Entanglement properties of quantum spin systems have been attracting much attention in quantum information theory and condensed matter physics. The entanglement entropy (EE), the von Neumann entropy of a subsystem, is a measure to quantify how much entangled a many-body ground state is. Recently the EE has been used to investigate the nature of quantum ground states such as the quantum phase transition and topological/quantum order. Vidal et al. conjectured that the EE of a large block of spins in gapped spin chains reaches saturation while that in critical spin chains shows a logarithmic divergence.

In this Letter we study the EE of gapped quantum spin chains with arbitrary integer-spin. After the Haldane conjecture that integer-spin antiferromagnetic Heisenberg chains have a finite gap but an $S = 2$ chain (MnCl$_3$(bipy)) in which the presence of the Haldane gap has been experimentally confirmed. We give the exact form of the EE in generic VBS states in this Letter. Then we explicitly confirm that the part of the conjecture proposed by Vidal et al. is true for all integer-spin VBS chains. The relationship between the EE and the correlation function is clarified and the physical meaning of the EE in gapped models is established. We also make a comparison between the analytical results for VBS chains and the numerical results for higher-spin antiferromagnetic Heisenberg chains. The obtained results indicate that the edge-state picture is valid not only for $S = 1$ Haldane chains but also for all the other integer spin-$S$ chains. This is a typical consequence of the non-trivial topological and/or quantum orders, where characteristic features are hidden in the bulk and appear only near the boundaries and impurities. We also discuss a potential application of the edge states as qubits for quantum computation.

Let us start with the Schwinger boson representation of generic VBS states. The spin operators are represented by the Schwinger bosons as

$$a_j^\dagger a_j = b_j^\dagger b_j$$

with $a_j^\dagger$ and $b_j$ satisfying the commutation relations $[a_j, a_k^\dagger] = [b_j, b_k^\dagger] = \delta_{ij}$ with the all the other commutators vanishing.

To reproduce the dimension of the spin-$S$ Hilbert space at each site, we must impose the constraint that the total boson occupation number $a_j^\dagger a_j + b_j^\dagger b_j = 2S$. Using the Schwinger boson representation, the VBS state has two spin-$S/2$'s on the boundary is written as

$$|\text{VBS}\rangle = \prod_{j=0}^L (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S |\text{vac}\rangle,$$

where $j = 1, 2, \ldots, N$ are bulk sites and 0 and $N + 1$ are end sites. $B_{ij} = a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger$ is a creation operator for the valence bond between $i$ and $j$.

The VBS state is a zero-energy ground state of the following Hamiltonian:

$$H = \sum_{j=1}^{N-1} \sum_{J=S+1}^{2S} A_{J} P_{J,j+1} + \pi_{0,1} + \pi_{N,N+1},$$

where the projection operator $P_{J,j+1}$ projects the bond spin $S_{j,j+1} = \frac{S_j + S_{j+1}}{2}$ onto the subspace of magnitude $J$. Here the coefficient $A_J$ can be an arbitrary positive value. The boundary terms describing interaction between spin $S/2$ and spin $S$ are explicitly written as

$$\pi_{0,1} = \sum_{J=S/2+1}^{3S/2} B_{J} P_{0,1}^J, \quad \pi_{N,N+1} = \sum_{J=S/2+1}^{3S/2} B_{J} P_{N,N+1}^J.$$
with $B_J > 0$. In order to calculate reduced density matrices, it is convenient to introduce a spin coherent state. For a point $\hat{\Omega} = (\sin \theta \cos \phi, \sin \sin \phi, \cos \theta)$ on the unit sphere, the spin coherent state at each site is defined as

$$\hat{\Omega} = \frac{(ua^\dagger + vb^\dagger)^{2S}}{\sqrt{(2S)!}},$$

where $(u, v) = (\cos(\theta/2)e^{i\phi/2}, \sin(\theta/2)e^{-i\phi/2})$ are spinor coordinates. Here we have already fixed the $U(1)$ gauge degree of freedom since it has no physical content. Using $\hat{\Omega}$, the trace of any operator $\mathcal{O}$ is written as $\text{Tr}\mathcal{O} = \frac{2^{S+1}}{4\pi} \int d\hat{\Omega} \langle \hat{\Omega} | \mathcal{O} | \hat{\Omega} \rangle$.

