

# Edge states of a spin- $\frac{1}{2}$ two-leg ladder with four-spin ring exchange

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A topological insulator and its spin analog as a gapped spin liquid have characteristic low-energy excitations (edge states) within the gap when the systems have boundaries. This is the bulk-edge correspondence, which implies that the edge states themselves characterize the gapped bulk spin liquid. Based on the general principle, we analyzed the vector chirality and rung-singlet phases of the spin- $\frac{1}{2}$  ladder with ring exchange by using the edge states and the entanglement entropy.

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## I. INTRODUCTION

Spontaneous symmetry breaking has been fundamental to characterize phases of matter. An example is a magnetic phase where a local-order parameter is defined as a quantum or thermal average of local combination of spins. Its ordered phase is not invariant against the symmetry operation which leaves the Hamiltonian invariant. In spite of enormous success of this concept, it has been also realized that there still exist many important phases that cannot be captured by the spontaneous symmetry breaking. Strong quantum fluctuation in low dimensions prevents such formation of the ordered state and makes it possible to realize states without any fundamental symmetry breaking. Such phases form a novel class of matter as quantum liquids and spin liquids. Typical examples of the quantum liquids are many of integer and fractional quantum Hall states. Spin analog of the quantum liquids is the spin liquid which includes the Haldane integer spin chain,<sup>1,2</sup> generic valence bond solid (VBS) states,<sup>3,4</sup> and some of the exactly solvable models that also have these spin liquid ground states (Kitaev model,<sup>5</sup> tensor category,<sup>6</sup> and so on).

As for an excitation of a quantum system, local characters of the order parameter and the symmetry breaking are fundamental. Generically speaking, one requires some mechanisms to have a gapless excitation. Typical machineries are the existence of the Fermi surface (formed by fermionic quasiparticles) and the Nambu-Goldstone bosons associated with the broken continuous symmetry. An example of the latter is the spin-wave excitation associated with the Neel order. Generically one may construct a gapless excitation by spatial modulation of the local-order parameter such as the Lieb-Shultz-Mattis-type spin twists.<sup>7</sup> In contrast, as for the quantum liquids and the spin liquids, it is natural to have a finite excitation gap unless one assumes exotic spinon Fermi surfaces.

To characterize such quantum liquids and the spin liquids, topological quantities such as the Berry phases and the Chern numbers are quite useful.<sup>8,9</sup> They do not have any symmetry breaking nor local-order parameter. Still, there are many kinds of interesting quantum states without characteristic low-energy excitation. Such nontrivial quantum phases are the topological insulator and its spin analog. A generic con-

cept to discuss such a phase is the topological order which was first considered for the quantum Hall states.<sup>10</sup> As in the quantum Hall states,<sup>11-14</sup> nontrivial topological insulators do have characteristic edge states or impurity states. The bulk is gapped and insulating. However the existence of boundaries or impurities brings low-energy excitations. The quantum Hall state of graphene also belongs to this topological insulator.<sup>15-17</sup> This is the bulk-edge correspondence where topologically nontrivial bulk guarantees the existence of localized modes and such low-energy localized excitations characterize the gapped bulk insulator<sup>13</sup> conversely.

Not only in the electronic systems but also in a quantum spin system such as the Haldane spin chain is the bulk-edge correspondence realized as the existence of the Kennedy triplet for an open chain,<sup>18</sup> which was confirmed experimentally as well.<sup>19</sup> As a novel theoretical tool, the entanglement entropy (E.E.) for the gapped topological insulators has been quite successful to classify the VBS states of the spin chains,<sup>4,20</sup> where this bulk-edge correspondence plays a fundamental role.

The spin- $\frac{1}{2}$  two-leg ladder with four-spin ring exchange has rich phase structure due to the frustration.<sup>21</sup> For this model, the static and dynamical properties have been intensively studied.<sup>21-29</sup> Although the ring exchange model is simple, due to the frustration, the ground state is quite involved, namely, in the vector-chirality (VC) phase. In this paper we consider the VC phase and the rung-single (RS) phase of this model to identify the ground state properties from the view point of the bulk-edge correspondence.

