Entanglement Entropy of 1D Gapped Spin Chains

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We investigate the entanglement entropy (EE) of gapped $S = 1$ and $S = 1/2$ spin chains with dimerization. We find that the effective boundary degrees of freedom as edge states contribute significantly to the EE. For the $S = 1/2$ dimerized Heisenberg chain, the EE of the sufficiently long chain is essentially explained by the localized $S = 1/2$ effective spins on the boundaries. As for $S = 1$, the effective spins are also $S = 1/2$ causing a Kennedy triplet that yields a lower bound for the EE. In this case, the residual entanglement reduces substantially by a continuous deformation of the Heisenberg model to that of the AKLT Hamiltonian.

KEYWORDS: Topological orders, Quantum phase transition, Entanglement entropy, Spin chains, Haldane gap, Edge states

1. Introduction

The concept of entanglement in quantum mechanics has significant importance in quantum information technologies, where quantum resources are used for processing information in novel ways. Recently, it has been clarified that the entanglement of a quantum state is one of the most important properties not only in quantum information science but also in condensed matter physics. Entanglement entropy (EE) measures the entanglement of a single quantum state, which is defined as the von Neumann entropy of a reduced density matrix of a subsystem. EE has been applied to a condensed matter system in order to understand quantum phases. There are several works¹–⁴ that have reported the EE near or at a quantum critical point. As for the system size dependence, the EE of gapped spin chains saturates, although that of critical spin chains shows a logarithmic divergence. Recently, the EE was used to detect the quantum dimension, which is a property of the topological order.⁵–⁷ The topological order is a new order that cannot be characterized by a classical local order parameter and a symmetry breaking by the conventional Ginzburg-Landau theory.⁸ Recently, one of the authors proposed the use of quantum objects such as quantized Berry phases to define the local order parameters that do not require classical symmetry breaking since they are gauge-dependent quantities unlike the classical ones.⁹–¹²

It is also interesting to study the EE from the viewpoint of bulk-edge correspondence. Although the EE is a physical quantity of the bulk, there is a relation between the EE and the edge states that appear in a topologically nontrivial system with boundaries. There are several works on the bulk-edge correspondence in many kinds of physical systems such as the 2D quantum Hall effect,¹³,¹⁴ polycrystalline,¹⁵,¹⁶ and the Haldane spin chain.¹⁷,¹⁸ The EE and the Berry phase of a topologically nontrivial system are closely related through the edge states.⁷

In this paper, we investigate the relation between the saturated EE in a gapped system and the corresponding edge state through the bulk-edge correspondence. The systems chosen are three different types of gapped quantum spin chains: (i) the $S = 1/2$ dimerized Heisenberg chain, (ii) the $S = 1$ XXZ Hamiltonian with the on-site anisotropic term $D \sum_{i=1}^{N} \langle S_i^z \rangle^2$, and (iii) the Affleck Kennedy Lieb Tasaki (AKLT) model.¹⁹

The $S = 1$ XXZ chain near the Heisenberg point is a typical Haldane spin chain, which has a finite gap in an appropriate range of the parameters. There are several other phases such as the “large-$D$ phase” and the “Néel phase.” They are characterized by the hidden $Z_2 \times Z_2$ symmetry breaking, which is nonlocal.²⁰,²¹ The string order parameter is a nonlocal order parameter;²² therefore, it is not a conventional classical order parameter. We see that the EE reflects these kinds of hidden symmetry breaking, which relates to the structure of the edge states.

2. EE of gapped system and edge state

The EE (the von-Neumann entropy) used in this paper is defined as follows:

$$ S = -\langle \log \hat{\rho}_A \rangle = -Tr[A \log \hat{\rho}_A], $$

where $\hat{\rho}$ is a density matrix of the pure state $|\psi\rangle$. We assume that the system consists of subsystems A and B. The reduced density matrix $\hat{\rho}_A$ is obtained by tracing out the degrees of freedom in subsystem B from the total density matrix $\hat{\rho}$. The EE quantifies the information about how much the state is entangled between the subsystems A and B. We consider $|\psi\rangle$ to be the ground state (GS), assuming that it is unique.

