Long-range string orders and topological quantum phase transitions in the one-dimensional quantum compass model

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Abstract
In order to investigate the quantum phase transition in the one-dimensional quantum compass model, we numerically calculate non-local string correlations, entanglement entropy and fidelity per lattice site by using the infinite matrix product state representation with the infinite time evolving block decimation method. In the whole range of the interaction parameters, we find that four distinct string orders characterize the four different Haldane phases and the topological quantum phase transition occurs between the Haldane phases. The critical exponents of the string order parameters $\beta = 1/8$ and the central charges $c = 1/2$ at the critical points show that the topological phase transitions between the phases belong to an Ising type of universality classes. In addition to the string order parameters, the singularities of the second derivative of the ground state energies per site, the continuous and singular behaviors of the Von Neumann entropy and the pinch points of the fidelity per lattice site manifest that the phase transitions between the phases are of the second-order, in contrast to the first-order transition suggested in previous studies.

Keywords: spin chain model, quantum phase transitions, entanglement

1. Introduction

Transition metal oxides (TMOs) with orbital degeneracies have been intensively studied for quantum phase transitions (QPTs) because they have shown extremely rich phase diagrams due to competitions between orbital orderings and complex interplays between quantum fluctuations and spin interactions [1–16]. In order to mimic such competitions between orbital ordering in different directions and directional natures of the orbital states with twofold degeneracy in the language of the pseudospin-1/2 operators, Kugel and Khomskii [17] first introduced the quantum compass model (QCM) in 1973. In this model, the pseudospin-1/2 operators characterize the orbital degrees of freedom and the anisotropic couplings between these pseudospins simulate the competition between orbital orderings in different directions. Furthermore, such an idea has been implemented to describe some Mott insulators with orbital degeneracy [18, 19], polar molecules in optical lattices [20] and ion trap systems [21], protected qubits for quantum computation in Josephson junction arrays [22] and so on.

Based on the one-dimensional QCM, physical properties and QPTs in TMOs have been explored in the absence [1–7] or in the presence [8–13] of a transverse magnetic field. Especially for its criticality, in 2007, Brzezicki et al [1] used the Jordan–Wigner transformation, mapping it to an Ising model, obtained an exact solution of the QCM and suggested that the system has the first-order transition occurring between two disordered phases. In 2008, You and Tian [2] supported Brzezicki et al’s result, i.e. the first-order transition by adopting the reflection positivity technique in the standard
phase transition in the one-dimensional QCM would suggest us to consider non-local long-range orders for its proper characterization. Interestingly, also, in a recent study on one-dimensional Hubbard model, it is shown that there are charge and spin parity string order parameters that determine their corresponding gapped phases [24] with vanishing Haldane-type string orders. Then, in order to characterize the phase transition properly, in this paper we investigate non-local string orders in the one-dimensional QCM. Actually, a string order as a non-local long-range order was introduced by Nijs and Rommelse [25] and Tasaki [26] and characterizes the Haldane phase in the spin-1 Heisenberg chain [27]. To calculate non-local string orders directly [28], in contrast to an extrapolated value for finite-size lattices, we employ the infinite matrix product state (iMPS) [29, 30] representation with the iTEBD algorithm developed by Vidal [30]. For a systematic study, the second derivative of ground state energy is calculated to reveal the phase transitions in the whole interaction parameter range. Its singularities indicate that there are the four phases separated by the second-order phase transitions. We find the four string order parameters that characterize each phase (see in figure 1), which means that all the four phases are a topologically ordered phase. Furthermore, the critical exponent from the string orders \( \beta = 1/8 \) and the central charges \( c \approx 1/2 \) at the critical points clarify that the topological quantum phase transitions (TQPTs) belong to the Ising-type phase transition. In addition, the continuous behaviors of the odd and even von Neumann entropies and the pinch points of the fidelity per lattice site (FLS) verify the second-order phase transitions between two topologically ordered phases.

