Critical Lines and Massive Phases in Quantum Spin Ladders with Dimerization

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We determine the existence of critical lines in dimerized quantum spin ladders in their phase diagram of coupling constants using the finite-size DMRG algorithm. We consider both staggered and columnar dimerization patterns, and antiferromagnetic and ferromagnetic inter-leg couplings. The existence of critical phases depends on the precise combination of these patterns. The nature of the massive phases separating the critical lines are characterized with generalized string order parameters that determine their valence bond solid (VBS) content.

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I. INTRODUCTION

The issue of the existence of massive or critical phases in quantum spin systems has motivated a great deal of study in strongly correlated systems since the seminal work on the Haldane conjecture [1]. This issue became a central problem when more complicated arrays of spins chains, known as quantum spin ladders, were discovered experimentally in cuprate materials that exhibit high-T_c superconductivity when they are appropriately doped [2], [3].

From a more fundamental viewpoint, the study of critical and massive phases in quantum spin ladders offer the possibility of a testing ground for studying complicated quantum many-body effects, that in some instances underly the physics of unconventional phases of matter [4]. A variety of spin ladders with different number of legs have been synthesized based on cuprate materials, like $SrCu_2O_3$, $Sr_2Cu_3O_5$ etc. [5], [6] or in other family of compounds $La_{4+4n}Cu_{8+2n}O_{14+8n}$ [7], and they present typically antiferromagnetic rung couplings among the legs of the spin ladders. It is also possible to find materials with less conventional ferromagnetic rung couplings as well like in certain chemical compounds like PNNNO and PIMNO [8]. In addition, the new tools to study strongly correlated systems based on optical lattices open the possibility of implementing a variety of quantum spin systems including ladders [9], [10].

The phase diagram of quantum spin ladders with staggered dimerization was conjectured on the basis of analytical non-perturbative methods [11] like the non-linear sigma model (NLSM) complemented with additional information from the weak and strong coupling limits in the rung coupling constants and dimerization parameters. Later, a series of different approximate analytical studies [12], [13] have been favorable for the existence of a critical line in the simplest case of a 2-leg spin ladder with staggered dimerization. Also, some preliminary numerical methods with the Lanczos algorithm [14], [15] have shown support for this fact for ladders with small size. Despite these several studies, a complete non-perturbative numerical analysis of these staggered low dimensional quantum spin systems have remained as an open problem.

In this paper we study a 3-leg quantum spin ladder with different types of rung couplings (either antiferromagnetic or ferromagnetic) and different dimerization patterns. These ladders are complex enough so as to serve as paradigmatic examples for testing the conjectured phase diagrams [11]. In order to achieve a conclusive answer to the conjectured phase diagrams for this system, we resort to a non-perturbative numerical tool like the DMRG method [16], [17], [18], [19], [20] in particular we employ its finite-size version based on the sweeping procedure to improve the convergence of the iterative steps. The characterization of the different phases separated by the critical lines is performed with a DMRG calculation of generalized string order parameters (SOP) [21] that were introduced to distinguish between massive phases in dimerized spin chains [22] even when the localized spins in the chain take on half-integer values. These SOPs are extensions of the originally non-local vacuum-expectation values introduced for integer spins and the like [23], [24].

The elucidation of the existence of a critical line in the phase diagram of quantum spin ladders with staggered dimerization is not straightforward when the ladders have end points as in the open boundary conditions geometry demanded by the standard DMRG method. Thus, we have to resort to numerical analysis of the low-lying spectrum of excitations in order to extract the correct gap in the bulk of the system when studying the universal properties of these ladders in the thermodynamic limit (length going to infinity) [25].

The string order parameter is a theoretical construct in condensed matter that allows the characterization of massive phases with a VBS structure. It has never been measured experimentally. However, with the engineering of optical lattices it would be possible to address a direct measurement of this important quantity [10].

This paper is organized as follows: in Sect.II we introduce the two patterns of dimerization in 3-leg ladders, one being columnar (1) with ferromagnetic rung couplings, while the other is alternating (2) with antiferromagnetic rung couplings. In the former, we establish a helpful connection with the $S = \frac{3}{2}$ antiferromagnetic alternating chain in a certain strong coupling limit. We

recall several conjetures about the phase diagram of both 3-leg Heisenberg models [11] that motivate their study with DMRG in order to clarify them. In Sect.III we perform the DMRG calculations of the low-energy gaps in both models of 3-leg ladders as a function of the various coupling constants. With this information we can establish the phase diagram and thus we establish the validity of the conjectured diagram [11]. In addition, we can give a precise location of the critical lines and we find qualitative differences between these critical lines in each model. In Sect.IV we introduce generalized string order parameter to characterize the nature of the massive phases separated by the critical lines found in the previous section. These string orders are measured with DMRG techniques and we show that they are a valuable tool for detecting VBS states in dimerized quantum spin ladders with different patterns of dimerization. Sect.V is devoted to conclusions. In appendix we study with DMRG the $S = \frac{3}{2}$ alternating spin ladder and its generalized string order parameters. This case appears as a limiting case in the study of the ferromagnetic 3-leg ladder with columnar dimerization and it is used as a guiding example to find the phase diagram.

