Search for quantum dimer phases and transitions in a frustrated spin ladder

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A two-leg spin-1/2 ladder with diagonal interactions is investigated numerically. We focus our attention on the possibility of columnar dimer phase, which was recently predicted based on a reformulated bosonization theory. By using density matrix renormalization group technique and exact diagonalization method, we calculate columnar dimer order parameter, spin correlation on a rung, string order parameters, and scaled excitation gaps. Carefully using various finite-size scaling techniques, our results show no support for the existence of columnar dimer phase in the spin ladder under consideration.

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Much effort has been devoted to understanding the effects of competing interactions on quasi-one-dimensional systems. The possibility of unconventionally ordered phases has been the focus of interest. For example, the one-dimensional extended Hubbard model (EHM) with nearest-neighbor repulsion V in addition to on-site repulsion U has been investigated intensively.[1–12] It had been considered for a long time that the ground-state phase diagram at half filling has only two phases, the spin-density-wave (SDW) and the charge-density-wave (CDW) states.[1–6] Moreover, the order of the phase transition at $U \simeq 2V$ can change from continuous to first order at a tricritical point, which was speculated to exist in the intermediate coupling regime.[2–4] Later, by using the level-spectroscopy method, Nakamura pointed out that there exists also a novel spontaneously dimerized phase, the so-called bond-order-wave (BOW) phase, in a narrow strip between the SDW and the CDW phases in the weak coupling region.[7] While this phase is absent in standard one-loop g-ology and bosonization calculations,[1,4] its existence was supported by a reformulated one,[8] where higher-order terms were included. The appearance of the BOW phase was subsequently confirmed by quantum Monte Carlo simulations,[9,10] density matrix renormalization group (DMRG) method,[11] and functional renormalization group calculations.[12]

Interestingly, same story may happen also in an antiferromagnetic two-leg spin ladder with diagonal frustrations. The Hamiltonian of this model reads as follows:

$$H = J\sum_{\alpha=1,2}\sum_{i}\mathbf{S}_{\alpha,i}\cdot\mathbf{S}_{\alpha,i+1} + J_{\perp}\sum_{i}\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i} + J_{\times}\sum_{i}(\mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i+1} + \mathbf{S}_{1,i+1}\cdot\mathbf{S}_{2,i}), \qquad (1)$$

where $\mathbf{S}_{\alpha,i}$ denotes a spin-1/2 operator at site i of the αth leg. J and $J_{\perp}$ are the exchange couplings on legs and rungs, respectively. We set $J \equiv 1$ hereafter. $J_{\times}$ denotes the next-nearest-neighbor interchain coupling. This model has been investigated for decades,[13–20] and considerable amount of knowledge has been accumulated. It has been believed that the ground state phase diagram consists of only two phases, the rung-singlet (RS) phase and the so-called Haldane phase. The earlier bosonization study predicted a direct transition between these two phases at $J_{\perp}=2J_{\times}$.[14] Various numerical calculations, such as series expansions,[18] DMRG,[19] and level-spectroscopy method,[20] showed the phase boundary to be shifted away from the $J_{\perp}=2J_{\times}$ line, with a larger RS phase. Moreover, the phase transition seems to be of second order at weak interchain couplings and becomes first order at stronger couplings.[18,19] Recently, it was suggested that there exists an intermediate, spontaneously dimerized phase, the so-called columnar dimer (DC) phase, lying between the Haldane and the RS phases at weak interchain couplings.[21] This remarkable proposal is based on a reformulated weak-coupling field theory, which is similar in spirit to that in Ref. 8 with success in the study of one-dimensional EHM. According to Ref. 21, for a given $J_{\times}$, the DC phase occurs within a narrow but finite region $(J_{\perp})_{c,T} \leq J_{\perp} \leq (J_{\perp})_{c,S}$ in the phase diagram. Here $(J_{\perp})_{c,T}=2J_{\times}-5J_{\times}^2/\pi^2$ and $(J_{\perp})_{c,S}=2J_{\times}-J_{\times}^2/\pi^2$ are two distinct critical points, given by vanishing mass gaps in the spin-triplet and the spin-singlet sectors, respectively. As mentioned before, this intermediate DC phase was not found in previous numerical calculations.[18–20] Thus the existence of this spontaneously dimerized DC phase is surprising and calls for thorough theoretical studies.

