Discord effects of inter-cluster interactions on a cluster-based Haldane state in a triangular spin tube

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Abstract. We have recently proposed a new concept of cluster-based Haldane states supported by an inherent chirality in a triangular spin tube with equivalent inter-cluster interactions. In this state, there appear spin-1/2 degrees of freedom consisting of a real spin and a scalar chirality as edge states. With applying a magnetic field, we can observe approximately a half of magnetization of $S = 1/2$ spin, i.e., a quarter spin magnetization, due to symmetrization of the real spin and the chirality. Here, we consider effects of discord between two types of inter-cluster interactions, inducing anisotropic biquadratic interactions of effective $S = 1$ spins. The discord brings the edge magnetization nearer to an exact value of quarter spin magnetization, whereas localization of the edge states becomes worse. These effects are also confirmed in a corresponding spin-1 model.

1. Introduction
Fractionalization of quantum degrees of freedom has opened the ways to new phenomena and effects in modern physics, e.g., quark model in particle physics and spin-charge separation in condensed-matter physics. Particularly, in condensed-matter physics, concepts of fractionalization have been applied to understand complicated many-body states, such as the fractional quantum Hall effects [1] and Majorana fermions in topological superconductors [2]. The Affleck–Kennedy–Lieb–Tasaki (AKLT) model [3] is an important example using fractionalization of quantum spin to give an intuitive picture of the Haldane state [4], which is the ground state of an $S = 1$ spin chain. Moreover, the Haldane state has recently attracted broader attention because of a possibility of holographic quantum computing [5].

To flexibly design the Haldane state with $S = 1/2$ spins, we have considered spin cluster chains (SCCs) where clusters of strongly interacting $S = 1/2$ spins line up and weakly interact with neighboring clusters [6, 7]. In addition, we have clarified general conditions for the Haldane state in SCCs, which we call cluster-based Haldane states (CBHS): (I) the ground state of a cluster is a triplet, (II) the inter-cluster interaction is weak enough as compared with any intra-cluster interactions, and (III) the effective inter-cluster interaction between clusters’ ground
states is mainly antiferromagnetic and XXZ-like (XY, Heisenberg, and weakly Ising types). The Kramers theorem allows the triplet ground state of a cluster (Condition I), composed by an even number of spins only with Hamiltonian terms keeping the time-reversal symmetry (TRS). However, the condition can be extended to SCCs whose clusters contain an odd number of spins, if there is a term breaking the TRS, e.g., magnetic fields and a scalar spin chirality. Both cases of the magnetic field and scalar chirality have been demonstrated with explicit spin Hamiltonians in our preceding works [7, 8]. Particularly, in the latter case, we have also shown an exotic edge state consisting of a real spin and a scalar chirality, which exhibits a quarter spin magnetization as a response to a magnetic field.

2. Model and Method

In this paper, we consider a CBHS supported by a chirality appearing in triangular spin tube (TST) defined by

\[ \mathcal{H}_{\text{TST}} = \sum_{j=1}^{L} \left( J \sum_{i<j'} s_{i,j} \cdot s_{i',j} - K s_{\text{tot},j} \cdot \chi_{j} \right) + \sum_{j=1}^{L-1} \left( J'_1 \sum_{i} s_{i,j} \cdot s_{i,j+1} + J'_2 \sum_{i \neq i'} s_{i,j} \cdot s_{i',j+1} \right) \]

where \( L \) is the number of clusters. The first (second) term represents intra-cluster (inter-cluster) interactions. The \( S = 1/2 \) local spin (the total spin) operator in a cluster is denoted by \( s_{i,j} \) (\( s_{\text{tot},j} = \sum_i s_{i,j} \)), where \( i = 1, 2, 3 \) (\( j = 1, 2, \cdots, L \)) denotes the site (cluster) index. The \( S = 1/2 \) pseudo spin operator \( \chi_{j} \) is constructed by the scalar chirality: \( \chi_j^x = (2/\sqrt{3}) s_{1,j} \cdot s_{2,j} \times s_{3,j}, \chi_j^z = (\chi_j^+ + \chi_j^-)/2, \chi_j^y = (\chi_j^+ - \chi_j^-)/(2i) \), where \( \chi_j^\pm \) represents the chirality ladder operators defined by \( \chi_j^\pm = \sum_{\sigma = \pm} |\sigma, \pm\rangle \langle \sigma, \mp| \) with the local eigenstates of the total spin and scalar chirality of a cluster, \( |s_{\text{tot},j}^z, \chi_j^z\rangle \).