This paper is organized as follows. In section 2, we introduce the one-dimensional QCM and discuss the second derivative of the ground state energy per site. In section 3, we display string correlations and define properly the four string order parameters characterizing the four topologically ordered phases. The critical exponents are presented. The phase transitions are discussed by employing the von Neumann entropy in section 4. The TQPTs are classified based on the central charge via the finite-entanglement scaling. In section 5, we discuss the pinch points of the FLS. Finally, our conclusion is given in section 6.

2. Quantum compass model and groundstate energy

We consider the one-dimensional spin-1/2 QCM [1] written as

\[
H = \sum_{i=-\infty}^{\infty} \left( J_x S^x_{2i} S^x_{2i+1} + J_y S^y_{2i} S^y_{2i+1} \right),
\]

where \( S^x_i \) and \( S^y_i \) are the spin-1/2 operators on the \( i \)th site. \( J_x \) and \( J_y \) are nearest-neighbor exchange couplings on the odd and the even bonds, respectively. In order to cover the whole range of the parameter \( J_x \) and \( J_y \), we set \( J_x = J \cos \theta \) and \( J_y = J \sin \theta \).

From the iMPS groundstate wavefunction, we obtain the groundstate energy of the QCM. In figures 2(a) and (b), we plot the groundstate energies \( e_{0,odd} \) on the odd bond and

![Figure 1. Groundstate phase diagram for the one-dimensional QCM in \( J_x-J_y \) plane. The four topologically ordered phases are characterized by the four distinct string orders (defined in the text). The critical lines are (i) \( J_x = J_y > 0 \) (\( \theta = \pi/4 \)), (ii) \( J_x = -J_y < 0 \) (\( \theta = 3\pi/4 \)), (iii) \( J_x = J_y < 0 \) (\( \theta = 5\pi/4 \)) and (iv) \( J_x = -J_y < 0 \) (\( \theta = 7\pi/4 \)). At the critical points, the central charges are \( c = 1/2 \) and the critical exponent of each string order is \( \beta = 1/8 \). The phase transitions between Haldane phases are a topological phase transition and belong to an Ising universality class. Here, the \( \theta \) is the interaction parameter from the setting \( J_x = J \cos \theta \) and \( J_y = J \sin \theta \) for the numerical calculation.](image)
θ derivative of the average energy corresponds to the critical point \( J_y \) in the QCM, the critical point order. As we introduced the controversy of the phase transition quantum phase transitions occur and they are of the second-order. The QCM has the different strengths of the spin exchange interaction depending on the odd and the even bonds. One can then define string correlations based on the bond alternation parameter \( \theta \) in our calculation. In \( \theta = 0 \) as an average value of the energies \( e_0 \) and \( e_0 \), i.e. \( e_0 = (e_{0, odd} + e_{0, even})/2 \). Here, the truncation dimension is chosen as \( \chi = 40 \). The energies are shown to be a periodic behavior as a function of the interaction parameter \( \theta \). One way to know whether there is a phase transition is to check the non-analyticity of the groundstate energy on the system parameters. Thus, in order to see any possible phase transition, we calculate the derivative of the energies over the interaction parameter \( \theta \). In the first derivative of the energies over the interaction parameter, no singular behavior is noticed in the whole parameter range. Then, in figure 2(c), we plot the second derivative of the energy \( e_0 \). Note that it exhibits the singular points at \( \theta = \pi/4, \theta = 3\pi/4, \theta = 5\pi/4 \) and \( \theta = 7\pi/4 \). This result means that, at the singular points, the quantum phase transitions occur and they are of the second-order. As we introduced the controversy of the phase transition in the QCM, the critical point \( \theta = \pi/4 \) in our calculation corresponds to the the critical point \( J_y = J_x \) investigated in previous studies. Consequently, our second derivative of the groundstate energy shows that the phase transition in the QCM should be of the second-order. Moreover, the critical lines separate the parameter space into the four regions (denoted by I, II, III and IV in figure 1), which may indicate four possible phases. Then, in order to characterize the four possible phases, we discuss string correlations in the next section.

