_f$ term and the result depends on $m + \bar{m}$ only. The remaining terms only depend on $\bar{m}$. Doing these, we obtain

$$\frac{1}{3} \sum_{\bar{m}} e^{-i\frac{2\pi}{a} \bar{m} i} \sum_{k,q'} e^{i\theta'(j-l)a\hat{x}} h^\alpha_i\langle -q' \rangle c^\dagger (k + q' + \frac{2\pi}{3a}\bar{m}\hat{x}) \frac{1}{2} \sigma^\gamma c(k)$$

$$\times \langle c^\dagger (k' - q') \frac{1}{2} \sigma^\gamma c(k' + \frac{2\pi}{3a}(m + \bar{m})\hat{x}) \frac{1}{2} \sigma^\alpha c(k' - q') \rangle t.$$  \hspace{6.2cm} (88)

Notice that in Eq. (88), the average $\langle \rangle_f$ is non-vanishing only when $\alpha = \gamma$. Hence the first line in Eq. (88) is simply $\int d\tau \sum_n h^\alpha_i(\tau, n)S^\alpha_i(\tau, n)$ as can be seen from Eq. (83). This confirms that the diagram in Fig. 13 indeed renormalizes $h^\alpha_i$. Since $q'$ is a slow wavevector, we can ignore $q'$ in the remaining part of Eq. (88) other than the field term. In summary, we conclude that Eq. (88) is equal to

$$\Delta \lambda_{ij} \delta_{ij} \ln b \cdot \int d\tau \sum_n h^\alpha_i(\tau, n)S^\alpha_i(\tau, n).$$  \hspace{6.2cm} (89)

The coefficient is

$$\lambda_{ij} \ln b = -\frac{a}{6} \sum_m e^{-i\frac{2\pi}{a} m(j-l)} \int_{[\Lambda/b, \Lambda]} d^2k G(k)G(k + \frac{2\pi}{3a}m\hat{x}),$$  \hspace{6.2cm} (90)

in which at zero temperature the sum over $k'$ is turned into an integral restricted within the momentum shell $[\Lambda/b, \Lambda]$, $"a"$ is the lattice constant, the minus sign comes from the fermion loop, and

$$G(k) = \frac{1}{i\omega - \epsilon(k)}$$  \hspace{6.2cm} (91)

is the free fermion Green’s function where $\epsilon(k)$ is the dispersion. In conclusion, the RG flow equation for the scaling field is

$$\frac{dh_{\alpha,n}^\alpha}{d\ln b} = h_{\alpha,n}^\alpha - \lambda_{ij} \Delta h_{\alpha,l}^\alpha,$$  \hspace{6.2cm} (92)

in which $\alpha = <ij>$.

Next we proceed to calculating the coefficients $\lambda_{ij}$ in the flow equations. At the free fermion fixed point, the dispersion is linear as shown in Fig. 14 (a). We ignore the nonlinear terms in the band structure since they are of higher dimensions hence irrelevant in the vicinity of the free fermion fixed point. The dispersion can be folded into a Dirac fermion with left and right movers as shown in Fig. 14 (a), in which the cutoff $\Lambda = \frac{\pi}{2a}$.

In momentum shell RG, the modes $(\omega, \hat{k})$ satisfying $\sqrt{\omega^2 + (v\hat{k})^2} \in [\Lambda/b, \Lambda]$ are integrated over, where $v = ta$ is the free fermion velocity and $t$ is the hopping strength. By rescaling $(\omega, \hat{k})$ to $(\omega/(v\Lambda), \hat{k}/\Lambda)$, Eq. (90) becomes

$$\lambda_{ij} \ln b = -\frac{1}{6t} \sum_m e^{-i\frac{2\pi}{a} m(j-l)} \ln b \sum_{\nu = \pm 1} \int \frac{d\theta}{4\pi^2} \frac{1}{i\cos \theta - \epsilon(\sin \theta + \nu) i\cos \theta - \epsilon(\sin \theta + \nu + \frac{1}{3}m)},$$  \hspace{6.2cm} (93)

