Energy-level ordering and ground-state quantum numbers for a frustrated two-leg spin-1/2 ladder

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The Lieb-Mattis theorem about antiferromagnetic ordering of energy levels on bipartite lattices is generalized to finite-size two-leg spin-1/2 ladder model frustrated by diagonal interactions. For reflection-symmetric model with site-dependent interactions, we prove exactly that the lowest energies in sectors with fixed total spin and reflection quantum numbers are monotone increasing functions of total spin. The nondegeneracy of most levels is also proven. We also establish the uniqueness and obtain the spin value of the lowest level multiplet in the whole sector formed by reflection-symmetric (antisymmetric) states. For a wide range of coupling constants, we prove that the ground state is a unique spin singlet. For other values of couplings, it may be also a unique spin triplet or may consist of both multiplets. Similar results have been obtained for the ladder with arbitrary boundary impurity spin. Some partial results have also been obtained in the case of periodical boundary conditions.

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I. INTRODUCTION

Nowadays, the frustrated spin systems are the subject of intensive study.[1–4] The interest on them is stimulated by recent progress in synthesizing corresponding magnetic materials.[5] In these models, due to competing interactions, the classical ground state cannot be minimized locally and usually possesses a large degeneracy. The frustration can be caused by the geometry of the spin lattice or by the presence of both ferromagnetic and antiferromagnetic interactions.

In contrast, the ground states of classical models on bipartite lattices are Néel ordered and are unique up to the global spin rotations. The bipartitness means that the lattice can be divided into two sublattices A and B, so that all interactions within the same sublattice are ferromagnetic while the interactions between different sublattices are antiferromagnetic. For the Néel state, all spins of A have the same direction while all spins of B are aligned in the opposite direction.

The quantum fluctuations destroy Néel state and the quantum model, in general, has more complicated ground state. However, for bipartite spin systems, the quantum ground state inherits some properties of its classical counterpart. In particular, Lieb and Mattis proved that the quantum ground state of a finite-size system is a unique multiplet with total spin $S_{gs}=|S_A-S_B|$, which coincides with the spin of the classical Néel state. Here, S_A and S_B are the highest possible spins on corresponding sublattices.[6,7] This feature of bipartite systems looks natural, since in the limit of large spin values the quantum model approaches the classical one. Moreover, a simple general rule that the energy increases with increasing spin, which is conventional for classical antiferromagnets, makes sense in this case, too. More precisely, the lowest-energy E_S in the sector, where the total spin is equal to S, is a monotone increasing function of the spin for any $S \geqslant S_{gs}$.[6] This property is known as Lieb-Mattis theorem about antiferromagnetic ordering of energy levels. Lieb-Mattis theorem is very important because it provides information about the ground state and spectrum of bipartite spin systems without exact solution or numerical simulation. Recently, it has been generalized to SU(n) symmetric quantum chain with defining representation and nearest-neighbor interactions.[8] A ferromagnetic ordering of energy levels has been formulated and proven also for XXX Heisenberg chains of any spin.[9]

More limited number of exact results is available for frustrated quantum spin systems. It is difficult to treat even their classical ground states as was mentioned above. The usual Lieb-Mattis theorem is no longer valid for frustrated systems. Recently, however, Lieb and Schupp proved rigorously that a reflection-symmetric spin system with antiferromagnetic crossing bonds possesses at least one spin-singlet ground state.[10,11] Moreover, under certain additional conditions, all ground states become singlets. A lot of frustrated spin systems satisfy the conditions of the Lieb-Schupp approach. Two-dimensional pyrochlore antiferromagnet having a checkerboard lattice structure is an example of such type of system.[10] Another example is the well-known two-dimensional antiferromagnetic J_1-J_2 model, namely, the Heisenberg model on square lattice with diagonal interactions, which has been studied recently.[12–15] Note that this approach does not provide any information about the degeneracy of ground states. Thus, for frustrated spin systems, this question still remains open. We also mention that the method used in Refs. 10 and 11 is restricted to the systems, which do not have a spin on their symmetry axis.

At the same time, recently, certain signs in favor of Lieb-Mattis theorem for frustrated spin systems have appeared. For the J_1-J_2 model, the number of arguments based on exact diagonalization and spin-wave approximation had been presented in support of the fact that the antiferromagnetic ordering of energy levels is preserved under weak frustration caused by diagonal couplings.[16] Recently, for the same model, the condition $S_{gs}=|S_A-S_B|$ for the ground-state spin has been tested numerically in Ref. 17. The authors came to the conclusion that it remains true provided that the frustration is sufficiently weak in order to destroy ground-state Néel order. The Lieb-Mattis property had been observed also at finite-size spectrum of the Heisenberg model on the triangular and Kagome lattices.[18] All these investigations suggest that in many cases, even a relatively strong frustration cannot destroy the antiferromagnetic ordering of energy levels.

On the other hand, recently, the spin ladder systems have attracted a lot of attention. The interest to them has been generated by significant progress made within the last years in fabrication of such type of compounds having a structure similar to the structure of two-dimensional high-temperature superconductors.[19] Ladder systems are simpler for study than their more complex two-dimensional counterparts. Moreover, the powerful theoretical and numerical methods, elaborated for one-dimensional models, can be applied to study them. The two-leg ladder frustrated by diagonal interactions is one of the simplest frustrated spin systems. It can be viewed as a quasi-one-dimensional analog of the J_1-J_2 model. Together with various generalizations, it has been investigated intensively during the last decade.[20–27] The ground-state phase diagram consists of two topologically distinct Haldane phases separated by the curve (or surface) of phase transition.

Inspired by the aforementioned activities, in this paper we generalize the Lieb-Mattis ordering theorem to two-leg spin-1/2 ladder model with diagonal interactions. We consider the system, which rests invariant under the reflection with respect to the longitudinal symmetry axis of the ladder.

In Sec. II, we formulate and prove an analog of Lieb-Mattis theorem for frustrated spin-1/2 ladder with free boundaries. The reflection symmetry splits the total space of states into two invariant sectors, composed correspondingly from reflection-symmetric and reflection-antisymmetric states. We establish the antiferromagnetic ordering of energy levels in symmetric and antisymmetric sectors separately for a wide range of the interaction constants. The nondegeneracy of most levels is also proven. In Sec. III, using the ordering rule and the results of Lieb and Schupp[10,11] on reflection-symmetric spin systems, the total spin and reflection quantum numbers of the ground state are derived. The results are tested and compared with numerical simulations. In Sec. IV, the validity of obtained results is checked in some particular cases, for which exact results are already known. Section V is devoted to the frustrated ladder with boundary impurity spin. Similar ordering of energy levels is established in this case, too. Some partial results are obtained for the model with periodic boundary conditions in Sec. VI. In the last section, we briefly summarize the results obtained in this paper. In the Appendix, we apply the general results for reflection-symmetric spin systems obtained in Refs. 10 and 11 to the frustrated ladder model.

II. ENERGY LEVEL ORDERING OF FINITE FRUSTRATED LADDER WITH OPEN BOUNDARIES

A. Frustrated ladder model

In this paper, we consider two finite identical antiferromagnetic spin-1/2 chains coupled by rung and diagonal interactions.[22,24] The Hamiltonian reads (see Fig. 1)

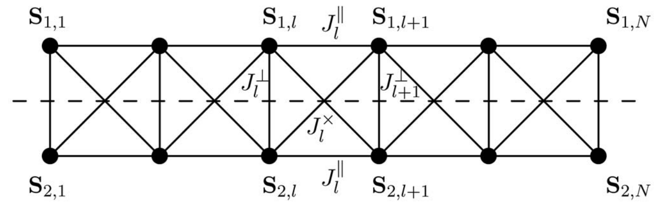

FIG. 1. Frustrated ladder with site-dependent couplings. Here $J_l^{\parallel}$ are intrachain couplings while $J_l^{\perp}$ and $J_l^{\times}$ are, respectively, rung and diagonal interchain couplings. The dashed line is the symmetry axis of the model.

$$H = \sum_{l=1}^{N-1} J_l^{\parallel}(\mathbf{S}_{1,l}\cdot\mathbf{S}_{1,l+1} + \mathbf{S}_{2,l}\cdot\mathbf{S}_{2,l+1}) + \sum_{l=1}^{N-1} J_l^{\times}(\mathbf{S}_{1,l}\cdot\mathbf{S}_{2,l+1} + \mathbf{S}_{1,l+1}\cdot\mathbf{S}_{2,l}) + \sum_{l=1}^{N} J_l^{\perp}\mathbf{S}_{1,l}\cdot\mathbf{S}_{2,l}, \tag{1}$$

where $\mathbf{S}_{1,l}$ and $\mathbf{S}_{2,l}$ are the spin operators of the first and second chains respectively. $J_l^{\perp}$ and $J_l^{\times}$ are rung and diagonal interchain couplings, while $J_l^{\parallel}$ are intrachain couplings. The open boundary conditions are applied here. All couplings depend on site. Their choice corresponds to a model possessing the reflection symmetry $\mathcal{R}$ with respect to the longitudinal symmetry axis. The reflection just permutes the spins of two chains: $\mathcal{R}\mathbf{S}_{1,l}=\mathbf{S}_{2,l}\mathcal{R}$.

We do not put any restriction on the rung couplings $J_l^{\perp}$ and consider antiferromagnetic intrachain couplings only. We suppose also that the diagonal spin interactions are weaker than intrachain interactions, i.e.,

$$J_l^{\parallel} > |J_l^{\times}|. \tag{2}$$

Note that the condition above is not too restrictive for antiferromagnetic values of $J_l^{\times}$ because the system remains invariant under the exchange of rung and diagonal couplings $J_l^{\parallel}\leftrightarrow J_l^{\times}$ belonging to lth box. The resulting model corresponds to a ladder obtained by permutation $\mathbf{S}_{1,l'}\leftrightarrow\mathbf{S}_{2,l'}$ of two spins in all rungs positioned on the right from lth rung (i.e., for all $l'>l$). It is topologically equivalent to the original model. Therefore, one can consider the couplings subjected to $J_l^{\parallel}\geqslant J_l^{\times}$ only without loss of generality. Note that condition (2) excludes the values of diagonal couplings $J_l^{\times}$ equal to $\pm J_l^{\parallel}$.

One must mention that we call model (1) a frustrated ladder, but, in fact, it becomes bipartite for some couplings. In particular, it is bipartite for ferromagnetic diagonal or rung interactions. These cases will be discussed in Sec. IV.