3. String order parameters and topological quantum phase transitions

The QCM has the different strengths of the spin exchange interaction depending on the odd bond and the groundstate energy per site \( e_0 \) as an average value of the energies \( e_{0, odd} \) and \( e_{0, even} \), i.e. \( e_0 = (e_{0, odd} + e_{0, even})/2 \). Here, the truncation dimension is chosen as \( \chi = 40 \). The energies are shown to be a periodic behavior as a function of the interaction parameter \( \theta \). One way to know whether there is a phase transition is to check the non-analyticity of the groundstate energy on the system parameters. Thus, in order to see any possible phase transition, we calculate the derivative of the energies over the interaction parameter \( \theta \). In the first derivative of the energies over the interaction parameter, no singular behavior is noticed in the whole parameter range. Then, in figure 2(c), we plot the second derivative of the energy \( e_0 \). Note that it exhibits the singular points at \( \theta = \pi/4, \theta = 3\pi/4, \theta = 5\pi/4 \) and \( \theta = 7\pi/4 \). This result means that, at the singular points, the quantum phase transitions occur and they are of the second-order. As we introduced the controversy of the phase transition in the QCM, the critical point \( \theta = \pi/4 \) in our calculation corresponds to the the critical point \( J_y = J_x \) investigated in previous studies. Consequently, our second derivative of the groundstate energy shows that the phase transition in the QCM should be of the second-order. Moreover, the critical lines separate the parameter space into the four regions (denoted by I, II, III and IV in figure 1), which may indicate four possible phases. Then, in order to characterize the four possible phases, we discuss string correlations in the next section.

![Figure 2](image_url) (a) Groundstate energies per site on odd-/even-bonds \( e_{0, odd} \), (b) average energy \( e_0 = (e_{0, odd} + e_{0, even})/2 \) and (c) second derivative of the average energy \( e_0 \) as a function of the interaction parameter \( \theta \). Here, the truncation dimension \( \chi = 40 \) is chosen for the IMPS calculation. In (c), note that the singular behaviors of the second derivative occur at the points \( \theta = \pi/4, \theta = 3\pi/4, \theta = 5\pi/4 \) and \( \theta = 7\pi/4 \).

[31, 32]. Let us first consider the string correlations defined as

\[
O_{x, odd}^\alpha(2i-1, 2j) = \left< S_{2i-1}^x \exp \left[ i\tau \sum_{k=2i}^{2j-1} S_k^\alpha S_{k+1}^\alpha \right] S_{2j}^x \right>
\]

\[
O_{x, even}^\alpha(2i, 2j + 1) = \left< S_{2i}^x \exp \left[ i\tau \sum_{k=2i+1}^{2j+1} S_k^\alpha S_{k+1}^\alpha \right] S_{2j+1}^x \right>
\]

where \( \alpha = x, y \) and \( z \). We observe numerically that the \( x \) components of the string correlations \( O_{x, odd/even}^\alpha \) decrease to zero within the lattice distance \(|i-j| = 6\) in the whole parameter range.

3.1. Behaviors of odd string correlations

In figure 3(a), we summarize the short- and long-distance behaviors of the odd string correlations \( O_{y, odd}^\alpha \) in \( J_y-J_z \) plane. (i) For \(|J_z| < |J_y|\) (the regions II and IV in figure 1), the odd...
\[ \theta = b \] are the fitting function \( a = -|\theta - j| + b \) for \( \theta \) by the asterisk in figure 3. For \( J_y > 0 \) [region I (Jy, \( \theta < 0 \) [region III]), \( O_{xy,odd}^2 \) shows a monotonic (oscillatory) saturation and \( O_{xy,odd}^2 \) displays an oscillatory (monotonic) decaying to zero.

