Quantum phase diagram of the frustrated spin ladder with next-nearest-neighbor interactions

Yan-Chao Li$^1$ and Hai-Qing Lin
Beijing Computational Science Research Center, Beijing 100084, People's Republic of China
E-mail: ycli@csrc.ac.cn

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Abstract. Using the density matrix renormalization group technique, we investigate the quantum phase diagram of a ferromagnetic frustrated two-leg spin-1/2 ladder with diagonal and in-chain next-nearest-neighbor (NNN) interactions. By analyzing the correlation function and four-site entropy, we obtain the quantum phase diagram of the system. We find that the system possesses a tetramer phase, a ferromagnetic phase and states I and II. Spin arrangements for states I and II are also determined. In addition, the influence of the in-chain NNN interaction $J_2$ on the phase transitions of the anti-ferromagnetic case is studied. We show the phase diagram and find that the stagger dimer phase exists only in a narrow parameter region. Meanwhile, the existence of the controversial columnar dimer phase at $J_2 = 0$ is carefully analyzed.

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$^1$ Author to whom any correspondence should be addressed.
1. Introduction

Due to the possibility of capturing Anderson’s resonating-valence-bond state scenario, which is related to the high-$T_c$ superconductivity mechanism, much attention has been focused on the frustrated spin ladder model [1–4]. Meanwhile, because of the existence of the frustrated effect, the system possesses a rich phase diagram. Given its special structure, the spin ladder is expected to serve as a relatively ideal model for revealing the transitional behavior between the quite different physical properties of one- and two-dimensional (1D and 2D) systems. Various methods have been applied to study this model [1, 5–16]. Lin et al [17] even obtained the exact solution of the so-called net spin ladder model for any spin $S$ under certain parameter conditions. They studied the ground state and the excitation gap of the system and found that there are distinct excitation phases in one and two dimensions.

However, a major part of the literature focuses on the anti-ferromagnetic frustrated (AFF) case. Very little is known about the properties of the ferromagnetic frustrated (FF) case. The discovery of FF $J_1$–$J_2$ chain compounds Rb$_2$Cu$_2$Mo$_3$O$_{12}$ [18] and LiCuVO$_4$ [19] has attracted much research attention [20, 21]. Some interesting properties are found in such materials; for example, inelastic neutron scattering measurements show the existence of a strong two-spinon continuum frustrated ferromagnetic spin-1/2 chain in LiCuVO$_4$ [22]. The FF $J_1$–$J_2$ chain is only a special case of the frustrated spin ladder model. We believe that a much richer phase diagram can be shown for the FF spin ladder case.

A previous paper [23] focuses on a ferromagnetic interchain FF spin ladder and demonstrates that the ferromagnetic interchain interaction stabilizes the columnar dimer (CD) phase. However, this is only one of the FF cases. The properties of another FF case—the nearest-neighbor (NN) interaction is ferromagnetic while the next-nearest-neighbor (NNN) interaction is anti-ferromagnetic—are still unknown. On the other hand, the introduction of the in-chain NNN interaction $J_2$ ($J_2$ and other interactions are shown in figure 1) further increases frustration among spins and may cause some interesting phenomena and quantum phases. The discovery of the in-chain NNN interaction in the quasi-1D magnetism of BiCu$_2$PO$_6$ [24] makes it even more necessary to reveal the interaction’s influence on quantum phase transitions (QPTs) of the system. However, there are a relatively few studies focused on this issue. The papers [15, 16] stress that the in-chain NNN interaction enhances the stability of the CD phase and causes another stagger dimer (SD) phase. However, because the calculations focus only on a special case $J_2 = \frac{1}{2} J_1$, more comprehensive results are needed.

Furthermore, there is another open question about the spin ladder: does an intermediate CD phase exist between the rung-singlet (RS) and the Haldane phases at $J_2 = 0$ and weak interchain couplings? Initially, some studies have shown that the phase transition between the RS and the Haldane phases is direct [1, 9, 12], but Starykh and Balents [25] proposed that there should be an intermediate quantum-disordered CD phase. This remarkable proposal has attracted much attention. Using the density matrix renormalization group (DMRG) algorithm, Huang et al [26] and Kim et al [27] studied the correlation functions and entanglement, but did not find any evidence for the CD state. Meanwhile, the papers [16, 23] give further support for the existence of the CD phase. However, because the predicted parameter region is very small and the number of kept states and the system size considered in the DMRG calculations are relatively small, calculation errors cannot be ignored. More convincing evidence is needed.
Therefore, in this paper, we investigate a two-leg spin-1/2 ladder with both diagonal and in-chain NNN interactions (SLDI). On the one hand, the phase diagram of the ferromagnetic-NN-interaction FF case in the presence of in-chain NNN interaction is emphatically studied. On the other, the influence of the in-chain NNN interaction on the quantum states of the AFF case is highlighted. Meanwhile, by investigating gradual changes in the behavior of entanglement with \( J_2 \) as well as the order parameter and entanglement behavior at \( J_2 = 0 \), we try to give an analysis of the controversial CD state.