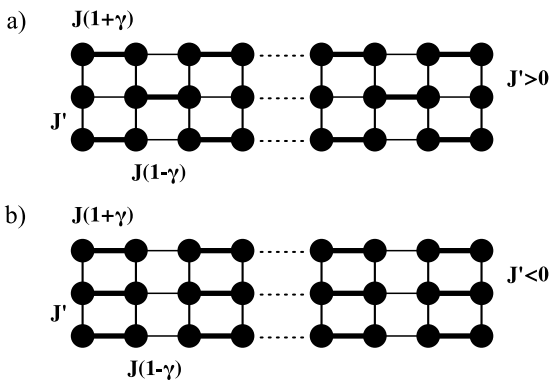

FIG. 1: Pictorial representation of the Hamiltonians corresponding *a)* to the completely antiferromagnetic ($J' > 0$) model (2) with alternated staggering and *b)* the ferromagnetic ($J' < 0$) model (1) with columnar staggering.

II. QUANTUM HAMILTONIANS FOR 3-LEG SPIN LADDERS WITH DIMERIZATION

One of the main interests established in [11] was the existence of an interplay between 3-leg ladders with a columnar dimerization pattern and ferromagnetic interleg, or rung, couplings on one side, and 3-leg ladders with alternating dimerization and antiferromagnetic rung couplings, on the other. The point was that both arrangements of 3-leg ladders should exhibit critical lines, while neither their precise location was known nor the nature of the massive phases they separated was determined. This is the open problem that we address here by means of the DMRG method. To this end, we start introducing both arrays of ladders since they are the candidates to exhibit critical lines.

Thus, we are mainly interested in studying a possible connection between two different arrangements of spins $\frac{1}{2}$ forming a 3-leg ladder which interact via Heisenberg terms. Both of them combine bonds of different strength parameterized by a constant γ and two different types of coupling constants, J for the Heisenberg interaction between spins along the legs, and J' for similar interactions between the rungs of the legs. Since the physics of the problem depends only on the ratio J'/J, the constant J will from now on be given a fixed antiferromagnetic value $J = 1$. The other constant J' will have positive sign in one of the models and negative in the other one. In addition to this difference, both models will also differ in the staggering pattern as we shall discuss below.

We next describe the model corresponding to the region with $J' < 0$, with the bond alternation pattern such that every one of the three legs begins with a strong bond followed by a weaker one, that is, the bond alternation follows a *columnar pattern*. The explicit Hamiltonian of this arrangement is

$$\begin{aligned} H_{\rm F} =& J \sum_{\ell=1,2,3} \sum_{i=1}^{L-1} (1-(-1)^i\gamma) \mathbf{S}_i(\ell) \cdot \mathbf{S}_{i+1}(\ell) \\ &+ J' \sum_{i=1}^{L} \mathbf{S}_i(1) \cdot \mathbf{S}_i(2) + J' \sum_{i=1}^{L} \mathbf{S}_i(2) \cdot \mathbf{S}_i(3), \end{aligned} \tag{1}$$

where L denotes the longitudinal length of the 3-leg ladder, $\mathbf{S}_i(\ell)$ is a spin-$\frac{1}{2}$ operator located at the site i of the ℓ-th leg with $0 < i \leq L$, γ is the dimerization parameter that sets the relative strength of the bonds that interact with Heisenberg coupling constant J along the leg of the ladder and J' on the rungs of the legs.

Since the coupling among legs is ferromagnetic, we know that for values $|J'| \gg 1$ this model converges to an effective $S = 3/2$ staggered spin chain. Studies with the NLσM method predicts [26] for this chain the existence of three critical points in the interval $\gamma \in [-1, 1]$ placed at $\gamma_c = \pm 2/3$ and $\gamma_c = 0$. Numerical studies showed that in fact these points correspond to $\gamma = \pm 0.42$ and $\gamma = 0$ [27], [28]. Since the $S = 3/2$ dimerized spin chain gives us valuable information about the expected massive phases of the ladder in the strong ferromagnetic regime, and since there exist some subtleties regarding the string order parameters that may lead to confusion, we have included a numerical study of this chain in appendix A.

For the completely antiferromagnetic regime $J' > 0$, we will use another staggering pattern that differs with respect to the previous one. In this case only the first and third leg begin with a strong bond, while the second one begins with a weak one, that is, the bond alternation is not columnar anymore but still follows a regular pattern that is called *alternating*. The Hamiltonian of this model

is

$$H_{\rm AF} = J \sum_{\ell=1,2,3} \sum_{i=1}^{L-1} (1+(-1)^{i+\ell}\gamma) \mathbf{S}_i(\ell)\cdot\mathbf{S}_{i+1}(\ell) + J' \sum_{i=1}^{L} \mathbf{S}_i(1)\cdot\mathbf{S}_i(2) + J' \sum_{i=1}^{L} \mathbf{S}_i(2)\cdot\mathbf{S}_i(3), \quad (2)$$

with the same conventions as before. A pictorial representation of this Hamiltonian together with the Hamiltonian of the ferromagnetic model is shown in fig. 1.