As an example, in figure 3(b), we plot the odd string correlations \( O_{xy,odd}^2 \) as a function of the lattice distance \(|i - j|\) for \( \theta = 0.2\pi \) (the range I) and \( \theta = 0.8\pi \) (the region III). The string correlations show a very distinct behavior. For \( \theta = 0.2\pi \), the \( O_{xy,odd}^2 \) has a minus sign, while the \( O_{xy,odd}^2 \) has an alternating sign depending on the lattice distance. In contrast to the case of \( \theta = 0.2\pi \), for \( \theta = 0.8\pi \), the \( O_{xy,odd}^2 \) has a minus sign, while the \( O_{xy,odd}^2 \) has an alternating sign depending on the lattice distance distance. From the short-distance behaviors, as shown in figure 3(b), it is hard to see whether the string correlations decay to survive in the long-distance limit (i.e. \(|i - j| \rightarrow \infty \)). In order to study the correlations in the limit of the infinite distance, one can then set a truncation error \( \epsilon \) rather than the lattice distance, i.e. \( O((i - j))/O((i - j - 1)) < \epsilon \). In this study, for instance, \( \epsilon = 10^{-8} \) is set. The insets of figure 3(b) show the string correlations for relatively very large lattice distances. We see clearly that the \( O_{xy,odd}^2 \)'s have a finite value while the \( O_{xy,odd}^2 \)'s decay to zero (around the lattice distance \(|i - j| \sim 5 \times 10^2 \)). As a consequence, the parameter regions I and III can be characterized by the odd string long-range order parameters. As discussed above, the odd string correlations have the two characteristic behaviors, i.e. one is a monotonic saturation for \( \theta = 0.2\pi \) and the other is an oscillatory saturation for \( \theta = 0.8\pi \). Such a distinguishable behavior of the string correlations allows us to say that the region I (\( J_y > 0 \)) and the region III (\( J_y < 0 \)) are at different phases each other and we call them the monotonic odd string order and the oscillatory odd string order, respectively.

In figure 4, we plot the odd string correlations \( |O_{xy,odd}^2(i, j)| \) as a function of \(|i - j|\) for the various parameter \( \theta \). The string correlations show a logarithmically decaying to their saturated values as the lattice distance increases. The fitting function of logarithmically decaying nonzero string correlations is \( |O_{xy,odd}^2(i, j)| = a \log |i - j| + b \) characterized by the fitting constants \( a \) and \( b \). By the numerical fitting, the fitting constants are given by (i) \( a = -0.0032 \) and \( b = 0.213 \) for \( \theta = 0.2\pi \), (ii) \( a = -0.0158 \) and \( b = 0.01672 \) for \( \theta = 0.24\pi \) and (iii) \( a = -0.0197 \) and \( b = 0.161 \) for \( \theta = 0.249\pi \), respectively. Figure 4 shows that the logarithmical decaying region increases as \( \theta \) approaches a critical point. Similar to the odd string correlations in the region I, the nonzero odd string correlations \( |O_{xy,odd}^2(i, j)| \) in region III have a similar logarithmical decaying behavior.

### 3.2. Behaviors of even string correlations

Similarly to the odd string correlations, the even string correlations show the two characteristic behaviors. In figure 5(a), we summarize the short- and long-distance behaviors of the even string correlations \( O_{xz,even}^2 \) in \( J_y \) plane. (i) For \(|J_y| < |J_z|\) (the regions I and III in figure 1), the even string correlations \( O_{xz,even}^2 \) decreases to zero within the lattice distance \(|i - j| \sim 80\). (ii) For \(|J_y| > |J_z|\) (the regions II and IV in figure 1), the absolute value of \( O_{xz,even}^2 \) saturates to a finite value while \( O_{xz,even}^2 \) decays to zero very slowly, which means \( O_{xz,even}^2 \) as a non-local long-range order parameter (indicated by an asterisk in figure 4(a)) characterizes a topologically ordered phase. Further, if \( J_z > 0 \) (region II) \((J_z < 0 \) [region IV]), \( O_{xz,even}^2 \) shows a monotonic (oscillatory) saturation and \( O_{xz,even}^2 \) displays an oscillatory (monotonic) decaying to zero.