We divide a one-dimensional chain into subsystems A and B (Fig.2) that denote the upper and lower parts, respectively. Since taking a partial trace over a spatially separated subsystem results in effective boundaries, it induces effective localizations of degrees of freedom as edge states. Then, we evaluate the EE as $S \sim S_{\text{bulk}} + S_{\text{edge}}$ where $S_{\text{bulk}}$ and $S_{\text{edge}}$ denote the contribution from the bulk and edge, respectively. This is because the degrees of
freedom originate not only from the edges but also from the bulk part of the system. We hypothesize that the edge state picture of the EE is valid for these systems. We obtain the ground state of the systems that from the bulk is essential in a gapless system because of the infinite correlation length.\textsuperscript{7, 23}

3. Evaluation of EE for several spin chains

We calculate the EE for the three spin chains and show that the edge state picture of the EE is valid for these systems. We obtain the ground state of the systems numerically using the Lanczos method in an invariant subspace with $S_{\text{total}}^{z} = 0$, where $S_{i}^{z}$ denotes the $z$-component of the spin operator on the $i$-th site. The EE is evaluated by diagonalizing $\hat{\rho}_{A}$ using the Householder method. We calculate the logarithm in base 2.

We impose periodic boundary conditions for the systems. These models exhibit various behaviors that can be distinguished as different quantum phases by the EE.

$S = 1/2$ Dimerized Heisenberg Model: The Hamiltonian of the $S = 1/2$ dimerized Heisenberg system is given by

$$H_{S=1/2,D} = \sum_{i=1}^{N/2} (J_{1}s_{2i-1} \cdot s_{2i} + J_{2}s_{2i} \cdot s_{2i+1}),$$

where $s_{i}$ are the $S = 1/2$ spin operators. $J_{1}$ and $J_{2}$ are parametrized as $J_{1} = \sin \theta$ and $J_{2} = \cos \theta$, respectively, where $\theta \in S^{1}$. We consider the case of $-\pi/2 < \theta < \pi/2$ in this paper. The ground state is unique in any $\theta$.\textsuperscript{26} In the case of $0 < \theta \ll \frac{\pi}{2}$, the ground state is composed of an ensemble of $N/2$ singlet pairs and the energy gap is finite ($\sim \frac{J_{1}}{\theta}$). The system is equivalent to the isotropic antiferromagnetic Heisenberg chain at $\theta = \frac{\pi}{2}$. This is the only gapless point. In the ferromagnetic strong coupling, $\theta \to -\frac{\pi}{2} + 0$, the system is effectively considered as the $S = 1$ Heisenberg chains.\textsuperscript{26}

We now discuss the EE of the system. Fig.1 shows the $\theta$ dependence of the EE. Fig.2 shows the subsystems considered in this study. As shown in Fig.2, a partial trace is performed across two $J_{2}$ coupling bonds. The EE tends to diverge as the system size increases at the critical point $\theta = \frac{\pi}{4}$ (isotropic Heisenberg point). This behavior of the EE has been discovered by Vidal et al.\textsuperscript{3} One can clearly observe the EE of the edge states, $2 \log 2$, near $\theta \sim 0$, while the EE converges to 0 in the region of $\theta \to \frac{\pi}{2}$. In the former limit, the system becomes a collection of $N/2$ singlet pairs with two almost free spins near the boundaries. Therefore, the EE in this region is given by that of the two free spins near the boundaries $2 \log 2$. In the latter limit, the system also becomes a collection of $N/2$ singlets; however, there are no free spins in this case. Then, the EE vanishes.

These results can be interpreted as follows. The EE reflects the local degrees of freedom that appear near the boundaries when the system gets truncated. Then, we speculate that a lower bound is obtained for EE as $S \geq \log g$, where $g$ denotes the above mentioned degrees of freedom near the edges. In this case, this local degree of freedom arises due to the two $S = 1/2$ spins localized on the edges as $g = 4$ as $|\alpha\rangle_{L} \otimes |\beta\rangle_{R} (\alpha, \beta = \uparrow, \downarrow)$.

