Frustrated mixed-spin ladders:  
An intermediate phase between rung-singlet and Haldane phases

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In frustrated spin ladders composed of antiferromagnetically coupled chains, homogeneous or inhomogeneous, the interplay of frustration and correlations causes the emergence of two phases, Haldane (H) phase and rung singlet (RS) phase, in which the transition between these two phases had been under debate. In this paper we investigate the ground state phase diagram of frustrated mixed-spin-(1, 1/2) ladders, using the notions from quantum information theory such as entanglement entropy, Schmidt gap and entanglement levels degeneracies, and also defining various local and nonlocal order parameters. Employing two numerical techniques, the infinite time-evolving block decimation (iTEBD) and density matrix renormalization group (DMRG) algorithms, we obtain the ground state phase diagram of the ladder, and demonstrate that there is an intermediate phase between RS and H phases, where the ground state is disordered and the entanglement spectrum follow no particular pattern.

I. INTRODUCTION

Low dimensional frustrated spin systems are one of the most active research fields in physics which have attracted a lot of attentions in the fields of topological quantum matters and cold atoms systems, aside from their pioneering importance on the understanding of quantum magnetism and emergent phenomena. Frustration causes different exotic orders such as topological orders, spin liquids, spin supersolids, helical and chiral orders and so on, to appear in the ground state phase diagram of the spin systems.1–6 Frustrated spin ladders are one of the low-dimensional systems that have received special attentions for several reasons; i) due to their low dimensionality, the interplay of frustration and quantum correlations causes many topological and nontopological phases such as the H phase, dimer orders, RS phase, spin liquids and Luttinger liquid to appear in their ground state phase diagram,7–22 ii) they are quasi-one dimension, and it is expected that they show characteristics of both one- and two-dimensional systems23, iii) and finally because of their low dimensionality there are various known numerical and analytical methods which can be employed to examine their ground state as well as their excitations behaviors.24,25 Mixed spin ladders are a group of materials that, despite their great importance, have received less attentions. The heterogeneity in these systems causes the emergence of behaviors that are not seen in homogeneous systems.26–31 The coexistence of different kinds of spins do not necessarily yield to magnetic ground states. Depending on the size of spins there could be three different possibilities. For a mixed-spin system with a unit cell consists of (τ, σ) spins, if τ > 2σ then the system mainly has a ferromagnetic character, if τ < 2σ, the system has a predominantly antiferromagnetic character, and in the case which τ = 2σ, the system shows a mixture of both ferromagnetic and antiferromagnetic characters. Therefore, mixed-spin-(1, 1/2) systems are expected to have interesting features.

In this paper we study the ground state phase diagram of a mixed-spin-(1, 1/2) ladder (illustrated in Fig. 1) in the presence of rung, leg and diagonal interactions. In a wide range of diagonal interactions, the system experiences two genetically disordered phases; a H phase and a RS phase, but there is no definite result in the type of phase transition between this two phases. Based on very few studies on this system, the H and the RS phases are interconnected by a first order phase transition. But whether or not there is an intermediate phase between these two phases is controversial. It has been shown that frustrated mixed-spin-(1,1/2) ladders can be mapped onto a frustrated spin-1/2 ladder32 where many efforts have been done in understanding the real nature of the phase transition between the rung-singlet and the H phase. It is not clear whether it is a first order phase transition19,33,34 or there is an intermediate phase between the RS and the H phases.21,22,35 In order to reach a definite conclusion we must carry on more sophisticated investigations.

In this paper, we examine the ground state phase diagram of the frustrated mixed-spin-(1,1/2) ladders, using basic notions from quantum information theory such as entanglement. Recent developments in constructing new algorithms to efficiently simulate quantum many-body wave functions has revealed the remarkable role of entanglement and provides astonishing tools to understand many body systems and quantum phase transitions.36–43 The most well-known measure of entanglement, is the Von Neumann entanglement entropy (EE) which is widely used to detect quantum phase transitions44 as well as topological properties of states.45,46 Moreover, the entanglement spectrum (ES),
Actually, the study of the low-lying part of the ES allows us to detect topological properties of a state or gives direct access to the excitation spectrum of edges. Using two numerical techniques, iTebD and DMRG, we obtain the EE and ES levels degeneracies, and demonstrate that the H and the RS phases are separated by an intermediate disordered phase characterized by a different ES levels degeneracies.

While examining the presence or absence of an intermediate phase in this system, we also compare both the results of iTebD and DMRG. We demonstrate that in the vicinity of the RS-H transition point, i.e., in the intermediate phase, in contrary to DMRG, the iTebD is very sensitive to initial conditions, and the ground state order predicted by iTebD can not be trusted.

This paper is organized as follows: In sec. II, we will introduce the Hamiltonian of the mixed-spin ladder and discuss its ground state properties by a perturbation theory. In Sec. III, the numerical iTebD technique and its generalization to the mixed-spin-$(1, 1/2)$ ladders will be explained. In Sec. IV, we will present a comprehensive study of the ground state phase diagram of the ladder in the absence of diagonal interactions, by introducing different local order parameters and investigating the behavior of the EE, ES levels degeneracies, and Schmidt gap. In Sec V, the effects of diagonal interactions will be discussed. Finally the summary and conclusion are presented in Sec. VI.