The Hamiltonian preserves the total spin $\mathbf{S}=\Sigma_l \mathbf{S}_{1,l}+\mathbf{S}_{2,l}$ of the system. Since $\mathcal{R}$ and $\mathbf{S}$ are compatible, the eigenstates of Eq. (1) can be chosen to be parametrized by the spin ($S=0,1,\ldots,N$), spin projection ($M=-N,-N+1,\ldots,N$), and reflection ($\sigma=\pm 1$) quantum numbers.

In order to make the use of the reflection symmetry easier, we introduce the symmetric and antisymmetric superposition, of two spins on each rung:

$$\mathbf{S}_l^{(s)} = \mathbf{S}_{1,l} + \mathbf{S}_{2,l}, \quad \mathbf{S}_l^{(a)} = \mathbf{S}_{1,l} - \mathbf{S}_{2,l}, \quad l = 1,2, \ldots, N. \quad (3)$$

The symmetrized spin $\mathbf{S}_l^{(s)}$ describes the total spin of lth rung. It remains unchanged under reflection, i.e., $\mathcal{R}\mathbf{S}_l^{(s)}\mathcal{R} = \mathbf{S}_l^{(s)}$, while the antisymmetrized rung spin acquires a minus sign, i.e., $\mathcal{R}\mathbf{S}_l^{(a)}\mathcal{R} = -\mathbf{S}_l^{(a)}$.

Now we express the Hamiltonian (1) in terms of these operators. After omitting the nonessential scalar term, the Hamiltonian takes the following simple form:

$$H = \sum_{l=1}^{N-1} (J_l^s \mathbf{S}_l^{(s)} \cdot \mathbf{S}_{l+1}^{(s)} + J_l^a \mathbf{S}_l^{(a)} \cdot \mathbf{S}_{l+1}^{(a)}) + \frac{1}{2}\sum_{l=1}^{N} J_l^{\perp} (\mathbf{S}_l^{(s)})^2. \quad (4)$$

Here, we have introduced the symmetrized and antisymmetrized couplings, which are antiferromagnetic due to condition (2) imposed above on the intrachain and diagonal couplings:

$$J_l^s = \frac{J_l^{\parallel} + J_l^{\times}}{2} > 0 \quad \text{and } J_l^a = \frac{J_l^{\parallel} - J_l^{\times}}{2} > 0. \quad (5)$$

Note that Eq. (4) does not contain terms which mix symmetrized and antisymmetrized spin operators. This fact is a consequence of the reflection symmetry of the model. We mention that similar decomposition for frustrated ladder Hamiltonian was also applied in Refs. 20 and 21.

In terms of lowering and rising operators $S_l^{(s)\pm} = S_l^{(s)x} \pm i S_l^{(s)y}$ and $S_l^{(a)\pm} = S_l^{(a)x} \pm i S_l^{(a)y}$, the Hamiltonian reads

$$\begin{aligned} H = \frac{1}{2}\sum_{l=1}^{N-1} (&J_l^s S_l^{(s)+} S_{l+1}^{(s)-} + J_l^s S_l^{(s)-} S_{l+1}^{(s)+} + J_l^a S_l^{(a)+} S_{l+1}^{(a)-} \\ &+ J_l^a S_l^{(a)-} S_{l+1}^{(a)+}) + \sum_{l=1}^{N-1} (J_l^s S_l^{(s)z} S_{l+1}^{(s)z} + J_l^a S_l^{(a)z} S_{l+1}^{(a)z}) \\ &+ \frac{1}{2}\sum_{l=1}^{N} J_l^{\perp} (\mathbf{S}_l^{(s)})^2. \end{aligned} \quad (6)$$

Further, in this section, we will show that for $J_l^{\parallel} > |J_l^{\times}|$ the minimal energy levels $E_{S,\sigma}$ in the symmetric ($\sigma=1$) as well as in the antisymmetric ($\sigma=-1$) spin-S sectors are nondegenerate and ordered antiferromagnetically, i.e., are increasing functions of S. This is an extension of Lieb-Mattis ordering theorem[6] to the frustrated ladder model. Here, we briefly outline the steps of the proof.

First, we construct a basis in which all nonzero off-diagonal matrix elements of the Hamiltonian become negative. In the next step, we show that the matrix of Hamiltonian being restricted to the subspace of states with fixed values of spin projection $S^z = M$ and reflection $\mathcal{R} = \sigma$ quantum numbers is connected. Then according to Perron-Frobenius theorem, the lowest-energy state in every such subspace, called a *relative ground state*, is nondegenerate. As we will show, the relative ground state in most cases has a total spin value equal to absolute value of its z projection ($S = |M|$). Together with the total spin symmetry of the Hamiltonian, this implies that the multiplet, to which the relative ground state belongs, possesses the lowest-energy value among all spin-S multiplets. The antiferromagnetic ordering between lowest-energy levels $E_{S,\sigma}$ then follows directly from their nondegeneracy.

B. Nonpositive basis

The existence of a basis, where all off-diagonal elements of the Hamiltonian are nonpositive, is not obvious as it is for nonfrustrated models. The spin flip applied on one sublattice[6,28] is adopted for bipartite systems and does not lead to the desired basis for frustrated systems. In this section, we construct a nonpositive basis for the frustrated ladder model. The first step is the use of the basis consisting of combined spin states on each rung instead of the standard Ising basis consisting of on-site spin-up and spin-down states. Then we apply a unitary shift to the Hamiltonian, which makes all nonvanishing off-diagonal elements arising from the symmetric part of Eq. (4) negative. In the final step, all basic states are multiplied by a sign factor making all nonvanishing off-diagonal matrix elements negative.

It is rather difficult to trace out the sign of matrix elements of H in the Ising basis, consisting of on-site spin states. Instead, we start with a more suitable basis consisting of combined spin states on every rung. Any rung state can be expressed as a superposition of three symmetric triplet states,

$$|1\rangle := |1,1\rangle = \left|\begin{matrix}\uparrow\\ \uparrow\end{matrix}\right\rangle, \quad |-1\rangle := |1,-1\rangle = \left|\begin{matrix}\downarrow\\ \downarrow\end{matrix}\right\rangle,$$

$$|\tilde{0}\rangle := |1,0\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right\rangle + \left|\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right\rangle\right), \quad (7)$$

and one antisymmetric singlet state,

$$|0\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right\rangle - \left|\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right\rangle\right). \quad (8)$$

We have used the above standard notations $\uparrow$, $\downarrow$ for on-site spin-up and spin-down states. For convenience, we mark the triplet states shortly by labels ± 1 and $\tilde{0}$.

The total space of states is spanned by the basic states

$$|m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_N\rangle, \quad m_l = \pm 1, \tilde{0}, 0. \quad (9)$$

Here $|m\rangle$ is one of the four rung states defined above. The reflection operator $\mathcal{R}$ is diagonal in this basis. Its quantum number is $(-1)^{N_0}$, where N_0 is the number of singlets in Eq. (9).

Now define the unitary operator, which rotates the odd-rung spins around the z axis on angle π, as follows:

$$U = \exp\left(i\pi \sum_{l=1}^{[(N+1)/2]} S_{2l-1}^{(s)z} \right), \quad (10)$$

where by $[x]$ we have denoted the integer part of x. Under the action of U, the odd-rung lowering-rising operators change the sign ($U S_{2l-1}^{(s,a)\pm} U^{-1} = -S_{2l-1}^{(s,a)\pm}$), while the others remain unchanged. Recall that for bipartite models, a similar unitary shift applied to the spins of one sublattice makes all off-diagonal elements of the Hamiltonian nonpositive.[6,28] In our case, the Hamiltonian (6) transforms to

$$\widetilde{H} = UHU^{-1} = \frac{1}{2}\sum_{l=1}^{N-1} (- J_l^s S_l^{(s)+} S_{l+1}^{(s)-} - J_l^s S_l^{(s)-} S_{l+1}^{(s)+} - J_l^a S_l^{(a)+} S_{l+1}^{(a)-} - J_l^a S_l^{(a)-} S_{l+1}^{(a)+}) + \sum_{l=1}^{N-1} (J_l^s S_l^{(s)z} S_{l+1}^{(s)z} + J_l^a S_l^{(a)z} S_{l+1}^{(a)z}) + \frac{1}{2}\sum_{l=1}^{N} J_l^{\perp} (\mathbf{S}_l^{(s)})^2. \tag{11}$$

It is easy to see that $J_\perp$ part of the Hamiltonian, presented by the last sum in Eq. (11), is diagonal in the basis (9) because it consists of the squares of rung spin operators.

The next observation is that $J^{(s)}$ part of the Hamiltonian $\widetilde{H}$ gives rise to negative off-diagonal elements. Indeed, the symmetrized spin operators describe the spin of rung states and act separately on singlet and triplet states in the usual way. All their off-diagonal matrix elements are positive:

$$\langle\widetilde{0}|S^{(s)+}|-1\rangle = \langle 1|S^{(s)+}|\widetilde{0}\rangle = \langle -1|S^{(s)-}|\widetilde{0}\rangle = \langle\widetilde{0}|S^{(s)-}|1\rangle = \sqrt{2}. \tag{12}$$

Taking into account the fact that the coefficients J_l^s are antiferromagnetic [see Eq. (5)], it is easy to see that all nonvanishing off-diagonal elements of the shifted Hamiltonian (11), which are generated by terms containing symmetrized spin operators, are negative.

