String order in spin liquid phases of spin ladders

G. Fáth, Ö. Legeza, and J. Sólyom
Research Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary
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Two-leg spin ladders have a rich phase diagram if rung, diagonal, and plaquette couplings are allowed for. Among the possible phases there are two Haldane-type spin liquid phases without local order parameter, which differ, however, in the topology of the short range valence bonds. We show that these phases can be distinguished numerically by two different string order parameters. We also point out that long-range string and dimer orders can coexist.

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I. INTRODUCTION

The properties of spin ladder systems attracted considerable interest in the past decade.[1] It was shown[2] that even-leg ladder models develop a gap in their excitation spectrum if the rung coupling is ferromagnetic. This result could be considered as a generalization of Haldane's conjucture[3] about the existence of a finite gap in integer spin Heisenberg chains, since for strong enough ferromagnetic rung coupling the spin ladder with spin-S on the legs is equivalent to a spin chain of spin-$2S$. In this case the ground state resembles that of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model,[4] in which short range valence bonds couple spins on neighboring rungs. Later it was demonstrated numerically,[5] that a gap is generated for antiferromagnetic rung coupling as well, in which case the singlet valence bonds are formed predominantly on the rungs. It may be called a *rung singlet* state. Both are Haldane-type spin liquids in which there are no broken local symmetries, and the excitations are coherent magnons with a finite gap.

A similar situation occurs if the two legs of the ladder are coupled not by rung couplings, but diagonally or by plaquette couplings.[6] When these couplings compete with each other, non-Haldane spin liquid phases, characterized by the absence of coherent magnon excitations and spontaneous dimerization,[6,7]may occur due to frustration effects. Although the thermodynamic properties of Haldane and non-Haldane spin liquids are identical, the correlation functions differ due to the difference in the excitations spectrum. The two phases could also be distinguished by a local dimer order parameter.

In addition to these spin liquid phases several other phases may occur, such as ferromagnetic or incommensurate phases. When drawing the phase diagram, it was thought for some time that the concept of Haldane-like spin liquids is unambiguous for spin ladders, and therefore the AKLT-like and rung singlet phases are identical not only thermodynamically, but also in the sense, that in a large parameter space, where rung, diagonal and plaquette couplings are all taken into account, one could go from one to the other without any discontinuity. In fact, it was argued[8] that there is a controlled way of changing the parameters gradually and interpolate continuously between two limiting cases belonging trivially to one or to the other phase. The procedure contains a shift of one of the legs of the ladder by one unit, thereby transforming a rung singlet into a diagonally situated valence bond, characteristic of the the AKLT-like state, or vice versa. However, as was pointed out by Kim *et al.*[9] this shift changes the topology of the system drastically. When we start from an open ladder, the above transformation deforms the usual straight-end ladder into a ''ladder'' whose ends are cut diagonally. Such a deformation has serious consequences on the degeneracy of the ground state for open boundary condition. In a usual ladder the AKLT state has a fourfold degeneracy due to the unpaired end spins, while the rung singlet state is unique. On the other hand, in the diagonally cut ladder the ground state is unique for the AKLT state, and fourfold degenerate in the rung singlet state. This is best seen in Figs. 1(a) and 1(b), where the typical valence-bond configurations of the AKLT-like state and the rung singlet state are shown. In Fig. 1(c) we also show a typical valence bond configuration of the dimer phase. In this phase the invariance of translation by one rung is broken spontaneously.

While in the AKLT state the number of valence bonds crossing an arbitrary vertical line between rungs is always odd, in the rung singlet state it is always even. This is true not only in this special configuration but remains valid generally, as long as the range of valence bonds is short compared to the size of the system.[10] The two states can be distinguished by a topological quantum number. Thus for topological reasons in a spin ladder the two Haldane-type spin liquid phases are different and in the space of couplings they must be separated by a phase transition hyperplane,[9,11] although extended gapless (critical) regions between them cannot be excluded *a priori* either.