This paper is organized as follows. In section 2, we briefly introduce the SLDI model and the DMRG method used in this paper. In section 3, the QPTs and the properties of each quantum state for the FF case are analyzed using DMRG and exact diagonalization techniques. The influence of \( J_2 \) on the QPTs of the system for the AFF case and the detection of the controversial CD state at \( J_2 = 0 \) are presented in section 4. Finally, in section 5, a brief summary is given.

2. The model and the method

The Hamiltonian of the SLDI model can be expressed as

\[
H = \sum_{\alpha=1,2} \sum_i \left( J_1 S_{\alpha,i} \cdot S_{\alpha,i+1} + J_2 S_{\alpha,i} \cdot S_{\alpha,i+2} \right) + \sum_i \left[ J_\perp S_{1,i} \cdot S_{1,i+1} + J \times \left( S_{2,i} \cdot S_{2,i+1} + S_{1,i+1} \cdot S_{1,i} \right) \right],
\]

where \( S_{\alpha,i} \) denotes spin-1/2 operators at site \( i \) of the \( \alpha \)th leg of the ladder and \( N \) is the number of rungs. Figure 1 shows the model. In this paper, we set the in-chain NN interaction \( |J_1| = 1 \) as the energy unit.

It is established that the CD and SD states can be detected by local order parameters defined by the difference in local spin correlations on legs [15, 16, 26]

\[
O_{CD} = \left| \sum_{\alpha=1,2} \left( S_{\alpha,i} \cdot S_{\alpha,i+1} - S_{\alpha,i+1} \cdot S_{\alpha,i+2} \right) \right|,
\]

\[
O_{SD} = \left| \left( S_{1,i} \cdot S_{1,i+1} + S_{2,i+1} \cdot S_{2,i+2} - S_{2,i} \cdot S_{2,i+1} + S_{1,i+1} \cdot S_{1,i+2} \right) \right|,
\]

respectively, where \( i \) denotes the site of rungs. To avoid boundary effects, sites in the middle of long chains are usually considered, i.e. \( i = N/2 \) is chosen. As mentioned in section 1, the CD
and SD states have been clearly detected in a specific case \((J_2 = J_1/2)\) of the SLDI model [16]. Therefore, we wish to analyze the two order parameters to detect the CD and SD states under different parameters.

In addition, the concept of entanglement, which captures information on a QPT by quantifying the strength of quantum correlations between subsystems of many-body systems [28–34], has been successfully used in detecting QPTs in various systems, such as in spin models [34–37], fermionic systems [31–33] and the Bose–Hubbard model [38]. Therefore, we also study entanglement entropy to detect QPTs in the system. The entropy of a subset \(A\) is defined as

\[
E_A = -\text{Tr}_A \rho_A \ln \rho_A,
\]

where \(\rho_A\) is the reduced density matrix of subsystem \(A\). According to the available results, we speculate that there might be a dimerized-like oligomer state in the system, and it has been pointed out that dimerization transition can easily be detected by the finite value of the difference of two-site entropies on neighboring sites at the center of a spin chain [33]. Therefore, we study four- and two-site entropies according to different characterizing lengths. By analyzing the individual behavior of different entropies and the differences between these entropies for two neighboring subsystems, we aim to give a confirmation of quantum states in the system.

Our calculations are based on the DMRG approach (for an overview, see [39]), in which the open boundary condition on the spin ladder is considered. For accuracy, \(m = 250\) states are kept for most cases, and we also use different \(m\) values to verify the accuracy for some cases (the largest number of retained states is \(m = 500\), where the truncation error is less than \(10^{-7}\)).