In this model, we assume the SCC condition (II), i.e., \( J, K \gg J'_1 \) (i=1,2), resulting in a triplet ground state obtained by symmetrization of the total spin and scalar chirality in a cluster. The low-temperature behavior is dominated by the triplet, corresponding to a pseudo spin-1 operator \( T_j \). Therefore, we can obtain an effective Hamiltonian for the \( S = 1 \) pseudo spins as follows,

\[ \mathcal{H}_{\text{eff}} = J'_1 \sum_{j=1}^{L-1} \left\{ Hs_j \left( \frac{5}{3} - \frac{2}{3} \alpha_{j'} \right) + \frac{8}{3} \left( 1 - \alpha_{j'} \right) Hs_j^2 \left( \frac{1}{2} \right) - \frac{8}{3} \left( 1 - \alpha_{j'} \right) I_{z,j} \right\} \]

with the anisotropic Heisenberg (XXZ) interaction and an additional \( z \) component interaction,

\[ Hs_j(\Delta) = T_j^x T_{j+1}^x + T_j^y T_{j+1}^y + \Delta T_j^z T_{j+1}^z, \quad I_{z,j} = \left[ 1 - (T_j^z)^2 \right] \left[ 1 - (T_{j+1}^z)^2 \right] \],

where we use the ratio of the inter-cluster interactions \( \alpha_{j'} = J'_2 / J'_1 \). Since an equivalent case \( \alpha_{j'} = 1 \) has been presented in the preceding paper [8], we concentrate on a discord case \( \alpha_{j'} \neq 1 \).

3. Discord effects of inter-cluster interactions

In this section, we show effects of the discord of two inter-cluster interactions \( J'_1 \neq J'_2 \) (\( \alpha_{j'} \neq 1 \)). As explained above, the equivalence of the inter-cluster interactions \( \alpha_{j'} = 1 \) effectively gives the Heisenberg spin chain of the \( S = 1 \) pseudo spins at low temperatures. On the other hand, if there is the discord \( \alpha_{j'} \neq 1 \), additional interactions appear in the effective Hamiltonian (2) such as an anisotropy and biquadratic interactions. To clarify effects of the additional terms as compared with a spin-1 chain, we consider an extended bilinear-biquadratic (eBLBQ) model of
Haldane gap \( \Delta = \Delta' = 1 \) in the spin-1 eBLBQ model \((A = 0)\). AKLT shows that at \( Q = 1/3 \), the Haldane gap is maximized and the edge states are most localized [3]. Therefore, in our model, the stabilization of the CBHS can be enhanced by the discord of the inter-cluster interactions \( \alpha J' \neq 1 \). To confirm the speculation, we have performed the variational matrix-product state (VMPS) calculation with \( L = 60, K = J/2, \) and \( \sqrt{(J'_1)^2 + (J'_2)^2} = J/10 \) in (1), and obtained the Haldane gap \( \Delta_2 \) as a function of the \( J' \) ratio defined by \( \theta_J = \tan^{-1} \alpha J' \).

Figure 1. (a) The Haldane gap \( \Delta_2 \) corresponding to the energy difference between the first \((M = 1)\) and second \((M = 2)\) excited states, and real (pseudo) magnetization \( M (M') \) of the \( \tilde{M} = 1 \) state, as a function of the \( J' \) ratio, \( \theta_J = \tan^{-1} \alpha J' \). The vertical dashed lines denote the equivalent condition \( \alpha J' = 1 \). The horizontal dashed line represents the zero-energy level, corresponding to the stable-unstable boundary of the Haldane state. The horizontal dotted line denotes the symmetric case \( M = M' \). (b) Local magnetization \( \langle S_j^z \rangle \) in the \( M = 1 \) state of the TST model. (c) Local magnetization \( \langle S_j^z \rangle \) in the \( M = 1 \) state of the spin-1 chain model. In (b), the \( J' \) ratio dependency is shown for \( \theta_J = \tan^{-1} \alpha J' = 0.25, 0.23, \) and 0.21 for a TST (1). In (c), effects of the \( Q \) and \( A \) terms including an anisotropy are presented for a spin-1 chain (4), where “Iso.” and “Aniso.” represent the isotropic case \( \Delta = \Delta' = 1 \) and an anisotropic case \( \Delta = 13/12, \Delta' = 1/2 \) for the bilinear-biquadratic term, respectively. The parameters of the orange diamonds in (c) correspond to the \( \alpha J' = 7/8 (\theta_J \cong 0.229\pi) \) in the effective model (4).