In this paper, we try to find numerical evidence for the possibility of the DC phase in a two-leg spin ladder of Eq. (1) in the vicinity of $J_{\perp}=2J_{\times}$. Here we take $J_{\times}=0.2$.[22] It is smaller than the value $J_{\times}=0.287$, where the transition changes to be first order.[19] Thus the proposed region for the DC phase becomes $0.38 \leq J_{\perp} \leq 0.396$. The values of $J_{\times}$ and $J_{\perp}$ under consideration should be small enough in accordance with the weak-coupling field theory in Ref. 21. Both the DMRG technique[23,24] under open boundary conditions up to $L=400$ rungs and the Lánczos exact diagonalization method with periodic boundary conditions up to $L=16$ are used. In our DMRG calculations, 500 states per block are kept, and the truncation error is of the order of 10^{-7}. To demonstrate the possibility of the DC phase, the most direct way is to show the corresponding order parameter being nonzero in the proposed region of the phase diagram. As far as we know, this order parameter has not yet been measured for the present model. We note that the critical point $(J_{\perp})_{c,T}$ in the spin-triplet sector is consistent with the phase boundary found previously.[18–20] Therefore, another support of the proposal in Ref. 21 is to show the existence of another critical point at $(J_\perp)_{c,S}$ with vanishing mass gap in the spin-singlet sector. Carefully using various finite-size scaling skills for the DC order parameter and other physical quantities defined below, our results fail to show the existence of the DC phase, but instead they indicate a direct transition between the RS and the Haldane phases.

By using the DMRG technique under open boundary conditions, we first analyze the DC order parameter. As shown in Ref. 25, due to the presence of open ends, weak dimerization profiles can be induced near the boundaries. In order to reduce the boundary effect, the DC order parameter is calculated by the difference of local spin correlation on legs

$$D \equiv \left| \left\langle \frac{1}{2} \sum_{\alpha=1,2} (\mathbf{S}_{\alpha,i} \cdot \mathbf{S}_{\alpha,i+1} - \mathbf{S}_{\alpha,i+1} \cdot \mathbf{S}_{\alpha,i+2}) \right\rangle \right|, \qquad (2)$$

where only the bonds in the middle of finite open ladder with length L are considered (i.e., $i=L/2$). $\langle \cdots \rangle$ means the ground-state expectation value. The DC order parameter in the thermodynamic limit is then $D_\infty \equiv \lim_{L\to\infty} D$. Our results of the DC order parameter D for various $J_\perp$ with $J_\times=0.2$ are shown in Fig. 1(a). We find that D always decreases to zero in the thermodynamic limit even for $J_\perp=0.39$, which lies within the suggested region for the DC phase. Figure 1(b) shows $\ln D$ versus L for various values of $J_\perp$. It is found that, for L being large, $D \approx c \exp(-L/\xi)$, where c is a constant and ξ is a kind of correlation lengths. Moreover, as shown in the inset of Fig. 1(b), $1/\xi \propto |J_\perp - (J_\perp)_c|$ with $(J_\perp)_c \approx 0.38$, which agrees with the value of the proposed critical point $(J_\perp)_{c,T} = 0.38$ in the spin-triplet sector. This indicates that the long-range DC phase may appear only at this phase boundary, rather than for a finite region in the phase diagram. In addition, it shows no evidence for the additional second-order quantum phase transition at $J_\perp=(J_\perp)_{c,S}=0.396$, since the correlation length ξ diverges only at a single critical point $(J_\perp)_{c,T}$, rather than at two points.

To be sure if we miss the critical point $(J_\perp)_{c,S}$ in the above analysis, a finite-size crossing method[26] is used, which is applicable to detect the critical points of second-order quantum phase transitions. It is noted that one can always decompose the Hamiltonian into two parts, i.e., $H \equiv \mathcal{H}_0 + g\mathcal{V}$, and consider the transition being driven by the parameter g. Based on the finite-size scaling analysis, it is shown that the curves of the mean value $O \equiv \langle \mathcal{V} \rangle / L$ at two successive values of size L as a function of g will cross at a single point g_L^* near each critical point g_c.[26] The value of the critical point g_c can be found numerically by extrapolating the sequence g_L^* to $L \to \infty$. In the present case, we take the driving parameter as $J_\perp$. Thus the corresponding transition-driving term becomes $\mathcal{V} = \Sigma_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}$, which gives $O = \langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} \rangle$ by translational invariance if periodic boundary conditions are used. In case of finite open ladders, to avoid boundary effects, sites in the middle of ladders (i.e., $i=L/2$) are used. In Fig. 2, we plot the curves of $\langle \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i} \rangle$ versus $J_\perp$ for various sizes L, which are calculated by the DMRG technique. It is found that there is only one crossing point $J_\perp^*(L)$ at $L \equiv (L_1 + L_2)/2$ for the curves at two subsequent sizes L_1 and L_2. This indicates that