As an example, in figure 5(b), we plot the even string correlations \( O_{xz,even}^2 \) as a function of the lattice distance \(|i - j|\) for \( \theta = 0.3\pi \) (the range II) and \( \theta = 1.3\pi \) (the region IV). For \( \theta = 0.3\pi \), the \( O_{xz,even}^2 \) has an alternating sign depending on the lattice distance, while the \( O_{xz,even}^2 \) has a minus sign. In contrast to the case of \( \theta = 0.3\pi \), for \( \theta = 1.3\pi \), the \( O_{xz,even}^2 \) has an alternating sign depending on the lattice distance, while the \( O_{xz,even}^2 \) has a minus sign. Similar to the odd string correlations, the short-distance behaviors of the even string correlations show the difficulty of seeing which string correlation survives in the long-distance limit (i.e. \(|i - j| \rightarrow \infty \)). By using the truncation error \( \epsilon = 10^{-8} \), we plot the string correlations for relatively very large lattice distance in the insets of figure 5(b). We see clearly that the \( O_{xz,even}^2 \)'s have a finite value while the \( O_{xz,odd}^2 \)'s decay to zero (around the lattice distance \(|i - j| \sim 2 \times 10^4 \)). As a result, the parameter regions II and IV can be characterized by the even string long-range order parameters. The even string correlations also have the two characteristic behaviors, i.e. one is a monotonic saturation for \( \theta = 0.3\pi \), the other is an oscillatory saturation for \( \theta = 1.3\pi \). The region II \((J_z > 0 \)) and the region IV \((J_z < 0 \)) are at different phases to each other and we call them the monotonic even string order and the oscillatory even string order, respectively. Similar to the odd string correlations, we have observed that the nonzero even string correlations \( |O_{xz,even}^2| \) logarithmically decay to the saturated values as the lattice distance increases, which is not presented here.
3.3. Phase diagram from string order parameters

As we discussed, the even and odd string correlations have shown two characteristic behaviors, i.e. one is monotonic, the other is oscillatory. Then, one may define a proper long-range string order based on the behaviors of the odd and the even string correlations. We define the long-range string order parameters as follows:

\[ O_{\text{str,odd}}^{y,z} = 0 \quad \text{for } \theta = 0.3\pi \] and \( \theta = 1.3\pi \). In the insets, note that \( O_{\text{str,even}}^{y,z} \)'s are saturated to a finite value, while \( O_{\text{str,even}}^{y,z} \)'s decay to zero for very large distance.

\[ O_{\text{str,odd}}^{y,z} = \lim_{|j-i|\to\infty} O_{\text{str,odd}}^{y,z} (2i - 1, 2j), \]

\[ O_{\text{str,odd}}^{-y,z} = \lim_{|j-i|\to\infty} (\pm 1)^{|j-i|+1} O_{\text{str,odd}}^{y,z} (2i - 1, 2j), \]

\[ O_{\text{str,even}}^{y,z} = \lim_{|j-i|\to\infty} O_{\text{str,even}}^{y,z} (2i, 2j + 1), \]

\[ O_{\text{str,even}}^{-y,z} = \lim_{|j-i|\to\infty} (\pm 1)^{|j-i|+1} O_{\text{str,even}}^{y,z} (2i, 2j + 1). \]

where, actually, the superscript + (−) of the string order parameters denotes the monotonic behavior (the oscillatory behavior).