Let us now calculate the EE of a block of $L$ contiguous bulk spins in the VBS state $|\text{VBS}\rangle$. For the density matrix of our ground state $\rho = |\text{VBS}\rangle\langle\text{VBS}|$, the reduced density matrix of the block of $L$ contiguous bulk spins is defined as $\rho_L = \text{Tr}_{\overline{\mathcal{B}}_L} \rho$. Here $\overline{\mathcal{B}}_L$ is a block of $L$ spins and $\overline{\mathcal{B}}_L$ is its complement. The EE $S_L = -\text{Tr}_L \rho_L \log_2 \rho_L$ is determined by eigenvalues of $\rho_L$. Suppose that the block of $L$ contiguous spins starting from site $k$ and stretching up to $k + L - 1$, where $k \geq 1$ and $k + L - 1 \leq N$ (Fig. 1). To obtain the reduced density matrix $\rho_L$, we take the trace over the sites $j = 0, 1, ..., k - 1$ and $j = k + L, ..., N, N + 1$. Using the spin coherent state representation, $\rho_L$ is formally written as

$$\rho_L = \frac{f(\prod_{j \in \overline{\mathcal{B}}_L} \frac{d\theta}{4\pi}) \prod_{j=0}^{L-1} \left(1 - \Omega_j \Omega_{j+1}\right)^S \prod_{j=k+L}^{N} \left(1 - \Omega_j \Omega_{j+1}\right)^S \prod_{j=0}^{L-1} \left(1 - \Omega_j \Omega_{j+1}\right)^S}{(2S)! L \int \prod_{j \in \overline{\mathcal{B}}_L} \frac{d\theta}{4\pi}) \prod_{j=0}^{L-1} \left(1 - \Omega_j \Omega_{j+1}\right)^S},$$

where $|\text{vac}\rangle\langle\text{vac}| = |0\rangle_0 \otimes |0\rangle_{L+1}\langle 0|_0$. The state $P_0^0|0\rangle_0$ in the numerator of (3) is explicitly given by $(a_0^\dagger a_0^\dagger - b_0^\dagger b_0^\dagger)|0\rangle_0$. From the definition of the spinor coordinates, we notice that $(u, v)$ changes to $(iv^*, -iv^*)$ when we change variables from $(\theta, \phi)$ to $(\pi - \theta, \phi + \pi)$. Then we can rewrite $P_0^0|0\rangle_0$ as $(-i)^S \sqrt{S!} |\Omega_0\rangle_0$. In the same way, $Q_j^0|0\rangle_{L+1}$ can be rewritten as $i^S \sqrt{S!} |\Omega_j\rangle_{L+1}$. Substituting these results into Eq. (3) and changing the variables of integration from $\Omega_j$ to $-\Omega_j$ ($j = 1, 2, ..., L$), we obtain

$$\rho_L = \frac{f(\prod_{j=1}^{L} \frac{d\theta}{4\pi}) \prod_{k=1}^{L-1} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S}{(2S)! L \int \prod_{j=1}^{L} \frac{d\theta}{4\pi}) \prod_{k=1}^{L-1} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S \prod_{k=1}^{L} \left(1 - \Omega_k \Omega_{k+1}\right)^S},$$

Now the physical meaning of $\rho_L$ is quite clear. Eq. (4) can be regarded as a correlation function between density matrices $|\Omega_1\rangle_1 \langle\Omega_1|_1$ and $|\Omega_L\rangle_L \langle\Omega_L|_L$. More precisely, the matrix elements of $\rho_L$ are completely determined by the two-point correlation functions of the corresponding one-dimensional classical statistical model $\mathcal{M}$. This can be checked by using the binomial expansion of $P_0$ and $Q_{L+1}$. While this interpretation enables us to understand the relation between the EE and the correlation functions, it is more convenient to use the form (4) for the calculation of the EE.

From now on, we follow Ref. [11] and obtain the eigenvalues of $\rho_L$. In Eq. (4), $T_{k,k+1} = \left(1 - \Omega_k \Omega_{k+1}\right)^S$ acts as a transfer matrix of the corresponding classical statistical model. Expanding $T_{k,k+1}$ in terms of Legendre polynomials and using the addition theorem for spherical harmonics, we find that $T_{k,k+1}$ can be expressed as a sum of Legendre polynomials $P_n$ with $n = 0, 1, 2, ..., S$.
Since the reduced density matrix \( \rho_{l} \) by the polynomials in monics, the transfer matrix can be rewritten as

\[
T_{k,k+1} = \frac{4\pi}{(S+1)^2} \sum_{l=0}^{S} \lambda(l) \sum_{m=-l}^{l} Y_{l}^{m}(\Omega_{k}) Y_{l}^{m}(\Omega_{k+1}) I_{l}^{m}(\Omega),
\]