3. Global phase diagram of the ferromagnetic frustrated case

When \(J_1, J_\perp < 0\) and \(J_2, J_\times > 0\), the system is the FF case mentioned in section 1. For convenience, we keep \(J_1 = -1.0\) and \(J_\perp = -0.5\) unchanged in the following. We calculate the four-site entropies \(E_{4L}\) and \(E_{4R}\). Here, \(E_{4L}\) and \(E_{4R}\) are taken from equation (3) by replacing \(A\) with the four spins on \(L\) in the middle of the chain and its four neighboring sites \(R\) (as indicated in figure 1), respectively. The results of the four-site entropies \(E_{4L}\) and \(E_{4R}\) as a function of \(J_\times\) at \(J_2 = 0.4\) are plotted in figure 2(a). Dramatic changes in \(E_{4L}\) and \(E_{4R}\) clearly separate the figure into three regions: I, II and III. Obviously, the three regions correspond to three different quantum phases. We see that there are clear differences between \(E_{4L}\) and \(E_{4R}\) in regions I and II, but the differences become smaller and smaller as \(N\) increases. Therefore, we analyze the finite-size scaling behavior of \(\Delta E_4\) \((\Delta E_4 = E_{4L} - E_{4R})\) in different regions as shown in figure 2(b). We find that \(\Delta E_4\) tends to zero in regions I and II as it approaches a certain finite value in region III in the thermodynamic limit. Therefore, we conclude that phase III must be a certain oligomer state.

To confirm the exact property of phase III, we turn to the correlation functions of the two arbitrary spins of \(L\) and \(R\). The results are shown in figure 3. The critical regions indicated by dramatic changes in the correlation functions are consistent with the results of entanglement. Furthermore, in region III, not only the correlation functions on legs, but also those on diagonals are separated (the inset in figure 3 gives a more precise picture), which further indicates the existence of the oligomer phase. We can confirm that this oligomer phase is actually a tetramer state.
Figure 2. (a) $E_{4L}$ and $E_{4R}$ as a function of $J_\times$ at $J_2 = 0.4$ under different rung numbers $N$. Dramatic changes in $E_{4L}$ and $E_{4R}$ separate the picture into three parts, I, II and III. (b) Finite-size scaling behavior of $\Delta E_4$ for different $J_\times$ values.

Figure 3. Correlation functions of the two different arbitrary spins of $L$ and $R$ as a function of $J_\times$ at $J_2 = 0.4$ for the FF case. The inset gives a refined picture of part III of the correlation functions.

According to the behavior of the mentioned correlation functions, we define the tetramer order parameter by the difference of local spin correlations on legs and diagonals as

$$O_T = \left| \sum_{\alpha,\beta=1,2} (S_{\alpha,i} \cdot S_{\beta,i+1} - S_{\alpha,i+1} \cdot S_{\beta,i+2}) \right|,$$

where $\alpha$ and $\beta$ indicate the number of legs and $i$ indicates the rung sites. To reduce the boundary effect, we consider the spins in the middle of the finite chain by setting $i = N/2$, i.e. spins on L and R are selected. $O_T$ as a function of $J_\times$ under different system sizes $N$ is shown in figure 4(a). The nonzero region of $O_T$ clearly reflects the existence of the tetramer phase. In figure 4(b), the finite size scaling behavior of $O_T$ is plotted for different $J_\times$ values. $O_T$ for $J_\times = 0.4265$ and
Figure 4. (a) The tetramer order parameter $O_T$ defined by the difference of local spin correlations on legs and diagonals under different $N$ values. (b) System size dependence of $O_T$ for different $J_\times$ values.

Figure 5. (a) $C^s_r$ and (b) $C^d_r$, which denote the correlation functions of spin 1 in L with the other spin on the same leg and on the other leg, respectively, as a function of $r$ ($r$ is the distance of the rungs to which spin 1 and the other spin belong). Panels (c) and (d) show the spin arrangements for states I and II, respectively.

0.4365 approaches certain finite values in the thermodynamic limit, which further confirms the existence of the tetramer phase III.

Next, we consider the properties of states I and II. To identify the spin arrangements of the two states, we calculate the correlation functions of spins under different distances. Figure 5(a) presents the correlation function $C^s_r$ of spin 1 of L with the spin on the same leg, whereas the correlation function $C^d_r$ of spin 1 with the spin on the other leg is shown in figure 5(b), where $r$ denotes the distance between the rungs where the two spins are located. The red dots denote the results for $J_\times = 0.6$, which belongs to state II, and the black circles represent the data for $J_\times = 0.2$, which is located in region I. The results for $J_\times = 0.6$ change monotonically
as $r$ increases, but $C_r^a$ and $C_r^d$ show different signs. This feature indicates that the interaction of the spins along the leg is ferromagnetic, whereas that between the legs is anti-ferromagnetic. When it comes to the data for $J_\times = 0.2$, the sign of the correlation function changes at a certain periodicity with $r$, and the results of figures 5(a) and (b) have a similar structure. Therefore, we conclude that the interaction between the legs is ferromagnetic, whereas that along the legs present some kind of periodic ferro- and anti-ferromagnetic arrangement. For direct sensing, we plot spin-arrangement sketches for the two states I and II in figures 5(c) and (d), respectively.