The defined string orders are calculated from the iMPS groundstate wave function. In figure 6, we display the string order parameters as a function of the interaction parameter \( \theta \). In figure 6(a), it is clearly shown that the odd string order parameters are finite for the region I (\(-\pi/4 < \theta < \pi/4\)) and the region III (\(3\pi/4 < \theta < 5\pi/4\)). Further, the monotonic odd string order parameter \( O_{\text{str,odd}}^{y} \) characterizes the region I and the oscillatory odd string order parameter \( O_{\text{str,odd}}^{z} \) characterizes the region III. Similarly to the odd string order parameters, the \( y \) component of the even string order parameters \( O_{\text{str,even}}^{y} \) and \( O_{\text{str,even}}^{z} \) are finite for the region II (\(\pi/4 < \theta < 3\pi/4\)) and the region IV (\(5\pi/4 < \theta < 7\pi/4\)). The monotonic even string order parameter \( O_{\text{str,even}}^{y} \) characterizes the region II and the oscillatory even string order parameter \( O_{\text{str,even}}^{z} \) characterizes the region IV. Consequently, the four regions in \( J_y-J_z \) plane (figure 1) are characterized by the four string order parameters \( O_{\text{str,odd}}^{y} \) and \( O_{\text{str,odd}}^{z} \), respectively, which implies that a different hidden \( Z_2 \times Z_2 \) breaking symmetry occurs in each phase. Therefore, the one-dimensional QCM has four distinct topologically ordered phases rather than disordered phases as suggested in previous studies. The system undergoes a topological quantum phase transition between two topological ordered phases as the interaction parameter crosses the critical lines \( |J_y| = |J_z| \). In addition, the continuous behaviors of the string order parameters across the critical lines show that the topological quantum phase transitions are of the continuous (second-order) phase transition rather than the discontinuous (first-order) phase transition.

In a previous study [7] on an EQCM, the existence of a string order has been noticed numerically for a relevant interaction parameter range. However, any characterization of phase has not been made in association with the one-dimensional QCM. However, the one-dimensional spin-1/2 Kitaev model [33], which is equivalent to the one-dimensional QCM, has shown to have two string order parameters [34] based on the dual spin correlation function [35] by using a dual transformation [36, 37] mapping the model into a...
one-dimensional Ising model with a transverse field. The actual parameter range in the one-dimensional Kitaev model studied in [34] corresponds to \( J_x > 0 \) and \( J_y > 0 \) in our one-dimensional QCM. The system was discussed to undergo a topological quantum phase transition at the critical point \( J_y = J_z > 0 \) (\( \theta = \pi/4 \)). In this sense, in the case of \( J_y, J_z > 0 \) in the one-dimensional QCM, we have numerically demonstrated and verified the existence of the string order parameters and the topological quantum phase transition as discussed in [34].

### 3.4. Critical exponents

In the critical regimes, as the order parameters, the string orders should show a scaling behavior to characterize the phase transitions. We plot the string order parameters \( O_{\text{str,even}}^{+/-} \) (figure 7(a)) and \( O_{\text{str,even}}^{-/-} \) (figure 7(b)) as a function of \( |\theta - \theta_c|^{1/4} \) with the critical points \( \theta_c = \pi/4, 3\pi/4, 5\pi/4 \) and \( 7\pi/4 \). It is shown that all the string order parameters nearly collapse onto one scaling fitting function in the critical regimes, i.e., they scale as \( O_{\text{str,even/odd}} \propto |\theta - \theta_c|^{1/4} \). As a result, the same critical exponents are given as \( \beta = 1/8 \) via \( O_{\text{str,even/odd}} \propto |\theta - \theta_c|^{2\beta} \) [38], which reveals that the TQPTs belong to the Ising-type phase transition.