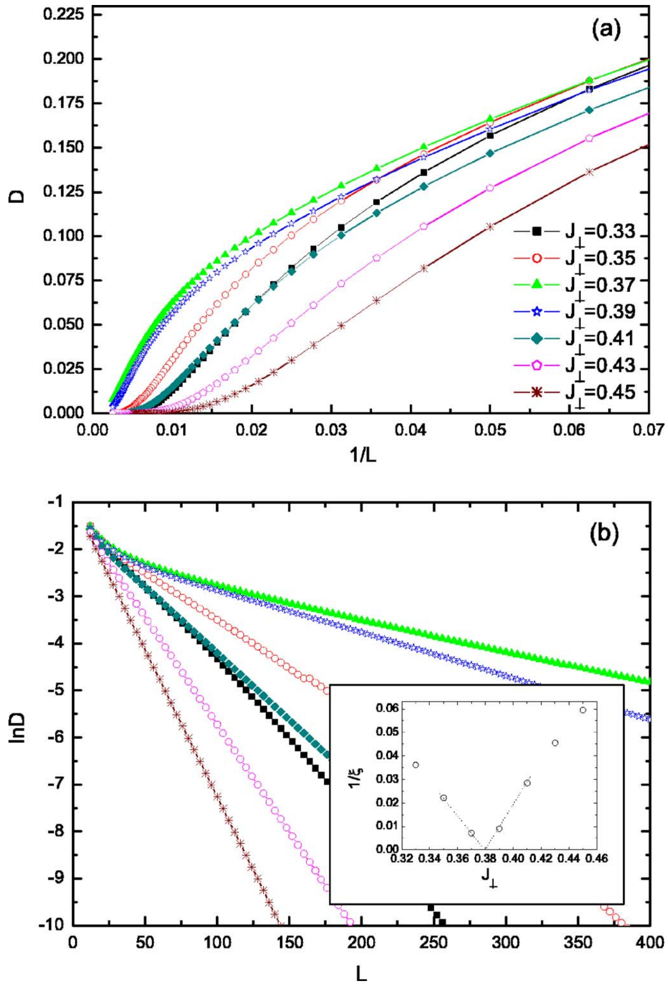

FIG. 1. (Color online) (a) Size dependence of the DC order parameter D for various $J_\perp$ with $J_\times=0.2$. (b) $\ln D$ versus L for various values of $J_\perp$ with $J_\times=0.2$. Labels for various $J_\perp$ are the same as those in (a). The inset shows the inverse of the correlation length ξ for various values of $J_\perp$.

there is *only one*, but not two, phase transition. Our conclusion is consistent with the picture provided by previous investigations,[13–20] where the complete phase diagram consists of only two phases with a single phase boundary. The scaling behavior of the crossing points is shown in the inset of Fig. 2. It is found that the crossing points converge to the value $(J_\perp)_c \simeq 0.378$ for the critical point. Our finding agrees well with that obtained by previous DMRG calculation[19] and is consistent with the predicted value for $(J_\perp)_{c,T}$.[21] Again, our results provide no support for the existence of another critical point at $(J_\perp)_{c,S}$ in the spin-singlet sector.

While our results show that there is no DC phase and there are only two phases in the complete phase diagram, the nature of these two phases has not yet been explored in the present study. According to previous investigations, these two phases should be the Haldane and the RS phases, and they can be identified by two distinct string order parameters O_{odd} and O_{even}.[15–17,27] These two string order parameters are given by