II. MODEL HAMILTONIAN AND SYMMETRIES

Let us consider a frustrated two-leg spin ladder composed of two different kinds of spin, $\sigma$ and $\tau$, describing by the following Hamiltonian:

$$ H = H_{\text{legs}} + H_{\text{rung}} + H_{\text{diag}}, $$

with

$$ H_{\text{legs}} = J_l \sum_{n=1,2} \sum_i (\sigma_i^{(n)} \cdot \tau_i^{(n)} + \tau_i^{(n)} \cdot \sigma_{i+1}^{(n)}), $$

$$ H_{\text{rung}} = J_r \sum_i (\sigma_i^{(1)} \cdot \sigma_i^{(2)} + \tau_i^{(1)} \cdot \tau_i^{(2)}), $$

$$ H_{\text{diag}} = J_d \sum_i (\sigma_i^{(1)} \cdot \tau_i^{(2)} + \sigma_i^{(2)} \cdot \tau_i^{(1)} + \tau_i^{(1)} \cdot \sigma_{i+1}^{(2)} + \tau_i^{(2)} \cdot \sigma_{i+1}^{(1)}), $$

where $n$ is the label of legs, and the summations run over unit cells (see Fig. 1). Here $J_l > 0$ is the intra-leg exchange interaction between spins $\sigma$ and $\tau$, and $J_r$ and $J_d > 0$ refer to the inter-legs interactions, the former is the rung coupling and the latter is the diagonal interaction between spins $\sigma$ and $\tau$. The Hamiltonian in Eq. (1) possesses the SU(2), time-reversal $T$ and leg-swap $s$ symmetries. Under time reversal and leg-swap symmetries the spin operators transform as:

$$ T \sigma_i^{(n)} T^{-1} = -\sigma_i^{(n)}, \quad T \tau_i^{(n)} T^{-1} = -\tau_i^{(n)}, $$

$$ s \sigma_i^{(1)} s^{-1} = \sigma_i^{(2)}, \quad s \tau_i^{(1)} s^{-1} = \tau_i^{(2)}. $$

Before examining the ground state phase diagram of this system in detail, it is intuitive to study the ground state properties of the system in the extreme limits of strong and weak rung couplings. In the absence of diagonal interactions the system is unfrustrated. In the limit of vanishing rung couplings, the ladder is decoupled into two equivalent mixed-spin-$(1, 1/2)$ chains. Mixed-spin chains are a special class of spin models which their universality class is completely different from the uniform spin models. According to the Lieb-Mattis theorem, the ground state of a mixed-spin-$(\sigma, \tau)$ chain has total spin $S_{\text{tot}} = (\tau - \sigma) L$ $(\tau > \sigma)$, with $L$ being the number of unit cells on the chain, and thus is necessarily long-range ferrimagnetic ordered. Since the elementary cell consists of two spins, linear spin wave theory yields two types of magnons: a gapless acoustical branch with $S^2 = L/2 - 1$ and a gapped optical branch with $S^2 = L/2 + 1$, respectively with the dispersions $\omega_k^\pm$ and $\omega_k^\tau$, given by $\omega_k^\pm = J_l = \pm \frac{1}{2} \pm \frac{1}{2} + 2 \sin^2 k$ $1/2$. Though the antiferromagnetic gap within the lowest-order spin-wave theory is $\Delta_\text{opt.} = J_l$. When rung couplings are switched on, in the case of $J_r > 0$, the gapless mode becomes linear reflecting the antiferromagnetic character of the ladder system, whereas the optical modes moves upward. Moreover, as soon as the antiferromagnetic rung couplings become non-zero the spin gap starts to open, it first increases quadratically till $J_r \sim 0.3$, and then grows linearly by increasing $J_r$.

In the limit of strong ferromagnetic rung couplings, i.e. for $J_r < 0$ and $J_l = 0$, the spins $\sigma$ ($\tau$) form rung-triplets (quintets) and the singlets (triplets) being much higher in energy. In this limit the ground state is a product of rung-triplet and rung-quintet states, separated by an energy gap of size $3/4 J_r$ (per total number of spins) with excited state. As soon as leg couplings are switched on, i.e. when $|J_r| \gg J_l$, the ladder behaves like a ferrimagnetic spin-$(1, 2)$ chain, with a long-range ferrimagnetic ground state of total spin $S_{\text{tot}} = L$. In this case, the antiferromagnetic gap within the lowest-order spin-wave theory is $\Delta = 2 J_r$. 

![FIG. 1. (Color online) Pictorial representation of a mixed-spin ladder with different intra- and inter-legs exchange couplings. The blue and red dots are representing the spin-$\sigma$ and spin-$\tau$. The index $i$ refers to cell number.](image-url)
As we mentioned, in the limit of weak ferromagnetic rung couplings there is also an antiferromagnetic gap of size $J_l$. Therefore, it appears that weak and strong ferromagnetic couplings are continuously related.

In the limit of strong antiferromagnetic rung couplings ($J_r > 0$, and $J_l \ll J_r$) the ground state is essentially a product of local rung-singlets, i.e.

$$|GS^0\rangle = \prod_i |S^\sigma_i\rangle \otimes |S^\tau_i\rangle,$$

where $|S^\sigma_i\rangle$ and $|S^\tau_i\rangle$, given by:

$$|S^\sigma_i\rangle = \frac{1}{\sqrt{2}} \left( \frac{1}{2} |t^+_i| - \frac{1}{2} |t^-_i| - | - \frac{1}{2} |t^+_{i+1} \right),$$

$$|S^\tau_i\rangle = \frac{1}{\sqrt{3}} \left( |t^+_{i+1}| |t^-_i| - |t^+_{i+1}| |t^+_i| + |t^-_{i+1}| |t^-_i| \right),$$