With this arrangement, it is also possible to effectively and approximately map the model onto a NLσM and again this formalism predicts a critical behaviour in the phase diagram of the couplings J'/J vs. γ [11]. However, this behaviour is only reliable in the strong coupling limit $J'/J \gg 1$.s More specifically, it predicts a critical curve running from the point $(\gamma = 2/3, J' = 0)$ to $(\gamma = 1, J' = 4/5)$ and another one which is the mirror reflection of the latter with respect to the J' axis. These predictions however shall be considered only as qualitative approximations of the real behaviour of the system. In this particular case, it is evident that the critical line must cut the γ axis exactly at $\gamma = 0$ since that point corresponds to two decoupled $S = 1/2$ staggered Heisenberg chains. However, this behaviour is missed by the NLσM technique. On the other hand, this model has not apparent limits which can give us a hint on the phases that give raise. In section III however, our DMRG computations will give strong evidence of their nature.

Despite the differences in both models, i.e. different sign of J' and different staggering pattern, there are various features that connect them. First of all and more important is that at least in the line $\gamma = 0$ both models are constinuosly related as we vary $J' < 0$ to $J' > 0$. On the other hand, according to NLσM, the first model is critical only in the region $J' > 0$ while the second one has only critical lines in the complementary part $J' < 0$. This dual-like behaviour combined with the expectation that the ground state of both models is a valence bond solid, rouse the belief about the possibility of establishing a connection among their phase diagrams [11]. We shall see to what extend these expectations are fulfilled with the help of the DMRG technique and the generalized string order parameters.

III. GROUND STATE DEGENERACY AND EXISTENCE OF CRITICAL LINES

Massive quantum phases are characterized by an energy gap from the ground state (degenerate or not) to the first excited state. On the contrary critical phases are characterized by a gapless spectrum between these energy levels. We have used the finite-size DMRG algorithm to compute the low energy levels and thus the corresponding gaps in order to identify the gap in the bulk of the system when we send the length of the 3-leg ladders to infinity (thermodynamic limit).

It is known that in the case of integer spin chains, some configurations of VBS states can break a hidden $Z_2 \times Z_2$ symmetry [21] that makes the ground state degenerate. This degeneration is a reflection of the spin-end effects in a antiferromagnetic Heisenberg chain of $S = 1$ spins [29]. In systems other than the parent Hamiltonians of the VBS states, but close enough to this picture and when using open boundary conditions, typically this degeneracy is approximate and the energy of the near-degenerate states decays with the size exponentially to a unique infinite volume ground state.

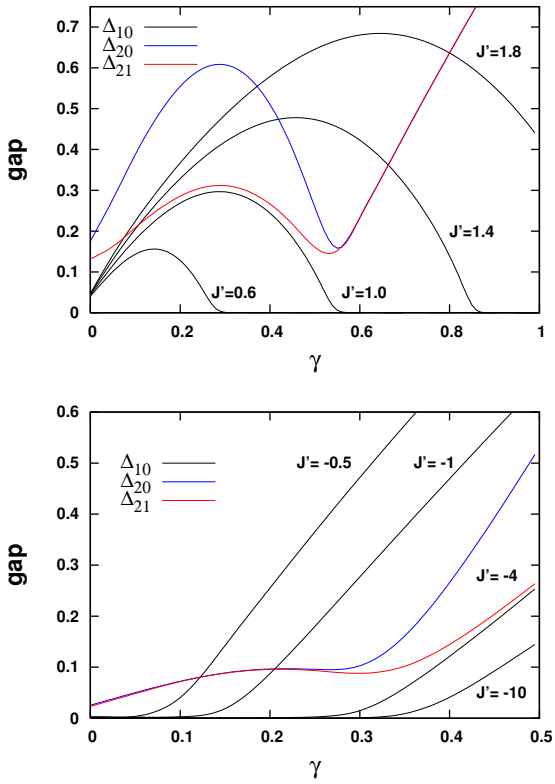

FIG. 2: (Color online)Energy gaps between the ground state and two first excited states in model (2) (*Up*) and model (1) (*Down*). For the sake of clarity Δ_{20} and Δ_{21} are shown only for one value of J'. Namely $J' = 1.0$ (*Up*) and $J' = -0.4$ (*Down*). It can be seen how the gap Δ_{21} indeed represents properly the gap of the spectrum irrespective of the degeneration of the ground state.

Fig. 2 shows the energy differences between the ground state and two first excited states in both models (1) and (2). We observe in this figure that Δ_{10} accounts for the degeneracy mentioned in the previous paragraph: in the completely antiferromagnetic model (2) the first excited state is clearly above the ground state in the phase corresponding to low values of γ, while it is degenerate in the rest of the γ interval. On the contrary, the ground state of the ferromagnetic model (1) is degenerate for low values of γ while it has a finite gap in the rest. As for Δ_{20}, it corresponds in fact to the gap of the spectrum in the