Finally, we consider the matrix elements produced by the antisymmetric local terms of Hamiltonian (11). In contrast to the symmetric case, the antisymmetrized spin operators mix triplet and singlet states. All their nonzero matrix elements are off-diagonal and have the following values:[29]

$$\langle 0|S^{(a)+}|-1\rangle = \langle -1|S^{(a)-}|0\rangle = \sqrt{2},$$

$$\langle 1|S^{(a)+}|0\rangle = \langle 0|S^{(a)-}|1\rangle = -\sqrt{2},$$

$$\langle\widetilde{0}|S^{(a)z}|0\rangle = \langle 0|S^{(a)z}|\widetilde{0}\rangle = 1. \tag{13}$$

Using the equations above, we can obtain all nontrivial matrix elements generated by $J^{(a)}$ part of the Hamiltonian. The nontrivial action of terms with operators $S^{(a)}$ on two adjacent spins is

$$S_1^{(a)\mp} S_2^{(a)\pm}|\pm 1\rangle \otimes |\mp 1\rangle = -2|0\rangle \otimes |0\rangle,$$

$$S_1^{(a)\pm} S_2^{(a)\mp}|0\rangle \otimes |0\rangle = -2|\pm 1\rangle \otimes |\mp 1\rangle, \tag{14a}$$

$$S_1^{(a)\pm} S_2^{(a)\mp}|0\rangle \otimes |\pm 1\rangle = 2|\pm 1\rangle \otimes |0\rangle,$$

$$S_1^{(a)\mp} S_2^{(a)\pm}|\pm 1\rangle \otimes |0\rangle = 2|0\rangle \otimes |\pm 1\rangle. \tag{14b}$$

The action of terms in Eq. (11) containing $S^{(a)z}$ reads

$$S_1^{(a)z} S_2^{(a)z}|0\rangle \otimes |0\rangle = |\widetilde{0}\rangle \otimes |\widetilde{0}\rangle, \quad S_1^{(a)z} S_2^{(a)z}|\widetilde{0}\rangle \otimes |\widetilde{0}\rangle = |0\rangle \otimes |0\rangle, \tag{15a}$$

$$S_1^{(a)z} S_2^{(a)z}|\widetilde{0}\rangle \otimes |0\rangle = |0\rangle \otimes |\widetilde{0}\rangle, \quad S_1^{(a)z} S_2^{(a)z}|0\rangle \otimes |\widetilde{0}\rangle = |\widetilde{0}\rangle \otimes |0\rangle. \tag{15b}$$

The subscripts 1 and 2 indicate the rung on which the spin operator acts.

Taking into account the positivity of antisymmetrized couplings $J_l^{(a)}$ [see Eq. (5)], we conclude that the elements generated by Eq. (14) acquire an overall minus sign in the shifted Hamiltonian matrix (11). At the same time, the elements corresponding to Eq. (15) enter in the Hamiltonian with the same sign. Hence, only the contribution from Eq. (14b) gives rise to negative matrix elements in the Hamiltonian $\widetilde{H}$, whereas Eqs. (14a) and (15) are responsible for unwanted positive off-diagonal elements. In order to alter their sign, we make the following observation.

Due to the reflection symmetry, the parity of singlet states, i.e., $(-1)^{N_0}$, is a conserved quantity under the action of each term in Eq. (11). The matrix elements (14a) and (15a) are the only ones which are responsible for the creation and annihilation of a singlet pair. Other elements rest singlet number unchanged. Thus, multiplying the basic states (9) on sign factor $(-1)^{\text{number of singlet pairs}} = (-1)^{[N_0/2]}$, one can make the elements arising from Eqs. (14a) and (15a) negative. The sign factor does not affect other matrix elements.

The remaining action (15b) just permutes the singlet and $S^z=0$ triplet states. In order to make this term negative, introduce the ordering between pairs of rung states $|0\rangle$ and $|\widetilde{0}\rangle$ inside multirung state (9). We say that a pair is ordered if $|\widetilde{0}\rangle$ is located on the left-hand side from $|0\rangle$. Denote by $N_{0\widetilde{0}}$ the number of disordered pairs in Eq. (9), i.e., the number of pairs $(|0\rangle, |\widetilde{0}\rangle)$, where $|0\rangle$ is on the left-hand side from $|\widetilde{0}\rangle$. Note that the nearest-neighbor actions (15b) change the ordering of only one pair. Therefore, if we multiply a basic state by another sign factor $(-1)^{N_{0\widetilde{0}}}$, all matrix elements generated by Eq. (15b) will change sign and become negative. At the same time, other matrix elements will hold unchained. Indeed, it is easy to see that the nearest-neighbor permutations $|\widetilde{0}\rangle|\pm 1\rangle \leftrightarrow |\pm 1\rangle|\widetilde{0}\rangle$ and $|0\rangle|\pm 1\rangle \leftrightarrow |\pm 1\rangle|0\rangle$ do not change the number of disordered pairs $N_{0\widetilde{0}}$ while pair creations and annihilations $(|\pm 1\rangle|\mp 1\rangle \leftrightarrow |\widetilde{0}\rangle|\widetilde{0}\rangle$ and $|\pm 1\rangle|\mp 1\rangle \leftrightarrow |0\rangle|0\rangle)$ change its value on *even* number. Note that a similar type of sign factor has been used in order to prove uniqueness of relative ground states for Heisenberg chains with higher symmetries.[8,30]

Finally, the basis in which all off-diagonal matrix elements of the Hamiltonian (11) are nonpositive is

$$|m_1, m_2, \ldots, m_N\rangle := (-1)^{[N_0/2]+N_{0\widetilde{0}}}|m_1\rangle \otimes |m_2\rangle \otimes \cdots \otimes |m_N\rangle. \tag{16}$$

C. Relative ground states in $S^z=M$, $\mathcal{R}=\sigma$ subspaces

Due to the spin projection and reflection symmetries, the Hamiltonian is invariant on each subspace with the definite values of spin projection and reflection operators: $S^z=M$, $\mathcal{R}=\sigma$, where $M=-N, -N+1, \ldots, N$ and $\sigma=\pm 1$. Keeping the terminology, we call it (M,σ) subspace. Below, we outline the proof that the matrix of the Hamiltonian in basis (16) being restricted on every (M,σ) subspace is connected.

Note that due to Eq. (5), all local actions considered in Eqs. (14) and (15) contribute in the Hamiltonian (6) with nonvanishing coefficients. It is easy to verify using Eqs. (12), (14), and (15) that any two adjacent states $|m_l\rangle\otimes|m_{l+1}\rangle$ and $|m_l'\rangle\otimes|m_{l+1}'\rangle$ are connected by the lth local terms of the Hamiltonian (11) provided that their quantum numbers are subjected to the conservation laws. In other words, both states must possess the same spin projection and reflection quantum numbers. This rule can be generalized by induction to any two basic states (11). In fact, any symmetric $(\sigma=1)$ basic state (16) after successive applications of the local terms in Eq. (11) can be transformed to state

$$|\underbrace{\pm 1,\ldots,\pm 1}_{|M|},\tilde{0},\ldots,\tilde{0}\rangle,$$

where plus (minus) sign holds for positive (negative) values of M. Similarly, any antisymmetric $(\sigma=-1)$ state is connected to state

$$|\underbrace{\pm 1,\ldots,\pm 1}_{|M|},\tilde{0},\ldots,\tilde{0},0\rangle.$$

This finishes the proof of the connectivity.

Now all conditions of Perron-Frobenius theorem[31] are fulfilled and one comes to the following result.

• The relative ground state $|\Omega\rangle_{M,\sigma}$ of $\tilde{H}$ in (M,σ) subspace is unique and is a positive superposition of all basic states:

$$|\Omega\rangle_{M,\sigma}=\sum_{\substack{\Sigma_l m_l=M\\(-1)^{N_0}=\sigma}}\omega_{m_1,\ldots,m_N}|m_1,m_2,\ldots,m_N\rangle,\quad \omega_{m_1,\ldots,m_N}>0. \tag{17}$$

The state $|\Omega\rangle_{M,\sigma}$ must have a definite value $S_{M,\sigma}$ of total spin quantum number. Otherwise, it could be presented as a superposition of independent states with different spins but the same energy. This would be in contradiction with the uniqueness condition established above. It is evident that if some spin-S state overlaps with the relative ground state $|\Omega\rangle_{M,\sigma}$ then $S_{M,\sigma}=S$. Below, we use this property in order to determine $S_{M,\sigma}$.

Due to the spin reflection symmetry $S_{M,\sigma}=S_{-M,\sigma}$. So, one can consider only non-negative values of M. First, we suppose that $M>0$.

If $\sigma=(-1)^{N-M}$, then the state

$$|\phi\rangle=|\underbrace{1,\ldots,1}_{M},\underbrace{0,\ldots,0}_{N-M}\rangle,$$

which is the highest weight state for a spin $S=M$ multiplet, contributes in the sum (17). Therefore, it overlaps with the relative ground state. According to the arguments above, $S_{M,\sigma}=M$ for this case.

Else if $\sigma=(-1)^{N-M-1}$, then both states

$$|\tilde{0},\underbrace{1,\ldots,1}_{M},\underbrace{0,\ldots,0}_{N-M-1}\rangle$$

and

$$|1,\tilde{0},\underbrace{1,\ldots,1}_{M-1},\underbrace{0,\ldots,0}_{N-M-1}\rangle$$

are also presented in the decomposition of $|\Omega\rangle_{M,\sigma}$ with *positive* coefficients. According to the definition (16) of basic states, their sum, up to a nonessential sign factor, can be presented as $|\psi\rangle=\sqrt{1/2}(|1\rangle\otimes|\tilde{0}\rangle+|\tilde{0}\rangle\otimes|1\rangle)\otimes|1,\ldots,1,0,\ldots,0\rangle$ and, of course, overlaps with Eq. (17). In fact, $|\psi\rangle$ has a definite spin value, which we will determine now. Remember we are currently working with the Hamiltonian (11), obtained from the original one by unitary shift (10). Turning back to H representation, we have to shift the states back. Thus, the original state is

$$U^{-1}|\psi\rangle=U|\psi\rangle\sim\sqrt{1/2}(-|1\rangle\otimes|\tilde{0}\rangle+|\tilde{0}\rangle\otimes|1\rangle)\otimes|\underbrace{1,\ldots,1}_{M-1},0,\ldots,0\rangle$$

up to an overall sign factor. The first term of the product is the highest state of the triplet in the decomposition of two triplets, while the second term is the highest state of $S=M-1$ multiplet. Together they form an $S=M$ multiplet. Therefore, $S_{M,\sigma}=M$ in the case of $\sigma=(-1)^{N-M-1}$, too.

Consider now the two subspaces with $M=0$. If $\sigma=(-1)^N$, the state constructed from rung singlets participates in the sum (17), so the relative ground state is a spin singlet too: $S_{0,\sigma}=0$. If $\sigma=(-1)^{N-1}$, the triplet state

$$|\tilde{0},\underbrace{0,\ldots,0}_{N-1}\rangle$$

enters in the sum, and, therefore, the relative ground state is a triplet, i.e., $S_{0,\sigma}=1$.

Summarizing the results, we arrive at the following conclusion.