are the rung-singlet states, respectively for the rungs with spins $\sigma$ and $\tau$ in the $i$-th unit cell. Here, $\pm 1/2$ are the eigenstates of $\sigma^z$, and $|\pm\rangle$ and $|0\rangle$ are the eigenstates of $\tau^z$. The ground state energy is $E_g/N = -\frac{1}{2}J_r$, where $N$ refers to the number of unit cells, and the first excited states are triplets, separated from the ground state by a finite energy gap of size $(J_r/2)$. By increasing leg couplings, the energy gap decreases monotonically. Using the non-degenerate perturbation theory, to first-order in $J_l/J_r$, the ground state is readily obtained as:

$$|GS^1\rangle = |GS^0\rangle + |1\rangle,$$

with

$$|1\rangle = \frac{J_l}{J_r} \sqrt{\frac{1}{6}} \sum_i \cdots \gamma^\tau_{-1,1} \cdots + \sum_i \cdots \gamma^\sigma_{i,i+1} \cdots,$$

where

$$\gamma^\tau_{i,j} = \frac{1}{3} \left( |t^+_i| |t^-_j| - |t^+_i| |t^+_j| + |t^-_i| |t^-_j| \right),$$

$$\gamma^\sigma_{i,j} = \frac{1}{3} \left( |t^+_i| |t^-_j| - |t^+_i| |t^+_j| + |t^-_i| |t^-_j| \right).$$

Here, $|t^\alpha_i\rangle$ with $\alpha = \pm, 0$ and $s = \sigma, \tau$ are the triplet states on the rung with spins $s$ defined as:

$$|t^+_s\rangle = -\frac{3}{2} \sum_{m=-s}^{s} \frac{(-)^{s-m} \sqrt{s(s+1) - m(m+1)}}{\sqrt{s(s+1)(2s+1)}} \times |m+1\rangle_i |m\rangle_i,$$

$$|t^-_s\rangle = \frac{3}{2} \sum_{m=-s}^{s} \frac{(-)^{s-m}}{\sqrt{s(s+1)(2s+1)}} |m\rangle_i |m+1\rangle_i,$$

As it is seen, to first order in $|J_l|/|J_r|$, the ground state of the ladder is given in terms of the rung-singlet and the rung-triplet states, and there is no contribution from the rung-quintets. This means that in the limit of weak leg coupling the quintet states can be projected out and the mixed-spin-(1,1/2) ladder is mapped onto a uniform spin-1/2 ladder with antiferromagnetic rung and leg couplings. However, when leg couplings become stronger we should take the rung-quintet states into account to write the true ground state of the ladder. To second order in $J_l/J_r$, the ground state of the ladder is given in terms of rung-singlets, rung-triplets and rung-quintets (see the Appendix A). According to the form of the second order ground state (see Eq. (A5)) we can see that the inhomogeneity of the system appears at stronger values of leg couplings. To see the ground state magnetic orders, we study the behavior of the expectation values of $\sigma_z^i$ and $\tau_z^i$ on the first and second order ground states. In these states all the local order parameters are vanishing and the ground state has no magnetic order.

As rung couplings between the mixed-spin chains are turned on, in the case of ferromagnetic rung couplings, the ground state order of the chains does not change essentially, and we still have a ferrimagnetic long-range order along the chains. However, when rung couplings are antiferromagnetic, even very small, according to the Marshall’s theorem the ferrimagnetic order of the chains is destroyed immediately. In next sections, we will carry out iTEBD and DMRG computations and investigate the ground state properties of our mixed-spin ladder in the vicinity of this point. We will show that in the limit of weak antiferromagnetic rung couplings these two techniques lead to different ground state orders.

Like the uniform spin ladders, our mixed-spin ladder is invariant under the exchange of the leg and diagonal couplings, i.e. $H(J_1, J_r, J_d) = H(J_d, J_r, J_1)$. Thus all the above discussions can be entirely applied to the case of $J_1 = 0$ and $J_d \neq 0$, by replacing $J_1$ with $J_d$.

### III. METHODS

Matrix product states (MPSs) provide an efficient representation for the ground state of one-dimensional systems which obey the area law in which the entanglement entropy grows with the boundary of a specific area rather than its volume. To use MPSs representation for our mixed-spin ladder, we map the ladder onto a chain and consider each rung as a supersite with a larger Hilbert space. In Vidal’s representation a generic translational invariant state of a one-dimensional system in thermodynamic limit can be described by the use of two sets of matrices in infinite system. However, in our case, we have considered a larger unit cell consists of four pairs of matrices $(\Gamma_A, \Gamma_B, \Gamma_C, \Gamma_D)$ and $(\lambda_A, \lambda_B, \lambda_C, \lambda_D)$, to make sure that the unit cell is sufficiently large to detect the dimer phases or phases with broken translational symmetry. In this representation an arbitrary
many-body quantum state of our ladder can be written as

$$\left| \psi \right> = \sum_{i_1, \ldots, i_N} \left[ \cdots \Gamma^{m_1}_{i_A} \lambda_A \Gamma^{m_2}_{i_B} \cdots \lambda_B \right] \Gamma^{m_3}_{i_C} \Gamma^{m_4}_{i_D} \cdots \left| i_1, i_2, \ldots, i_N \right> ,$$

where \( |i_1, i_2, \ldots, i_N \rangle \) is a product state with \( i_k \), being the \( i \)-th state of the rung \( n \), 4 states for spin-\( \frac{1}{2} \) rungs while 9 for spin-1. This state is diagrammatically shown in Fig. 2, where \( \lambda \)'s are positive, real and square diagonal matrices. The matrix elements of \( \lambda \) are nothing but the Schmidt coefficients, and \( \lambda^2 \) are the eigenvalues of the reduced density matrix \( \rho_{\text{red}} = Tr_{B(A)}(\left| \psi \right> \left< \psi \right|) \), where \( A \) and \( B \) are two halves of the ladder). The full set of these eigenvalues are the ES, and the EE is directly connected to this eigenvalues thorough

$$S = - \sum \lambda^2 \log \lambda^2 .$$

The tensors \( \Gamma \) are matrices of dimension \( \chi \) which correspond to changes of basis between the different Schmidt basis. \( \chi \) is a key parameter in tensor network states, called bond dimension, and the accuracy of the state (5) is controlled by this quantity. For partially entangled states by choosing a fairly small bond dimension one can reach to valid results.