The low energy behavior of this system is identical to that of the $S = 1$ Heisenberg model in the region of $\theta \to -\frac{\pi}{2} + 0$.\textsuperscript{26} We expect that the edge states of the $S = 1/2$ dimer phase are similar to those of the $S = 1/2$ dimer phase as the EE is larger than $2 \log 2$, which gives the lower bound.

$S = 1$ XXZ Chain with D-term: The Hamiltonian of the $S = 1$ XXZ chains with an on-site anisotropic term is given by

$$H_{S=1} = J \sum_{i=1}^{N} (S_{i}^{x}S_{i+1}^{x} + S_{i}^{y}S_{i+1}^{y} + \Delta S_{i}^{z}S_{i+1}^{z}) + D \sum_{i=1}^{N} (S_{i}^{z})^{2},$$

where $S_{i}$ are the $S = 1$ spin operators. The energy gap as a Haldane gap is finite near the point $\Delta = 1$ and $D = 0$.\textsuperscript{27} There are several phases known as the “Haldane phase,” the large-$D$ phase and the Néel phase in the range of $\Delta > 0$ with a gapped-gapped transition (Gaussian transition) between the Haldane phase and the large-$D$ phase and the Ising transition between the Néel phase and the Haldane phase. These three phases are distinguished by local and nonlocal order parameters\textsuperscript{22} or by the breaking of the hidden $Z_{2} \times Z_{2}$ symmetry that appears on performing a non-local unitary transformation.\textsuperscript{20, 21} Quantum order parameters to characterize the states are also defined.\textsuperscript{9–11} A system with open boundary condition has the localized effective spin-$1/2$ edge state in the Hal-
dane phase, and the low energy effective Hamiltonian can be written by an effective coupling of the two $S = 1/2$ edge spins.

Fig. 3(a) shows the EE of the XXZ spin chain with the $D$ term, which is calculated in the subspace $S^z_{total} = 0$ by changing the anisotropies $\Delta$ and the coefficient of the $D$ term $D$ with a system size $N = 10$. Figs. 3(b) and (c) show the cross section of Fig. 3(a) along the corresponding planes (indicated by lines A and B in Fig. 3(a)) and the system size dependence of the EE.

From Fig. 3(a), it can be observed that there are three regions. The EE is larger than $2 \log 2$, which can be interpreted as the effect of the edge states created by taking a partial trace. We notice that the EE is lower than $2 \log 2$ in the Haldane phase, and it also relates to the edge states. In summary, the Haldane phase is a quantum liquid. The EE is larger than $2 \log 2$, which can be interpreted as the contribution from the edge state. The rest of the contribution $S = 2 \log 2$ comes from the bulk. This interpretation is consistent with the result. The EE reflects the spontaneous breaking of the hidden $Z_2 \times Z_2$ symmetry, which plays an essential role in Haldane spin chains and it also relates to the edge states. In summary, the EE has a lower bound of $\log g$, where $g$ is the number of elements in the group of spontaneously broken symmetry ($g = 1$ for the large-$D$ phase, $g = 2$ for the Haldane phase, and $g = 2^2$ for the Haldane phase), at least in the calculated regions.

We notice that the EE is lower than $2 \log 2$ in the Haldane phase when total system size is small, as shown in figs. 3(b) and (c). This low value of the EE is due to the correlation length of the system and the system size. When the correlation length is long as compared to the total system size, $S_L$ and $S_R$ are effectively coupled. Then, the degrees of freedom on the edges decrease because both the sides of the edge states are not independent in the presence of substantial coupling.

As discussed above, the bulk-edge correspondence is confirmed through the trace-out operation, and the EE shows the degrees of freedom in the subsystem. An edge state in the open boundary condition is one of the important characteristics of the Haldane materials. The above-mentioned phases of the periodic spin chains are well characterized by the EE that reflects the edge state of each corresponding open spin chain. We found that the bulk and edge are inextricably linked in these kinds of spin chains. We confirmed that the Haldane phase can be distinguished by the EE intermediate the information of the edge states.

