Quantum antiferromagnetic Heisenberg half-odd integer spin model as the entanglement Hamiltonian of the integer spin Affleck-Kennedy-Lieb-Tasaki states

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Applying a symmetric bulk bipartition to the one-dimensional Affleck-Kennedy-Lieb-Tasaki valence bond solid (VBS) states for the integer spin-S Haldane gapped phase, we can create an array of fractionalized spin-S/2 edge states with the super unit cell l in the reduced bulk system, and the topological properties encoded in the VBS wave functions can be revealed. The entanglement Hamiltonian (EH) with \( l = \text{even} \) corresponds to the quantum antiferromagnetic Heisenberg spin-S/2 model. For the even integer spins, the EH still describes the Haldane gapped phase. For the odd integer spins, however, the EH just corresponds to the quantum antiferromagnetic Heisenberg half-odd integer spin model with spinon excitations, characterizing the critical point separating the topological Haldane phase from the trivial gapped phase. Our results thus demonstrate that the topological bulk property not only determines its fractionalized edge states, but also the quantum criticality associated with the topological phase, where the elementary excitations are precisely those fractionalized edge degrees of freedom confined in the bulk of the topological phase.

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INTRODUCTION

Topological phases of matter including those require symmetry protection have been the subject of intense interest in quantum information science, condensed matter physics and quantum field theory. Much effort has been devoted to classification of these topological phases, and tremendous success is achieved in our understanding of quantum Hall states[1], topological insulators[2–4], and symmetry protected topological (SPT) phases[5–7]. The SPT phases possess bulk energy gaps and do not break any symmetry, but have robust gapless edge excitations. These SPT states can not be continuously connected to a trivial gapped state without closing the energy gap. So there exists a topological phase transition between a SPT phase and its adjacent trivial phase, and the corresponding critical theory does not belong to the conventional Landau-Ginzburg-Wilson paradigm[8–11]. Such a critical point is a prototype of “deconfined quantum critical point (QCP)” with fractionalized elementary excitations[12]. A crucial question is how to extract the critical properties from the ground state wave function of the SPT phases.

In one dimension, Haldane[13] predicted that quantum antiferromagnetic Heisenberg spin chains are classified into two universality classes: half-odd integer spins with gapless excitations and integer spins with gapped excitations. Recent studies[14, 15] indicated that the Haldane gapped phase for odd integer spin chains is a typical SPT phase, while the even integer spin chains correspond to the topologically trivial phase, because their edge states are not protected by the projective representation of the bulk SO(3) symmetry. According to the classification theory[2], there exists only one nontrivial SPT phase for the SO(3) symmetric quantum Heisenberg spin model, whose fixed point wave function is given by the Affleck-Kennedy-Lieb-Tasaki (AKLT) valence bond solid state (VBS)[16]. Since the symmetry protection of the SPT phase in the bulk can be analyzed in terms of symmetry protection of the fractionalized edge spins, it motivates us to question if there exists a general connection between the SPT phase and the quantum critical phases of the quantum antiferromagnetic Heisenberg half-odd-integer spin chains.

In this paper, we first review the entanglement property of a single block in the one-dimensional integer spin-S AKLT VBS states, and prove that the entanglement Hamiltonian can be expressed in terms of the Heisenberg exchange of two edge spin-S/2’s. By using a symmetric bulk bipartition[9, 17, 18], we can create an array of fractionalized spin-S/2 edge states with super unit cell l in the reduced bulk system. Then the reduced density matrix and entanglement Hamiltonian (EH) can be derived in terms of the fractionalized edge spins, leading to the quantum antiferromagnetic Heisenberg spin-S/2 model when the super unit cell l includes even number of lattice sites. For \( S = 4n + 2 \) with integer n, the EH still describes the nontrivial Haldane gapped phase with odd integer spins, and for \( S = 4n \) the EH corresponds to the even integer Haldane gapped phase. For the odd integer spin-S, however, the quantum antiferromagnetic Heisenberg half-odd integer spin model emerges, characterizing the quantum critical point separating the nontrivial Haldane phase from the trivial phase. So our re-
sults demonstrate that the topological bulk property not only determines its fractionalized edge states, but also the critical point at the continuous phase transition to its nearby trivial phase.