When $J_2$ or $J_\times$ is very small, the structural feature of the entanglement entropy is quite different. Figures 6(a) and (b) present the four-site entropy $E_{4L}$ for $J_\times = 0.1$ and $J_2 = 0.1$, respectively. The dramatic change point in figure 6(a) and the jump in figure 6(b) clearly indicate two critical points. Comparing our results with the previous ones, we find that the phases on the right side of the two critical points in figures 6(a) and (b) are states II and I, respectively, whereas phase IV is a new quantum state. Because the anti-ferromagnetic interactions $J_2$ and $J_\times$ are relatively small compared with the ferromagnetic interactions $|J_1|$ and $|J_\perp|$ for case IV, the ferromagnetic order is dominant and phase IV should be a ferromagnetic state. This conjecture is later confirmed by the $2N+1$-fold degenerate ground-state result with $S_{\text{tot}} = 2N$ of this phase ($S_{\text{tot}}$ is the total spin quantum number and $2N$ is the total spin number) obtained using the exact diagonalization method. In addition, we find that ground-state level crossings occur at the two critical points. Given the discontinuous nature of $E_{4L}$, we conclude that the two phase transitions are of first order.

Now, we apply the methods and results presented above to draw a full phase diagram for the FF case at $J_\perp = -0.5$. Figure 7 summarizes our results. We can distinguish four different quantum states. When $J_2$ and $J_\times$ are small, the system is in the ferromagnetic phase (ferro). States I and II (their spin arrangements are shown as insets in figure 7) appear at large $J_\times$ and $J_2$, respectively. Between these two phases, there exists a tetramer state for relatively large $J_\times$ and $J_2$ due to competition among different interactions. We determine that the transition from tetramer to II is of second order, while the other phase transitions are of first order.

One of the transitions in figure 7—that between the ferro and I states occurring near $J_\times = 0.25$ when $J_2 = 0$—can be understood easily from the following simple consideration. For ferromagnetic chains, the interchain coupling can be written as $(-|J_\perp| + 2J_\times)M_1 \cdot M_2$, where $M_{1,2}$ represents the slowly varying expectation value of the site spins $(S)$ in chain 1 (2) correspondingly. Hence, the negative value of $(-|J_\perp| + 2J_\times)$ implies the ferromagnetic order of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6}
\caption{(a) $E_{4L}$ as a function of $J_2$ at $J_\times = 0.1$ and (b) $E_{4L}$ as a function of $J_\times$ at $J_2 = 0.1$ for the FF case.}
\end{figure}
Figure 7. Ground-state phase diagram for the FF case at \( J_\perp = -0.5 \) and \( J_1 = -1.0 \). The black arrows show the arrangement of spins on the ladder for states I and II, respectively.

\( M_1 \) and \( M_2 \), whereas the positive value results in the anti-ferromagnetic (\( M_1 \) opposite to \( M_2 \)) arrangement, which is exactly the structure of state I. In figure 7, \( J_\perp = -0.5 \) implies transition at \( J_\times = 0.25 \), which is sufficiently close to our DMRG result.

4. Global phase diagram of the anti-ferromagnetic frustrated case

When all the interactions are anti-ferromagnetic, the system is the AFF case. We first consider the \( J_2 = 0 \) case. As mentioned in section 1, the existence or non-existence of the CD state is a big issue in this case. We find that the \( J_\perp \) parameter interval for the order parameter \( O_{CD} \) studied in [26] is beyond the CD region predicted in [25], which, we think, is the main cause of the failure of CD state detection. Therefore, we calculate the CD order parameter \( O_{CD} \) in more refined parameter regions. At the same time, we also consider the entanglement as in [26], but keep more states in the DMRG calculations.