One of the efficient MPSs-based algorithm for simulating one-dimensional quantum many-body systems is iTEBD technique. In iTEBD, by considering the imaginary time evolution of a quantum state we can find the ground state of the Hamiltonian through the relation

$$\left| GS \right> = \lim_{T \rightarrow \infty} \exp(-TH) \left| \psi_0 \right> ,$$

where \( \left| \psi_0 \right> \) is an arbitrary state which we call it initial guess state. In the vicinity of the phase transition points, the final results obtained by iTEBD are strictly dependent to this initial guess, and it is of crucially important to choose suitable guess states to reach the true ground state of the system. By dividing the time \( T \) into \( N \) infinitesimal periods (\( \delta t \)), rewriting the Hamiltonian as

$$H = H_{\text{odd}} + H_{\text{even}} ,$$

$$H_{\text{odd}} = J_d (\sigma_i^1 \cdot \sigma_{i+1}^1 + \tau_i^1 \cdot \tau_{i+1}^1) + J_l (\sigma_i^1 \cdot \tau_i^1 + \sigma_{i+1}^1 \cdot \tau_{i+1}^1),$$

$$H_{\text{even}} = J_r (\tau_i^1 \cdot \tau_{i+1}^2 + \sigma_i^1 \cdot \sigma_{i+1}^2) + J_l (\sigma_i^1 \cdot \tau_i^1 + \tau_{i+1}^1 \cdot \sigma_{i+1}^2) ,$$

and performing Suzuki-Trotter decomposition, the time evolution operator can be approximated as:

$$U(\delta t) \approx \prod_{i_{\text{odd}}} e^{-i\delta t h[i,i+1]} \prod_{i_{\text{even}}} e^{-i\delta t h[i,i+1]} ,$$

where \( h[i,i+1] \) are the two-rung operators which their summation will construct \( H_{\text{odd}}(H_{\text{even}}) \). This operator is applied severally to the state \( \left| \psi_0 \right> \) in Eq. (5) in order to update the infinite MPSs representation, until the ground state energy or entropy converge. A key feature of the iTEBD algorithm is that it directly treats the infinite system by exploiting the translational invariance, so it is free of finite-size effects.

In our ladder system, we used second order Suzuki-Trotter decomposition, and the simulations are started with a time step \( \delta t = 0.5 \), then it is gradually decreased up to \( \delta t = 10^{-5} \). As we mentioned, close to the RS-H phase transition point, the iTEBD can lead to the results, not compatible with fundamental theories in condensed matter physics such as Mermin-Wagner and Lieb-Mattis theorems. Therefore, we use DMRG technique to obtain the correct ground state of the system. Unlike iTEBD, DMRG is a variational method but these two methods have many steps in common. We iteratively optimize the MPSs of two neighboring sites to minimize the ground state energy. Then project the Hamiltonian onto the variational space and use an iterative algorithm such as Lanczos to lower the energy. Repeating this two-site update for each pair of neighboring sites, the wave function converges to the ground state. In our computations, we used a finite DMRG technique, and considered systems with 120, 180 and 240 rungs. Also, the bond dimension has been increased up to 1000.

IV. RESULTS: UNFRUSTRATED MIXED-SPIN LADDERS

In the absence of the diagonal interactions, i.e., for \( J_d = 0 \), our mixed-spin ladder (1) is unfrustrated and, as seen by perturbation theory, in the two extreme limits of strong FM and vanishing rung couplings, the ground state is ferrimagnetically long-range ordered, while in the limit of strong AF rung couplings it is RS disordered. In order to obtain the ground state phase diagram we introduce a dimensionless parameter as \( R = J_r / (J_l + |J_r|) \), where \( R = -1 \) (+1) indicates the strong FM (AF) rung couplings regime, and \( R = 0 \) corresponds to two decoupled mixed-spin chains.

Before finding the ground state phase diagram, it is insightful to study the behavior of the ground state energy. We have plotted in Fig. 3, the ground state energy per unit cell versus the parameter \( R \), obtained by iTEBD with two different bond dimensions, \( \chi = 100 \) and 120. As it is obviously seen, the energy obtained with \( \chi = 100 \) and 120 are almost the same, meaning that \( \chi = 120 \) is a suitable bond dimension. The discontinuity at \( R = 0 \) implies that a phase transition of first order occurs in the
This might be caused by the dependency of
− \( R \) chain, and at the energy coincides with the energy of a mixed-spin-(1,1/2)
to − \( R \) triplet and a spin-1 rung-quintet, at \( R = 0 \) (\( J_1 = 1 \), \( J_2 = 0 \))
the energy coincides with the energy of a mixed-spin-(1,1/2)
chain, and at \( R = 1 \) (\( J_1 = 0 \), \( J_2 = 1 \)) the ground state energy is \(- \frac{1}{4} \), the total energy of spin-1/2 and spin-1 rung-singlets.