**SINGLE BLOCK ENTANGLEMENT**

The spin-$S$ AKLT VBS state as the fixed point state of the Haldane gapped phase is defined by

$$|\text{VBS}\rangle = \prod_{i=0}^{N} \left( a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger \right)^S |\text{vac}\rangle,$$

where $a_i^\dagger$ and $b_i^\dagger$ are the Schwinger boson creation operators with a local constraint $a_i^\dagger a_i + b_i^\dagger b_i = 2S$, and the spin operators are expressed as $S_i^+ = a_i^\dagger b_i$, $S_i^- = b_i^\dagger a_i$, and $S_i^z = \left(a_i^\dagger a_i - b_i^\dagger b_i\right)/2$. In this construction, each physical spin is composed of two spin-$S/2$'s projected into a total spin-$S$ state, while each neighboring sites are linked by spin-$S/2$ singlet, see Fig. 1(a).

To consider the entanglement properties, we choose a block of $l$ sites denoted by the part A. With the help of the spin coherent state representation, the reduced density matrix $\rho_A$ can be obtained by tracing out the degrees of freedom without the part A, and its nonzero eigenvalues $\lambda_j$ with degeneracy $2j + 1$ have been derived\[^1\] \[^2\]

$$\lambda_j = \frac{1}{(S + 1)^2} \sum_{k=0}^{S} (2k + 1) |f(k)|^{l-1} \cdot \frac{1}{2} \cdot \frac{1}{4} (S + 2)^j,$$

where $j = 0, 1, \ldots, S$ and the recursion function $I_k[x]$ is defined by

$$I_{k+1}[x] = \frac{2k + 1}{(S + k + 2)^2} \left( k + \frac{4x}{k + 1} \right) I_k[x]$$

$$- \frac{k}{(S - k + 1)^2} \left( S - k + 1 \right) \frac{1}{S + k + 2} I_{k-1}[x],$$

with $I_0[x] = 1$ and $I_1[x] = \frac{4x}{S + 2}$. Since the function $|f(k)|$ decreases with $k$ very quickly, only the first two terms ($k = 0, 1$) dominate in the summation for a long block length $l$. Thus the eigenvalues are approximated as

$$\lambda_j \approx \frac{1}{(S + 1)^2} + 3 \left( \frac{-S}{S + 2} \right)^{l-1} \frac{2j + 1}{S + 2}.$$

and up to the first order of $\delta = \left( \frac{S - S}{S + 2} \right)^l$ the entanglement spectrum is thus derived as

$$\xi_j \approx J(l) \left[ \frac{1}{2} j (j + 1) - \frac{1}{2} \left( \frac{S}{2} + 1 \right) \right].$$

with $J(l) = \frac{12}{S(S + 2)} \left( \frac{-S}{S + 2} \right)^l$. Then the corresponding EH can be recognized as: $H_E = J(l) s_1 \cdot s_2$ where $s_1$ and $s_2$ are the fractionalized edge spins. Therefore, for a long block length $l$, the entanglement properties of the single block are just described by the quantum Heisenberg spin model, and the corresponding entanglement spectra are displayed in Fig. 1(b).

**SYMMETRIC BULK BIPARTITION**

The symmetric bulk bipartition is the most effective tool to generate an extensive array of fractionalized edge spin-$S/2$'s in the bulk subsystem, i.e., the spin chain is divided into two subsystems both including the same number of disjoint blocks\[^3\] \[^4\]. The fractionalized edge spins can thus percolate in the reduced bulk system and emerge as coherent elementary excitations of the effective field theory of the subsystem. It is convenient to write the AKLT VBS wave function in the form of matrix product state (MPS) representation shown in Fig. 2(a).

$$|\text{VBS}\rangle = \sum_{\{s_i\}} \text{Tr} A^{[s_1]} A^{[s_2]} A^{[s_N]} |s_1, s_2, \ldots, s_N\rangle,$$

where $A^{[s_i]}$ are the $(S + 1)\times(S + 1)$ local matrices, whose elements can be obtained from the Schwinger boson representation, and the periodic boundary condition are assumed. When we group each continuous $l$ lattice sites into a block, all the even blocks are denoted by the part A and the rest by the part B. Then by tracing out the part B, the reduced density matrix $\rho_A$ and the EH ($H_E = -\ln \rho_A$) can be derived. The general procedure is described as the following four steps.