The \( O_{CD} \) results are shown in figure 8. \( O_{CD} \) bends upward as \( N \) increases and approaches a finite value in the thermodynamic limit for several parameters, indicating the existence of the CD long-range order. This result is consistent with the finding in [26] and the expectation in [23, 25], and it gives an explicit proof that the CD state exists in a narrow parameter region. This result further negates the suspicion in [26] that the CD long-range order may appear only at the phase boundary \( J_\perp = 0.38 \) and not in a finite region.

The four-site entropies \( E_{4,L} \) and \( E_{4,R} \) as well as their differences \( \Delta E_4 = E_{4,L} - E_{4,R} \), as a function of \( J_\perp \) under different system sizes \( N \), are shown in figures 9(a) and (b), respectively. The regimes to which \( E_{4,L} \) and \( E_{4,R} \) belong are separated clearly as shown in figure 9(a), which reflects the oligomerization property of the regime. The \( \Delta E_4 \) results in figure 9(b) give a much clearer picture. Although \( \Delta E_4 \) becomes smaller and smaller as \( N \) increases, some points around \( J_\perp = 0.38 \) move toward certain finite values. Even in the thermodynamic limit, the maximal value is larger than 0.3. Obviously, the left and right regions of the middle separated
regime are the Haldane and the RS states, respectively, and the separation state corresponds to the CD state.

As to the tetramer phase in the FF case, we also give an analysis here for the CD property of the separated regime. We compare the difference of the two-site entropies $E_{2,L}$ (for spins 1 and 3 of L) and $E_{2,R}$ (for spins 3 and 5 of R) $\Delta E_2$ with $\Delta E_4$ as shown in figure 10. The consistency of $2 \times \Delta E_2$ and $\Delta E_4$ clearly indicates that the difference between $E_{4,L}$ and $E_{4,R}$ completely comes from the dimerization of the spins on the legs of the chain; $\Delta E_4$ reflects the existence of the CD phase.

Our result is different from that in [27]. By analysis, we find that although the accuracy $10^{-8}$ in [27] is higher than ours ($10^{-7}$), the bending-up behavior only becomes clear because $N$ is large enough as shown in the $O_{CD}$ results. Therefore, we believe that system size is very important in determining the extrapolation property; it can change the final conclusion. A very recent work presents results consistent with ours from the correlation point of view. The work focuses on the influence of calculation accuracy on determining the CD state and demonstrates that the limiting value for $N \to \infty$ depends strongly on the functional form used for the extrapolation [40]. Thus, the work does not give a definite conclusion. To solve this issue, further analysis or other methods are needed, but our entanglement result at least gives a more obvious distinction for the dimer phase compared with the $O_{CD}$ results. We hope that it can serve as a guide for future research.

We then consider the influence of $J_2$ on the QPTs of the system. According to previous studies, the system may present richer quantum states when $J_\times$ is a weak coupling [15, 16, 26]. Therefore, we consider the weak-coupling case and set $J_\times = 0.2$. $E_{4,L}$ and $O_{CD}$ as a function of $J_\perp$ under different $J_2$ values are presented in figures 11(a) and (b), respectively. The middle uplifted region of $E_{4,L}$ and the nonzero regime of $O_{CD}$, which reflect the CD phase, become wider and higher as $J_2$ increases. This feature shows the clear and gradual change process of the quantum states with increasing $J_2$ and further confirms the conclusion in [15, 16] that $J_2$ enhances the stability of the CD phase. Meanwhile, the curve for $J_2 = 0$ has a structure similar

Figure 8. Scaling behavior of $O_{CD}$ as a function of $1/N$ at $J_2 = 0$ and $J_\times = 0.2$ for different $J_\perp$. The dotted line is a guide to the eyes.
Figure 9. (a) Four-site entropies $E_{4L}$ and $E_{4R}$ as a function of $J_\perp$ for $J_2 = 0$ under different $N$ values. The results for L are displayed only for $N = 240$ and 360. (b) $\Delta E_4 = E_{4L} - E_{4R}$ under different $N$ values.

to those of $J_2 \neq 0$ for both $E_{4L}$ and $O_{\text{CD}}$. From this point of view, we may also conclude that the CD phase does exist at $J_2 = 0$.