In order to capture the ground state orders in both sides of this point we introduce the following order parameters:

\[
O_{FiM-F} = \frac{1}{2} \left( \langle \sigma_i^{(1)z} - \sigma_i^{(1)z} \rangle + \langle \tau_i^{(2)z} - \sigma_i^{(2)z} \rangle \right),
\]

\[
O_{FiM-N} = \frac{1}{2} \left( \langle \sigma_i^{(1)z} - \sigma_i^{(1)z} \rangle - \langle \tau_i^{(2)z} - \sigma_i^{(2)z} \rangle \right) \tag{9}
\]

where \( \langle \ldots \rangle \) is the expectation value of "\( \ldots \)" on the ground state of the system. In the phase with non-vanishing FiM-F (FiM-N) order parameter, the system orders ferrimagnetically along the legs (as in ferrimagnetic chains) and ferromagnetically (antiferromagnetically) along the rungs (see the schematic pictures in the inset of Fig. 4). In both these phases the time reversal symmetry is broken, but the leg-swap breaks only in the FiM-N phase. We have plotted in Fig. 4 the ground state order parameters versus \( R \), obtained by iTEBD. In the entire region of \(-1 < R < 0 \), the FiM-F order parameter is non-zero and the ladder is ferrimagnetically ordered. In this region the ground state is in the sector \([1, 2, 1, 2, \ldots, 1, 2] \), where the numbers are the values of \( \sigma \) and \( \tau \) in the sector \([\sigma_1, \tau_1, \sigma_2, \tau_2, \ldots, \sigma_{N-1}, \tau_{N-1}, \sigma_N, \tau_N] \) of the Hilbert space. At \( R = 0 \), the ladder is decoupled to two equivalent mixed-spin-(1,1/2) chains and the system is ferrimagnetically ordered, and the ground state is in the sector \([1/2, 1, \ldots, 1/2, 1] \). For large values of \( R > 0 \), all local order parameters are exactly zero, and the system is in the RS disordered phase. By decreasing \( R \), although the leg couplings change the ground state of the system (as seen by our perturbation theory), but according to the Mermin-Wagner theorem, we expect the ground state order does not change and the ladder shows no long-range order in the entire region of \( R > 0 \). But amazingly we see that in a narrow interval near the \( R = 0 \)
point, i.e., in the region of \( 0 < R \leq 0.08 \), our iTEBD predicts a ground state with FiM-N long-range order. The

![Image](image-url)
Although the discontinuous change in EE indicates exactly the phase transition point from the FiM-F state to the RS, it fails to characterize the ground state phases, individually. Since changes in the degeneracy of the ES levels is associated with a quantum phase transition, we use the ES as a tool to identify these phases. We have shown in Fig. 6, the degeneracy of the ES levels in both the FiM-F and the RS phases. As seen, by changing the parameter $R$ from $-1$ to $+1$, the degeneracy of the ES levels varies such that in the RS phase ($0 < R < 1$) the ES levels have odd degeneracies, while in the FiM-F phase ($-1 < R \leq 0$), they have no degeneracy.

V. RESULTS: FRUSTRATED MIXED-SPIN LADDER

In this section, we introduce the diagonal interactions ($J_d > 0$) to the system, and investigate the impact of frustration on the ground state phase diagram of the mixed-spin-(1, 1/2) ladder. In the case of ferromagnetic rung couplings, in the limits of weak leg and weak diagonal couplings, i.e., for $J_d, J_l \ll |J_r|$, the ground state can be obtained using a perturbation theory. To this end, we write the legs and rungs Hamiltonians as:

$$H_{\text{legs}} + H_{\text{diag}} = \sum_{m=+,-} J^m \sum_i \left[ \sigma_i^m \cdot \sigma_{i+1}^m + \gamma_{i}^m \cdot \tau_{i+1}^m \right],$$

(10)

with $\gamma_{+} = \sigma_i^{(1)} + \sigma_i^{(2)}$ and $\gamma_{-} = \sigma_i^{(1)} - \sigma_i^{(2)}$, and $J^\pm = J_l \pm J_d$. Here, the "+" term preserves the total spin in each rung while the "−" term changes the triplets and quintets to singlets. In the case of antiferromagnetic legs and diagonal interactions the "+" term gives a nonzero contribution at the first order perturbation and lifts the ground state degeneracy of the Hamiltonian $H_{\text{rung}}$. The effective Hamiltonian turns out to be

$$H = J \sum_i (S_i \cdot T_i + T_i \cdot S_{i+1}).$$

(11)

where $S_i$ and $T_i$ are respectively the spin-1 and spin-2 operators and $J = \frac{1}{2} (J_l + J_d)$. Therefore the ground state is ferrimagnetically long-range ordered. By increasing the strengths of leg and diagonal couplings, no phase transition happens in the system and the ferrimagnetic order is preserved.

In the case of antiferromagnetic rung couplings, the situation is completely different and the ground state experiences various phase transitions. For antiferromagnetic leg coupling, as seen in the previous section, in the absence of weak diagonal interactions the system is in the RS disordered phase, but what happens when diagonal interactions are switched on. By an analysis of the different spin-spin correlations within unit cells, on can shown that for $J_l = J_d = 1$, in the region of $0 \leq J_d < 0.845$, we have $(\tau_r^1, \tau_i^2) = (\sigma_i^1, \sigma_i^2) - \frac{1}{2}$, which implies that the weight of the rung-quintet states on the spin-1 rungs is negligible in this interval. Therefore, one can project the quintet states, and map the frustrated mixed-spin-(1, 1/2) ladder onto a frustrated uniform spin-1/2 ladder with AF leg, rung and diagonal couplings. Different analytical approaches and numerical methods, like bosonization, renormalization groups, DMRG and exact diagonalization techniques, have been used to examine the existence of an intermediate phase between the RS and the H phases in the ground state phase diagram of frustrated spin-1/2 ladder with AF couplings. It has been demonstrated that, in the weak coupling regime, there is a columnar-dimer phase in a very narrow neighborhood of $J_{\perp} = 0.38$ (for $J_q = 1$ and $J_x = 0.2$) between the RS and the H phases. However, the spin-1/2 ladder which our mixed-spin ladder mapped onto, does not belong to the mentioned region, and consequently it was concluded that there is not any intermediate phase between the RS and the H phases. In order to reach a definite conclusion we must carry on more sophisticated investigations.