in which $\nu = \pm 1$ corresponds to left and right movers, and $\epsilon(x) = \text{sgn}(x) - 1, -2 \leq x \leq 2$ ($x$ is mod 4). Thus

$$\lambda_{ij} = \frac{1}{24\pi^2 t} \sum_{m = 0, \pm 1} e^{-i\frac{2\pi}{a} m(j-l)} \sum_{\nu = \pm 1} \int_0^{2\pi} d\theta \frac{1}{\cos^2 \theta + \epsilon^2(\sin \theta + \nu) \cos^2 \theta + \epsilon^2(\sin \theta + \nu + \frac{1}{3}m)}$$

$$\times [\cos^2 \theta - \epsilon(\sin \theta + \nu)\epsilon(\sin \theta + \nu + \frac{4}{3}m) - i \cos \theta(\epsilon(\sin \theta + \nu) + \epsilon(\sin \theta + \nu + \frac{4}{3}m))].$$  \hspace{6.2cm} (94)
The imaginary part vanishes, as can be seen by performing a change of variable \( \theta \to \pi - \theta \) under which \( \sin \theta \) is invariant but \( \cos \theta \) changes a sign. The \( m = 0 \) term also vanishes. This is because the \( \theta \)-integral for both the left and right movers is equal to \( \int d\theta (\cos^2 \theta - \sin^2 \theta) = 0 \). Thus we obtain

\[
\lambda_{jl} = \frac{1}{2\pi} \sum_{m=\pm 1} e^{-i\frac{2\pi}{3}m(j-l)} \sum_{\nu=\pm 1} \int_0^{2\pi} d\theta \frac{\cos^2 \theta - \bar{\epsilon}(\sin \theta + \nu)\bar{\epsilon}(\sin \theta + \nu + \frac{4}{3}m)}{[\cos^2 \theta + \bar{\epsilon}^2(\sin \theta + \nu)] \cdot [\cos^2 \theta + \bar{\epsilon}^2(\sin \theta + \nu + \frac{4}{3}m)]}.
\]  

(95)

Using \( \bar{\epsilon}(x) = \bar{\epsilon}(-x) \), it can be further shown that in Eq. (95), \((m = 1, \nu = 1)\) is equal to \((m = -1, \nu = -1)\), and \((m = 1, \nu = -1)\) is equal to \((m = -1, \nu = 1)\). Hence we get

\[
\lambda_{jl} = \frac{1}{t} E \cos(\frac{2\pi}{3}(j-l)),
\]

(96)
in which

\[
E = \frac{1}{12\pi^2} \sum_{\nu=\pm 1} \int_0^{2\pi} d\theta \frac{\cos^2 \theta - \bar{\epsilon}(\sin \theta + \nu)\bar{\epsilon}(\sin \theta + \nu + \frac{4}{3})}{[\cos^2 \theta + \bar{\epsilon}^2(\sin \theta + \nu)] \cdot [\cos^2 \theta + \bar{\epsilon}^2(\sin \theta + \nu + \frac{4}{3})]}.
\]

(97)

The numerical evaluation of \( E \) gives \( E = 0.14 \).

The flow equation of \( h^x_u \) now becomes

\[
\frac{dh^x_{u,1}}{d\ln \beta} = h^x_{u,1} - \lambda_{23} \Delta h^x_{u,2} - \lambda_{23} \Delta h^x_{u,3}
= h^x_{u,1} - E \frac{\Delta}{t} h^x_{u,2} - E \cos(\frac{2\pi}{3}) \frac{\Delta}{t} h^x_{u,3}.
\]

(98)

Comparing with the flow equation in the main text, we see that

\[
\lambda = \frac{1}{t} E > 0,
\]

\[
\nu = \frac{1}{t} E \cos(\frac{2\pi}{3}) < 0.
\]

(99)

Finally we discuss the flow of the staggered part \( h^\alpha_{s,i} \). We give a quick derivation for the flow equation of \( h^\alpha_{s,i} \), only highlighting the difference from the derivation for the flow of the uniform part.