When $J_2$ is further increased to $J_2 = 0.5$, except for the CD phase indicated by the separation of $E_{4L}$ and $E_{4R}$, there appears another dramatic change near $J_\perp = 0.11$ as shown in figure 12(a). Comparing our result with those in [16], we find that the quantum phase in the region $0.11 \leq J_\perp \leq 0.16$ is the SD state. Because of the specific symmetry between L and R, $E_{4L}$ and $E_{4R}$ are equal and do not show the dimerization property. According to the dimer structure property of the SD state, we calculate different two-site entropies on the legs of L and R as shown in figure 12(b). We can clearly see that $E_{13} = E_{24}$ and $E_{35} = E_{46}$ in the CD region, whereas $E_{13} = E_{46}$ and $E_{24} = E_{35}$ in the SD region. Here, the numbers represent the places of spins on L and R. Based on this property, we define order parameters for the SD and CD states, respectively, from the entanglement point of view as shown in figure 12(c). The red dots represent the SD order parameter $E_{\text{SD}} = (E_{13} + E_{46}) - (E_{24} + E_{35})$, and the crosses represent the CD order parameter $E_{\text{CD}} = (E_{13} + E_{24}) - (E_{35} + E_{46})$. The phase transition points indicated here
Figure 10. \( \Delta E_4 \) and \( 2 \times \Delta E_2 \) as a function of \( J_\perp \), where \( \Delta E_2 = E_{13} - E_{35} \) is the difference between the two-site entropies for spins on L and R.

Figure 11. (a) Four-site entropy \( E_{4,L} \) and (b) order parameter \( O_{\text{CD}} \) as a function of \( J_\perp \) for different \( J_2 \) values.

are consistent with those of \( O_{\text{CD}} \) and \( O_{\text{SD}} \) in [16]. \( E_{\text{SD}} \) and \( E_{\text{CD}} \) clearly describe the dimerization of the SD and CD states, respectively.

Using the above methods of analysis, we obtain the ground-state phase diagram in the parameter plane for the AFF case. The result is shown in figure 13. We determined that the critical points for the Haldane–CD and CD–RS transitions are \( J_{\perp HC}^c = 0.372 \) and \( J_{\perp CR}^c = 0.385 \), respectively, when \( J_2 \) is absent. The width of the CD phase \( \delta J_\perp = 0.013 \) here agrees very well with the analytical predictions in [25], which yield \( \delta J_\perp = (2J_\perp/\pi)^2 = 0.016 \). In addition, the CD phase becomes wider and wider as \( J_2 \) increases, indicating the enhancement effect of \( J_2 \) on the CD state. Furthermore, when \( J_2 > 0.544 \), the Haldane phase disappears and a new SD phase appears. These results agree with the expectations in [15]. Due to the competition between different interactions, the SD phase exists only in a narrow parameter region \( 0.473 < J_2 < 0.544 \).
Figure 12. (a) $E_{4L}$ and $E_{4R}$ for $J_2 = 0.5$ and $N = 360$. (b) Two-site entropy as a function of $J_\perp$ for different NN sites on L and R. (c) Order parameters defined by the difference of these two-site entropies $E_{CD} = (E_{13} + E_{24}) - (E_{35} + E_{46})$ and $E_{SD} = (E_{13} + E_{46}) - (E_{24} + E_{35})$.

5. Summary

In summary, we first study the QPTs of the FF case of the SLDI model. The results of the four-site entropy and the correlation functions clearly indicate the existence of an interesting tetramer phase when $J_2$ and $J_\times$ are located at some regions. We identify the tetramer order parameter using the difference in local spin correlations on legs as well as on diagonals. When $J_2$ and $J_\times$ are small, the exact diagonalization results show that the system presents a $2N + 1$-fold degenerate ferromagnetic state. When a significant difference exists between $J_2$ and $J_\times$, the system presents state I or II. By analyzing correlation functions on the same and different legs with different rung distances, we give their possible spin-arrangement structures. The phase diagram for the FF case is shown.

In addition, QPTs for the AFF case are considered. Entanglement results at the weak coupling $J_\times = 0.2$ show that when $J_2$ is considered, the stability of the CD state is enhanced. It becomes wider and wider as $J_2$ increases, and replaces the Haldane phase when $J_2 > 0.544$, which is consistent with the expectation in [15, 16]. The SD phase, on the other hand, only exists in a very narrow parameter region. Furthermore, the gradual change in the behavior of
Figure 13. Ground-state phase diagram for the AFF case at $J_\times = 0.2$. The SD state only exists in a narrow parameter region.

the entanglement and correlation functions with $J_2$ indicate that when $J_2 = 0$, the controversial CD state might really exist. Aiming at this point, we analyze the order parameter defined by correlation functions and the difference between two neighboring four-site entropies and their finite-size scaling behavior. Then we further confirm the existence of the CD state. The phase diagram for the AFF case is given as well.

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