## II. MODEL

The Hamiltonian is given by

$$\mathcal{H}_{\text{cyc}} = J \left[ \sum_{x=1}^{N/2} \sum_{y=1,2} \mathbf{S}_{x,y} \cdot \mathbf{S}_{x+1,y} + \sum_{x=1}^{N/2} \mathbf{S}_{x,1} \cdot \mathbf{S}_{x,2} \right] + K \sum_{x=1}^{N/2} (P_x + P_x^{-1}). \quad (1)$$

Hereafter, we parametrize the exchange parameter  $(J, K)$  as  $(J, K) = (\cos \theta, \sin \theta)$ . The four-spin cyclic exchange consists of the two- and four-spin exchange interactions as<sup>22</sup>

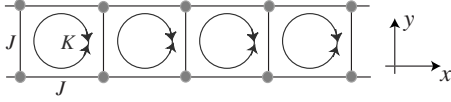


FIG. 1. Lattice structure:  $J$  is the exchange interaction in the leg or rung direction and  $K$  is the four-spin cyclic interaction.  $x$ - ( $y$ -) axis is defined as the leg (rung) direction.

$$\begin{aligned}
 P_x + P_x^{-1} = & \mathbf{S}_{x,1} \cdot \mathbf{S}_{x,2} + \mathbf{S}_{x+1,1} \cdot \mathbf{S}_{x+1,2} \\
 & + \mathbf{S}_{x,1} \cdot \mathbf{S}_{x+1,1} + \mathbf{S}_{x,2} \cdot \mathbf{S}_{x+1,2} + \mathbf{S}_{x,1} \cdot \mathbf{S}_{x+1,2} \\
 & + \mathbf{S}_{x,2} \cdot \mathbf{S}_{x+1,1} + 4(\mathbf{S}_{x,1} \cdot \mathbf{S}_{x+1,1})(\mathbf{S}_{x+1,1} \cdot \mathbf{S}_{x+1,2}) \\
 & + 4(\mathbf{S}_{x,1} \cdot \mathbf{S}_{x+1,1})(\mathbf{S}_{x,2} \cdot \mathbf{S}_{x+1,2}) \\
 & - 4(\mathbf{S}_{x,1} \cdot \mathbf{S}_{x+1,2})(\mathbf{S}_{x,2} \cdot \mathbf{S}_{x+1,1}) + 1/4. \quad (2)
 \end{aligned}$$

Here,  $\mathbf{S}_{x,y}$  denotes a spin- $\frac{1}{2}$  operator at site  $(x,y)$  (see Fig. 1). We assume the system-size  $N$  to be even.

### III. EDGE STATES

The Berry phases as topological order parameters classify the rung-singlet and the VC and RS phases of the model.<sup>29</sup> In the VC phase, Hamiltonian (1) is adiabatically connected to a decoupled vector-chiral model  $\mathcal{H}_{\text{dvc}} = \sum_{x=\text{even}} (\mathbf{S}_{x,1} \times \mathbf{S}_{x,2}) \cdot (\mathbf{S}_{x+1,1} \times \mathbf{S}_{x+1,2})$ , whose ground state is a direct product of plaquette singlets  $|\psi_a\rangle$  [see Fig. 2(a)], which is defined as

$$\begin{aligned}
 |\psi_a\rangle = & [(1,1), (2,2)] \otimes [(1,2), (2,1)] \otimes [(3,1), (4,2)] \\
 & \otimes [(3,2), (4,1)] \otimes \cdots. \quad (3)
 \end{aligned}$$

Here, we have introduced a singlet at two sites  $\vec{\alpha}$  and  $\vec{\beta}$ ,  $[\vec{\alpha}, \vec{\beta}] = [(\alpha_x, \alpha_y), (\beta_x, \beta_y)]$ , as

$$[\vec{\alpha}, \vec{\beta}] = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{\vec{\alpha}} |\downarrow\rangle_{\vec{\beta}} - |\downarrow\rangle_{\vec{\beta}} |\uparrow\rangle_{\vec{\alpha}}). \quad (4)$$