### 4. Entanglement entropy and central charge

Quantum entanglement in many-body systems can be quantified by the von Neumann entropy that is a good measure of bipartite entanglement between two subsystems of a pure state [39, 40]. Generally, for one-dimensional quantum spin lattices, at critical points, the von Neumann entropy exhibits its logarithmic scaling conforming conformal invariance. Its scaling is governed by a universal factor, i.e., a central charge \( c \) of the associated conformal field theory. The central charge allows us to classify a universality class [41] of quantum phase transition. In our iMPS representation, a diverging entanglement at quantum critical points gives simple scaling relations for (i) the von Neumann entropy \( S \) and (ii) a correlation length \( \xi \) with respect to the truncation dimension \( \chi \) [42] as follows:

\[
\xi(\chi) \propto \xi_0 \chi^\kappa \quad (4a)
\]

\[
S(\chi) \propto \frac{c}{6} \log_2 \chi \quad (4b)
\]

where \( \kappa \) is a so-called finite-entanglement scaling exponent and \( \xi_0 \) is a constant. Thus, one can calculate a central charge by using equations (4a) and (4b).

In order to obtain the von Neumann entropy, we partition the spin chain into the two parts denoted by the left semi-infinite chain \( L \) and the right semi-infinite chain \( R \). In terms of the reduced density matrix \( \rho_L \) or \( \rho_R \) of the subsystems \( L \) and \( R \), the von Neumann entropy can be defined as \( S = -\text{Tr} \rho_L \log_2 \rho_L = -\text{Tr} \rho_R \log_2 \rho_R \).

In the iMPS representation, the iMPS groundstate wavefunction can be written by the Schmidt decomposition \( |\Psi\rangle = \sum_{\alpha=1}^{4} \phi_L^{\alpha} |\phi_R^{\alpha}\rangle \), where \( |\phi_L^{\alpha}\rangle \) and \( |\phi_R^{\alpha}\rangle \) are the Schmidt bases for the semi-infinite chains \( L(\infty, \cdots, i) \) and \( R(i+1, \cdots, \infty) \), respectively. \( \lambda^{\alpha} \) are actually eigenvalues of the reduced density matrices for the two semi-infinite chains \( L \) and \( R \). In our four-site translational invariant iMPS representation, we have the four Schmidt coefficient matrices \( \lambda_A, \lambda_B, \lambda_C \) and \( \lambda_R \), which means that there are four possible ways for the partitions. Due to the two-site translational invariance of the QCM, in fact, we have \( \lambda_A = \lambda_C \) and \( \lambda_B = \lambda_D \), i.e., one partition is on the odd sites, the other is on the even sites. From the \( \xi_{\text{even}} \) and \( \xi_{\text{odd}} \), one can obtain the two von Neumann entropies depending on the odd- or even-site partitions as

\[
S_{\text{even/odd}} = -\sum_{\alpha=1}^{4} \lambda_{\text{even/odd,} \alpha} \log_2 \lambda_{\text{even/odd,} \alpha}^2 \quad (5)
\]

where \( \lambda_{\text{even/odd,} \alpha} \)'s are diagonal elements of the matrix \( \lambda_{\text{even/odd}} \).

In figure 8(a), we plot the von Neumann entropies \( S_{\text{odd,} \theta} \) and \( S_{\text{even,} \theta} \) as a function of the control parameter \( \theta \). One can easily notice that there are four singular points \( \theta = \pi/4, 3\pi/4, 5\pi/4 \) and \( 7\pi/4 \) in both the odd-bond and the even-bond entropies. The four singular points of the von Neumann entropies indicate a quantum phase transition at those points. It should be noted that the detected transition points from the von Neumann entropies correspond to the critical points from the second derivative of the groundstate energy and the string order parameters. The continuous behaviors of von Neumann entropies around critical points also indicate the occurrence of the continuous (second-order) quantum phase transition as the system crosses the transition points. Hence, it is shown that the von Neumann entropy can detect the topological quantum phase transitions.