• The relative ground state $|\Omega\rangle_{M,\sigma}$ always belongs to a spin-$|M|$ multiplet except $M=0$ and $\sigma=(-1)^{N-1}$ cases when it belongs to a spin triplet. In other words,

$$S_{M,\sigma}=\begin{cases}1 & \text{if } M=0 \text{ and } \sigma=(-1)^{N-1},\\ |M| & \text{for other values of } M \text{ and } \sigma.\end{cases} \tag{18}$$

D. Ordering rule among the lowest levels in sectors with different value of total spin

Consider now the restriction of the Hamiltonian to the sector containing states with fixed values of the total spin and reflection quantum numbers. Apparently, the relative ground state $|\Omega\rangle_{M,\sigma}$ is also the lowest-energy state in the sector characterized by $S=S_{M,\sigma}$ and $\mathcal{R}=\sigma$. Denote by $E_{S,\sigma}$ the lowest-energy level in that sector. According to the previous section, the relative ground state is unique on (M,σ) subspace. Therefore, the level $E_{S,\sigma}$ with $S=S_{M,\sigma}$ must be nondegenerate, i.e., it must contain only one spin-S multiplet with parity σ. This is just the multiplet, which encloses the state $|\Omega\rangle_{M,\sigma}$ itself. Using Eq. (18), it is easy to see that any level $E_{S,\sigma}$ is nondegenerate, in this regard, except perhaps the one with $S=0$ and $\sigma=(-1)^{N-1}$.

Moreover, every (M,σ) subspace contains a representative from any multiplet with parity σ and spin $S\geqslant|M|$.

Therefore, the state $|\Omega\rangle_{M,\sigma}$ has the minimum energy for all these multiplets. According to Eq. (18), its spin has the value $S_{M,\sigma}=|M|$ provided that $\sigma=(-1)^N$. The uniqueness of relative ground state then implies that all levels $E_{S,\sigma}$ with spin $S > S_{M,\sigma}$ are higher than the level with $S=S_{M,\sigma}$. Consequently, $E_{S,\sigma}$ is a monotone increasing function of S. If $\sigma=(-1)^{N-1}$, then the last equation is true for $|M|>0$ only and, hence, $E_{S,\sigma}$ increases in the range $S\geq 1$.

Finally, we arrive at the following conclusion.

• The minimum-energy levels $E_{S,\sigma}$ are nondegenerate [except perhaps the one with $S=0$ and $\sigma=(-1)^{N-1}$] and are ordered according to the rule:

$$E_{S_1,\sigma} > E_{S_2,\sigma}: \begin{cases} \text{for } \sigma=(-1)^N & \text{if } S_1 > S_2, \\ \text{for } \sigma=(-1)^{N-1} & \text{if either } S_1 > S_2 \geq 1 \quad \text{or } S_1 = 0, \quad S_2 = 1. \end{cases} \tag{19}$$

The ordering rule above enables to determine the total spin of the minimum-energy states in the symmetric and antisymmetric sectors.

• The ground state in the entire $\sigma=(-1)^N$ sector is a spin singlet while in the $\sigma=(-1)^{N-1}$ sector it is a spin triplet. In both cases, it is unique.

In other words, for a frustrated ladder with an even number of rungs, the ground state in the symmetric sector is a singlet state, while in the antisymmetric sector it is formed by the three states of a triplet. In contrast, for the odd number of rungs, it is a singlet in the antisymmetric sector, while in the symmetric sector, it consists of three triplet states.

III. GROUND STATE

A. Exact results

The ordering rule (21) does not compare energy levels in the symmetric ($\sigma=1$) sector with the levels in the antisymmetric ($\sigma=-1$) sector. It is clear that the total ground state coincides with the minimum-energy state in either symmetric or antisymmetric sector. If the lowest levels in both sectors coincide, the total ground state becomes degenerate. Using the results of the previous section, we come to the following conclusion. The ground state of a frustrated ladder with couplings obeying Eq. (2) may be: (a) a unique $\sigma=(-1)^N$ spin singlet; (b) a unique $\sigma=(-1)^{N-1}$ spin-triplet; (c) any superposition of both of them, i.e., singlet ⊕ triplet.

The frustrated ladder (1) in certain parameter regions belongs to a large class of reflection-symmetric models considered recently by Lieb and Schupp.[11] In the Appendix, the rigorous results obtained in Ref. 11 are applied to the frustrated spin ladder case. It appears that *all* ground states of the Hamiltonian (1) are spin *singlets* if the couplings satisfy $J_l^{\perp} > |J_{l-1}^{\times}| + |J_l^{\times}|$, where $J_0^{\times}=J_N^{\times}=0$ is supposed. The nonstrict inequality sign can be set instead of a strict one for antiferromagnetic values of diagonal couplings. The details are given in the Appendix. Note that the aforementioned result is true for any values of intrachain couplings $J_l^{\parallel}$ including ferromagnetic ones.

From the other side, for $J_l^{\parallel} > |J_l^{\times}|$, our results established in the previous section become valid, too. Setting together both Lieb-Schupp and our results, we come to the conclusion that *only* case (a) above can take place. This means that the ground state is a unique $\sigma=(-1)^N$ singlet, provided that the couplings satisfy

$$J_l^{\perp} > |J_{l-1}^{\times}| + |J_l^{\times}| \quad \text{and } J_l^{\parallel} > |J_l^{\times}|.$$

Consider separately the most familiar case of a ladder with site-independent couplings. According to the discussions above and in the Appendix, we come to the following conclusion. The ground state of finite-size frustrated ladder model with antiferromagnetic rung $J^{\perp}$ and intrachain $J^{\parallel}$ interactions is a unique spin singlet with $\sigma=(-1)^N$ reflection symmetry if the couplings satisfy $J^{\perp} \geq 2J^{\times} > -J^{\perp}$ and $J^{\parallel} > |J^{\times}|$.

It must be emphasized that this result is rigorous for finite-size ladders only, which are the main objects of study in this particle.

B. Thermodynamic limit, comparison with other approaches and numerical test

The results obtained above are in good agreement with the ground-state properties of a frustrated ladder model, which have been investigated intensively in the literature so far. From our results, it is unclear whether or not the singlet-triplet degeneracy takes place for finite-size ladders. Moreover, in the thermodynamic limit $N \to \infty$, the additional degeneracy of energy levels can occur and, in principle, the strict inequality in Eq. (19) must be replaced by a nonstrict one. The investigations carried out by different methods suggest that all three possibilities for the ground state described in the previous section may take place. In fact, the ground-state degeneracy happens at critical points only, while in most cases, the ground state is a unique $\sigma=(-1)^N$ singlet or $\sigma=(-1)^{N-1}$ triplet. This property remains true in the thermodynamic limit. The rest of this section is devoted to the testing of our exact results and more detailed comparison with data obtained by other methods.

The weak interchain coupling analysis ($J^{\perp}, J^{\times} \ll J^{\parallel}$) based on the conformal field theory approach shows that for $J^{\perp} > 2J^{\times}$, the ground state has a tendency to form singlets along the rungs and triplets along the diagonals, while for $J^{\perp} < 2J^{\times}$, it has a tendency to form triplets along the rungs and singlets along the diagonals.[23] The former ground state

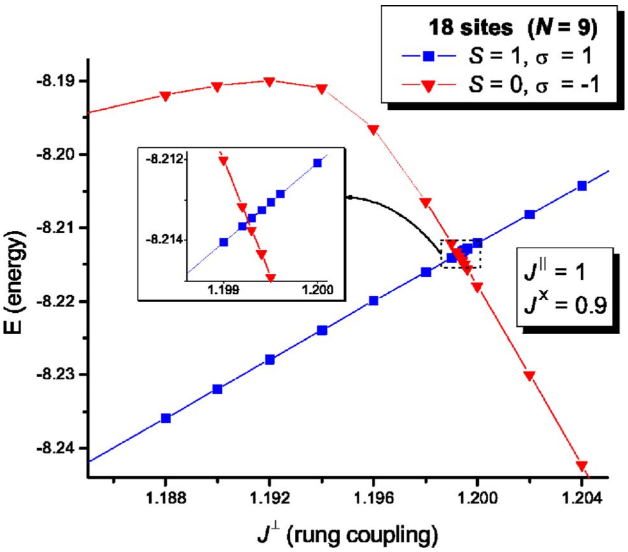

FIG. 2. (Color online) Two lowest-energy levels, obtained by exact diagonalization of frustrated ladder with 18 sites ($N=9$), are plotted as a function of rung coupling. Corresponding states have different spin S and reflection σ quantum numbers. The level crossing happens at some point.

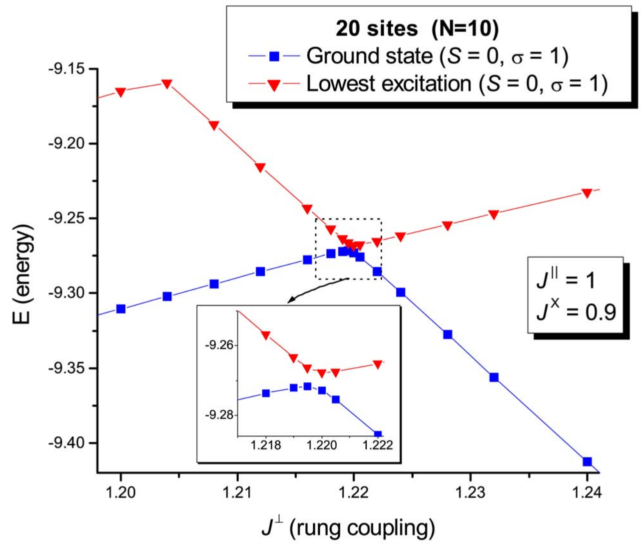

FIG. 3. (Color online) The ground state and lowest excitation of frustrated ladder with 20 sites ($N=10$) obtained by exact diagonalization for different values of rung coupling. Both states have the same quantum numbers. The level crossing does not happen in agreement with our exact results.

corresponds to the usual ladder or rung-dimer phase, while the last one corresponds to spin-1 Haldane chain. In both cases, it is nondegenerate. The two phases belong to the same universality class because a continuous path connecting them exists and it does not contain any critical point.[32] The distinction between them has a topological character.[25,26] For $J^{\perp}=2J^{\times}$, both types of dimerized ground states exist leading to twofold degeneracy.[23]

Numerical simulations[24,26] strongly support this picture and extend the phase transition curve out of the weak coupling region. The transition curve obeys the relation $J^{\perp}<2J^{\times}$ and approaches to the line $J^{\perp}=2J^{\times}$ at the weak coupling limit.