By taking into account of the translational invariance, we consider the linear combination of  $|\psi_a\rangle$  and  $|\psi_b\rangle$  as shown in Fig. 2(b). State  $|\psi_b\rangle$  is defined as

$$\begin{aligned}
 |\psi_b\rangle = & [(2,1), (3,2)] \otimes [(2,2), (3,1)] \otimes [(4,1), (5,2)] \\
 & \otimes [(4,2), (5,1)] \otimes \cdots. \quad (5)
 \end{aligned}$$

Notice that the two dimerized plaquette-singlet states  $|\psi_a\rangle$  and  $|\psi_b\rangle$  are not orthogonal to each other, but their overlap is exponentially small for large  $N$ . For  $N/2$  being even, the

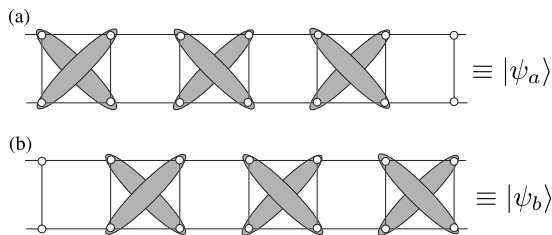


FIG. 2. Two types of the dimerized plaquette-singlet states. Shaded links denote the singlet of the two  $S=1/2$  spins.

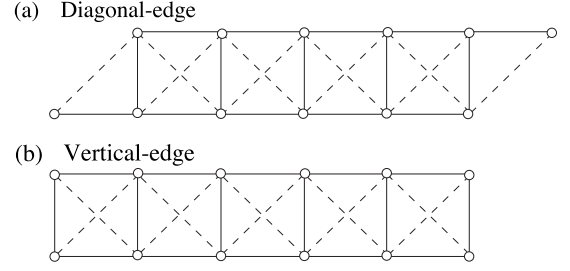


FIG. 3. Two types of open boundary conditions (OBCs).

overlap is obtained as  $\langle \psi_a | \psi_b \rangle = 2^{2-N/2}$ . As described later, the state  $|\psi_s\rangle \propto |\psi_a\rangle + |\psi_b\rangle$  can be a good trial state to understand the edge states and the entanglement entropy for the vector-chirality state.<sup>30</sup>

In the VC phase, the bulk itself has a finite gap in the thermodynamic limit.<sup>21,24</sup> We introduce two types of boundaries—(a) diagonal edge and (b) vertical edge (see Fig. 3).<sup>31</sup> We diagonalized the Hamiltonian numerical by the Lanczos method. In Fig. 4 we show the size dependence on the energy gap of the total  $S^z=0$  sector for  $\theta=4\pi/5$ , where the bulk spin gap is relatively large. The system with the vertical edges has almost the same excitation energy as that of the periodic one. In contrast, there exist additional low-energy excited states with an exponentially small energy gap when the system has the diagonal edges. The appearance of

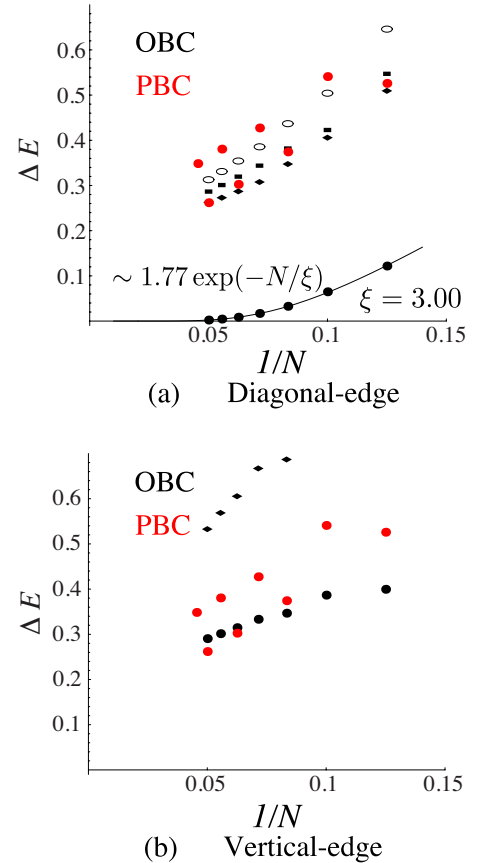


FIG. 4. (Color online) System-size dependence of low-excitation energy for  $\theta=4\pi/5$  with the two OBCs compared with the energy gap under the periodic boundary condition (PBC).