In figures 8(b) and (c), we plot the correlation length \( \xi(\chi) \) as a function of the truncation dimension \( \chi \) and the von Neumann entropy \( S(\chi) \) as a function of \( \chi \) at the critical points \( C_1(J_1, J_2) = (1, 1), C_2 = (-1, 1), C_3 = (-1, -1), \) and \( C_4 = (1, -1) \), respectively. The truncation dimensions are taken as \( \chi = 12, 16, 20, 24, 28, 32, 40, \) and 44. The correlation length \( \xi(\chi) \) and the von Neumann entropy \( S(\chi) \) diverge as the truncation dimension \( \chi \) increases. Using the numerical fitting function \( \xi(\chi) = \xi_0 \chi^\kappa \) in equation (4a), the fitting constants are...
function of the truncation dimension from the string order parameters. (the critical points. = 1, (i) Neumann entropy

the critical exponent = 4, 3.

0 = 0.04 and κ = 2.071 at C1, (ii) ξ0 = 0.041 and κ = 2.068 at C2, (iii) ξ0 = 0.039 and κ = 2.087 at C3 and (iv) ξ0 = 0.041 and κ = 2.065 at C4. In order to obtain the central charge, we use the numerical fitting function of the von Neumann entropy $S(\chi) = (c/6) \log_2 \chi + S_0$. As shown in figures 8(c), the linear scaling behaviors of the entropies give (i) $c = 0.5079$ with $S_0 = 0.331$ at $C_1$, (ii) $c = 0.4992$ with $S_0 = 0.3464$ at $C_2$, (iii) $c = 0.5048$ with $S_0 = 0.314$ at $C_3$ and (iv) $c = 0.4983$ with $S_0 = 0.34$ at $C_4$. Our central charges are very close to the value $c = 0.5$, respectively. Consequently, the topological quantum phase transitions at all the critical points belong to the same universality class, i.e. the Ising universality class. This result is consistent with the universality class from the critical exponent $\beta = 1/8$ of the string order parameters.

5. Fidelity per lattice site

Similarly to the von Neumann entropy, the fidelity per lattice site (FLS) [43] is known to enable us to detect a phase transition point as an universal indicator without knowing any order parameters. From our iMPs groundstate wave function $|\Psi(\theta)\rangle$ with the interaction parameter $\theta$, we define the fidelity as $F(\theta, \theta') = |\langle \Psi(\theta)|\Psi(\theta')\rangle|$. Following [43], the ground-

state FLS $d(\theta, \theta')$ can then be defined as

$$\ln d(\theta, \theta') = \lim_{L \to \infty} \frac{\ln F(\theta, \theta')}{L},$$

where $L$ is the system size.

In figure 9, the groundstate FLS $d(\theta, \theta')$ is plotted in $\theta-$ $\theta'$ parameter space. The FLS surface reveals that there are four pinch points $\theta = \pi/4, 3\pi/4, 5\pi/4$ and $7\pi/4$. Each pinch point corresponds to each phase transition point from the second-order derivative of the ground-state energy, the string order parameters and the von Neumann entropy. In addition, the continuous behavior of the groundstate FLS verifies that the second-order quantum phase transitions occur at the pinch points.

6. Conclusion

We have investigated the quantum phase transition in the one-dimensional QCM by using the iMPs representation with the iTEBD algorithm. To characterize quantum phases in the one-dimensional QCM, we introduced the odd and the even string correlations based on the alternating strength of the exchange interaction. We have observed that there are the two distinct behaviors of the odd and the string correlations, i.e. one is of the monotonic, the other is of the oscillatory. Based on the topological characterization, we find that there are the four topologically ordered phases in the whole interaction parameter range (figure 1). In the critical regimes, the critical exponents of the string order parameters are obtained as $\beta = 1/8$, which implies that the topological quantum phase transitions belong to the Ising type of universality class. Consistently, we obtain the central charges $c = 1/2$ from the entanglement entropy. In addition, the singular behaviors of the second-order derivatives of groundstate energy, the string order parameters characterizing the four Haldane phases, the continuous behaviors of the von Neumann entropy and the FLS allow us to conclude that the phase transitions in the one-dimensional QCM are of the second-order, in contrast to previous studies.
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