Here, we study the ground state phases of the frustrated mixed-spin-(1, 1/2) ladder by examining the behavior of the EE, the ES and the string orders. We utilize both the iTEBD and the DMRG techniques and investigate the existence of any intermediate phase between the RS and the H phases. It has been demonstrated that, in the weak coupling regime, there is a columnar-dimer phase in a very narrow neighborhood of $J_{\perp} = 0.38$ (for $J_q = 1$ and $J_x = 0.2$) between the RS and the H phases. However, the spin-1/2 ladder which our mixed-spin ladder mapped onto, does not belong to the mentioned region, and consequently it was concluded that there is not any intermediate phase between the RS and the H phases. However, in order to reach a definite conclusion we must carry on more sophisticated investigations.

In this section, we introduce the diagonal interactions ($J_d > 0$) to the system, and investigate the impact of frustration on the ground state phase diagram of the mixed-spin-(1, 1/2) ladder. In the case of ferromagnetic rung couplings, in the limits of weak leg and weak diagonal couplings, i.e., for $J_d, J_l \ll |J_r|$, the ground state can be obtained using a perturbation theory. To this end, we write the legs and rungs Hamiltonians as:

$$H_{\text{legs}} + H_{\text{diag}} = \sum_{m=+,-} J^m \sum_i \left[ \sigma_i^m \cdot \sigma_{i+1}^m + \gamma_{i}^m \cdot \tau_{i+1}^m \right],$$

(10)

with $\gamma_{+} = \sigma_i^{(1)} + \sigma_i^{(2)}$ and $\gamma_{-} = \sigma_i^{(1)} - \sigma_i^{(2)}$, and $J^\pm = J_l \pm J_d$. Here, the "+" term preserves the total spin in each rung while the "−" term changes the triplets and quintets to singlets. In the case of antiferromagnetic legs and diagonal interactions the "+" term gives a nonzero contribution at the first order perturbation and lifts the ground state degeneracy of the Hamiltonian $H_{\text{rung}}$. The effective Hamiltonian turns out to be

$$H = J \sum_i (S_i \cdot T_i + T_i \cdot S_{i+1}).$$

(11)

where $S_i$ and $T_i$ are respectively the spin-1 and spin-2 operators and $J = \frac{1}{2} (J_l + J_d)$. Therefore the ground state is ferrimagnetically long-range ordered. By increasing the strengths of leg and diagonal couplings, no phase transition happens in the system and the ferrimagnetic order is preserved.

In the case of antiferromagnetic rung couplings, the situation is completely different and the ground state experiences various phase transitions. For antiferromagnetic leg coupling, as seen in the previous section, in the absence of weak diagonal interactions the system is in the RS disordered phase, but what happens when diagonal interactions are switched on. By an analysis of the different spin-spin correlations within unit cells, on can shown that for $J_l = J_d = 1$, in the region of $0 \leq J_d < 0.845$, we have $(\tau_r^1, \tau_i^2) = (\sigma_i^1, \sigma_i^2) - \frac{1}{2}$, which implies that the weight of the rung-quintet states on the spin-1 rungs is negligible in this interval. Therefore, one can project the quintet states, and map the frustrated mixed-spin-(1, 1/2) ladder onto a frustrated uniform spin-1/2 ladder with AF leg, rung and diagonal couplings. Different analytical approaches and numerical methods, like bosonization, renormalization groups, DMRG and exact diagonalization techniques, have been used to examine the existence of an intermediate phase between the RS and the H phases in the ground state phase diagram of frustrated spin-1/2 ladder with AF couplings. It has been demonstrated that, in the weak coupling regime, there is a columnar-dimer phase in a very narrow neighborhood of $J_{\perp} = 0.38$ (for $J_q = 1$ and $J_x = 0.2$) between the RS and the H phases. However, the spin-1/2 ladder which our mixed-spin ladder mapped onto, does not belong to the mentioned region, and consequently it was concluded that there is not any intermediate phase between the RS and the H phases. In order to reach a definite conclusion we must carry on more sophisticated investigations.

Here, we study the ground state phases of the frustrated mixed-spin-(1, 1/2) ladder by examining the behavior of the EE, the ES and the string orders. We utilize both the iTEBD and the DMRG techniques and investigate the existence of any intermediate phase between the RS and the H phases. It has been demonstrated that, in the weak coupling regime, there is a columnar-dimer phase in a very narrow neighborhood of $J_{\perp} = 0.38$ (for $J_q = 1$ and $J_x = 0.2$) between the RS and the H phases. However, the spin-1/2 ladder which our mixed-spin ladder mapped onto, does not belong to the mentioned region, and consequently it was concluded that there is not any intermediate phase between the RS and the H phases. However, in order to reach a definite conclusion we must carry on more sophisticated investigations.
For $0.74 \leq J_d \leq 0.88$, all ES levels have even degeneracies, and all local order parameters are vanishing. The even degeneracies in the ES levels is a characteristic of the H phase. In the region $0.88 < J_d \leq 1.5$, ES levels are nondegenerate, and the FIM-F order parameter is finite, but its magnitude discontinuously changes at $J_d = 1.17$, where a first-order phase transition occurs in the system. For $(0.88 \leq J_d \leq 1.17)$ the ground state belongs to the sector $[1, 2, \cdots, 1, 2]$ whereas for $J_d > 1.17$, the translational symmetry of the ladder breaks and the ground state belongs to the sector $[1, 1, 1, 2, \cdots, 1, 1, 1, 2]$. As seen, the iTEBD predicts an intermediate phase between the RS and the H phases where the ES levels degeneracies do not follow the specific patterns of the RS and the H phases. It also predicts that in this narrow interval

FIG. 7. (Color online) The ground state energy of the frustrated mixed-spin-(1, 1/2) ladder per unit cell versus $J_d$, obtained by iTEBD with $\chi = 100$ and 120. Inset: the ground state energy for the region $0.65 < J_d < 1$.