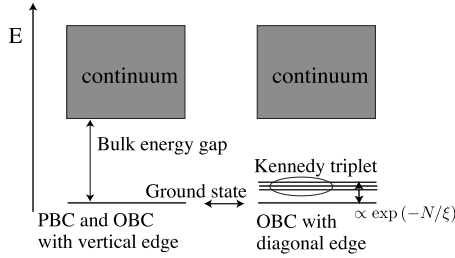
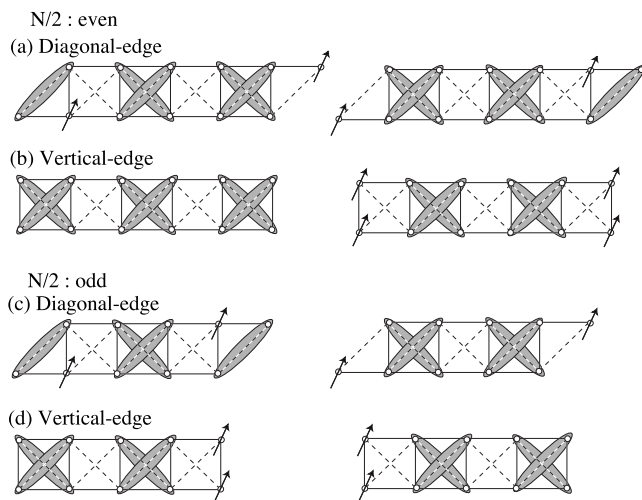
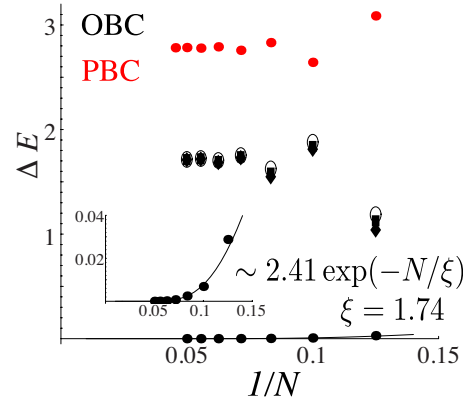


FIG. 5. Schematic of the low-energy excitations.

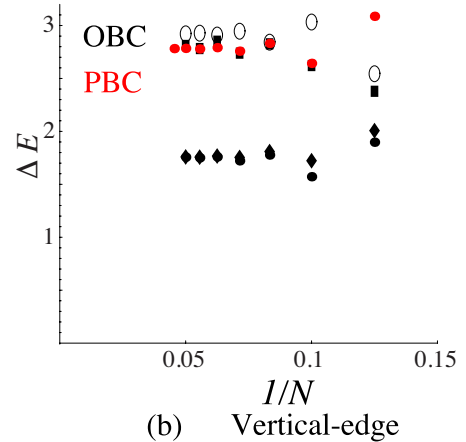
such a localized mode indicates the feature of the *bulk-edge correspondence*. In fact, this mode is a triplet excitation and can be interpreted as the Kennedy triplet (see Fig. 5)—triplet excitation between the effective boundary spins at both sides.<sup>18</sup> We confirmed that this mode is really a triplet excitation from the diagonalization on the different  $S^z$  sector. This mode is observed also in the different  $(J, K)$ 's in VC phase.<sup>32</sup> Note that the Kennedy triplet in this model was also discussed in a different context before.<sup>27</sup>

When we introduce the boundary for the trial state  $|\psi_s\rangle$ , i.e., the linear combination of the two dimerized plaquette singlets, the isolated spins appear near the boundaries (see Fig. 6). In the system with diagonal edges they appear at each boundary, while in the system with vertical edges they appear as a pair at one side of the edge. Although a pair of localized spins behaves freely in the decoupled vector chiral model  $\mathcal{H}_{\text{dev}}$ , the pair of the spins couples each other in the original model  $\mathcal{H}_{\text{cyc}}$  with vertical edges. Therefore, the Kennedy triplet excitation does not appear in the system with the vertical edges. Thus the trial state  $|\psi_s\rangle$  gives consistent understanding for the low-energy spectra of the VC phase.