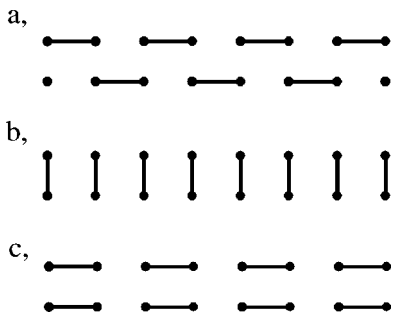

FIG. 1. Representative valence-bond configurations without quantum fluctuations in different gapped phases of spin ladders. (a) The AKLT-like state, (b) rung singlet state, (c) dimerized state. State (a) is odd, while states (b) and (c) are even under our topological classification.

Since the topological quantum number is not accessible to direct computation, a generalization of the hidden order parameter of the spin-1 chain[12] was proposed,[9] that could distinguish between the even and odd topological sectors of the Haldane phase. Although the relationship between the two new string order parameters and the two types of Haldane phases was made plausible by looking at special configurations, it was not possible to calculate their value, since the bosonization procedure applied to obtain the phase transition lines did not distinguish between the two parameters.

The aim of this paper is to do a numerical study of the relationship between the possible spin liquid phases of the spin ladders and the string order parameter, using the density matrix renormalization group (DMRG) procedure.[13] The setup of the paper is as follows. In Sec. II we give a short description of the ladder models and a brief account of what is known about the possible phases. The results of our numerical calculations are presented in Sec. III. Finally Sec. IV contains a brief summary.

II. GAPPED PHASES IN LADDER MODELS

Following the notations of Ref. 14 we will write the most general form of the Hamiltonian for isotropic two-leg spin ladder models if only spins on the same and neighboring rungs interact, as

$$\mathcal{H}=\sum_{i=1}^{N} h_{i,i+1}, \tag{1}$$

where

$$\begin{aligned} h_{i,i+1}=&J_l\vec{\sigma}_i\cdot\vec{\sigma}_{i+1}+J_l'\vec{\tau}_i\cdot\vec{\tau}_{i+1}+\tfrac{1}{2}J_r\vec{\sigma}_i\cdot\vec{\tau}_i+\tfrac{1}{2}J_r'\vec{\sigma}_{i+1}\cdot\vec{\tau}_{i+1}\\ &+J_d\vec{\sigma}_i\cdot\vec{\tau}_{i+1}+J_d'\vec{\tau}_i\cdot\vec{\sigma}_{i+1}+V_{ll}(\vec{\sigma}_i\cdot\vec{\sigma}_{i+1})(\vec{\tau}_i\cdot\vec{\tau}_{i+1})\\ &+V_{rr}(\vec{\sigma}_i\cdot\vec{\tau}_i)(\vec{\sigma}_{i+1}\cdot\vec{\tau}_{i+1})+V_{dd}(\vec{\sigma}_i\cdot\vec{\tau}_{i+1})(\vec{\tau}_i\cdot\vec{\sigma}_{i+1}). \end{aligned} \tag{2}$$

In Eq. (2) σ_i and τ_i are spin-1/2 operators corresponding to spins sitting on the two legs of the ladder. The schematic plot of the spin couplings in $h_{i,i+1}$ between the spins on the two legs of the ladder are shown in Fig. 2.

The terms with J_l and J_l' couple neighboring spins on the same legs, the terms with J_r and J_r' spins on the same rung, while the terms with J_d and J_d' spins that are situated diagonally. In addition to these bilinear terms there could be three biquadratic terms with couplings V_{ll}, V_{rr}, and V_{dd}.

In order to decrease the number of parameters from now on we only consider the case when $J_R\equiv J_r=J_r'$, $J_L\equiv J_l=J_l'$, and $J_D\equiv J_d=J_d'$. The energy scale will be set by fixing $J_L=1$.