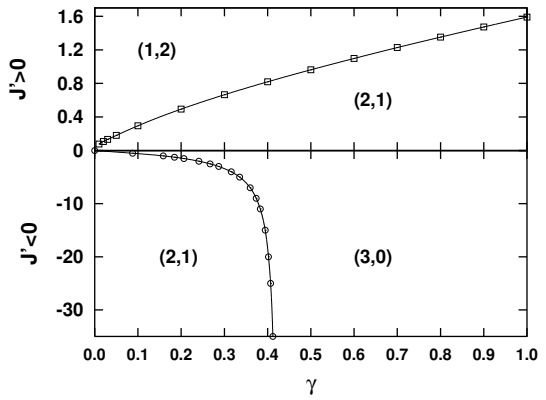

FIG. 3: Critical curves of model (1) with $J' > 0$ and alternated staggering, and model (2) with $J' < 0$ and columnar staggering. Each point in the critical lines has been obtained keeping one parameter fixed and finding the value of the other parameter that minimizes the gap Δ_{21}. Computations have been performed on ladders of size $L = 3 \times 150$ retaining $m = 400 (J' > 0$ region) and $m = 450 (J' < 0$ region) states of the density matrix.

degenerate regions while it clearly differs from the gap Δ_{10} in the non degenerate regions. Finally, the energy difference Δ_{21} coincides in both regions and both models with the gap of the massive phases. This holds true up to slight deviations due to finite size effects and irrespective of the degeneracy of the ground state, Thus, we may conclude that this gap Δ_{21} is in fact the same one that survives when using periodic boundary conditions.

As mentioned in the previous section, the existence of critical lines (characterized by a gapless spectrum) in both models (1) and (2) is supported by arguments coming from the strong coupling limit in the case of model (1), and NLσM valid in both of them. These arguments are however not conclusive. In this section we will prove numerically that these lines exist and we give an accurate estimation of its shape and location. To this end, we will find the critical values $\gamma_c(J')$ that make the gap $\Delta_{21}(\gamma_c(J'))$ vanish. It is very important at this point to emphasize that an exactly vanishing value of the gap shall only be attained in the thermodynamic limit. For finite size systems, the magnitude of the gap remains finite and gets closer and closer to zero as we increase the size. In our case however, critical points are separating massive gapped phases and therefore, for large enough sizes but still computationally feasible, the gap at these points attain a local minimum value and can be accurately computed.

Fig.3 shows the critical region computed for both models (2) and (1). In order to compute this curves, we have used the finite DMRG algorithm in ladders of $L = 3 \times 150$ sites. For the completely antiferromagnetic model (2) we retained $m = 400$ states of the density matrix and a Lanczos tolerance equal to 10^{-9}. The ferromagnetic model (1) turned out to be numerically more demmanding and we set $m = 450$ and the tolerance equal to 10^{-10}. Two sweeps of DMRG were enough in both models to make the energies converge. These results clearly confirm the conjectured phase diagrams for these 3-leg models [11].

The solid lines in fig. 3 are only a guide for the eye. We have however used our numerical data to stimate the best fit to that critical lines. For the region $J' > 0$ we have used a simple potential function of the form

$$J'_c = a\gamma_c^r \tag{3}$$

The best value of each parameter has been obtained performing a least square fit and are equal to $a = 1.59 \pm 0.01$ and $r = 0.72 \pm 0.01$. As for the critical line in the semiplane $J' < 0$, we have used for the region close to the vertical asymptota a relation of the form

$$J'_c = \frac{C}{(\gamma_c - a)^s} \tag{4}$$

And the values that best fit the data have been found to be $C = 0.38 \pm 0.02$, $s = 1.07 \pm 0.02$ and $a = 0.427 \pm 0.001$. Notice that the value of this last parameter is in good agreement with previous computations of the critical point of the $S = 3/2$ alternating dimerized chain.

IV. MASSIVE PHASES AND GENERALIZED STRING ORDER PARAMETERS

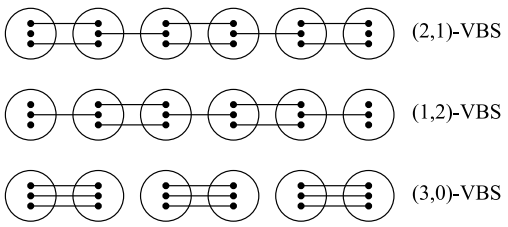

FIG. 4: Valence bond solid diagrams of the phases that give raise the models discussed in this paper. Each small solid circle and line represents both spin-1/2 variable and a singlet pair repectively. The large open circles represent the symmetrization of the spin 1/2-variables on each leg to create a spin-3/2 variable.

In this section we will characterize the quantum phases that appear in the phase diagram in Fig.3. To achieve this goal, we will resort to the generalized string order parameter [21], [24], which are able to detect the VBS state character of dimerized spin systems even when the local spins take on half-integer values. These parameters are generalizations for arbitrary complex phase of the original string order [23], [24] parameter first proposed for the case of integer spin $S = 1$. Resorting to the VBS picture, massive phases corresponding to valence bond solids can be denoted according to the number of valence bonds formed with the contiguous sites, i.e, one

particular valence bond solid can be denoted as (m,n)-VBS with $m+n=2S$.

For instance, we have already mentioned in the previous section that in the strong coupling limit, the columnar dimerized 3-leg ladder (1) effectively becomes a $S=\frac{3}{2}$ alternating spin chain. Thus, in this case we have $m+n=3$.