By replacing \( h^\alpha_i(\tau,n) \) by \((-)^n h^\alpha_{s,i}(\tau,n)\) in Eq. (83), we obtain

\[
\int d\tau \sum_n h^\alpha_i(\tau,n) S^\alpha_i(\tau,n) = \frac{1}{3} \sum_{kq} \sum_m e^{i\ell_{c} m} e^{i\frac{2\pi}{3} m} (-)^l h^\alpha_{s,i}(-q) c^l(k + \frac{2\pi}{3a} m, \tilde{k} + \frac{2\pi}{3a} \tilde{m}) \frac{1}{2} \sigma^\alpha c(k - q).
\]

(100)
In what follows, we will drop the subscript “s” for simplicity. The renormalization expression in Eq. (84) becomes
\begin{align*}
\Delta \frac{1}{3N\beta} \sum_m e^{-i\frac{2\pi}{3}m\lambda} \sum_{kqy} e^{i\hat{q}(i-j)\hat{a}_x} c^\dagger(k+q) \frac{1}{2} \tilde{\sigma}^c c(k) \cdot \frac{1}{3} \sum_{k'q'm'} e^{i\hat{q}'(i\hat{a}_x^\dagger)} e^{i\hat{q}'(m'+\frac{1}{2})\hat{a}_x^\dagger} c(k') \frac{1}{2} \tilde{\sigma}^c c(k') \frac{1}{2} \tilde{\sigma}^c c(k' - q') t, \tag{101}
\end{align*}
and the momentum conservations in Eq. (86) are now
\begin{align*}
m' &= m + \hat{m} \\
p &= k' + \frac{2\pi}{3a} m + \frac{\pi}{3a} \\
q &= q' + \frac{2\pi}{3a} \hat{m} + \frac{\pi}{3a}. \tag{102}
\end{align*}
Then Eq. (103) becomes
\begin{align*}
\frac{1}{3} \sum_m e^{i\frac{2\pi}{3}(m+\frac{1}{2})\lambda} (-i)^l \sum_{kq'} e^{i\hat{q}'\hat{a}_x} c^\dagger(k+q') \frac{1}{2} \tilde{\sigma}^c c(k) \cdot \frac{1}{3} \sum_m e^{-i\frac{2\pi}{3}(m+\frac{1}{2})(j-l)} c^\dagger(k' - q') \frac{1}{2} \tilde{\sigma}^c c(k') \frac{1}{2} \tilde{\sigma}^c c(k' - q') t. \tag{103}
\end{align*}
Instead of Eq. (96), Eq. (103) leads to an RG coefficient
\begin{align*}
\lambda_{jl} \ln b &= -\frac{a}{6} (-i)^{-l} \sum_m e^{-i\frac{2\pi}{3}(m+\frac{1}{2})(j-l)} \int_{A/b} d^2 k G(k) G(k + 2\pi \frac{3a}{m} \hat{m}) x. \tag{104}
\end{align*}
Correspondingly, Eq. (95) is changed to
\begin{align*}
\lambda_{jl} &= \frac{1}{2 \pi \pi^2} (-i)^{-l} \sum_{m=0,\pm1} e^{-i\frac{2\pi}{3}(m+\frac{1}{2})(j-l)} \int_0^{2\pi} \int_0^{2\pi} \frac{\cos^2 \theta - \epsilon \sin \theta + \nu}{\cos^2 \theta + \epsilon^2 \sin \theta + \nu + 4(m+\frac{1}{2})} \right] \right], \tag{105}
\end{align*}
where in particular, the $m = 0$ term does not vanish in the current situation. Define $E_m$ as
\begin{align*}
E_m = \frac{1}{2 \pi \pi^2} \sum_{\nu = \pm 1} \int_0^{2\pi} \frac{\cos^2 \theta - \epsilon \sin \theta + \nu}{\cos^2 \theta + \epsilon^2 \sin \theta + \nu + 4(m + \frac{1}{2})} \right] \right], \tag{106}
\end{align*}
we have
\begin{align*}
\lambda_{jl} &= \frac{1}{k} (-i)^{-l} \sum_{m=0,\pm1} e^{-i\frac{2\pi}{3}(m+\frac{1}{2})(j-l)} E_m. \tag{107}
\end{align*}
The values of $E_m$ can be evaluated numerically as
\begin{align*}
E_0 &= -0.069, \quad E_{+1} = 0.053, \quad E_{-1} = -0.069. \tag{108}
\end{align*}
Notice that $\lambda_{jl}$ only depends on $j-l$, where $j-l = 0, \pm 1 \mod 3$. It is straightforward to obtain $\lambda_{ij} = -0.039/t$, $\lambda_{i,\pm1} = 0.060/t$.