It is known from previous studies[6] that all the interleg couplings $J_R, J_D, \ldots, V_{dd}$, when acting alone, generate a Haldane-like phase. This is an AKLT-like phase with odd topology of the number of valence bonds if $J_R<0$, $J_D>0$, $V_{ll}>0$, $V_{rr}<0$, or $V_{dd}>0$, while for opposite sign of the couplings a rung singlet like state with even topology is generated.

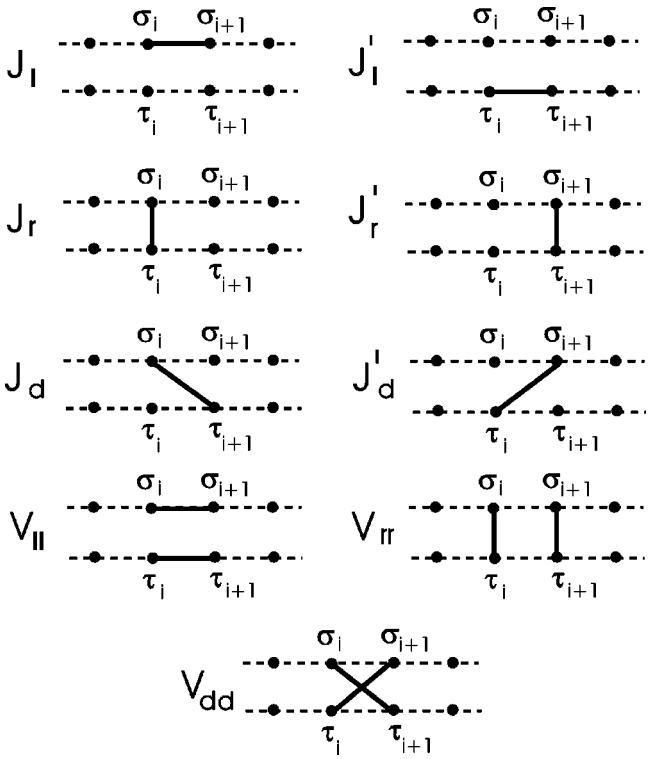

FIG. 2. Schematic plot of the Hamiltonian.

As mentioned before, the goal of the present paper is to identify an appropriate order parameter that can characterize the spin liquid phases. Starting from the string order parameter of the $S=1$ chain proposed by den Nijs and Rommelse,[12] it is natural to generalize it to spin ladders by defining the order parameter of AKLT-like Haldane state as

$$\mathcal{O}^{\alpha}_{\rm odd}=-\lim_{|i-j|\to\infty}\left\langle S_i^{\alpha}\exp\left(i\pi\sum_{l=i+1}^{j-1}S_l^{\alpha}\right)S_j^{\alpha}\right\rangle, \tag{3}$$

where S_i^{α} is the total spin on rung i, $S_i^{\alpha}=\sigma_i^{\alpha}+\tau_i^{\alpha}$, $\alpha=x,y,z$.

Since in the extreme limits the pure rung singlet state can be related to the AKLT state by a shift of one of the legs, the string order parameter of the Haldane state with even topological quantum number is expected to be

$$\mathcal{O}^{\alpha}_{\rm even}=-\lim_{|i-j|\to\infty}\left\langle S_i^{\alpha}\exp\left(i\pi\sum_{l=i+1}^{j-1}S_l^{\alpha}\right)S_j^{\alpha}\right\rangle, \tag{4}$$

where S_i^{α} is now the sum of two diagonally situated spins, $S_i^{\alpha}=\sigma_i^{\alpha}+\tau_{i+1}^{\alpha}$.[9,15]

In what follows we will calculate the order parameters for the z component only, they will be denoted as $\mathcal{O}_{\rm odd}$ and $\mathcal{O}_{\rm even}$, respectively. We will show, that these two order parameters are mutually exclusive. $\mathcal{O}_{\rm odd}$ is finite for the AKLT-like Haldane state, while $\mathcal{O}_{\rm even}$ is finite for the rung singlet-like Haldane phase. Moreover the order parameter goes to zero continuously at the transition point when the transition is of second order, while it vanishes with a jump in case of first order transitions.