The definition of the generalized string order parameter extended to our particular three leg ladder with arbitrary size $L=3\times\ell$ is

$$O_{\rm str}(\theta)=\Big|\lim_{j-i\to\infty}\langle S^z_{2i}\exp(i\theta\sum_{k=2i}^{2j-1}S^z_k)S^z_{2j}\rangle\Big| \qquad (5)$$

with $0<i<j<\ell/2$ and $S^z_i=S^z_i(1)+S^z_i(2)+S^z_i(3)$. It is actually not necessary to consider $j-i\gg 1$ to obtain accurate values of the parameter and typically a value of $i-j$ of some few tens is enough to give values very close to the infinite limit value, considered that i and j are well within the bulk and far away from the edges. Thereby, for convenience we will work with the parameter defined as

$$O_{\rm str}(2i,2j,\ell,\theta)=\Big|\langle S^z_{2i}\exp(i\theta\sum_{k=2i}^{2j-1}S^z_k)S^z_{2j}\rangle\Big| \qquad (6)$$

with i,j and S^z_i defined as before.

It has been shown [21] that the generalized string order parameter evaluated in $\theta=\pi$ acts as an order parameter since it vanishes or not depending on the number of bonds n being odd or even. Moreover, the shape of the string order parameter in the region $\theta\in[0,2\pi]$ provides us with valuable information about the VBS character of the phases since the number of zeros in this range coincides with the number of bonds m [21].

Fig. 5 shows the parameter $O_{\rm str}$ computed in the completely antiferromagnetic model (2) in the whole range of γ for various values of J'. The operator clearly distinguishes regions where it is finite from others where it vanishes. Moreover for a fixed value of J', the value of γ where it decays to zero coincides [30] with the critical value γ_c corresponding to that value of J' in the critical line of Fig. 3. On the other hand, Fig. 6 shows $O_{\rm str}$ computed in the ferromagnetic model (1) in the strong coupling regime. For strong values of the ferromagnetic coupling J' we should expect that our ladder behave like an effective $S=3/2$ alternating spin chain. Indeed, we can observe that the string order parameter is clearly non-vanishing above $\gamma=0.42$, the critical point of the chain. As for the region below this point, the tendency of the string order parameter is to decay to zero as we increase the size of the system, except for the point $\gamma=0$ and its vicinity. In fact, this behaviour is anomalous since $\gamma=0$ is critical in the chain and therefore the string order parameter should vanish. In the appendix we have addressed this issue with the pure $S=3/2$ alternating dimerized chain. Our study in the chain explains the behaviour of the ladder and shows that indeed the string order parameter decays to zero also at this point. The decay rate is however slower and it is not enough to increase the size of the ladder. Fig. 8 (down) shows that we have additionaly to consider sites i and j further and further apart to make the string order parameter decay at $\gamma=0$.

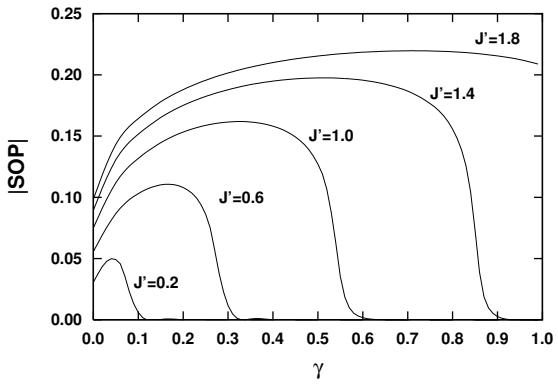

FIG. 5: Generalized string order parameter $O_{\rm str}(i=20,j=42,\ell=80,\theta=\pi)$ computed in the completely antiferromagnetic model (2) with alternated staggering for several fixed values of J'. Regions where the string order parameter vanishes correspond to a different quantum phase from that where it is non null. Notice that there exists a certain J' above which the system only exhibit one quantum phase irrespective of the value of γ. This value corresponds to the J' coordinate with $\gamma_c=1$ of the critical line of figure 3.

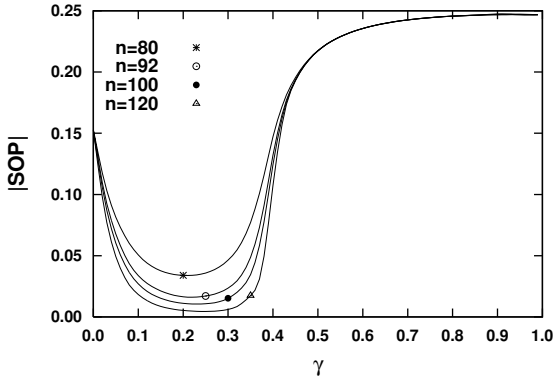

FIG. 6: Generalized string order parameter $O_{\rm str}(i=\ell/2-24,j=\ell/2+26,\ell=n,\theta=\pi)$ computed in the strong ferromagnetic regime $J'=-25$ of the ferromagnetic model (1) with columnar staggering. See the text for explanations.