Next we consider the RS phase. In Fig. 7, we show the size dependence on the energy gap of the total  $S^z=0$  sector for  $\theta=-\pi/5$ . Combining with the calculation on different  $S^z$  sector we obtain the Kennedy triplet mode as in the VC phase in the case with diagonal edge. This is consistent with the naive picture of the rung singlet, which is obtained by the


 FIG. 6. Linear combination of the dimerized plaquette singlets  $|\psi_s\rangle$  with OBCs.


(a) Diagonal-edge



(b) Vertical-edge

 FIG. 7. (Color online) System-size dependence of low-excitation energy for  $\theta=-\pi/5$  with the two OBCs compared with the energy gap under the PBC. The inset is the extended figure for the first excitation state energy.

Berry phase (see Fig. 8). This mode is confirmed also in the different  $(J, K)$ 's in the RS phase.

#### IV. ENTANGLEMENT ENTROPY

In this section, let us consider entanglement entropy for the VC state. Define the density matrix of the state  $|\psi\rangle$  as  $\hat{\rho}=|\psi\rangle\langle\psi|$  and divide the system into two subsystems  $A$  and  $B$  [see Figs. 9(a) and 9(b)]. Then the entanglement entropy is defined as<sup>33</sup>

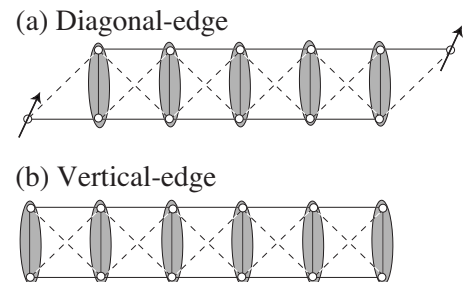


FIG. 8. Rung singlets with OBCs.

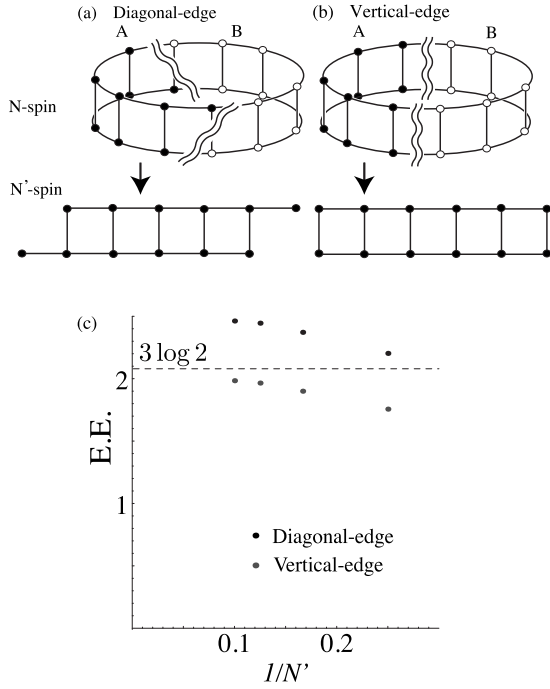


FIG. 9. Two types of the reduction to the subsystem  $A$  with (a) diagonal edge and (b) vertical edge. (c) Entanglement entropy of subsystem for  $\theta=4\pi/5$  with  $N'$  spins by reduction from  $N=20$  spin system.

$$\text{E.E.} = -\langle \log \hat{\rho}_A \rangle_A = -\text{Tr}[\hat{\rho}_A \log \hat{\rho}_A].$$

Here the reduced density matrix  $\hat{\rho}_A$  is given as  $\hat{\rho}_A = \text{Tr}_B \hat{\rho}$ . It represents how much state  $|\psi\rangle$  is entangled between subsystems  $A$  and  $B$ .