III. NUMERICAL RESULTS

To investigate this problem we performed numerical calculations applying the DMRG method[13] on the model defined by the Hamiltonian in Eq. (1). Since the DMRG procedure is more accurate for systems with free ends, we consider our ladder model with open boundary condition. In order to eliminate the fourfold degeneracy of the ground state in the conventional Haldane phase due to the free $S=1/2$ spins at the ends of the ladder, we exploited the left-right reflection symmetry of the system. Out of the four degenerate ground state we have selected the one with $S^z_{\rm tot}=0$ and positive parity. The calculations were done for chains with up to 150 sites keeping 100 to 200 states per block. The truncation error varied in the range 10^{-5} to 10^{-7}. In most of the calculations we used the finite-lattice method with two or three iteration cycles.

In order to reduce the undesirable boundary effects we fixed site i in Eqs. (3) and (4) at the center of the chain and let site j run through half of the chain. The finite size scaling procedure was used to determine the thermodynamic limit of the quantitities measured.

In what follows we present our numerical results for the string order parameters for various choices of the coupling constants. Since our aim was not to explore the full phase diagram, but rather to check how the string order parameters $\mathcal{O}_{\rm even}$ and $\mathcal{O}_{\rm odd}$ vary as we go from one Haldane-like phase to another, topologically different gapped phase, we calculated the string order parameters along specially chosen paths connecting points in the parameter space, where the model is known to belong to different phases. It is worth pointing out that since the ground state wave function and therefore the ground state expectation values of operators can be calculated more accurately than those of excited states, the order parameters provide a better way to obtain phase diagrams than investigating the energy spectrum.

A. Haldane phases due to rung, diagonal, or plaquette couplings alone

The effect of J_R alone was analyzed numerically for short systems in Ref. 15. It was found there that for $J_R<0$ the order parameter $\mathcal{O}_{\rm odd}$ is finite, while for $J_R>0$ the other order parameter $\mathcal{O}_{\rm even}$ is finite. Our results with the DMRG method confirmed these results.

From earlier works[6] it is known, that not only the rung but also the diagonal and plaquette interleg couplings are relevant perturbations which generate a gap and drive the system into phases with topological order. Depending on the sign of the perturbation the emerging phases belong to one of the two possible topological sectors.

We have therefore investigated the effect of these couplings by doing calculations at two specialy chosen values. The finite size scaling analysis of the results obtained for couplings $J_d=\pm 1$ or $J_D=\pm 1$ indicated that irrespective whether only one or both diagonal couplings are present, $\mathcal{O}_{\rm odd}\neq 0$ and $\mathcal{O}_{\rm even}=0$ for positive J_d or J_D, while we have $\mathcal{O}_{\rm even}\neq 0$ and $\mathcal{O}_{\rm odd}=0$ for negative J_d or J_D.

Similarly, calculations for the values ± 1 of the couplings V_{ll}, V_{rr}, and V_{dd} (the other couplings set to zero) convinced us that the even order parameter is finite, $\mathcal{O}_{\rm even}>0$, for $V_{ll}<0$, or $V_{rr}>0$, or $V_{dd}<0$, while the odd order parameter is finite, $\mathcal{O}_{\rm odd}>0$, for opposite signs of the couplings, i.e., for $V_{ll}>0$, $V_{rr}<0$, or $V_{dd}>0$. Our results obtained for the string order parameters allows us to conclude that the topology of the valence bond structure can be identified directly by calculating the order parameters $\mathcal{O}_{\rm odd}$ or $\mathcal{O}_{\rm even}$, since they mutually exclude each other.