With the considerations explained in the previous paragraph, we have proved that the string order parameter (6) evaluated in $\theta=\pi$ is valid to identify quantum phase transitions in both models (1) and (2). Now we want to extend the study to the whole θ domain to test the nature of the massive phases. In fact, from definition (6) $O_{\rm str}(i,j,\ell,\theta)=O_{\rm str}(i,j,\ell,\theta+\pi)$ and hence we can restrict the study to the range $\theta\in[0,\pi]$. We will study first the ferromagnetic model (1) with columnar stag-

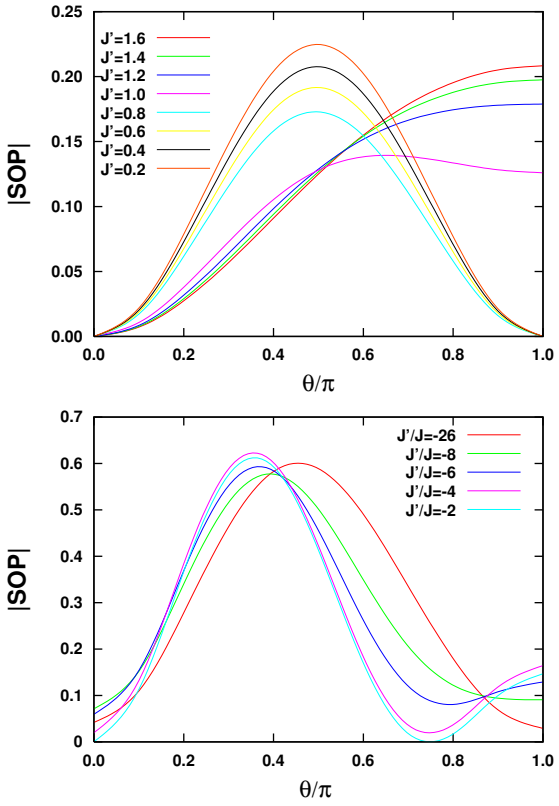

FIG. 7: (Color online)Generalized string order parameter $O_{\rm str}(i=20, j=42, \ell=80, \theta)$ computed in the completely antiferromagnetic model at $\gamma = 0.5$ (*Up*) and the ferromagnetic model at $\gamma = 0.35$ (*Down*). According to fig. 3 this values cut the critical lines at $(\gamma_c = 0.5, J_c' = 0.96)$ and $(\gamma_c = 0.35, J_c' = -6.1)$ respectively. It can be observed that both graphs show a change in the number of zeros near these points.

gering. As we commented in the previous sections, we can guess the phases of the diagram going to the strong coupling limit $|J'| \gg 1$. In this regime the ferromagnetic coupling among rungs is the leading interaction and the ladder transforms into an effective $S = 3/2$ alternating spin chain. Resorting to continuity arguments, the phases of the ladder must be the same that appears in the strong coupling limit, i.e, a $(2,1)$-VBS in the region $0 < \gamma < \gamma_c$ and a $(3,0)$-VBS when $\gamma_c < \gamma \leq 1$. In fig.7 (down) we show $O_{\rm str}$ computed in the θ domain. All the curves appearing in the figure correspond to a fixed $\gamma = 0.35$. According to Fig. 3 this value of γ cuts the critical line in a certain value of J' and so we should notice a qualitative change in the curves in Fig. 7. This change can be observed since plots corresponding to very negative J' have a local minimum at $\theta = \pi$, while it changes to become a maximum as we move towards J' close to zero. Hence, the number of zeroes in the domain $\theta \in [0, 2\pi)$ moves from one to two. In fact, the string order parameter is not strictly equal zero in our graphs, but this fact has been already pointed out in spin chains [28] and conclusively proved that it was due to finite size effects. The values closer to zero are attained considering larger sizes. According then to the VBS notation and our DMRG results, we can label the phases of model (1) as $(2,1)$-VBS in the region $0 < \gamma < \gamma_c$ and $(3,0)$-VBS for $\gamma_c < \gamma \leq 1$ as expected from the knowledge of the $S = 3/2$ chain.

The completely antiferromagnetic model is more difficult to guess a priori the quantum phases that gives raise to or even if its ground states are valence bond solids. We have used again the generalized string order parameters to check the nature of the phases. Fig.7 (up) shows the string order parameter as a function of θ and a fixed value $\gamma = 0.5$ which cuts the critical line. It can be seen that indeed the SOP behaves as expected for a valence bond solid VBS state and two phases can be identified attending to the number of zeros in this domain. For higher values of J' the SOP has a maximum at $\theta = \pi$ and only one zero in the region $0 \leq \theta < 2\pi$. As we consider lower values of J', more precisely in the interval from $J' = 1.0$ to $J' = 0.8$, the SOP at $\theta = \pi$ falls abruptly to zero and therefore the SOP has two vanishing values in the aforementioned interval. From these results we can conclude firstly, that both massive phases can be properly described as valence bond solids and also they can be identified as a $(1,2)$-VBS for $0 \leq \gamma < \gamma_c$ and a $(2,1)$-VBS for $\gamma_c < \gamma \leq 1$.