**The $S = 1$ Heisenberg Model to the AKLT Model:** We also calculate the EE of the AKLT model numerically by modifying the parameter $\beta$ (Fig.4). The Hamiltonian
is given by

\[ H_{\text{AKLT}} = J \sum_{i=1}^{N} \left( S_i \cdot S_{i+1} + \beta (S_i \cdot S_{i+1})^2 \right), \]

(4)

where \( S_i \) are the \( S = 1 \) spin operators. There are solvable points at \( \beta = 1/3 \) and \( \beta = \pm 1. \) The ground state can be explicitly written as the valence-bond solid (VBS) state at the point \( \beta = 1/3. \)

Fig. 4 shows the EE of the AKLT model obtained by changing the parameter \( \beta. \) The result shows that the value of EE is minimum at the point \( \beta = 1/3, \) at which the ground state is the VBS state. The EE is lower than \( 2 \log 2 \) when the system size is \( N = 4, 6, 8, 10. \) This is due to the correlation between the edge spins \( (S_L \text{ and } S_R), \) which is also discussed in the previous model. According to the edge state picture of the EE, \( S \geq 2 \log 2 \) when the substantial coupling of the spins vanishes (in the large \( N \) limit), as speculated from the numerical results; however, one cannot observe this relation from the numerical calculations. To confirm this relation, we evaluate the exact form of the EE of the periodic VBS state analytically.

The EE of the periodic VBS state is obtained analytically by using a transfer matrix technique as follows:

\[ S_{N,L} = -3\lambda_A \log \lambda_A - \lambda_B \log \lambda_B, \]

(5)

\[ \lambda_A = \frac{1}{4} \left( 1 - p^L \right) \left( 1 - p^{N-L} \right), \]

(6)

\[ \lambda_B = \frac{1}{4} \left( 1 + 3p^L \right) \left( 1 + 3p^{N-L} \right), \]

(7)

\( p = -\frac{1}{4}, \) where \( N \) and \( L \) denote the total system size and the length of the subsystem, respectively. It is evident that this expression is invariant under the replacement \( L' = N - L, \) i.e., \( S_{N,L} = S_{N,N-L}, \) which is a general property of the EE.

In the limit \( N \to \infty, \) the EE reduces to the expression

\[ \lim_{N \to \infty} S_{N,L} = 2 \log 2 - \frac{3}{4} (1 - p^L) \log (1 - p^L) \]

\[ - \frac{1}{4} (1 + 3p^L) \log (1 + 3p^L), \]

(8)

which is exactly the same as the EE of the VBS state with two spin-1/2s on the boundary.

Next, we consider the thermodynamic limit of \( S_{N,L} \) with \( \alpha = L/N \) fixed. We obtain \( \lim_{N \to \infty} S_{N,N\alpha} = 2 \log 2 \) \( (\alpha = L/N \) fixed). We can see that the EE does not diverge. This result is consistent with the equation \( S \geq 2 \log 2 \) as a consequence of the edge state picture. According to the edge state picture, the EE in the AKLT model receives no contribution from the bulk, while the contribution from the two edges is present. Therefore, this is the point at which the EE is lowest in the Haldane phase, as long as the edge state picture of the EE is valid.

4. Conclusion

We have explored new aspects of the bulk-edge correspondence in spin systems on the basis of quantity obtained from the quantum information, namely, the entanglement entropy (EE). The tracing out can be interpreted as the truncation of the system, and the EE includes the information regarding how many degrees of freedom the truncated state has. In the case of the \( S = 1 \) XXZ spin chain with the \( D \) term and the AKLT model, it is the degrees of freedom of the effective \( S = 1/2 \) spins localized at the edges of the chain, which are known as the characteristics of the ground state in the Haldane phase with an open boundary condition. Further, we speculate that the EE has a lower bound of \( \log g, \) reflecting the effective boundary degrees of freedom \( g. \)

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