**Solving the flow equations**

In this section, we solve the flow equations
\begin{align*}
\frac{dh_1^\epsilon}{dt} &= (1-\nu \Delta) h_1^\epsilon - \lambda \Delta h_2^\epsilon - \nu \Delta h_3^\epsilon, \\
\frac{dh_2^\epsilon}{dt} &= (1-\nu \Delta) h_2^\epsilon - \lambda \Delta h_1^\epsilon - \nu \Delta h_3^\epsilon, \\
\frac{dh_3^\epsilon}{dt} &= h_3^\epsilon, \tag{109}
\end{align*}
in which \( t = \ln b \), and the subscripts \( u, s \) are dropped in \( h \) for simplicity. The initial conditions are \( h^x_j(t = 0) = h^x_j(0) \), \( j = 1, 2, 3 \).

The equation for \( h^x_3(t) \) is easily solved as

\[
h^x_3(t) = e^t h^x_3(0).
\]

The sum and difference of the equations for \( h^1, h^2 \) are

\[
\frac{d(h^1 + h^2)}{dt} = (1 - (\nu + \lambda)\Delta)(h^x_3 + h^x_2) - 2\nu \Delta h^x_3,
\]
\[
\frac{d(h^1 - h^2)}{dt} = (1 - (\nu - \lambda)\Delta)(h^x_3 - h^x_2).
\]

The second equation in Eq. (111) can be readily solved as

\[
h^1(t) - h^2(t) = e^{(1-\nu-\lambda)\Delta t}(h^1(0) - h^2(0)).
\]

To solve the first equation in Eq. (111), let

\[
h^1(t) + h^2(t) = u(t)e^{(1-(\nu+\lambda)\Delta)t}.
\]

The equation for \( u(t) \) is

\[
\frac{du}{dt} = -2\nu \Delta h^x_3(0)e^{(\lambda+\nu)\Delta t},
\]

which can be solved as

\[
u(t) = h^1(0) + h^2(0) + \frac{2\nu}{\nu+\lambda}h^x_3(0)(1 - e^{(\nu+\lambda)\Delta t}).
\]

Keeping terms only up to first order in \( \Delta \), we get

\[
h^1(b) = b[(1 - \nu \Delta \ln b)h^x_3(0) - \lambda \Delta \ln bh^x_2(0) - \nu \Delta \ln bh^x_3(0)],
\]
\[
h^2(b) = b[(1 - \nu \Delta \ln b)h^x_2(0) - \lambda \Delta \ln bh^x_1(0) - \nu \Delta \ln bh^x_2(0)],
\]
\[
h^x_3(b) = bh^x_3(0).
\]

## MORE ON AFM PHASE

### Numerical study on the \( \pi/3 \)-oscillating components of the correlation functions

In this section, we study the momentum \( \pm \pi/3 \) oscillating components of the spin-spin correlation functions. An angle \( \phi = 1.05\pi \) is chosen as a representative example. The correlation functions \( \langle S^a_i S^a_{i+r} \rangle \) are calculated from DMRG numerics on a system of \( L = 144 \) sites with a periodic boundary condition. As throughout the manuscript, to reach numerical convergence, up to \( m = 1000 \) DMRG states were kept and tens of finite size sweeps were performed with a final truncation error of \( 10^{-6} \). We will neglect the uniform and momentum \( \pm 2\pi/3 \) oscillating components of the correlation functions, since they decay faster than the staggered and momentum \( \pm \pi/3 \) oscillating components at long distances. We denote the staggered component as \( s_{aa}(r) \) and the two momentum \( \pm \pi/3 \) oscillating components as \( p_{aa}(r) \) and \( q_{aa}(r) \). We expect that all of these nine correlation functions \( s_{aa}, p_{aa}, q_{aa} (\alpha = x, y, z) \) behave as \( \sim \ln^{1/2} \left( \sin(\pi r/L) \right) / \sin(\pi r/L) \) at long distances. Since \( s_{aa} \) has already been studied in the maintext, here we focus on \( p_{aa} \) and \( q_{aa} \). A representative direction \( \alpha = x \) is chosen for \( p_{aa} \) and \( \alpha = z \) is chosen for \( q_{aa} \).