V. CONCLUSIONS

We have given a precise meaning to the conjectured phase diagrams [11] corresponding to 3-leg Heisenberg ladders with columnar dimerization and ferromagnetic rung couplins on one side, and similarly for alternating dimerization with antiferromagnetic couplings among the rungs. Although both models exhibit critical lines, their qualitative form is different: in the former, the critical line approaches an asymptota at the critical value $\gamma_c = 0.42$ were it effectively becomes an alternating $S = \frac{3}{2}$ spin ladder. On the contrary, the latter model does not exhibit any asymptota but the critical line meets the wall $\gamma = 1$ of the phase diagram.

Moreover, we have also clarified the valence-bond-solid nature of the massive phases separated by the critical lines in the phase diagram. In this regard, we have found that the generalized string order parameters are a very good tool for characterizing VBS state phases in ladders with a variety of dimerization patterns. Our results are based on extensive calculations using the finite-size DMRG technique.

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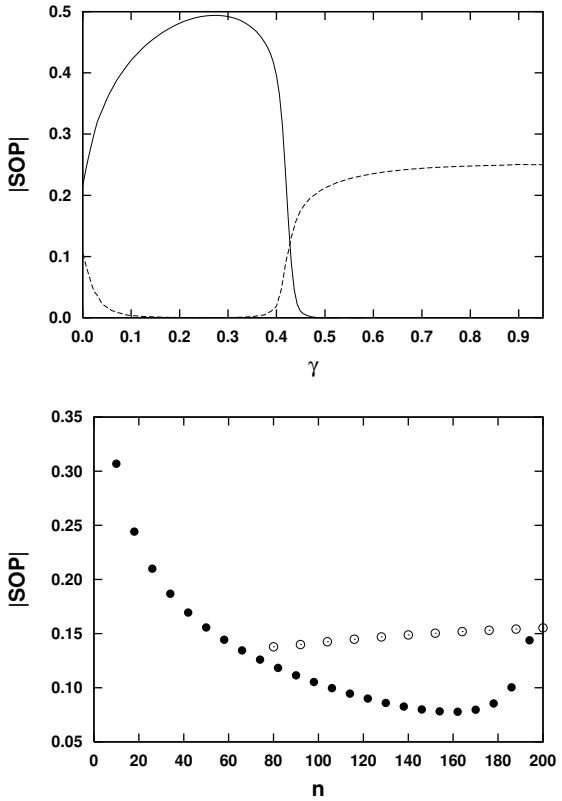

FIG. 8: *Up*: string order parameters $O^{\rm odd}_{\rm str}(i=51, j=131, L=180, \theta=\pi)$ (solid line) and $O^{\rm even}_{\rm str}(i=52, j=130, L=180, \theta=\pi)$(dashed line) computed in a $S=3/2$ alternating dimerized chain. *Down*: string order parameter $O^{\rm even}_{\rm str}$ at $\gamma=0$ varying the total length of the chain $O^{\rm even}_{\rm str}(i=n/2-24, j=n/2+26, L=n, \theta=\pi)$ (empty circles) and varying the distance $i-j$, $O^{\rm even}_{\rm str}(i=(L-n+1)/2+1, j=i+n-1, L=200, \theta=\pi)$ (solid circles).

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APPENDIX A: THE $S=3/2$ STAGGERED SPIN CHAIN

It was already pointed out by Oshikawa [21] that half-integer systems are amenable to have many order parameters. We want to compare in this section two order parameters which despite differing slightly in their definition have in fact quite different behaviour and may even lead to confusion. We will see that both parameters capture the quantum phase transition of the chain, but only one can go further and give evidences of the quantum phases themselves.

The string order parameters are defined as

$$O^{\rm even}_{\rm str}(\theta, L) = \Big| \lim_{j-i\to\infty} \langle S^z_{2i} \exp(i\theta \sum_{\ell=2i}^{2j-1} S^z_\ell) S^z_{2j} \rangle \Big| \qquad \text{(A1)}$$

with $0 < i < j \leq L/2$, and

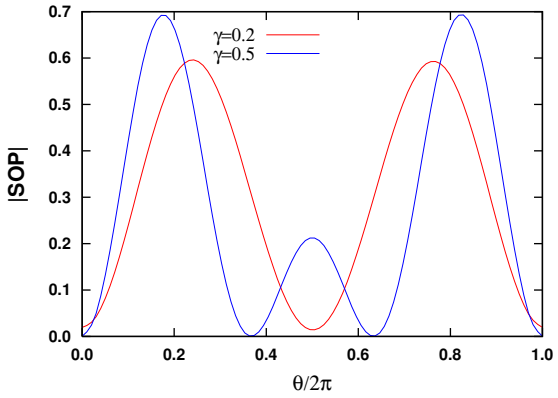

FIG. 9: (Color online) string order parameter $O^{\rm even}_{\rm str}(i=22, j=80, L=100, \theta)$ computed below and above the critical point $\gamma_c = 0.42$ of a $S=3/2$ alternating dimerized chain. The number of zeros of this parameter determines the nature of the valence bond solid at each phase.

$$O^{\rm odd}_{\rm str}(\theta, L) = \Big| \lim_{j-i\to\infty} \langle S^z_{2i+1} \exp(i\theta \sum_{\ell=2i+1}^{2j} S^z_\ell) S^z_{2j+1} \rangle \Big| \qquad \text{(A2)}$$

with $0 \leq i < j < L/2$.