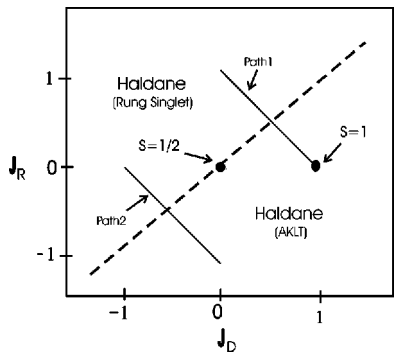

FIG. 3. The J_R-J_D phase diagram. Phase boundary is indicated by dashed line and the two trajectories of the calculation by solid lines.

B. The J_R-J_D phase diagram

Next we consider the subspace spanned by J_R and J_D. According to the recent bosonization study[9] the phase transition line separating the two topological sectors is of first order in the quadrant $J_R>0$, $J_D>0$, while of second order in the quadrant $J_R<0$, $J_D<0$. In order to check the behavior of the string order parameter, we have calculated them along two paths in the (J_R, J_D) parameter space.

Path 1 is defined by $J_R=1-J_D$ with $0<J_D<1$, and path 2 is parametrized by $J_R=-1-J_D$ with $-1<J_D<0$. They are indicated by solid lines on Fig. 3.

Our numerical results for $\mathcal{O}_{\rm even}$ and $\mathcal{O}_{\rm odd}$ obtained in the thermodynamic limit along path 1 is plotted on Fig. 4. The lines connecting the points are only guides to the eye. It is apparent from the figure that $\mathcal{O}_{\rm even}$ is finite in one particular region while $\mathcal{O}_{\rm odd}$ in the other.

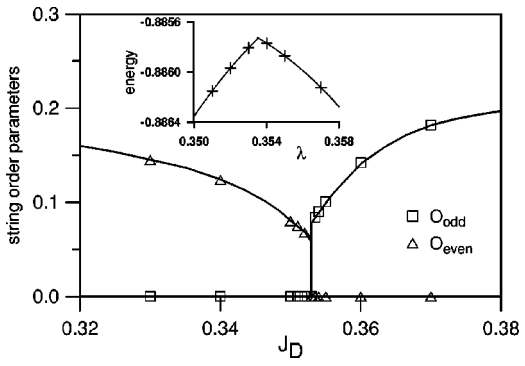

FIG. 4. The $N\to\infty$ extrapolated values of the string order parameters $\mathcal{O}_{\rm even}$ and $\mathcal{O}_{\rm odd}$ calculated along path 1. The inset of the figure shows the cusp singularity of the ground state energy indicating a first order transition.

As one sees from the figure the string order parameters, extrapolated to the infinite ladder limit, have a jump discontinuity at the transition point. In order to further support the first order nature of the phase transition we have also investigated the low lying energy spectrum. We found that there is a sudden change in the degeneracy of the ground state at the transition point. In the case of open ladders the fourfold degeneracy of the AKLT phase associated with spin-1/2 endspins disappear, and the ground state becomes unique as a rung-dimer-like structure emerges. Moreover, by examining higher lying energy levels we found that the energy gap remains finite throughout the transition. The ground state energy shows a cusplike singularity, a characteristic feature of first order transitions, as is shown on the inset of Fig. 4. Note, however, that for finite chains there is no observable level crossing in the ground state due to hybridization.

Next we consider the behavior of the order parameters calculated along path 2 in the negative J_R and J_D quadrant. Our results are plotted in Fig. 5. In this case again, only one of the order parameters is finite in a particular phase, however, the gap vanishes continuously at the phase boundary, which is a characteristic features of second order phase transitions. It is worth noting that there is an order of magnitude difference in the scale of Fig. 4 and Fig. 5 as a function of J_D. Since the phase transition points were located on two special trajectories only, the phase boundary that separates the two types of Haldane-like phases is drawn by dashed line in Fig. 3 to indicate that its exact shape was not determined.