Step 1. Conduct the coarse graining and distill relevant states within each block\[^5\]. We pick out a block with $l$
sites, and perform the singular value decomposition

$$R_{\alpha,\beta} = \sum_{p=0}^{\kappa-1} X_{\{s_i\},p} \Lambda_p Y_{p,(\alpha,\beta)},$$

(7)

where the number of nonzero singular values $\kappa$ records the number of relevant states in the block. For the spin-$S$ AKLT VBS state, $\kappa = (S + 1)^2$, and the relevant states $|p\rangle$ are effectively composed by two edge spin-$S/2$'s:

$$|p\rangle = \sum_{m,n} \chi^p_{m,n}|m,n\rangle,$$

which are the combination of the degenerate edge states $|m, n\rangle$ with $m, n \in [-S/2, S/2]$. Then we can rewrite the original VBS wave function into the blocked MPS form, see Fig. 2(b)

$$|\Psi\rangle = \sum_{\{p_i\}} \text{Tr} \left( B[p_1] B[p_2] \ldots B[p_{N/l}] \right) |p_1, p_2, \ldots, p_{N/l}\rangle,$$

(8)

where the block matrices are given by $B[p] = \Lambda_p \rho_p Y_{p,(\alpha,\beta)}$.

Step 2. Trace out the degrees of freedom in the part B. Such a procedure can be presented elegantly by a graphical notation described in Fig. 2(c). The contribution of the subsystem B is represented by the transfer matrix $T = \sum_p B[p] \otimes B[p]$. The expression $\rho_A$ can be written into a matrix product operator form, which is displayed in Fig. 2(c)

$$\rho_A = Tr \left( \prod_j R_j \right),$$

(9)

$$R_j = \sum_{p_j, q_j} |p_j\rangle \langle q_j| \left( B[p_j] \otimes B[q_j] \right) T.$$

(10)

Step 3. To derive the EH, we have to express the projection operator $|p_j\rangle \langle q_j|$ in terms of product of spin operators. Note that each $|p_j\rangle$ is composed of two edge-spin-$S/2$'s and we can write an expansion $|m\rangle\langle n| = \sum_{\Gamma} \Gamma_{(m,n),i} O^i$, where $O^i$ ($i = 1, 2, 3$) are the spin-$S/2$ operators with $O^0 = I$. With these considerations, the full expression $R_j$ is written as

$$R_j = \sum_{\{p_j, q_j\}} \sum_{\{m, n\}} \left( B[p_j] \otimes B[q_j] \right) T \chi_{m_1, n_1} \chi_{m_2, n_2} \times \Gamma_{(m_1, n_1),a_{1j}-1} \Gamma_{(m_2, n_2),a_{2j}-1} O^{a_{1j}} \cdot$$

(11)

It is emphasized that no approximation has been made so far.

Step 4. Since the form $R_j$ is complicated, a controlled approximation can be introduced. For a long block length $l$, the only dominant coupling in $\rho_A$ is $\delta = \left( \frac{S}{S+2} \right)^l$, which implies that the exchange coupling between two edge spins decays exponentially. Then $R_j$ can be separated into two individual edge spins, and the final result for $H_E$ is given by

$$H_E \approx \frac{12}{S(S + 2)} \left( \frac{-S}{S + 2} \right)^l \sum_i s_i \cdot s_{i+1},$$

(12)

where $s_i$ is the fractionalized edge spin-$S/2$'s in the reduced system. The detailed derivations for $S = 1$ and $S = 2$ cases are included in the supplementary material.

Therefore, the resulting entanglement properties can be divided into three categories: (i) For $l = odd$, $H_E$ represents a ferromagnetic ordered phase with spin wave excitations (the numerical result for $S = 1$ is included in the supplementary material); (ii) For $l = even$ and $S = even$, $H_E$ describes the Haldane gapped phase with integer spins. In particular, for $S = 4n + 2$ with integer $\eta$, it represents the SPT phase of the odd integer spin Haldane phase even though the original VBS state corresponds to the topologically trivial state. (iii) For $l = even$ and $S = odd$, $H_E$ is just the quantum Heisenberg antiferromagnetic half-odd integer spin model with quantum critical ground state [22]. The corresponding effective field theory for $S > 1$ describes a multicritical point characterized by the 1+1 (space-time) dimensional SU(2) level-5 Wess-Zumino-Witten (WZW) theory, but the stable fixed point of these critical phases is determined by the SU(2) level-1 WZW theory [22, 23]. These are the important properties encoded in the AKLT VBS states with integer spins.