Let us assume state  $|\psi\rangle$  as a unique ground state under the PBC in the VC state. We take subsystem  $A$  as the subsystem with the diagonal (vertical) edges with  $N'$  spins by the reduction from  $N=20$  spin system with the PBC. Similarly as for the energy gap, we consider two types of open boundaries, we calculate the entanglement entropy numerically for the cases with vertical edge and diagonal edge as shown in Figs. 9(a) and 9(b). Figure 9(c) shows the  $N'$  dependence of the entanglement entropy. In both cases, the obtained E.E. contains a contribution around  $3 \log 2$ . The contribution  $3 \log 2$  can be understood by the trial state  $|\psi_s\rangle$  (see the Appendix).

In the naive picture, in the RS phase the isolated single on the rung is a good trial state. Therefore we expect that  $\text{E.E.} = 2 \log 2$  for the diagonal edge and that  $\text{E.E.} = 0$  for the vertical edge. We have qualitative agreement that the E.E. for the diagonal edge is larger than that for the vertical edge, although there is strong  $\theta$  dependence and large deviation from the  $2 \log 2$ . This is due to the relatively large overlap on the leg direction.

## V. SUMMARY

In summary, it has been shown that in the vector-chirality state the dimerized plaquette-singlet state  $|\psi_s\rangle$  can be a good trial state to understand the numerical results for the topo-

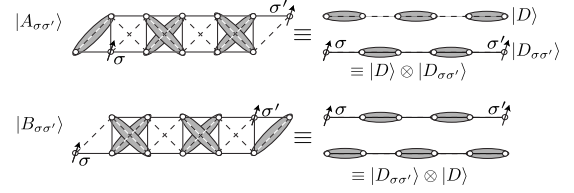


FIG. 10. Two types of the tensor products of the two dimerized states in Eq. (A6) with diagonal edges for even  $N'/2$  case ( $N'=12$ ), which corresponds to Fig. 6(a).

logical properties—the edge states and the entanglement entropy. The entanglement entropy of  $|\psi_s\rangle$  has been obtained as  $3 \log 2$  for both types of the reduced systems while the appearance of the edge states depends on the type of boundaries. These *boundary-dependent* low-energy excitations as the generic edge states characterize the vector-chirality phase. This boundary-dependent edge state is also observed in the rung-singlet phase. Such localized modes in the boundary are expected to be observed experimentally through the impurity or surface effect.

## ACKNOWLEDGMENTS

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## APPENDIX: ENTANGLEMENT ENTROPY FOR THE TRIAL STATE

For example, we calculate the entanglement entropy of  $|\psi_s\rangle$  in the diagonal-edge case for even  $N/2$  and  $N'/2$  cases. The reduced density matrix  $\hat{\rho}_A$  can be obtained as (see Fig. 10)

$$\hat{\rho}_A = \frac{1}{4m} \sum_{\sigma, \sigma' = \uparrow, \downarrow} [|A_{\sigma\sigma'}\rangle\langle A_{\sigma\sigma'}| + |B_{\sigma\sigma'}\rangle\langle B_{\sigma\sigma'}|] + \frac{m'}{4m} [|A_{\uparrow\downarrow}\rangle\langle B_{\downarrow\uparrow}| - |A_{\uparrow\downarrow}\rangle\langle B_{\downarrow\uparrow}| + (A \leftrightarrow B)], \quad (\text{A1})$$

where  $m = 2 + 2^{3-N/2}$  and  $m' = 2^{1-(N-N')/2}$ . States  $|A_{\sigma\sigma'}\rangle$  and  $|B_{\sigma\sigma'}\rangle$  are represented as the tensor product of the dimerized states in the zigzag chains (see Fig. 10),