The properties of the ground state differ for ladders with odd and even values of the rung number. First, we consider odd-rung ladders. Small values of rung coupling $J^{\perp}$ give rise to Haldane-type ground state, which is a spin triplet with $\sigma=1$ [case (b) in the previous section], while large values lead to rung-singlet-type ground state with $\sigma=-1$ [case (a)]. At some intermediate point, the level crossing happens, which corresponds to the aforementioned case (c) with degenerate singlet-triplet ground state. The level crossing point approaches to the critical line in the thermodynamic limit. The numerical investigation of small size ladder Hamiltonians supports this picture. In Fig. 2, the two lowest levels of a frustrated ladder with 18 sites ($N=9$) obtained by exact diagonalization are plotted for different values of rung coupling. The figure clearly indicates that both levels cross at some point.

On the contrary, for even-rung ladders, both Haldane and rung-dimmer states are singlets and located in the $\sigma=1$ sector. The level crossing is forbidden in this case because our results exclude the existence of degenerate double-singlet ground state for finite-size systems. In Fig. 3, we present the two lowest levels obtained by numerical diagonalization of the system with 20 sites ($N=10$) close to the composite spin point $J^{\parallel}=J^{\times}$. Both levels approach each other but do not intersect. The level crossing is absent. It occurs at the composite spin point, which is out of the parameter space (2) considered in this paper. This model will be discussed in the next section. In the thermodynamic limit, the closest point of both levels approaches the level crossing point of odd-rung ladders and the level crossing picture recovers.

Similar behavior is observed for ferromagnetic interchain couplings ($J^{\perp}<0$ and $J^{\times}<0$). Large values of $|J^{\perp}|$ correspond to Haldane phase and its small values put the system in rung-dimmer phase. The phase transition curve in the thermodynamic limit is remarkably close to the line $J^{\perp}=2J^{\times}$ (Ref. 33) and coincides with it in the weak interchain interaction limit.[23] This curve has been traced out with high precision by applying different boundary conditions for each phase.[26] A slight deviation from it is observed close to the ferromagnetic phase only.

IV. COMPARISON WITH KNOWN RESULTS

In this section, we compare the properties of the generalized ladder Hamiltonians (1) and (2) established in the previous section with those obtained earlier for some particular values of couplings.

A. Ferromagnetic rung interactions

If we set all rung couplings to be ferromagnetic and others to be antiferromagnetic, the ladder model (1) becomes *bipartite*. The two sublattices A and B, forming the ladder, consist of spins of even and odd rungs correspondingly. Then the conditions of standard Lieb-Mattis ordering theorem[6] are fulfilled. The Ising basis after the unitary shift (10) becomes negative. Thus the relative ground state $|\Omega\rangle_M$ is unique in whole subspace $S^z=M$. Apparently, it is an eigenstate of the reflection operator. The corresponding eigenvalue is $\sigma=1$ because $|\Omega\rangle_M$ is a positive superposition of shifted basic states[6] and the shift operator (10) remains invariant with respect to the reflection. Thus, in this case the minimal energy in the symmetric sector is lower than the corresponding one in the antisymmetric sector: $E_S=E_{S,1}<E_{S,-1}$. As was mentioned in the Introduction, the ground state is unique and has spin $S_{gs}=|S_A-S_B|$,[6,7] i.e., is a singlet for even values of N and triplet for odd values of N. In both cases, $\sigma=1$. This is in agreement with our results, which claim that $\sigma=(-1)^N$ for singlet ground state and $\sigma=(-1)^{N-1}$ for the triplet one. All mentioned properties are similar to the properties of spin-1 Haldane chain because due to ferromagnetic rung couplings, which make preferable rung triplet states, the low-energy properties are well described by Haldane chain.[34,35]

B. Ferromagnetic diagonal interactions

Consider now the ladder with ferromagnetic diagonal couplings and antiferromagnetic rung and intrachain couplings. The low-energy properties of this system have been investigated recently in Ref. 33. The model contains a standard antiferromagnetic ladder as a particular case. The frustration is lost in this case, too. The lattice becomes bipartite of checkerboard-type and the Lieb-Mattis theorem can be applied in this case, too. The sublattice A consists of the odd sites of the first chain and the even sites of the second chain, while the sublattice B consists of the even sites of the first chain and the odd sites of the second one. The spin-rotation operator leading to a nonpositive basis is given by $U'=\exp(i\pi S_A^z)$, where $S_A^z=\Sigma_l(S_{1,2l-1}^z+S_{2,2l}^z)$ is the spin projection operator of A sublattice.[6] As in the previous case, the relative ground state $|\Omega\rangle_M$ in M subspace is expressed as a positive superposition of the shifted basic states $\left|{m_{1,1},\dots,m_{1,N} \atop m_{2,1},\dots,m_{2,N}}\right\rangle=U'\left(\left|{m_{1,1} \atop m_{2,1}}\right\rangle\otimes\dots\otimes\left|{m_{1,N} \atop m_{2,N}}\right\rangle\right)$, where $m=\uparrow,\downarrow$ labels on-site spins. Now using the definition of $\mathcal{R}$ and U' after a simple algebra, we obtain

$$\mathcal{R}\left|\begin{matrix} m_{1,1},\dots,m_{1,N} \\ m_{2,1},\dots,m_{2,N}\end{matrix}\right\rangle = e^{i\pi(S^z-2S_A^z)}\left|\begin{matrix} m_{2,1},\dots,m_{2,N} \\ m_{1,1},\dots,m_{1,N}\end{matrix}\right\rangle = (-1)^{N-M}\left|\begin{matrix} m_{2,1},\dots,m_{2,N} \\ m_{1,1},\dots,m_{1,N}\end{matrix}\right\rangle.$$

Hence, we have $\mathcal{R}|\Omega\rangle_M=(-1)^{N-M}|\Omega\rangle_M$. Thus, among two (M,σ) subspaces with different values of σ, the minimal energy level in the subspace with $\sigma=(-1)^{N-M}$ is the lowest: $E_S=E_{S,\sigma}<E_{S,-\sigma}$. The total ground state is a spin singlet with $\sigma=(-1)^N$ reflection quantum number in accordance with our results in Sec. II.

C. Composite spin model

The equal values of diagonal and intrachain couplings $(J_l^{\times}=J_l^{\|})$ correspond to a so-called composite spin model.[36] These values of coupling parameters are out of the range (2), where the results of Sec. II are valid. However, due to continuity, some results still remain true in this limiting case. In particular, the ordering rule is fulfilled after replacing the strict inequality sign in Eq. (19) by the nonstrict one like in the thermodynamic limit.

In contrast, the results related to the uniqueness of relative ground states cannot be applied here. Indeed, in this case, $J_l^{(a)}=0$ and the antisymmetrized term, which is responsible for the exchanges between singlet and triplet rung states, is absent in the Hamiltonian (11). The spins of individual rungs are now conserved quantities.[20] Therefore, all singlets remain frozen at their sites and the Hamiltonian is *not connected* on (M,σ) subspaces anymore. For site-independent values of couplings, the ground state has been obtained explicitly.[20] For small values of $J^{\perp}$, it is reduced to the ground state of Haldane chain ($S=0$ for even N, $S=1$ for odd N and $\sigma=1$ always), while the large values lead to the rung-singlet state $|0\rangle\otimes\dots\otimes|0\rangle$ [$S=0$ and $\sigma=(-1)^N$]. This agrees with our results in Sec. III. Both states are eigenstates of the composite spin Hamiltonian, which makes the level crossing at some critical point $J_c^{\perp}(N)<2J^{\times}$ inevitable. For even values of N, the degeneracy disappears under a weak deviation from the composite spin point, as has been discussed in Sec. III. However, the two lowest levels still approach closely, as is shown in Fig. 3.

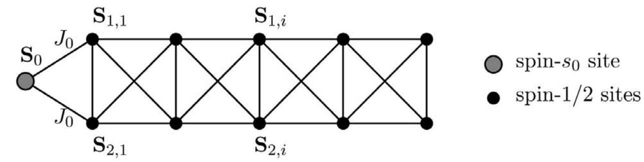

FIG. 4. Spin-1/2 frustrated ladder with boundary impurity spin s_0.

V. ORDERING IN FRUSTRATED LADDER WITH BOUNDARY IMPURITY

Consider frustrated spin-1/2 ladder (1) with an impurity spin s_0 coupled antiferromagnetically to two spins of the first rung, as is shown in Fig. 4. The original Hamiltonian (1) is supplemented by boundary term $H_{\text{imp}}=J_0\mathbf{S}_0\cdot\mathbf{S}_1^{(s)}$, $J_0>0$, which preserves the reflection symmetry.

A. Relative ground states

After the rotation of odd-rung spins on angle π around z axis by means of unitary operator (10), the impurity-ladder interaction term acquires the form

$$\widetilde{H}_{\text{imp}}=UH_{\text{imp}}U^{-1}=-\frac{J_0}{2}(S_0^+S_1^{(s)-}+S_0^-S_1^{(s)+})+J_0S_0^zS_1^{(s)z}.$$

We will work here in a basis, which is a natural extension of the basis (16), used before for the ladder with free boundary conditions:

$$|m_0\rangle\otimes|m_1,\dots,m_N\rangle=(-1)^{[N_0/2]+N_0\tilde{0}}|m_0\rangle\otimes|m_1\rangle\otimes\cdots\otimes|m_N\rangle. \tag{20}$$

Here $|m_0\rangle:=|s_0,m_0\rangle$ $(m_0=-s_0,\dots,s_0-1,s_0)$ is the usual basis of spin-s_0 multiplet. All nonvanishing matrix elements of $S_0^{\pm}$ are positive: $\langle m_0|S_0^+|m_0-1\rangle=\langle m_0-1|S_0^-|m_0\rangle=\sqrt{(s_0+m_0)(s_0-m_0+1)}>0$. It is easy to see that the spin exchanges due to the boundary term do not affect the sign factor $(-1)^{[N_0/2]+N_{0\tilde{0}}}$. This, together with Eq. (12), implies that $\tilde{H}_{\text{imp}}$ has only nonpositive off-diagonal elements in the basis (20).

The bulk part (11) of the Hamiltonian is also nonpositive in this basis as was proved already in Sec. II. Thus, the entire Hamiltonian $\tilde{H}+\tilde{H}_{\text{imp}}$ has no positive off-diagonal elements, too.

It is easy to ensure that its restriction to any (M,σ) subspace with fixed spin projection M and reflection σ quantum numbers is connected. This can be shown using the arguments similar to those applied before for the ladder without impurity spin.