In Fig. 15 (a) and (c), \( p_{xx}(r) \) and \( q_{zz}(r) \) are plotted against \( \sin(\pi r/L) \) on a log-log scale, both exhibiting a good linear relation with a slope \( \sim -0.9 \) which is close to \(-1\) within \( 10\% \) error. Due to the logarithmic correction, it is expected that the observed exponent is slightly smaller than the predicted value 1. To study the logarithmic factor, in Fig. 15 (b) and (d), \( (p_{xx}(r)\sin(\pi r/L))^2 \) and \( (q_{zz}(r)\sin(\pi r/L))^2 \) are plotted against \( \log \left( \sin(\pi r/L) \right) \). If the logarithmic factor is \( \ln^{1/2} \left( \sin(\pi r/L) \right) \), then a linear relation will be observed. We see from Fig. 15 (b) and (d) that the linearity is not good due to an oscillation with a six-site periodicity. In fact, such six-site oscillation is not unexpected. When applying the nine-point formula, the uniform component and the momentum \( \pm 2\pi/3 \) components are neglected.
These naturally introduce oscillations into the extracted values of $s_{\alpha\alpha}, p_{\alpha\alpha}, q_{\alpha\alpha}$ with a six-site periodicity. On the other hand, since $C_2/C_1$ is still close to 1 even very far away from the SU(2) symmetric point $\phi = 5\pi/4$, $s_{\alpha\alpha}$ dominates over $p_{\alpha\alpha}, q_{\alpha\alpha}$. The smallness of $p_{\alpha\alpha}, q_{\alpha\alpha}$ means that they are more sensitive to the influence of the uniform and the momentum $\pm 2\pi/3$ components. Indeed, Fig. 3 (d) in the main text also contains oscillations, but much less prominent than those in Fig. 15 (b) and (d). We expect that the oscillations in Fig. 15 (b) and (d) can be reduced by going to larger system sizes.

**Finite size scaling of $C_1/C_2$**

In this section, we study the dependence of the ratio $C_1/C_2$ on the system size for different angles $\phi$. Here we use a method independent from the one used in the main text. An open boundary condition is adopted here, and spin-spin correlations are evaluated between the sites at $r_1 = L/4$ and $r_2 = 3L/4$. To reach numerical convergence, $m = 800$ DMRG states are used and up to 10 finite size sweeps are performed with a final truncation error of $10^{-9}$.

Given the above setup, $\langle S^\alpha_{r_1} S^\alpha_{r_2} \rangle$ are computed for different $L$. As shown in Fig. 16 when displayed in a log-log scale, a perfect linear behavior is observed as in the main text for the staggered part of the correlation functions. Similarly to Fig. 3 in the main text, $x$ and $y$ correlations numerically coincide at large distances, while the $z$ correlation appears as a parallel straight line with approximately the same slope but different intercept compared with the other two correlations.

By extrapolating the intercepts with the y-axis, the ratio $C_1/C_2$ can be extracted. Fig. 16 (c) shows a very weak dependence of $C_1/C_2$ on system sizes for all the values of $\phi$ within the AFM phase of the model. We have verified that the results are consistent with those obtained using chains with periodic boundary conditions, and therefore provide further evidence that the numerical results do not depend on the choice of boundary conditions.
FIG. 16: $\langle S_{L/4}^\alpha S_{3L/4}^\alpha \rangle$ ($\alpha = x, y, z$) as functions of system size $L$ in a log-log plot at (a) $\phi = 0.7\pi$ and (b) $\phi = 0.85\pi$, and (c) $C_1/C_2$ extracted from the spin-spin correlations as a function of $\phi$ within the AFM phase.