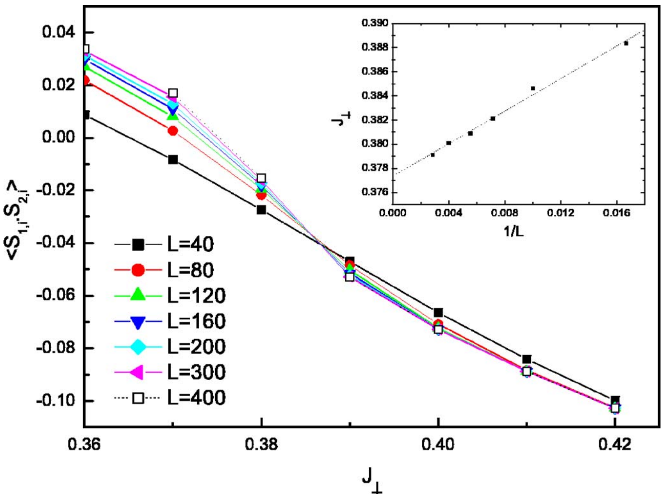

FIG. 2. (Color online) Spin correlation on the $(N/2)$-th rung as a function of $J_\perp$ for various sizes L with $J_\times=0.2$. The inset shows the L^{-1} scaling behavior of the crossing points.

$$O_P = -\lim_{|i-j|\to\infty}\left\langle \tilde{S}^z_{P,i}\exp\left(i\pi\sum_{l=i+1}^{j-1}\tilde{S}^z_{P,l}\right)\tilde{S}^z_{P,j}\right\rangle, \qquad (3)$$

where P = odd, even. The composite spin operators are defined as $\tilde{S}^z_{\text{odd},i}=S^z_{1,i}+S^z_{2,i}$ and $\tilde{S}^z_{\text{even},i}=S^z_{1,i}+S^z_{2,i+1}$. Because of spin isotropy, we calculate the string order parameters for the z-component spins only. In case of finite ladders, it turns out that the intersection of the curves of two distinct string order parameters implies the critical point.[17] In order to reduce the undesirable boundary effects, we fix site j in Eq. (3) at the center of the chain and let site $i=20$ in our calculations. Our DMRG results of O_{odd} and O_{even} for various sizes L as functions of $J_\perp$ with $J_\times=0.2$ are shown in Fig. 3. For smaller $J_\perp$, one has $O_{\text{odd}}\neq 0$ and $O_{\text{even}}=0$, which implies the Haldane phase; while $O_{\text{odd}}=0$ and $O_{\text{even}}\neq 0$ for larger $J_\perp$, which implies the RS phase. The finite size scaling procedure is used

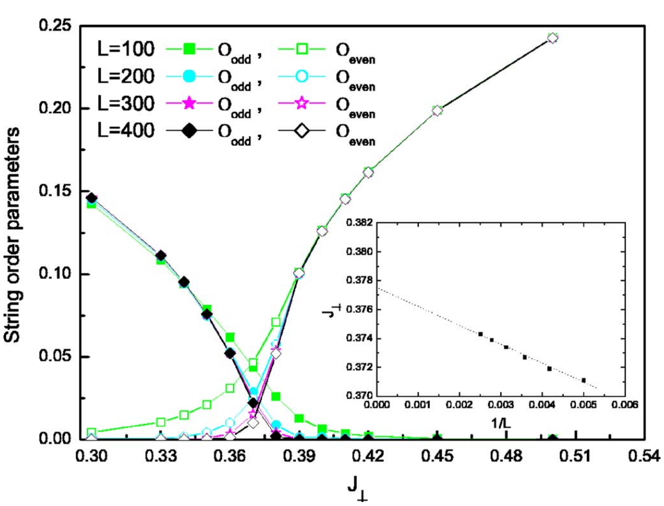

FIG. 3. (Color online) String order parameters for ladders with various sizes L as functions of $J_\perp$ with $J_\times=0.2$. The inset shows the L^{-1} scaling behavior of the crossing points.