C. The role of plaquette couplings

In order to consider the influence of the plaquette couplings we have chosen the special values $K \equiv J_R = V_{ll} = V_{dd}$, $V_{rr} = 0$, since the phase diagram has already been studied for this parametrization.[6] This choice has been motivated by the possible mapping of the ladder model to the spin-1 bilinear-biquadratic chain for $K = 1$.[6] Here we calculate string order parameters along four lines going through the expected phase boundaries shown by solid lines in Fig. 6.

Calculations along path 1 have revealed that $\mathcal{O}_{\text{odd}}$ is finite in the AKLT-like Haldane phase, but it vanishes in the dimerized phase. On the other hand, $\mathcal{O}_{\text{even}}$ becomes finite in the dimerized phase, thus the two phases are well distinguished by the order parameters. Examining the trajectory (path 2) going through the phase boundary between the rung singlet like Haldane and dimerized phases, we have found that $\mathcal{O}_{\text{even}}$ remains finite and $\mathcal{O}_{\text{odd}}$ scales to zero everywhere. This shows that the string order parameter does not uniquely characterize the Haldane phase, it is rather an indicator of the topology of the valence bond structure, since both the rung singlet and the dimerized phases have even topological quantum numbers.

Thus when $\mathcal{O}_{\text{even}} \neq 0$, the string order is not sufficient to classify unambiguously the ground state. Another order parameter, the so-called *dimer order* parameter has to be measured. Taking the difference of the local energy on neighboring bonds in the middle of the ladder this order parameter is defined as

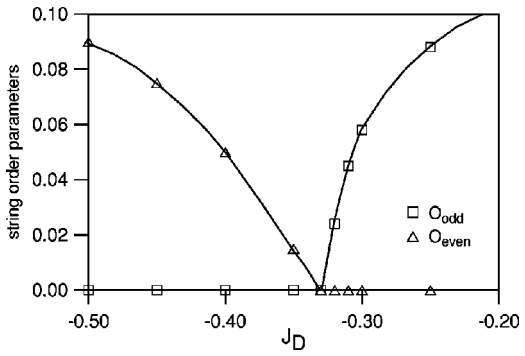

FIG. 5. The $\mathcal{O}_{\text{even}}$ and $\mathcal{O}_{\text{odd}}$ string order parameters calculated along path 2.

$$D = \frac{\langle h_{i,i+1}\rangle - \langle h_{i+1,i+2}\rangle}{\frac{1}{2}\left[\langle h_{i,i+1}\rangle + \langle h_{i+1,i+2}\rangle\right]}. \tag{5}$$

In the Haldane-type spin liquids D vanishes, but there exists an extended region in the parameter space, where the dimer order parameter scales to finite value in the thermodynamic limit, signaling a dimerized phase with spontaneously broken translational symmetry.

Next let us consider the $K > 0$ half-plane focusing on the $J_D = 0$ half-line and its vicinity. Calculation of the order parameters along path 3, defined by $K = 1 + J_D$ with $-1 < J_D < 1$ revealed that $\mathcal{O}_{\text{even}}$ is finite for $J_D < 0$, while $\mathcal{O}_{\text{odd}}$ is finite for $J_D > 0$. At $J_D = 0$ all order parameters including D vanish as is shown in Fig. 7. Since the string order parameters become finite for arbitrary small finite value of J_D the two types of spin liquids are separated by a critical line and the extended critical phase reported earlier[6] does not exist.