(5)

with \( \lambda(l) \equiv (-1)^{l} S! (S+1)! / [(S-l)! (S+l+1)!] \). Then we substitute (5) into (4), recall the orthornormality of spherical harmonics, i.e., \( \int d\Omega Y_{l}^{m}(\Omega) Y_{l}^{m'}(\Omega) = \delta_{mm'} \), and obtain

\[
\rho_{l} = \frac{4\pi}{(S+1)^2} \sum_{l=0}^{S} \lambda(l) I_{l}^{m-1} \sum_{m=-l}^{l} [T_{l}^{m}(\Omega) \otimes (T_{l}^{m}(\Omega))]^{l},
\]

where irreducible \( l \)-th order spherical tensor operators \( T_{l}^{m}(\Omega) \) are defined as \( T_{l}^{m}(\Omega) \equiv \frac{2S/2+1}{4\pi} \int d\Omega Y_{l}^{m}(\Omega) \hat{\Omega}^{l} \). We should note here that \( T_{l}^{m}(\Omega) \) acts on the Hilbert space of the left-end spin-\( S/2 \) while \( (T_{l}^{m}(\Omega))^{l} \) acts on that of the right-end spin-\( S/2 \). Let us now introduce the following formula found in (11):

\[
I_{j+1}(X) = \frac{2j+3}{(S+j+2)^{2}} \left( \frac{X}{j+1} + j \right) I_{j}(X) - \frac{j}{j+1} \frac{2j+3}{(S+j+2)^{2}} \left( \frac{S-j+1}{S+j+2} \right)^{2} I_{j-1}(X),
\]

with \( I_{0}(X) = \frac{1}{4X} \) and \( I_{1}(X) = \frac{3}{4X} \). The isotropic two site tensor operators \( I_{j}(\tilde{S}_{0} \cdot \tilde{S}_{L+1}) \) are mutually orthogonal with respect to the trace inner product \( Tr_{0,L+1}(I_{j}I_{k}) \). Since Eq. (6) is completely determined by the polynomials in \( \tilde{S}_{0} \cdot \tilde{S}_{L+1} \), the reduced density matrix \( \rho_{L} \) is diagonal in the basis which diagonalizes the total spin operator \( J_{0,L+1}^{2} = \tilde{S}_{0} + \tilde{S}_{L+1} \). Therefore, the eigenvalues of \( \rho_{L} \) are given by

\[
\rho_{L}(J) = \frac{4\pi}{(S+1)^2} \sum_{l=0}^{S} \lambda(l) I_{l}^{m-1} \left( \frac{3}{2} \right) I_{l}^{m}(\Omega) \sum_{m=-l}^{l} [T_{l}^{m}(\Omega) \otimes (T_{l}^{m}(\Omega))]^{l},
\]

where \( J(=0,1,2,...,S) \) is a magnitude of the total spin and each \( \rho_{L}(J) \) is \((2J+1)\)-fold degenerate. Finally, the EE of a block of \( L \) contiguous bulk spins is explicitly written as

\[
S_{L} = - \sum_{j=0}^{S} (2J+1) \rho_{L}(J) \log_{2} \rho_{L}(J).
\]

Since the reduced density matrix \( \rho_{L} \) approaches a \((S+1)^{2}\)-dimensional identity matrix in the thermodynamic limit \( L \rightarrow \infty \), we can see that \( S_{L} \leq \log_{2}(S+1) = \log_{2}(S) \) and approaches this upper bound exponentially fast in \( L \). This saturation can be observed in Fig. 1 where the EE \( S_{L} \) for various spin-\( S \) VBS chains are plotted as a function of the block size \( L \). Here we confirm that the conjecture proposed by Vidal et al. is valid for all integer-spin VBS chains.

Next we make a comparison between the above results for the VBS chains and numerical results for the integer-spin Heisenberg models. Since \( S = 1 \) systems have recently been extensively studied \(^{24} \), we study numerically the EE and the energy spectra of the \( S = 2 \) Heisenberg model and its continuous deformations. One of the simplest \( S = 2 \) Hamiltonian which interpolates between these two models can be written as

\[
H = \sum_{i=1}^{N} \hat{S}_{i}^{T} \cdot \hat{S}_{i+1} + \alpha \left( \frac{2}{9} (\tilde{S}_{i} \cdot \tilde{S}_{i+1})^{2} + \frac{1}{63} (\tilde{S}_{i} \cdot \tilde{S}_{i+1})^{3} + \frac{10}{7} \right),
\]

where \( \alpha = 0 \) and \( \alpha = 1 \) correspond to the Heisenberg model and the \( S = 2 \) AKLT model, respectively.