NUMERICAL CALCULATIONS

Spin-1 AKLT state

In order to put the above analytical results on a solid ground, we perform the exact numerical diagonalization
for the reduced density matrix $\rho_A$ for the spin-1 AKLT state without any approximations. The full entanglement spectrum (ES) for the block length $l = 4$ is displayed in Fig. 3(a). We use the effective length $L_A$ to denote the reduced system length, independent of the block length in the original scale. The degeneracies of each levels correspond to 1, 3, 5, etc for every system length. The density of entanglement entropy $S_A / L_A$ saturates to 0.6929 very quickly, close to the value $\ln 2 = 0.6931$. The entanglement spectral gap $\xi_1 - \xi_0$ is found to scale linearly with the inverse subsystem length $\xi_1 - \xi_0 = k_1 L_A^{-1}$ shown in Fig. 3(b), suggesting the bulk ES is gapless in the thermodynamic limit. Moreover, the second excited entanglement level is also fitted as $\xi_2 - \xi_0 = k_2 L_A^{-1}$ displayed in Fig. 3(b), and the ratio of these two excited levels is determined as $k_2/k_1 = 1.975 \sim 2$, implying the difference of scaling dimensions for these two excited levels is 2.

To determine the universality class of this spectrum, we focus on the wave function of the lowest level $|\psi_0\rangle$. By further cutting the reduced system into two halves with lengths $l_a$ and $(L_A - l_a)$, respectively, we calculate the entanglement entropy: $s(l_a, L_A) = \text{Tr}_{l_a+1, l_a+2, L_A}(|\psi_0\rangle\langle\psi_0|)$. Fitting to the Calabrese-Cardy formula[24],

$$s(l_a, L_A) = \frac{c}{3} \ln \left[ \frac{L_A}{\pi} \sin \left( \frac{\pi l_a}{L_A} \right) \right] + s_0,$$

we obtain the central charge $c = 1.02 \pm 0.02$ in Fig. 3(c). This result confirms that the obtained ES belongs to the universality class of the 1+1 (space-time) dimensional SU(2)$_1$ WZW conformal field theory, which is the same as the quantum antiferromagnetic Heisenberg spin-1/2 chain. The corresponding EH describes the critical point separating the spin-1 Haldane phase from the trivial gapped phase[9]. Such a critical point differs the critical point between the Haldane phase and dimerized phase in the SO(3) bilinear-biquadratic spin-1 chain from that the dimerized phase has spontaneously translation symmetry breaking[25]. It is a multicritical point described by the 1+1 dimensional SU(2)$_2$ WZW theory with $c = 3/2$.

When the block includes the odd number of lattice sites, e.g. $l = 3$, the bulk ES is calculated and displayed in Fig. 3(a). The entanglement entropy density is found to saturate to 0.691, which is within 0.3% to the value of $\ln 2$. The lowest entanglement level $\xi_0$ is linear with system size. However, the lowest entanglement level has the degeneracy $L_A + 1$ in each system size. We computed the magnetization distribution $m_{2m} = \sum_i m_i^2$ for these states and found they are well located in $[-L_A/2, L_A/2]$, indicating that a large spin-$L_A/2$ is formed. This can only be achieved in the ferromagnetic interacting between edge spins, and the bulk ES thus describes a ferromagnetical long-range ordered state. For more evidence, we evaluate the entanglement gap scales as $\xi_1 - \xi_0 \sim L_A^{-2}$, which is a direct sign of spin-wave excitations. To further confirm the this spectrum, we fit the second excitation level $\xi_2 - \xi_0 \sim L_A^{-2}$, as dictated in Fig. 3(b). If we take the Heisenberg interaction as the EH, the coupling constant is fitted to be $J \sim -0.037$, while in our analytical analysis it is $J = (-1/3)^2 = -0.038$. Thus, our analytical derivation is confirmed.