Finally, it can be seen on the figure that for $J_D > 0.6$ both order parameters vanish and a new phase appears. In order to analyze the question whether the new phase develops just above the *VBS* point, we investigated the vicinity of the *VBS* point along path 4. We found that $\mathcal{O}_{\text{odd}}$ remains finite up to $K \sim 1.9$ while $\mathcal{O}_{\text{even}}$ vanishes for the whole regime. Investigating the low lying energy spectra we found a multiply degenerate ground state. In order to decide whether this

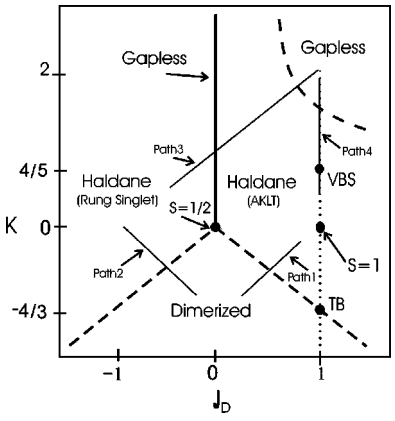

FIG. 6. The K vs J_D phase diagram. Phase boundaries are indicated by dashed lines and the various trajectories of the calculation by solid lines.

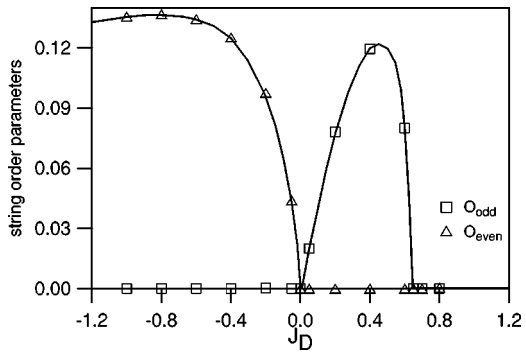

FIG. 7. The $\mathcal{O}_{\text{even}}$ and $\mathcal{O}_{\text{odd}}$ string order parameters calculated along path 3.

phase extends to the J_D axis we made test calculations at $J_D=0.05$, $K=1.5,2$ and found a finite $\mathcal{O}_{\text{odd}}$ but vanishing $\mathcal{O}_{\text{even}}$ order parameters. This suggests the schematic phase boundary shown by a dashed line in the figure.

IV. CONCLUSIONS

In the present paper we have studied the relationship between various gapped Haldane and non-Haldane spin liquid phases and the two different string order parameters in the general two-leg spin ladder model, containing rung, diagonal and plaquette couplings as well. The string order parameters have been calculated numerically using the DMRG method.

It has been found that there are two kinds of Haldane-type massive spin liquids characterized by finite O_{even} or O_{odd} string order parameters, respectively. It was shown that $\mathcal{O}_{\text{odd}}$ is finite in the AKLT-like phase, while $\mathcal{O}_{\text{even}}$ is finite in the rung-singlet-like phase. Examining the transition from the AKLT-like to the rung-singlet-like phases the type of phase transition can be first or second order depending on the path in parameter space, and this shows up in the abrupt or continuous vanishing of the order parameter.

When plaquette couplings are allowed for, non-Haldane-like spin liquid phases can occur, and the string order parameters are not sufficient to characterize the phases. $\mathcal{O}_{\text{even}}$ remains finite in the dimerized phases, too. Thus the string order parameter reflects the topology of the valence bond structure and does not characterize uniquely the Haldane-type phases. A dimer order parameter can, however, be defined, which is finite in a non-Haldane-type dimer phases but vanishes in Haldane-type spin liquids.

It was found previously that there exists a small range of the parameters where the combination of perturbing operators is irrelevant and the spectrum remains massless. Investigating the vicinity of $J_D=0,K>0$ axis we have found that both string order parameters vanish on this critical line, but $\mathcal{O}_{\text{even}}$ or $\mathcal{O}_{\text{odd}}$ becomes finite immediately as we move away from this axis. Therefore, we conclude that the two kind of spin liquids are separated by a critical line and not by an extended gapless regime reported earlier. In addition, around the $J_D=1$ line for $K>1.8$ we have found a new phase. This phase is characterized by multiply degenerate ground state and vanishing order parameters. The detailed analysis of this region is left for future investigation.

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