Applying again Perron-Frobenius theorem, we come to the conclusion that the relative ground state of $\tilde{H}+\tilde{H}_{\text{imp}}$ of each (M,σ) subspace is unique and is a positive superposition of *all* basic states (20):

$$|\Omega\rangle_{M,\sigma}=\sum_{\substack{\Sigma_l m_l=M\\(-1)^{N_0}=\sigma}}\omega_{m_0,\ldots,m_N}|m_0\rangle\otimes|m_1,\ldots,m_N\rangle,$$

$$\omega_{m_0,\ldots,m_N}>0. \tag{21}$$

Now turn to the determination of the spin $S_{M,\sigma}$ of this state. As before, in order to do this, we will construct a state with certain value of spin and positive or vanishing coefficients in its decomposition over the basic states (20). In this case, it will overlap with the relative ground state (21). Then the uniqueness of the relative ground state would indicate that both states have the same spin value.

Due to the spin reflection symmetry, both states $|\Omega\rangle_{\pm M,\sigma}$ have the same spin quantum number. Thus, without any restriction, we can consider $M\geqslant 0$ values only. First, we consider the values $M\geqslant s_0$ and will prove below that $S_{M,\sigma}=M$.

In $\sigma=(-1)^{N-M+s_0}$ sector, there is a simple highest state

$$|s_0\rangle\otimes|\underbrace{1,\ldots,1}_{M-s_0},0,\ldots,0\rangle$$

of a multiplet with spin $S=M$. It coincides up to an unessential sign factor with one of the basic states (20). Therefore, $S_{M,\sigma}=M$ for this case.

For the opposite values of the reflection quantum number $[\sigma=(-1)^{N-M+s_0-1}]$, we take as an indicator the state

$$|\psi'\rangle=\left(\sqrt{\frac{s_0}{s_0+1}}|s_0\rangle\otimes|\tilde{0}\rangle+\frac{1}{\sqrt{s_0+1}}|s_0-1\rangle\otimes|1\rangle\right)\otimes|\underbrace{1,\ldots,1}_{M-s_0},0,\ldots,0\rangle,$$

which can be considered as a generalization of the state $|\psi\rangle$ used before for the bulk ladder. Again, $|\psi'\rangle$ is a positive superposition of two basic states from Eq. (20). As has been done before for state $|\psi\rangle$, its spin can be detected going back to the original H representation: $|\psi'\rangle\rightarrow U^{-1}|\psi'\rangle$. As a result, just the sign of the second term in the brackets is changed. It is easy to check that $\sqrt{\frac{s_0}{s_0+1}}|s_0\rangle\otimes|\tilde{0}\rangle-\sqrt{\frac{1}{s_0+1}}|s_0-1\rangle\otimes|1\rangle$ is the highest state of spin-s_0 multiplet, which appears in the decomposition of the tensor product of two multiplets with spins s_0 and 1. Thus, the spin of the entire shifted state $U^{-1}|\psi'\rangle$ is again M.

Next, we consider the values $0\leqslant M<s_0$, which are essential for $s_0\geqslant 1$. We will show that in this case the relative ground state in (M,σ) subspace belongs to a spin $S_{M,\sigma}=s_0$ multiplet if $\sigma=(-1)^N$; otherwise it belongs to a spin $S_{M,\sigma}=s_0-1$ multiplet. The first case is easy to prove using for the test the basic state $|M\rangle\otimes|0,\ldots,0\rangle$ of spin s_0. For the second case, we choose as a test the state

$$|\psi''\rangle=|\chi\rangle\otimes\underbrace{|0\rangle\otimes\ldots\otimes|0\rangle}_{N-1},$$

where

$$|\chi\rangle=\sqrt{\frac{(s_0-M+1)(s_0-M)}{2s_0(2s_0+1)}}|M-1\rangle\otimes|1\rangle+\sqrt{\frac{(s_0-M)(s_0+M)}{s_0(2s_0+1)}}|M\rangle\otimes|\tilde{0}\rangle+\sqrt{\frac{(s_0+M+1)(s_0+M)}{2s_0(2s_0+1)}}|M+1\rangle\otimes|-1\rangle.$$

It is easy to see that $|\psi''\rangle$ is a positive superposition of three states from the basic set (20). The action of U^{-1} on $|\psi''\rangle$ changes only the sign of the first and last terms of $|\chi\rangle$ giving rise to a state of spin $S=s_0-1$ multiplet, as is easy to verify by applying $(\mathbf{S}_0+\mathbf{S}_1^{(s)})^2$ to it.

Finally, summarizing the results obtained above, we arrive at the following conclusion.

• For the ladder with diagonal interactions obeying Eq. (2) and antiferromagnetically coupled boundary impurity s_0 the relative ground state in (M,σ) subspace is nondegenerate and belongs to a multiplet with the spin

$$S_{M,\sigma}=\begin{cases}|M| & \text{if } |M|\geqslant s_0\\ s_0 & \text{if } |M|<s_0 \text{ and } \sigma=(-1)^N\\ s_0-1 & \text{if } |M|<s_0 \text{ and } \sigma=(-1)^{N-1}.\end{cases} \tag{22}$$

Note that for $s_0=1/2$ value of impurity spin, only the first line holds and we have simply $S_{M,\sigma}=|M|$.

B. Ordering rule and ground state

Using the spin value of the relative ground state (22) and its uniqueness proved above, one can compare the minimal energy levels $E_{S,\sigma}$ of the sectors with fixed spin and reflection quantum numbers and study their degeneracy just in the same way as was done above for the open ladder.

For $\sigma=(-1)^N$, it is clear from Eq. (22) that the energy level $E_{S,\sigma}$ is nondegenerate for any $S\geqslant s_0$. The uniqueness of the relative ground state suggests that all levels with spin $S>S_{M,\sigma}$ are above the level with $S=S_{M,\sigma}$, which contains the state $|\Omega\rangle_{M,\sigma}$ itself. Thus, $E_{S,\sigma}$ is a monotone increasing function of spin in the range $S \geqslant s_0$. For $S < s_0$, the level degeneracy and ordering are not clear. All relative ground states $|\Omega\rangle_{M,\sigma}$ with $|M| \leqslant s_0$ constitute a spin-s_0 multiplet having the lowest-energy value among all states with the reflection parity $\sigma=(-1)^N$.

For $\sigma=(-1)^{N-1}$, the level $E_{S,\sigma}$ is nondegenerate for any $S \geqslant s_0-1$. The lowest-energy $E_{S,\sigma}$ is a monotone increasing function of spin in the range $S \geqslant s_0-1$. In the case of $s_0 \geqslant 1$, all relative ground states $|\Omega\rangle_{M,\sigma}$ with $|M| \leqslant s_0-1$ are combined into $S=s_0-1$ multiplet having the minimal energy among the states with $\sigma=(-1)^{N-1}$. For $s_0=1/2$, the lowest level increases with spin everywhere. The following statement sums up the discussions above.

• For the ladder with diagonal interactions obeying $J_l^{\parallel} > |J_l^{\times}|$ and antiferromagnetically coupled boundary impurity s_0 the lowest-energy levels in sectors with fixed value of spin S and reflection σ quantum numbers are ordered according to the rule:

$$E_{S_1,\sigma} > E_{S_2,\sigma}: \begin{cases} \text{for } \sigma = (-1)^N & \text{if either } S_1 > S_2 \geqslant s_0 \text{ or } S_1 < S_2 = s_0 \\ \text{for } \sigma = (-1)^{N-1} & \text{if either } S_1 > S_2 \geqslant s_0 - 1 \text{ or } S_1 < S_2 = s_0 - 1 . \end{cases} \tag{23}$$

•The ground state of the model in the entire $\sigma=(-1)^N$ sector is a $S=s_0$ multiplet, while in the entire $\sigma=(-1)^{N-1}$ sector it is a $S=|s_0-1|$ multiplet. In both cases, it is unique.

The absolute value sign is used in order to take into consideration the impurity with $s_0=1/2$ also. In that case, the ordering rule (23) is simplified because in that case $S=1/2$ is the lowest value of the total spin and the relation $E_{S_1,\sigma} > E_{S_2,\sigma}$ holds for any σ and any two spins obeying $S_1 > S_2$. The lowest-energy states in both symmetric and antisymmetric sectors are unique spin doublets.

As for the ladder model without impurity, one cannot compare energy levels related to different reflection quantum numbers. Nevertheless, one can gain information about the total ground state of the model from the ordering rule established above. The total ground state is nondegenerate and either belongs to $\sigma=(-1)^N$ sector and, hence, has spin value $S=s_0$ or belongs to $\sigma=(-1)^{N-1}$ and has spin $S=|s_0-1|$. If the lowest-energy levels in both sectors coincide, which can occur, for example, due to some additional symmetry presented in the model, then the ground state becomes degenerate and is the superposition of two multiplets with spin values s_0 and $|s_0-1|$. Therefore, the ground state could be *at most* doubly degenerate.

In contrast to the model with free boundary conditions studied in Sec. II, here we cannot apply the Lieb-Schupp results[10,11] in order to choose the valid quantum numbers for the ground state. The reason is that their approach cannot be used for a reflection-symmetric spin system if some spins are positioned on the symmetry axis.

C. An example: Periodic spin-1/2 chain with odd number of spins

The translationally invariant periodic spin-1/2 chain with *odd* $N'=2N+1$ number of spins is a particular case of the general class of frustrated ladders with boundary spin considered in this section. It corresponds to $s_0=1/2$ and $J_0=J_l^{\parallel}=J_N^{\perp}$ with vanishing values for other coupling coefficients. The model is integrable by Bethe ansatz[37] like its more familiar even-site counterpart, but many of its properties differ from those of even-site chain.[38] In particular, the even-site chain is bipartite and Lieb-Mattis theorem is valid in this case, while the odd-site chain is a frustrated system. Recently, the classical ground state of the last model has been constructed and the lowest energy has been obtained exactly.[39]

The system possesses an additional symmetry: it remains invariant with respect to the cyclic translation by one site T. The translation and reflection operators satisfy the commutation relation $\mathcal{R}T=T^{-1}\mathcal{R}$. Thus, if $|\psi\rangle$ is an eigenstate of T with eigenvalue $e^{i\phi}$ then the reflected state $\mathcal{R}|\psi\rangle$ is also an eigenstate with eigenvalue $e^{-i\phi}$. Hence, for all values of momentum except $\phi=0,\pi$, the energy levels of periodic chain are at least twofold degenerate.