THE FM PHASE

Spin orientations with $O_h \rightarrow D_8$ symmetry breaking

We discuss the $O_h \rightarrow D_8$ symmetry breaking. We show that the spin orientations

$$\langle \vec{S}_1 \rangle = S' \hat{z}, \langle \vec{S}_2 \rangle = S'' \hat{z}, \langle \vec{S}_3 \rangle = S'' \hat{z},$$

are invariant under $< R_a T_a R(\hat{z}, \pi) R T_a R(\hat{z}, \pi) > \sim D_8$.

Consider a general spin configuration within a unit cell,

$$\vec{S}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}, \vec{S}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}, \vec{S}_3 = \begin{pmatrix} x_3 \\ y_3 \\ z_3 \end{pmatrix}. $$
Under $R_aT_a \cdot R(\tilde{z}, \pi) \cdot R_I I \cdot R(\tilde{z}, \pi)$, Eq. [118] is mapped to

$$
R_aT_a \cdot R(\tilde{z}, \pi) \cdot R_I I \cdot R(\tilde{z}, \pi) : 
\begin{align*}
\vec{s}_1 & \rightarrow \begin{pmatrix} -x_1 \\ -y_1 \\ z_1 \end{pmatrix} \rightarrow \begin{pmatrix} z_3 \\ y_3 \\ x_3 \end{pmatrix} \rightarrow \begin{pmatrix} z_3 \\ -y_3 \\ -x_3 \end{pmatrix} \rightarrow \begin{pmatrix} y_1 \\ -x_1 \\ z_1 \end{pmatrix}, \\
\vec{s}_2 & \rightarrow \begin{pmatrix} -x_2 \\ -y_2 \\ z_2 \end{pmatrix} \rightarrow \begin{pmatrix} z_2 \\ y_2 \\ x_2 \end{pmatrix} \rightarrow \begin{pmatrix} z_2 \\ -y_2 \\ -x_2 \end{pmatrix} \rightarrow \begin{pmatrix} y_3 \\ -x_3 \\ z_3 \end{pmatrix}, \\
\vec{s}_3 & \rightarrow \begin{pmatrix} -x_3 \\ -y_3 \\ z_3 \end{pmatrix} \rightarrow \begin{pmatrix} z_1 \\ y_1 \\ x_1 \end{pmatrix} \rightarrow \begin{pmatrix} z_1 \\ -y_1 \\ -x_1 \end{pmatrix} \rightarrow \begin{pmatrix} y_2 \\ -x_2 \\ z_2 \end{pmatrix},
\end{align*}
$$

in which the arrows indicate subsequent applications of the operators in $R_aT_a \cdot R(\tilde{z}, \pi) \cdot R_I I \cdot R(\tilde{z}, \pi)$ separated by dot. Under $T \cdot (R_aT_a)^{-1} \cdot R_I I \cdot R_aT_a$, Eq. [118] is mapped to

$$
T \cdot (R_aT_a)^{-1} \cdot R_I I \cdot R_aT_a : 
\begin{align*}
\vec{s}_1 & \rightarrow \begin{pmatrix} z_2 \\ x_2 \\ y_2 \end{pmatrix} \rightarrow \begin{pmatrix} -x_2 \\ -z_2 \\ -y_2 \end{pmatrix} \rightarrow \begin{pmatrix} -y_1 \\ -x_1 \\ -z_1 \end{pmatrix} \rightarrow \begin{pmatrix} y_1 \\ x_1 \\ z_1 \end{pmatrix}, \\
\vec{s}_2 & \rightarrow \begin{pmatrix} z_3 \\ x_3 \\ y_3 \end{pmatrix} \rightarrow \begin{pmatrix} -x_1 \\ -z_1 \\ -y_1 \end{pmatrix} \rightarrow \begin{pmatrix} -y_3 \\ -x_3 \\ -z_3 \end{pmatrix} \rightarrow \begin{pmatrix} y_3 \\ x_3 \\ z_3 \end{pmatrix}, \\
\vec{s}_3 & \rightarrow \begin{pmatrix} z_1 \\ x_1 \\ y_1 \end{pmatrix} \rightarrow \begin{pmatrix} -x_3 \\ -z_3 \\ -y_3 \end{pmatrix} \rightarrow \begin{pmatrix} -y_2 \\ -x_2 \\ -z_2 \end{pmatrix} \rightarrow \begin{pmatrix} y_2 \\ x_2 \\ z_2 \end{pmatrix}.
\end{align*}
$$