### Spin-2 AKLT state

Another important calculation is performed for the spin-2 AKLT VBS state. The ES with $l = 6$ under open boundary condition is presented in Fig. 3(a). The lowest level is singlet and the first excited level is triplet. However, the level spacing between these two states is fitted as an exponential decay with the subsystem size: $(\xi_l - \xi_0)/J(\ell) \sim e^{-L_A/\Delta}$ with $\Delta = 4.769$, displayed in Fig. 3(b). Here the antiferromagnetic Heisenberg coupling strength $J(\ell)$ is fitted to be 0.0230, very close to our analytical value 0.0234. In the thermodynamic limit, the lowest entanglement level becomes four-fold degenerate. These results are consistent with the defining property of the topological spin-1 Haldane phase. Moreover, $(\xi_2 - \xi_0)/J(\ell)$ shown in Fig. 3(c) approaches to the finite value 0.274, smaller than the Haldane gap value 0.41 from
FIG. 4: (a) The bulk ES with $S = 1$ and the block length $l = 3$, the lowest level is $(L_A + 1)$-fold degenerate. (b) The entanglement spectral gap is linear with square of the inverse subsystem size, indicating a spin-wave excitation for the ferromagnetic Heisenberg spin chain. The second excited level is also plotted, but the data from small sizes slightly deviate from the line.

FIG. 5: (a) The bulk ES with $S = 2$ and the block length $l = 6$ for an open chain. The lowest level is singlet, and the first excited level is triplet. (b) The first excited level decays exponentially with the subsystem size. (c) The bulk excitation energy $(\xi_2 - \xi_0)/J(l)$ saturates to a finite value in thermodynamic limit.

FIG. 4: (a) The bulk ES with $S = 1$ and the block length $l = 3$, the lowest level is $(L_A + 1)$-fold degenerate. (b) The entanglement spectral gap is linear with square of the inverse subsystem size, indicating a spin-wave excitation for the ferromagnetic Heisenberg spin chain. The second excited level is also plotted, but the data from small sizes slightly deviate from the line.

FIG. 5: (a) The bulk ES with $S = 2$ and the block length $l = 6$ for an open chain. The lowest level is singlet, and the first excited level is triplet. (b) The first excited level decays exponentially with the subsystem size. (c) The bulk excitation energy $(\xi_2 - \xi_0)/J(l)$ saturates to a finite value in thermodynamic limit.

The difference can be improved when the longer length of the effective spin chain is calculated.

**DISCUSSION AND CONCLUSION**

The symmetric bulk bipartition allows us to establish a general description of QCP separating the SPT phase from its trivial gapped phase directly from the fixed point wave function of the topological phase. For the one-dimensional SPT phase with the protecting symmetry of $G = SO(3)$ Lie group, its fundamental group is $\Pi_1(G) = Z_2$. So there are only two different phases: the odd integer spin Haldane gapped phase and its trivial gapped phase adiabatically connected to the even integer spin Haldane gapped phase. A QCP exists to separate these two phases, and the effective model Hamiltonian for this QCP is just given by the quantum antiferromagnetic Heisenberg half-odd integer spin chain. The corresponding critical theory is characterized by the 1+1 (space-time) dimensional $SU(2)_1$ WZW conformal field theory with the Lie group $\tilde{G} = SU(2)$, where $\tilde{G}$ is just the universal covering group of $G$ and has a trivial fundamental group, $\Pi_1(\tilde{G}) = 1$. Our results may thus generalize the widely discussed bulk-edge correspondence: the bulk topological property of the topological phase not only determines its symmetry-protected edge degrees of freedom, but also the critical properties of the second order phase transition to the trivial phase. Furthermore, the fundamental degrees of freedom of the critical theory are precisely these edge degrees of freedom *confined* in the bulk of the topological phase. As a result this QCP is a typical deconfined critical point. These results can be generalized for other SPT phases with the protecting symmetry of continuous Lie group.

To summarize, we have applied a symmetric bulk bipartition to the one-dimensional AKLT VBS states for the integer spin-$S$ Haldane gapped phase, and an array of fractionalized spin-$S/2$ edge spins can be created in the reduced bulk system. Via the calculations of the bulk entanglement spectra for the reduced system, the topological properties encoded in the original VBS wave
functions are revealed.

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