The relative ground states of even-site translationally invariant chain have just the exceptional values of momenta (0 or π), which is in agreement with their uniqueness. In contrast, for odd-site chain, the exact solution shows that relative ground state in $S^z=M$ subspace is *exactly* doubly degenerate with two opposite momenta $\phi=\pm\pi(M+1/N')$.[37] This is in agreement with our results, which assert that it should be *at most* doubly degenerate. Therefore, the relative ground states in symmetric and antisymmetric M subspaces have the same energy levels. The reason of the degeneracy is the translation symmetry, which mixes these two states. Hence, the lowest levels in symmetric and antisymmetric sectors coincide ($E_{S,1}=E_{S,-1}=E_S$) except, of course, $M=\pm N'/2$ subspaces, where only one ferromagnetic state presents. Moreover, antiferromagnetic ordering rule ($E_{S_1} > E_{S_2}$ if $S_1 > S_2$) is fulfilled for even-site chains. The total ground state is the combination of two spin doublets with different reflection quantum numbers.

VI. PERIODIC LADDER

Consider now the frustrated ladder with periodic boundary conditions. The bulk Hamiltonian (1) is supplemented by the term

$$H_{\text{per}} = J_N^{\parallel}(\mathbf{S}_{1,N}\cdot\mathbf{S}_{1,1} + \mathbf{S}_{2,N}\cdot\mathbf{S}_{2,1}) + J_N^{\times}(\mathbf{S}_{1,N}\cdot\mathbf{S}_{2,1} + \mathbf{S}_{1,1}\cdot\mathbf{S}_{2,N}),$$

which describes the interactions between the spins of the first and last rungs. Following Eq. (2), we set the condition $J_N^{\perp}$

$>|J_N^{\times}|$ on the boundary coupling constants. In the expression of the Hamiltonian, in terms of symmetrized and antisymmetrized spin operators (4), the boundary term contributes as $H_{\text{per}}=J_N^s\mathbf{S}_N^{(s)}\cdot\mathbf{S}_1^{(s)}+J_N^a\mathbf{S}_N^{(a)}\cdot\mathbf{S}_1^{(a)}$, where the coefficients J_N^s, and J_N^a are given in Eq. (5). Both are antiferromagnetic.

Under the action of unitary shift operator (10), the total Hamiltonian acquires the form $\tilde{H}+\tilde{H}_{\text{per}}$, where $\tilde{H}$ is derived already in Eq. (11) and

$$\tilde{H}_{\text{per}} = UH_{\text{per}}U^{-1} = \frac{(-1)^{N-1}}{2}(J_N^s S_1^{(s)+}S_N^{(s)-} + J_N^s S_1^{(s)-}S_N^{(s)+} + J_N^a S_N^{(a)+}S_1^{(a)-} + J_N^a S_N^{(a)-}S_1^{(a)+}) + J_N^s S_1^{(s)z}S_N^{(s)z} + J_N^a S_1^{(a)z}S_N^{(a)z}. \tag{24}$$

The boundary term $\tilde{H}_{\text{per}}$ produces positive off-diagonal elements in the basis (16), in which the bulk part $\tilde{H}$ of the total Hamiltonian is negative. One reason is the sign factor $(-1)^{N-1}$ in Eq. (24) due to which positive off-diagonal elements appear for even values of N. Another more important reason is that the sign factor $(-1)^{N_{0\tilde{0}}}$ in front of basic states (16) is essentially nonlocal. Remember that $N_{0\tilde{0}}$ counts the number of such $(|0\rangle, |\tilde{0}\rangle)$ pairs that $|0\rangle$ is positioned on the left-hand side from $|\tilde{0}\rangle$. The exchange between the first and last rung spins can produce an uncertain sign factor, which depends on intermediate rung states. Below, we will derive the conditions under which the basis (16) nevertheless remains nonpositive.

The term $S_1^{(s)z}S_N^{(s)z}$ is diagonal in the basis (16). The other terms produce off-diagonal elements. First, consider the matrix elements, which are generated by the terms with $S^{(a)z}$. They do not depend on the parity of N. Using Eqs. (15) and (16), it is easy to check that

$$\langle\tilde{0},\ldots,\tilde{0}|S_1^{(a)z}S_N^{(a)z}|0,\ldots,0\rangle = \langle 0,\ldots,\tilde{0}|S_1^{(a)z}S_N^{(a)z}|\tilde{0},\ldots,0\rangle = (-1)^{N_0+N_{\tilde{0}}+1}, \tag{25}$$

where the dots indicate all intermediate rung states, which have to be the same for the bra and ket states to ensure that the matrix element is nonzero. Here, N_0 and $N_{\tilde{0}}$ are the numbers of rung-singlet and $S^z=0$ triplet states correspondingly.

Next, we consider the matrix elements generated by lowering-rising spin operators in Eq. (24). Taking into account Eqs. (12), (14), and (16), we obtain

$$\langle\tilde{0},\ldots,\tilde{0}|S_1^{(s)\mp}S_N^{(s)\pm}|\pm 1,\ldots,\mp 1\rangle = \langle\pm 1,\ldots,\tilde{0}|S_1^{(s)\pm}S_N^{(s)\mp}|\tilde{0},\ldots,\pm 1\rangle = (-1)^{N_0}\cdot 2,$$

$$\langle 0,\ldots,0|S_1^{(a)\mp}S_N^{(a)\pm}|\pm 1,\ldots,\mp 1\rangle = \langle\pm 1,\ldots,0|S_1^{(a)\pm}S_N^{(a)\mp}|0,\ldots,\pm 1\rangle = (-1)^{N_{\tilde{0}}}\cdot 2. \tag{26}$$

The matrix elements (25) and (26), together with their transpositions, are the only off-diagonal elements generated by $\tilde{H}_{\text{per}}$. They will be negative if $(-1)^{N_{\tilde{0}}+N_0}=(-1)^{N+N_0}=(-1)^{N+N_{\tilde{0}}}=1$ because the values of couplings J_N^s and J_N^a are positive. Using the relations $\sigma=(-1)^{N_0}$ for reflection quantum number σ and $(-1)^M=(-1)^{N-N_{\tilde{0}}-N_0}$ for the spin projection quantum number M, we can rewrite the last equations as

$$\sigma = (-1)^N = (-1)^M. \tag{27}$$

Remember now that the bulk part of the Hamiltonian has only nonpositive off-diagonal elements in the basis (16) for any M and σ (see Sec. II). Therefore, the entire Hamiltonian is nonpositive only on those (M,σ) subspaces (where $S^z=M$ and $\mathcal{R}=\sigma$), which are subjected to the condition (27). Moreover, in any such subspace, its matrix is connected because $\tilde{H}$ is connected as was already proven. Thus, according to Perron-Frobenius theorem, the relative ground state in each (M,σ) subspace with quantum numbers obeying Eq. (27) is nondegenerate and is a positive superposition of all basic states (17). The last fact has been used in Sec. II in order to determine the spin $S_{M,\sigma}$ of the relative ground state for the open ladder. So, here, the formula (18) can be applied too, and, actually, it is reduced just to $S_{M,\sigma}=|M|$ since Eq. (27) exclude the exceptional case of $M=0$ and $\sigma=(-1)^{N-1}$. The outcome is as follows.

- For the periodic frustrated ladder with even number of rungs, the relative ground state in any $(M=\text{even},\sigma=1)$ subspace is unique and belongs to a spin-$|M|$ multiplet. For the ladder with odd number of rungs, the same is true in any $(M=\text{odd},\sigma=-1)$ subspace.

As a consequence, the lowest-energy levels $E_{S,\sigma}$ among all states with fixed spin S and reflection σ quantum numbers are nondegenerate for $\sigma=1$ and even values of S as well as for $\sigma=-1$ and odd values of S. Moreover, we get a partial antiferromagnetic ordering of the lowest-energy levels $E_{S,\sigma}$.

- For the periodic frustrated ladder with even number of rungs, the relation $E_{S_1,1}>E_{S_2,1}$ holds for any even spin S_2 and any spin S_1 such that $S_1>S_2$. The ground state in an entire symmetric $(\sigma=1)$ sector is a unique spin singlet.
- For ladder a with an odd number of rungs, $E_{S_1,-1}>E_{S_2,-1}$ for any odd spin S_2 and any spin S_1 satisfying $S_1>S_2$.

For odd N, the lowest state in the antisymmetric may be a unique spin-triplet, a spin-singlet(s), or a singlet(s)$\oplus$ triplet representation.

Remember that in this paper we consider the ladders with coupling obeying $J_l^{\parallel}>|J_l^{\times}|$. The ladder with periodic boundary term under a certain supplementary condition on coupling constants becomes a part of a more general class of reflection-symmetric models investigated recently by Lieb and Schupp.[10,11] This fact has been used in Sec. II in the case of free boundaries and is discussed in detail in the Appendix. For the coupling values obeying $J_l^{\perp}>|J_{l-1}^{\times}|+|J_l^{\times}|$, all ground states become spin singlets, and among them there is one with $\sigma=(-1)^N$. Moreover, for antiferromagnetic diagonal interactions (i.e., if all $J_l^{\times}>0$) the nonstrict inequality sign can be used in the last inequality instead of the strict one [see Eq. (A7) in the Appendix]. In particular, the translationally invariant frustrated ladder with the antiferromagnetic couplings obeying $J^{\perp}\geqslant 2J^{\times}$ and $J^{\parallel}>J^{\times}$ has only spin-singlet ground states as well as is subjected to the ordering rule proved in this section.

For the ladders with an even-rung number, the aforementioned properties are in good agreement with our results obtained in this section. For the ladders with odd rungs, they even strengthen the partial ordering rule. The relation $E_{S_1,-1} > E_{S_2,-1}$, holding for any odd S_2 and any S_1 such that $S_1 > S_2$, becomes valid for $S_2=0$, too. The question of the degeneracy of the level $E_{0,-1}$ still remains open.

Unlike in the open ladder case, here we did not obtain definite exact results related to the degeneracy degree and spin quantum number of the total ground state. The main reason is the absence of exact results related to the $\sigma=(-1)^{N-1}$ sector in the case when the periodic boundary term presents.

VII. SUMMARY AND CONCLUSION

We have generalized Lieb-Mattis energy level ordering rule for spin systems on bipartite lattices[6] to the frustrated spin-1/2 ladder model. The model consists of two coupled antiferromagnetic chains frustrated by diagonal interactions and possesses reflection symmetry with respect to the longitudinal axis. The spin exchange coupling constants depend on site and are subjected to the relations (2). We have considered the finite-size system with free boundaries, the system with any impurity spin attached to one boundary as well as the ladder with periodic boundary conditions. Below, we describe briefly the results obtained in this paper.