$$\begin{aligned} |A_{\sigma\sigma'}\rangle &= [(1,1), (2,2)] \otimes |\sigma\rangle_{(2,1)} \otimes [(3,1), (4,2)] \\ &\otimes [(3,2), (4,1)] \otimes \cdots \otimes [(N'/2 - 1, 1), (N'/2, 2)] \\ &\otimes [(N'/2 - 1, 2), (N'/2, 1)] \otimes |\sigma'\rangle_{(N'/2+1, 2)}, \quad (\text{A2}) \end{aligned}$$

$$\begin{aligned}
|B_{\sigma\sigma'}\rangle &= |\sigma\rangle_{(2,1)} \otimes [(2,1), (3,2)] \otimes [(2,2), (3,1)] \otimes \cdots \\
&\otimes [(N'/2 - 2, 1), (N'/2 - 1, 2)] \\
&\otimes [(N'/2 - 2, 2), (N'/2 - 1, 1)] \otimes |\sigma'\rangle_{(N'/2, 2)} \\
&\otimes [(N'/2, 1), (N'/2 + 1, 2)]. \quad (\text{A3})
\end{aligned}$$

We introduce the dimerized states  $|D\rangle$  and  $|D_{\sigma\sigma'}\rangle$  on the chain with length  $N'/2$ ,

$$|D\rangle = [1, 2] \otimes [3, 4] \otimes \cdots \otimes [N'/2 - 1, N'/2], \quad (\text{A4})$$

$$|D\rangle_{\sigma\sigma'} = |\sigma\rangle_1 \otimes [2, 3] \otimes \cdots \otimes [N'/2 - 2, N'/2 - 1] \otimes |\sigma'\rangle_{N'/2}. \quad (\text{A5})$$

Changing site indexes to decouple the ladder into two chains, we have equivalences  $|A_{\sigma\sigma'}\rangle = |D\rangle \otimes |D\rangle_{\sigma\sigma'}$  and  $|B_{\sigma\sigma'}\rangle = |D\rangle_{\sigma\sigma'} \otimes |D\rangle$  (see Fig. 10). Here we have introduced the normalized state  $|\tilde{D}\rangle \propto |D\rangle - \langle D_{\uparrow\downarrow} | D \rangle |D_{\uparrow\downarrow}\rangle - \langle D_{\downarrow\uparrow} | D \rangle |D_{\downarrow\uparrow}\rangle$

by the Gram-Schmidt orthogonalization method. Then we have the following relation:

$$\begin{aligned}
\hat{\rho}_A &\approx \frac{1}{8} \sum_{\sigma, \sigma' = \uparrow\downarrow} [ (|\tilde{D}\rangle \otimes |D_{\sigma\sigma'}\rangle) (\langle \tilde{D} | \otimes \langle D_{\sigma\sigma'} |) \\
&+ (|D_{\sigma\sigma'}\rangle \otimes |\tilde{D}\rangle) (\langle D_{\sigma\sigma'} | \otimes \langle \tilde{D} |)]. \quad (\text{A6})
\end{aligned}$$

The approximation holds up to the order  $\mathcal{O}(2^{-N'/2}) + \mathcal{O}(2^{-(N-N')/2})$  and the eight summands correspond to the states shown in Fig. 6(a). Thus, the entanglement entropy is obtained as E.E.  $\approx -8 \times \frac{1}{8} \log \frac{1}{8} = 3 \log 2$ . In a similar manner, we can calculate the entanglement entropy in the case of the other geometry. The entanglement entropy counts the degrees of freedom of the spins around the edges, although the Kennedy triplet does not appear in the system with vertical edge due to the short-range residual interaction between the localized effective spins.

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- <sup>30</sup>The phase factor can be arbitrary on  $|\psi_b\rangle$ .
- <sup>31</sup>We make a boundary by truncating all terms  $\mathbf{S}_i \cdot \mathbf{S}_j$  and  $(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l)$  whose bond crosses the boundary. Note that some terms of  $P_x + P_x^{-1}$  in Eq. (2) do not cross the boundary even in the vertical-edge case.
- <sup>32</sup>Close to the phase boundary, the correlation length becomes large and the bulk spin gap is very tiny. In this case, ‘‘Kennedy triplet’’ is hardly observed.
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