The edge-state picture in general \( S \) Haldane systems allows us to interpret the spectra as follows. The low-lying \((S+1)\)-multiplets have \((2S_{total}+1)\)-fold degeneracy in each sector when the system has open boundaries. These generalized Kennedy triplet states are almost degenerate, and are completely degenerate at the AKLT point. This can be understood from the VBS picture. It would be valid for the Heisenberg model by some results from numerical calculations \(^{22,23} \). Let us now show that the ground state properties remain unchanged through the adiabatic continuation from the AKLT to the Heisenberg model. Fig. 2(a) shows the low-energy behaviors of the system are adiabatically equiva-
SU(2)-invariant models with integer-spin.

EE takes a minimum value at the AKLT point in general. This implies that the EE at the AKLT point has contributions not only from the edges created by taking partial trace. This fact is related to the minimum value of $S_{\infty}(2) = 2 \log_2 3 = 3.16993$ as the system size increases. This value coincides with our analytically calculated one with open boundary conditions (See Fig. 1). The lower bound of the EE in the calculated region is given by $S \geq 2 \log_2 3$, and this is the contribution from the boundaries of the system created by taking partial trace over the subsystem. This lower bound is equal to the EE at the AKLT point.

Finally, let us discuss the EE in our system. The obtained results of the EE from exact diagonalizations are shown in Fig. 2 (b). The EE at the AKLT point has a tendency to converge to the value $S_{\infty}(2) = 2 \log_2 3$ as far as the boundary conditions are satisfied with each other in this parameter region.

The authors are grateful to K. Azuma, H. Song, S. Murakami, S. Todo and N. Nagaosa for fruitful discussions. This work was supported Grant-in-Aids (Grant No. 15104006, No. 16076205, and No. 17105002) and NAREGI Nanoscience Project from the Ministry of Education, Culture, Sports, Science, and Technology. HK was supported by the Japan Society for the Promotion of Science. YH was supported by Grant-in-Aids for Scientific Research, No. 17540347 from JSPS, No.18043007 on Priority Areas from MEXT and the Sumitomo Foundation.

* Electronic address: katsura@appi.t.u-tokyo.ac.jp
† Electronic address: hirano@pothos.t.u-tokyo.ac.jp
‡ Electronic address: hatsugai@pothos.t.u-tokyo.ac.jp

[1] G. Vidal et al., Phys. Rev. Lett. 90, 227902 (2003).
[2] M. Levin and X. G. Wen, Phys. Rev. Lett. 96, 110405 (2006).
[3] A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006).
[4] S. Ryu and Y. Hatsugai, Phys. Rev. B 73, 245115 (2006).
[5] Y. Hatsugai, J. Phys. Soc. Jpn. 74, 1374 (2005); 75, 123601 (2006).
[6] F. D. M. Haldane, Phys. Lett. A93, 464 (1983).
[7] F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983).
[8] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987).
[9] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Commun. Math. Phys. 115, 477 (1988).
[10] F. Verstraete and J. I. Cirac, Phys. Rev. A 70, 060302(R) (2004).
[11] W. D. Freitag and E. Müller-Hartmann, Z. Phys. B - Condensed Matter 83, 381 (1991).
[12] F. Verstraete, M. A. Martín-Delgado, J. I. Cirac, Phys. Rev. Lett. 92, 087201 (2004).
[13] H. Fan, V. Korepin, and V. Roychowdhury, Phys. Rev. Lett. 93, 227203 (2004).
[14] J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod and W. G. Stirling, Europhys. Lett. 3, 945 (1987).
[15] K. Katsumata, H. Hori, T. Takeuchi, M. Date, A. Yamagishi and P. Renard, Phys. Rev. Lett. 63, 86 (1989).
[16] C. E. Granroth et al., Phys. Rev. Lett. 77, 1616 (1996).
[17] Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993).
[18] A. Auerbach, Interacting Electrons and Quantum Magnetism, (Springer, New York, 1998).
[19] D. P. Arovas, A. Auerbach and F. D. M. Haldane, Phys. Rev. Lett. 60, 531 (1988).
[20] H. Fan, V. Korepin and V. Roychowdhury, quant-ph/0511150.
[21] H. Hagiwara, K. Katsumata, I. Affleck, B. I. Halperin and J. P. Renard, Phys. Rev. Lett. 65, 3181 (1990).
[22] S. Miyashita and S. Yamamoto, Phys. Rev. B 48, 913 (1993).
[23] S. Qin, T. K. Ng and Z. B. Su, Phys. Rev. B 52, 12844 (1995).
[24] T. Hirano and H. Hatsugai, unpublished.