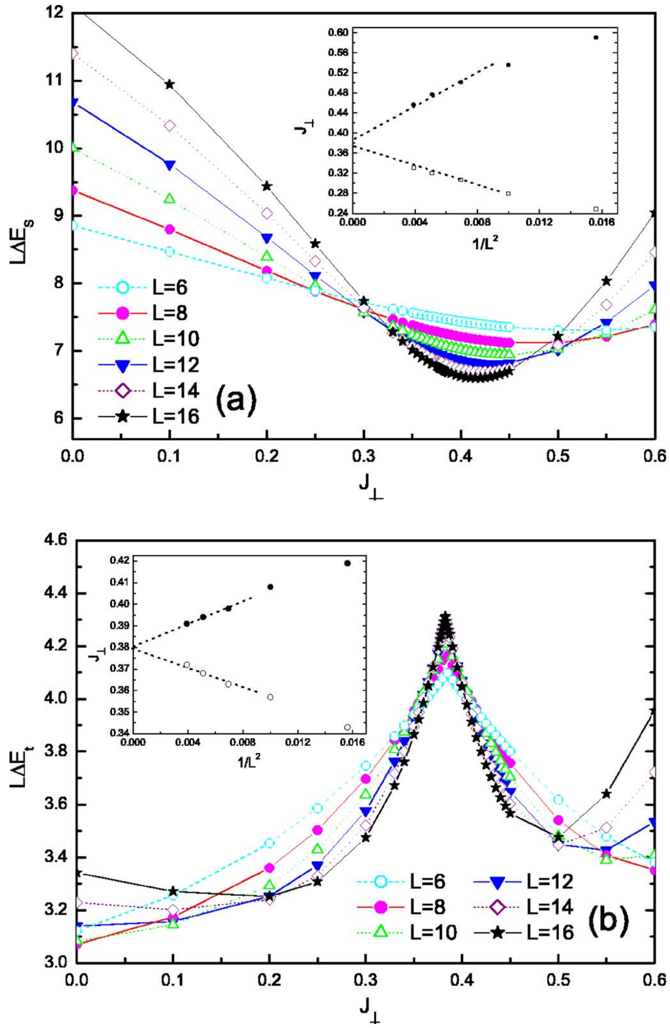

FIG. 4. (Color online) Scaled gaps (a) $L\Delta E_s$ for spin-singlet excitation and (b) $L\Delta E_t$ for spin-triplet excitation as functions of $J_\perp$ for various sizes L with $J_\times=0.2$. Insets show the L^{-2} scaling behavior of the left and the right crossing points represented by open and solid circles, respectively. Dotted lines are guides to the eye. They are straight lines fitted to the last few points.

to determine the thermodynamic limit of the value of the critical point. As shown in the inset of Fig. 3, the crossing points converge to the value of $(J_\perp)_c\simeq 0.378$, which agrees quite well with that found in the inset of Fig. 2.

Finally, we provide a further examination of the possibility of another critical point $(J_\perp)_{c,S}$ with vanishing gap in the spin-singlet sector. According to the phenomenological renormalization-group (PRG) method,[28] second-order phase transition points can be determined by the crossing points of the curves of the scaled gaps $L\Delta E_\nu$ at two successive sizes L and $L+2$, where ΔE_ν denote the excitation gaps in the spin-singlet and the spin-triplet sectors for $\nu=s$ and t, respectively. Here the gaps are calculated by using exact diagonalization method with periodic boundary conditions up to $L=16$. In the present case, the ground state is unique for any $J_\times$ and $J_\perp$, and it has total spin $S=0$ and momentum $k=0$. The spin-triplet (-singlet) excitation gap ΔE_t (ΔE_s) is determined by the energy difference between the ground state and the lowest level with total spin $S=1$ (with total spin $S=0$ and $k=\pi$). Our results for the scaled gaps $L\Delta E_\nu$ as functions of $J_\perp$ for various sizes L with $J_\times=0.2$ are exhibited in Fig. 4. For both cases of $L\Delta E_s$ and $L\Delta E_t$, there are two crossing points of the curves at subsequent sizes. However, it implies only one, but not two, critical point, because the extrapolation of the left and the right crossing points tend to a single value in the thermodynamical limit as shown in the insets of Fig. 4. The limiting values for the spin-singlet and the spin-triplet sectors are almost the same, and both give $(J_\perp)_c \simeq 0.38$. Our findings indicate that only one phase transition at $(J_\perp)_c \simeq 0.38$ occurs in the present system, and then the spin-singlet and the spin-triplet gaps vanish simultaneously. We note that simple linear extrapolations from data of systems of small sizes may be somewhat dangerous. Nevertheless, because our results based on PRG are consistent with that obtained by the above DMRG analysis and that given by earlier DMRG calculation,[19] they may lead to true physics in the thermodynamical limit.

In summary, we study numerically a two-leg spin ladder with diagonal frustrations for weak interchain couplings. All our results indicate that the transition from the RS to the Haldane phases is direct, without any phase in between. This conclusion is consistent with the picture obtained by all previous investigations,[13–20] except that proposed in Ref. 21 based on a reformulated weak-coupling field theory. It is not clear why a reformulated bosonization analysis works for one-dimensional EHM, but could fail for the present two-leg spin ladder. Further theoretical investigations are necessary to clarify this issue.

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