FIG. 8. (Color online) The EE (top) and the Schmidt gap (bottom) for the frustrated mixed-spin-(1, 1/2) ladder versus $J_d$, obtained by iTEBD with $\chi = 100$ and 120.

FIG. 9. (Color online) The degeneracies of the ES levels of the frustrated mixed-spin ladder versus $J_d$, obtained by iTEBD with $\chi = 120$. The RS phase is characterized by odd degeneracies in ES levels, while in the H phase ES levels have even degeneracies. In the ferrimagnetic phases ES levels are nondegenerate.

FIG. 10. (Color online) The different order parameters defined in Eq. (9) versus $J_d$, obtained by iTEBD with $\chi = 120$. The FiM-N order parameter is nonzero in a narrow interval between the RS and the H phases, and the FiM-F order parameter is non-zero for $J_d \geq 0.88$. The discontinuity at the H-FiM phase transition point, shows that this phase transition is of first-order.
the ground state has long-range FIM-N order. However, as we discussed the ground state must be a singlet state below $J_d < 0.88$. In order to reach the true ground state, we repeat our iTEBD computations using various initial guess states and different bond dimensions (not shown). Although by changing the initial state the energy of the resulted ground state changes, but its long-range order didn’t disappear. As the former section, we employed DMRG which is less dependent on the initial guess.

Using DMRG we achieved interesting results: consistent with the above discussions, all local order parameters are zero ($\langle \sigma_i^{(1,2)} \rangle = \langle \tau_i^{(1,2)} \rangle = 0$) below $J_d < 0.89$, indicating that the ground state belongs to $s_i^\text{tot} = 0$ and it is a singlet state, but as it is obviously seen from the EE and also the ES levels degeneracies (Fig. (11, 12)), there is still a different phase between the RS and the H phases in which the ES levels do not follow the specific degeneracies of the RS and the H phases. In this intermediate phase the EE is much larger than its values in the RS and the H phases. We name this intermediate phase as ”disordered (D) phase”. This naming can be meaningful because in this phase all the local parameters are zero, and the ES levels do not follow a specific pattern. The very sharp and continuous increase of EE at $J_d \approx 0.71$ implies that a phase transition of second-order occurs from the RS to the D phase in the system. Also, on the other side, i.e., at $J_d \approx 0.73$, the rapid and discontinuous growth of the EE, by decreasing $J_d$, indicates the system undergoes a phase transition of first-order from the H phase to the D phase.

In order to understand the nature of this D phase, we analyze the short-range correlation functions inside a unit cell. At the RS phase for an specific $J_d$, the correlations of two spins along the rungs are constant and for both $\sigma$ and $\tau$ rungs $\langle \sigma(\tau)_{i}^{(1)} \sigma(\tau)_{i}^{(2)} \rangle < 0$. At H phase again for an specific $J_d$ the correlations along the rung is almost constant and by changing the diagonal coupling it change smoothly. In this phase $\langle \sigma_{i}^{(1)} \sigma_{i}^{(2)} \rangle > 0$ and $\langle \tau_{i}^{(1)} \tau_{i}^{(2)} \rangle < 0$. However, in the intermediate phase, there is no similar pattern and when we are moving along different rungs the correlations change, and in contrary to the RS and the H phases we can not find a unique behavior for the correlations along the rungs in the D phase.

In the absence of magnetic orders, the different gapped phases can be distinguished by non-local string order parameters. Here, we define the following string order parameters which depend on the spins located at the end sites of the string:

$$
\mathcal{O}_{\sigma_{\text{Odd}}}^{\sigma} = \lim_{|i-j| \to \infty} |\langle \sigma_{o,i}^{z} e^{i\pi \sum_{k=1}^{-1} \sigma_{o,k}^{z} \sigma_{o,j}^{z}} \rangle|,
$$

$$
\mathcal{O}_{\sigma_{\text{Odd}}}^{\tau} = \lim_{|i-j| \to \infty} |\langle \tau_{o,i}^{z} e^{i\pi \sum_{k=1}^{-1} \tau_{o,k}^{z} \tau_{o,j}^{z}} \rangle|,
$$

$$
\mathcal{O}_{\sigma_{\text{Even}}}^{\sigma} = \lim_{|i-j| \to \infty} |\langle \sigma_{e,i}^{z} e^{i\pi \sum_{k=1}^{-1} \sigma_{e,k}^{z} \tau_{e,j}^{z}} \rangle|,
$$

$$
\mathcal{O}_{\sigma_{\text{Even}}}^{\tau} = \lim_{|i-j| \to \infty} |\langle \tau_{e,i}^{z} e^{i\pi \sum_{k=1}^{-1} \tau_{e,k}^{z} \tau_{e,j}^{z}} \rangle|,
$$

with

$$
\sigma_{o,i}^{z} = \sigma_{i}^{z} + \sigma_{i+1}^{z}, \quad \tau_{o,i}^{z} = \tau_{i}^{z} + \tau_{i+1}^{z},
$$

$$
\sigma_{e,i}^{z} = \sigma_{i}^{z} + \tau_{i+1}^{z}, \quad \tau_{e,i}^{z} = \tau_{i}^{z} + \sigma_{i+1}^{z}.
$$