Clearly, Eq. [117] is invariant under $R_aT_a \cdot R(\tilde{z}, \pi) \cdot R_I I \cdot R(\tilde{z}, \pi)$ and $T \cdot (R_aT_a)^{-1} \cdot R_I I \cdot R_aT_a$. In addition, the invariant spin configurations under both operations can only be of the form given in Eq. [117].

Next we prove that $<R_aT_a R(\tilde{z}, \pi) R_I I R(\tilde{z}, \pi), T(R_aT_a)^{-1} R_I I R_aT_a>$ is isomorphic to $D_8$. The generator-relation representation of $D_8$ is

$$
D_8 = \langle a, b | a^4 = b^2 = (ab)^2 = e \rangle. 
$$

We make the following identification: $a = R_aT_a \cdot R(\tilde{z}, \pi) \cdot R_I I \cdot R(\tilde{z}, \pi)$, and $b = T \cdot (R_aT_a)^{-1} \cdot R_I I \cdot R_aT_a$. We show that $a$ and $b$ satisfy the relations in Eq. [121]. Since the actions of $a$ and $b$ in the spin space are $R(\tilde{z}, \pi/2)$ and the reflection to the plane $ACA'\prime C'$ shown in Fig. 17 respectively, it is straightforward to verify that the relations in Eq. [121] are satisfied by restricting the actions to the spin space. Then it is enough to verify the relations for the spatial components. Firstly, for $a^4$ we have

$$
(TaI)^4 = Ta(IaITaI)Ta(IaITaI) = TaT_{-a}TaT_{-a} = e. 
$$

Secondly, for $b^2$, we have

$$
(Ta^{-1}ITa)^2 = Ta^{-1}I(TaT_{-a})ITa = Ta^{-1}T_{-a}Ta = T_{-a}Ta = e. 
$$

Thirdly, for $(ab)^2$, we have

$$
(TaITa^{-1}ITa)^2 = T_{3a}^2, 
$$

which is $e$ modulo $T_{3a}$. This shows that $<R_aT_a R(\tilde{z}, \pi) R_I I R(\tilde{z}, \pi), T(R_aT_a)^{-1} R_I I R_aT_a>$ is isomorphic to a subgroup of $D_8$. On the other hand, by only considering the actions within the spin space, one can show that there are at least eight elements within the group $<R_aT_a R(\tilde{z}, \pi) R_I I R(\tilde{z}, \pi), T(R_aT_a)^{-1} R_I I R_aT_a>$. Thus we conclude that it is isomorphic to $D_8$.

**ED results on the ground state degeneracies**

The model is equivalent to a ferromagnetic Heisenberg model at $\phi = 0.25\pi$. We have verified numerically that the ferromagnetic phase extends in the region $0.12\pi \lesssim \phi < \phi_c \approx 0.33\pi$. Therefore, without loss of generality, in this section we investigate the low energy properties of the model for $\phi = 0.2\pi$. 
TABLE III: Energies of several lowest lying states computed with Lanczos Exact Diagonalization. Numerics are performed on a system containing $L = 21$ sites with a periodic boundary condition.