Notice that, including the edges, both definitions involve an odd number of spins between sites $2i$ and $2j$ or $2i+1$ and $2j+1$ and an even number of antisymmetric operators under spin flip. This condition is required to obtain a value of the mean value different from zero.

It has been commented in the previous sections that the $S=3/2$ alternating dimerized chain has three critical points at $\gamma_c = 0$ and $\gamma_c = \pm 0.42$ in the interval $\gamma \in [-1, 1]$. The phase diagram is symmetric respect $\gamma = 0$ and therefore we can constrain our study to the region $0 \leq \gamma$.

As regards the interval $0 < \gamma < \gamma_c$ the ground state is known to be a $(2,1)$-VBS while for $\gamma_c < \gamma \leq 1$ it is a $(3,0)$-VBS. The first issue we have to check is wether or not the parameters defined above can make explicit this quantum phase transition. In fig. 8 (up) we have plotted both parameters $O^{\rm odd}_{\rm str}(\pi, L)$ and $O^{\rm even}_{\rm str}(\pi, L)$ in the range $0 \leq \gamma \leq 1$. This graph shows that both operators are finite at one side of the critical point while thay vanish at the other. We can conclude then that they act as proper order parameters in the phase transition. However a clear major difference can be noticed from this figure since each one of these order parameters in fact vasnishes on differents sides of the critical point.

On the other hand, the behaviour of the string order parameters at the critical point $\gamma = 0$ requires further insight. We know that critical points correspond to critical ground states where the hidden order measured by string order parameters must vanish. In fig. 8 (up) it is not however clear that the value of the string order parameters decays to zero at this critical point. We have

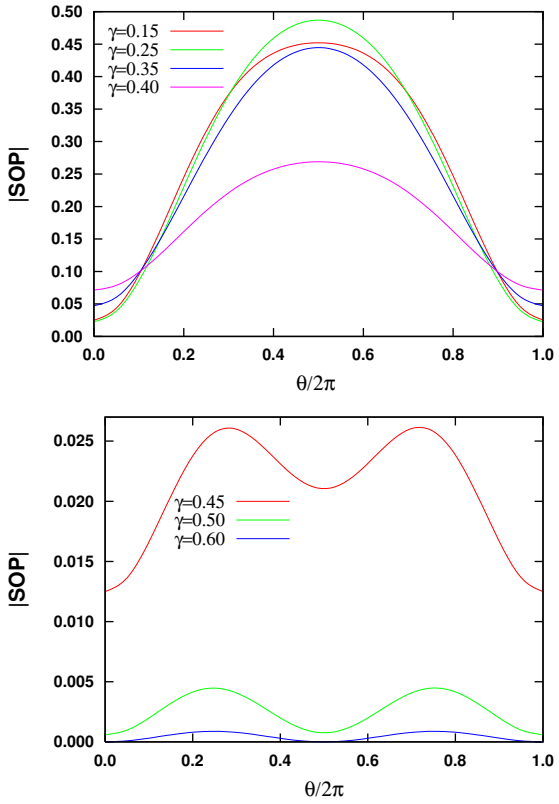

FIG. 10: (Color online) string order parameter $O_{\rm str}^{\rm odd}(i = 21, j = 79, L = 100, \theta)$ computed below (*Up*) and above (*Down*) the critical point $\gamma_c = 0.42$ of a $S = 3/2$ alternating dimerized chain. In this case the string order parameter in the θ does not clearly determine the valence bond phases of the chain. Notice also the appreciable change of scale from one phase to the other.

addressed deeper this issue in fig. 8 (down). This graph shows a finite size scaling analysis of the string order parameter $O_{\rm str}^{\rm even}$ at the critical point $\gamma = 0$. It can be observed that the scaling and decay of the parameter is more influenced by the distance $i-j$ than the total length of the chain. The rise of the string order parameter for large distances $i - j$ close to the total lenght L is expected due to finite size effects. For values far enough of the edges the tendency of the string order parameter is however to vanish as expected increasing the distance $i - j$.

A regards the shape of these parameters for arbitrary θ, fig. 9 shows $O_{\rm str}^{\rm odd}(\theta, L)$ for two different values of γ below and above the critical point.From the knowledge that we have of the phases of the chain we can see that this order parameter behaves as pointed out in [21] and the number of zeros identifies the valence bond phase ocurring. In effect, for values $\gamma < \gamma_c$ the number of vanishing values in $0 \leq \theta < 2\pi$ is two and coincides with a $(2, 1)$-VBS while for $\gamma > \gamma_c$ there are three null values corresponding to the $(3, 0)$-VBS phase.

On the other hand $O_{\rm str}^{\rm even}(\theta, L)$ is plotted for various values of γ in fig. 10. Two features can be remarked of this parameter: it also shows a qualitative change in its shape as we move from one phase to the other. In this case however the relation of the number of zeros with the nature of the phase is not clear. Besides, the characteristic scale of the parameter differs significantly in both phases.

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[30] With less precision since computations in fig. 5 were performed in shorter ladders.