As it is seen from Fig. 14, in the RS phase $\mathcal{O}_{\text{odd}} = 0$ but $\mathcal{O}_{\text{Even}} \neq 0$, while in the H phase $\mathcal{O}_{\text{odd}} \neq 0$ and $\mathcal{O}_{\text{Even}} = 0$. Therefore, we can label these two disordered phases with non-vanishing even or odd string order parameters. Typical configuration of the RS and the H phases are demonstrated in Fig. 13. In the D phase, however, both the odd and even string order parameters are non-zero (based on our iTEBD calculations).
phase also emerges in a narrow interval between the RS and the H phases. In this D phase all local order parameters are zero, and in contrary to the RS and the H phases where the ES levels possess respectively odd and even degeneracies, in this region the ES levels have no specific pattern, i.e., they have mixed odd-even degeneracies. In order to understand the nature of this phase, we also examined the behavior of the short-range spin correlation functions along the rungs, and showed that in contrary to the RS and the H phases there is no a unique behavior for the correlations in the D phase.

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Appendix A: Second order correction of ground state

In this Appendix we will obtain the ground state of the unfrustrated mixed-spin-(1,1/2) ladder up to second order in $J_l/J_r$. For a spin-s system the quintet states can be represented as:

$$|q^+^2\rangle_i = Q(s) \sum_{m=-s+1}^{s-1} (-1)^{s-m} \sqrt{s(s+1) - m(m-1)}$$

$$\times \sqrt{s(s+1) - m(m+1)} |m+1\rangle_i^{(1)} |-m+1\rangle_i^{(2)},$$

$$|q^{+1}\rangle_i = Q(s) \sum_{m=-s}^{s-1} (-1)^{s-m} \sqrt{s(s+1) - m(m+1)}$$

$$\times (2m+1) |m+1\rangle_i^{(1)} |-m\rangle_i^{(2)},$$

$$|q^0\rangle_i = Q(s) \sum_{m=-s}^{s} (-1)^{s-m} (s(s+1) - 3m^2)$$

$$\times |m\rangle_i^{(1)} |-m\rangle_i^{(2)},$$

$$|q^{-1}\rangle_i = Q(s) \sum_{m=-s}^{s-1} (-1)^{s-m} \sqrt{s(s+1) - m(m+1)}$$

$$\times (2m+1) |m\rangle_i^{(1)} |-m-1\rangle_i^{(2)},$$

$$|q^{-2}\rangle_i = Q(s) \sum_{m=-s+1}^{s-1} (-1)^{s-m} \sqrt{s(s+1) - m(m-1)}$$

$$\times \sqrt{s(s+1) - m(m+1)} |m-1\rangle_i^{(1)} |-m-1\rangle_i^{(2)},$$

(A1)
where

\[ Q(s) = \frac{-\sqrt{15/2}}{\sqrt{s(s+1)(2s+1)(2s+3)(2s-1)}}. \]

The second order correction of the ground state is readily obtained as follows:

\[
|2\rangle = -\left( \frac{J_i}{J_{r}} \right)^2 \frac{2a}{3} |J_0\rangle + F(i, j) + \frac{b}{J_{r}} \sum_i \left( \cdots \gamma_{i,i+1}^1 \cdots + \cdots \gamma_{i-1,i}^1 \cdots \right) + (\cdots \gamma_{i,i+1}^2 \cdots + \cdots \gamma_{i-1,i}^2 \cdots ) + \frac{c}{15J_{r}} \gamma_{i,i+1}^2 \cdots + \cdots \gamma_{i-1,i}^2 \cdots ) + \frac{d}{15J_{r}} \gamma_{i,i+1}^2 \cdots + \cdots \gamma_{i-1,i}^2 \cdots ) .
\]

(A2)

Finally the ground state of the ladder up to second order in \( J_i/J_r \) is given by:

\[
|GS(2)\rangle = |GS(0)\rangle + (1 + |2\rangle).
\]

(A5)

Appendix B: Different initial guesses in iTEBD algorithm

Since the iTEBD algorithm is very sensitive to the initial guess for the ground state, in the vicinity of phase transition points it may lead to results which are not compatible with fundamental theories in condensed matter physics such as Mermin-Wagner theorem. For example, in our unfrustrated mixed-spin ladder, in the region \( 0 < R < 0.08 \), the iTEBD results predict the presence of a long-range ferrimagnetic order. We examined the ground state of the system using various initial states and the result has been summarized in the following table. As it is obvious the state with minimum energy shows a magnetic long-range order.

| Initial guess | Ground state energy \( E_{FJM-N} \) | \( x \) | \( \chi \) |
|---------------|---------------------------------|-----|-----|
| Random       | -28.686389927308               | -0.871082587742 | 120 |
| Random       | -28.686389927308               | -0.089252552437 | 140 |
| Random       | -28.686389927308               | -0.86653753846  | 160 |
| Random       | -28.686389927308               | 0.750641229902  | 180 |
| Random       | -28.686389927308               | 0.322147931627  | 200 |
| Random       | -28.686389927308               | 0.61149290830   | 220 |
| FM           | -28.686389927308               | 0.0322147931627 | 240 |
| Haldane      | -28.686389927308               | 0.903698521454  | 260 |
| RS           | -28.686389927308               | -0.706567415176 | 280 |
| Columnar dimer | -28.686389927308               | 0.29916032904   | 300 |
| Staggered dimer | -28.686389927308               | -1.018585788427 | 320 |
| RS           | -28.686389927308               | 0.18966530778   | 340 |
| SU(2)        | -28.686389927308               | -0.009413096230 | 360 |
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