The total spin S and reflection parity $\sigma=\pm 1$ are good quantum numbers. So, the Hamiltonian remains invariant on individual sectors with fixed values of both quantum numbers. For the open ladder and ladder with impurity, we have established that the lowest-energy levels $E_{S,\sigma}$ of these sectors with the same value of σ are ordered antiferromagnetically. More precisely, the relation $E_{S_1,\sigma} > E_{S_2,\sigma}$ holds for any two spins satisfying $S_1 > S_2 \geqslant S_{\text{gs}}(\sigma)$. Here, $S_{\text{gs}}(\sigma)$ is the spin value of the *unique* lowest level multiplet among all multiplets with the reflection parity σ:

$$S_{\text{gs}}(\sigma) = \begin{cases} s_0 & \text{if } \sigma = (-1)^N \\ |s_0 - 1| & \text{if } \sigma = (-1)^{N-1}, \end{cases}$$

where N is the number of rungs and s_0 is the impurity spin value. The case $s_0=0$ corresponds to the open ladder without impurity. We have also proven that all levels $E_{S,\sigma}$ with $S \geqslant S_{\text{gs}}(\sigma)$ are nondegenerate, which means that only one multiplet exists on the corresponding level. Note that $S_{\text{gs}}(\sigma)$ coincides for $\sigma=1$ with the ground-state spin S_{gs} of the Haldain chain obtained after replacing each rung with the spin $s=1$. The last model is bipartite and the Lieb-Mattis formula $S_{\text{gs}} = |S_A - S_B|$, mentioned in the Introduction, gives just the value of $S_{\text{gs}}(1)$.

In contrast to bipartite spin systems, the lowest levels in the symmetric ($\sigma=1$) and antisymmetric ($\sigma=-1$) sectors cannot be compared with each other, at least by means of our approach. Therefore, in general, the total ground state of the model is a unique multiplet with spin s_0 or $|s_0-1|$. If the lowest levels in both sectors coincide, then the degeneracy occurs and the ground state is the superposition of both multiplets. In this regard, our results claim that the ground state can be *at most* doubly degenerate.

For more restrictive values of couplings given in the Appendix, the frustrated ladder with free boundaries ($s_0=0$) fits the class of reflection-symmetric spin systems, all ground states of which are spin singlets.[10,11] Combining with our results, this implies that the ground state is a unique spin singlet in this case. This property is true, in particular, for frustrated ladder with site-independent antiferromagnetic couplings obeying $J^{\perp} \geqslant 2J^{\times}$ and $J^{\parallel} > J^{\times}$.

For a ladder with periodic boundary conditions, we have prove a weaker ordering rule. Namely, for the ladder with even (odd) number of rungs the ordering $E_{S_1,\sigma} > E_{S_2,\sigma}$ if $S_1 > S_2$ is established exactly for $\sigma=1$ ($\sigma=-1$) and even (odd) values of spin S_2 only. The degeneracy of the ground state and its total spin value remain open questions in this case.

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APPENDIX: APPLICATION OF LIEB-SCHUPP APPROACH TO FRUSTRATED SPIN LADDER

Recently, Lieb and Schupp[11] proved exactly that a reflection-symmetric spin system with antiferromagnetic crossing bonds has at least one spin-singlet ground state. Moreover, under certain additional conditions, all ground states become singlets. Frustrated spin-1/2 ladder (1) is an example of reflection-symmetric system (see Fig. 1). The Hamiltonian in the Lieb-Schupp form is

$$H = \sum_{l=1}^{N} \gamma_l^2 \mathbf{S}_{1,l} \cdot \mathbf{S}_{2,l} + \sum_{l=1}^{N} (\alpha_l \mathbf{S}_{1,l} + \beta_l \mathbf{S}_{1,l+1}) \cdot (\alpha_l \mathbf{S}_{2,l} + \beta_l \mathbf{S}_{2,l+1}) + \sum_{l=1}^{N} J_l (\mathbf{S}_{1,l} \cdot \mathbf{S}_{1,l+1} + \mathbf{S}_{2,l} \cdot \mathbf{S}_{2,l+1}). \quad \text{(A1)}$$

Here, $\alpha_l, \beta_l, \gamma_l, J_l$ are arbitrary real coefficients. The boundary conditions are $\alpha_N = \beta_N = J_N = 0$ for open ladder and $\mathbf{S}_{\delta,N+1} = \mathbf{S}_{\delta,1}$ ($\delta=1,2$) for periodic ladder. There are two kinds of bonds in Eq. (A1): the first sum consists of rung bonds while the second sum contains square bonds. Comparing Eq. (A1) with Eq. (1) one can express the spin coupling constants in Eq. (1) in terms of Lieb-Schupp coefficients:

$$J_l^{\parallel} = J_l, \quad J_l^{\perp} = \alpha_l^2 + \beta_{l-1}^2 + \gamma_l^2, \quad J_l^{\times} = \alpha_l \beta_l. \quad \text{(A2)}$$

In the second equation above the boundary conditions, $\beta_0=0$ and $\beta_0=\beta_N$ are used for open and periodic ladders correspondingly. Note that the value of interchain rung coupling is always antiferromagnetic.

Exploiting the reflection symmetry, Lieb and Schupp proved that there is a ground state of Eq. (A1), which overlaps with rung-singlet state $|0,\ldots,0\rangle$ (Ref. 10) and, more generally, with the canonical singlet state.[11] This means that the spin ladder Hamiltonian with diagonal interactions (1) possesses a spin-singlet ground state with $\sigma=(-1)^N$ reflection symmetry for any value of $J_l^{\|}$ provided that the remaining two couplings are subjected to the relation

$$J_l^{\perp} \geqslant \alpha_l^2 + \beta_{l-1}^2, \quad J_l^{\times} = \alpha_l \beta_l \tag{A3}$$

for some α_l, β_l. Setting several restrictions on auxiliary parameters $\alpha_l, \beta_l, \gamma_l$, one can simplify Eqs. (A2) and (A3) significantly and get the constraints containing interaction couplings only. Of course, those restrictions narrow the total region in phase space, where the Lieb-Schupp result is valid.

Consider the simplest and most familiar case of ladder with site-independent couplings. We set $\alpha_l=\alpha$, $\beta_l=\beta$, $\gamma_l=0$ for periodic ladder, where α,β are some real parameters. For open ladder, we choose the boundary values of γ_l parameter as $\gamma_1=\beta, \gamma_N=\alpha$. It is easy to verify that for both open and periodic boundary conditions, all values of interchain couplings satisfying $J^{\perp}=\alpha^2+\beta^2$, $J^{\times}=\alpha\beta$ lie inside the general region in phase space defined by Eq. (A3). Hence, there is a $\sigma=(-1)^N$ singlet among the ground states if two interchain coupling constants satisfy

$$J^{\perp} \geqslant 2|J^{\times}|. \tag{A4}$$

This relation can be generalized to the ladder model with site-dependent couplings. Setting $\alpha_l=\pm\beta_l$, one reduces the general region (A3) to

$$J_l^{\perp} \geqslant |J_{l-1}^{\times}| + |J_l^{\times}|. \tag{A5}$$

Here, as before, the boundary conditions $J_0^{\times}=J_N^{\times}=0$ and $J_0^{\times}=J_N^{\times}$ are applied for open and periodic ladders correspondingly.

Another important property of reflection-symmetric spin systems established exactly in Refs. 10 and 11 is that for any crossing bond, the expectation of the spin of its all sites, weighted by their coefficients, vanishes for *any* ground state $|\Omega\rangle$. Using this feature of ground states, it was proven that in a system with sufficient symmetry, so that every spin can be considered to be involved in a crossing bond, all ground states are spin singlets.

As was already mentioned, for a frustrated ladder, there are rung bonds and square bonds, which are described correspondingly by the first and second terms in Eq. (A1). The aforementioned condition means that $\langle\Omega|\mathbf{S}_l^{(s)}|\Omega\rangle=0$ if $\gamma_l\neq 0$ and $\langle\Omega|\alpha_l\mathbf{S}_l^{(s)}+\beta_l\mathbf{S}_{l+1}^{(s)}|\Omega\rangle=0$, where $\mathbf{S}_l^{(s)}$ is the spin operator of lth rung (3). Therefore, if $\alpha_l=\beta_l\neq 0$, then the expectation of total spin of each square bond vanishes also, i.e., $\langle\Omega|\mathbf{S}_l^{(s)}+\mathbf{S}_{l+1}^{(s)}|\Omega\rangle=0$. Applying this to the ladder with site-independent spin exchange, one can ensure that all its ground states are singlets provided that the interchain couplings satisfy

$$J^{\perp} \geqslant 2J^{\times} > -J^{\perp}. \tag{A6}$$

Indeed, using the aforementioned parametrization of $J^{\perp},J^{\times}$ and taking sum over all square bonds, we get $(\alpha+\beta)\langle\Omega|\mathbf{S}|\Omega\rangle=0$ for periodic ladder and any ground state $|\Omega\rangle$. For the open ladder, one must add two boundary rung bonds with coefficients β and α in order to obtain the last equation. So, if $\alpha\neq-\beta$, then any ground state is a singlet.

Consider now the ladder with site-dependent spin exchange and set again $\alpha_l=\pm\beta_l$ in Eq. (A2). Note that if all $\gamma_l\neq 0$, which makes strict the inequality sign in Eq. (A5), then due to the discussions above the mean value of the spin of every rung vanishes for any ground state. Therefore, all ground states are singlets if $J_l^{\perp}>|J_{l-1}^{\times}|+|J_l^{\times}|$. In fact, the inequality is nonstrict for positive values of diagonal couplings. This becomes apparent if we perform the sum over square bonds instead of rung bonds using the parametrization $\alpha_l=\beta_l$. Then the ground-state mean value of the total spin of each such bond vanishes as has been mentioned above. Taking the sum over all square bonds for the periodic ladder and the sum over half of square bonds in checkerboard order for the open ladder with even number of rungs, we obtain the zero expectation for the total spin of the model provided that

$$J_l^{\perp} \geqslant J_l^{\times} + J_{l-1}^{\times}, \quad J_l^{\times} > 0. \tag{A7}$$

For the open ladder with an odd number of rungs, one of the boundary rung spins must be added to that sum. The ground state then is a singlet if the corresponding coefficient [γ_1 or γ_N in Eq. (A1)] is nonzero. This means that the inequality in one of the two boundary relations in Eq. (A5) must be strict, i.e., $J_1^{\perp}>J_1^{\times}$ or $J_N^{\perp}>J_{N-1}^{\times}$.

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