ED on spin $S = 1/2$ chain with periodic boundary conditions finds a degenerate ground state subspace with dimension 6 at zero field as shown by the blue box under the $h = 0$ column in Table III This subspace is separated from the excited states by a relatively small gap $\sim 10^{-3}$ for a chain with length $L = 21$ sites. These results are compatible with a symmetry breaking pattern from $O_h \to D_8$. The 6-fold degeneracy of $O_h \to D_8$ symmetry breaking is equivalent to the number of faces of a cube shown in Fig. 17, with normal directions pointing along the cartesian axes directions $\hat{\alpha} = \pm \hat{x}, \pm \hat{y}, \pm \hat{z}$.

To further test the symmetry breaking patterns, we apply a small uniform magnetic field in such a way that the low lying sextet do not hybridize with excited states above the gap in the spectrum. In particular, we have applied a magnetic field of strength $h \hat{y} = 5 \times 10^{-6}$ along the $y$-direction such that the constraint $10^{-6} \ll h \hat{y} L \approx 10^{-4} \ll 10^{-3}$ is fulfilled. The column of $h \hat{y}$ in Table III shows that there is a unique ground state separated by a gap $E_2 - E_1 \approx 5 \times 10^{-5}$ from a quartet of excited states. Above the first 6 states, there is a gap $E_7 - E_6 \approx 10^{-3}$ as without field, showing that the field is just acting within the low energy sextet.

We finally apply a small magnetic field along the direction of one of the 8 corners of the cube, $h_\hat{n} = \frac{1}{\sqrt{3}} (1, 1, 1)$. As shown in the column $h_\hat{n}$ in Table III, the 6-fold degenerate manifold splits into two triplet of states: Three states pointing to the directions $+\hat{x}, +\hat{y}, +\hat{z}$ and the other three to opposite direction $-\hat{x}, -\hat{y}, -\hat{z}$. This is again consistent with the symmetry breaking pattern shown in Fig. 17.

**DMRG results on the correlation functions in the FM phase**

![Graph showing correlation functions](image)

**FIG. 18:** $\langle S^z_1 S^z_{r+1} \rangle$ at $h_z = 10^{-4}$ along $\hat{z}$. All other correlation functions vanish including $\langle S^\alpha_1 S^\alpha_{r+1} \rangle$ ($\alpha = x, y$) and all cross correlations. Hence, they are not displayed.

We have numerically computed the correlation functions under different fields using DMRG numerics on a system with $L = 24$ sites with a periodic boundary condition. Fig. 18 shows $\langle S^z_1 S^z_{r+1} \rangle$ with $h_z = 10^{-4}$ along $\hat{z}$, and the pattern is consistent with Eq. (117). All other correlation functions vanish, including $\langle S^z_1 S^x_{r+1} \rangle$, $\langle S^y_1 S^y_{r+1} \rangle$, and all
cross correlations \( \langle S_1^{\alpha} S_{r+1}^{\beta} \rangle (\alpha \neq \beta) \). The results are again consistent with the \( O_h \to D_8 \) symmetry breaking.

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[7] Let \( V_1 \) and \( V_2 \) be two \( \mathbb{R} \)-linear irreducible representations of the group \( F \). Let \( \phi : V_1 \times V_2 \to \mathbb{R} \) be a bilinear form satisfying \( \phi(fv_1, v_2) = \phi(v_1, f^{-1}v_2) \) for any \( v_1 \in V_1, v_2 \in V_2, f \in F \). Then \( \phi \) induces a map \( \phi^* : V_1 \to V_2^* \), in which \( V_2^* \) is the dual space of \( V_2 \), i.e., \( V_2^* \) consists of all \( \mathbb{R} \)-linear functions on \( V_2 \). Note that \( V_2^* \) is naturally a representation of \( F \). The property of \( \phi \) ensures that \( \phi^* \) commutes with \( F \). Then by Schur’s lemma, \( \phi^* \) is either 0 or an isomorphism. Thus if \( V_1 \) and \( V_2^* \) are two different irreducible representations, \( \phi^* \) has to be zero, hence \( \phi = 0 \). Since \( \mathbb{C} \)-linear spaces are also \( \mathbb{R} \)-linear and the inner product on a complex Hilbert space is bilinear in \( \mathbb{R} \) by restricting the coefficients in \( \mathbb{C} \) to \( \mathbb{R} \), the above conclusion holds also for complex irreducible representations.