Figure 1(a) shows the Haldane gap defined by the energy difference between the \( \tilde{M} = 1 \) and \( \tilde{M} = 2 \) ground states, where the total pseudo magnetization is defined by \( \tilde{M} = M + M' \) with the real and pseudo magnetizations, \( M = \sum_j \langle s_{\text{tot},j}^z \rangle \) and \( M' = \sum_j \langle \chi_{\text{tot}}^z \rangle \). As we can see, the Haldane gap has a peak at \( \theta_J \cong 0.215\pi \), whereas the \( \theta_J = \pi/4 \) represents the equivalent point of \( J'_1 = J'_2 \) denoted by the vertical dashed line. In the effective Hamiltonian (2), we cannot find the AKLT condition \( [Q = 1/3, A = 0, \Delta = \Delta' = 1] \) due to a necessarily finite anisotropy and another term. If we ignore effects of the anisotropy and the additional term, an AKLT-like condition \( \alpha J' = 7/8 \) corresponds to \( \theta_J = \tan^{-1} \alpha J' \cong 0.229\pi \), which is not so far from the point \( \theta_J \cong 0.215\pi \) showing the peak of the Haldane gap in Fig. 1(a).

Next, we have also investigated the difference between the real and pseudo magnetizations, \( M \) and \( M' \), at the \( \tilde{M} = 1 \) ground state as a function of the \( J' \) ratio [see Fig. 1(a)].
Interestingly, symmetrization of the real and pseudo magnetizations recovers with decreasing $\theta_{J'}$, i.e., approaching the AKLT-like point. Since the real magnetization corresponds to the sum of magnetization of the two edge states, the quasi-fractionalization of $S = 1/2$ spin magnetization shows nearly an exact half value, that is, an $S = 1/4$ spin magnetization for $\theta_{J'} \lesssim 0.2\pi$, while the CBHS becomes unstable for $\theta_{J'} \lesssim 0.175\pi$ due to a negative Haldane gap.

Furthermore, to check the localization of the edge state, we have calculated the local magnetization, $\langle s_{\text{tot},j}^z \rangle$ in the $\tilde{M} = 1$ state of the TST model with various $J'$ ratios [see Fig. 1(b)]. With approaching the most stable point $\theta_{J'} \cong 0.215\pi$, the edge state surprisingly extends to the bulk, so that the localization becomes worse. To clarify which term dominates the extension in the effective Hamiltonian (2), we have also obtained the local magnetization in the spin-1 eBLBQ model (4). Figure 1(c) shows effects of the additional terms and anisotropy. We can confirm that the isotropic additional terms prevent the edge state from extending, while the anisotropy automatically appearing in the effective Hamiltonian (4) makes the localization worse. Therefore, we conclude that in the TST model, the discord of the inter-cluster interactions stabilizes the CBHS and brings the edge magnetization nearer to the exact value of the quarter spin magnetization, whereas the localization of the edge states simultaneously becomes worse.

4. Summary
In this paper, we have investigated the discord effects of the inter-cluster interactions on the edge state of the CBHS in the TST model. In this model, the edge state shows an approximately half of spin-1/2 magnetization in the equivalent case of the inter-cluster interactions [8]. On the other hand, if the equivalence is broken, some additional terms such as the biquadratic interactions appear in the effective Hamiltonian. To confirm the effects, we have performed the VMPS calculations for the TST model, together with the spin-1 eBLBQ model for comparison. In conclusion, we have clarified that the biquadratic interactions certainly stabilize the CBHS and brings the edge magnetization nearer to the exact value of the quarter spin magnetization, while the localization of the edge states simultaneously becomes worse due to the anisotropy automatically appearing with the biquadratic terms.

Acknowledgments
This work was partly supported by a Grant-in-Aid for Scientific Research (C) (Grant No. 20K03840). Numerical computation was carried out on the supercomputers at JAEA and the Supercomputer Center at the Institute for Solid State Physics, University of Tokyo.

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