Dimerized ground states in spin-$S$ frustrated systems.

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We study a family of frustrated anti-ferromagnetic spin-$S$ systems with a fully dimerized ground state. This state can be exactly obtained without the need to include any additional three-body interaction in the model. The simplest members of the family can be used as a “building block” to generate more complex geometries like spin tubes with a fully dimerized ground state. After presenting some numerical results about the phase diagram of these systems, we show that the ground state is robust against the inclusion of weak disorder in the couplings as well as several kinds of perturbations, allowing to study some other interesting models as a perturbative expansion of the exact one. A discussion on how to determine the dimerization region in terms of quantum information measures is also presented. Finally, we explore the relation of these results with the case of the a 4-leg spin tube which recently was proposed as the model for the description of the compound Cu$_2$Cl$_4$D$_8$C$_4$SO$_2$, delimiting the region of the parameter space where this model presents dimerization in its ground state.

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I. INTRODUCTION

In physics, exact results have proved to be extremely useful from a conceptual point of view. As an example, the case of the exact ground state of the $S = 1$ AKLT model$^2$ has been very important in the confirmation of Haldane’s prediction$^2$. Although solvable models usually are somewhat artificial, they are very useful as the starting point in the study of the features of more realistic systems, when their exact solution are not available. In this way, one of the paradigms in the physics of one dimensional spin chains is the Majumdar-Gosh (MG) model$^3$. This model represents one of the first examples of gapped spectrum where the exact ground state (GS) is exactly known. Although the exact results are valid only in the point $J_2 = J_1/2$, this point is representative of an extended phase. Generalizations of the MG point to come up with more realistic models are extremely important for the theoretical description of frustrated magnets like Cs$_2$CuCl$_4$$^4$, KCuCl$_3$$^5$, TlCuCl$_3$$^5$, NH$_4$CuCl$_6$$^6$, etc, which are being currently under experimental investigation.

In this paper we present a family of anti-ferromagnetic models with an exact dimer product state as its ground state. As in the case of the MG model, where the GS represents an extended phase, the manifold in the parameter space where the GS can be analytically determined is representative of an extended phase, that cover a large region of the parameter space. A dimerized phase corresponds to a non-magnetic phase without “classical analog”, characterized by short range, strong quantum correlations. This property, for gapped systems, could be exploited as a resource for quantum information processing$^7$-$9$. Hence, a suitable parameter order for this phase have to take into account the presence of these quantum correlations. For this reason, in this work we employ both measures of likelihood as the global and local fidelities to the fully dimerized state, as well as pair-wise and block measures of quantum entanglement. On these basis, we show that the fully dimerized state can be seen as the starting point to characterize non magnetic phases like such one observed in KCuCl$_2$$^3$. This material has a zigzag structure of Cu-ions and corresponds to a particular limit of the model studied in the present work.

Later, we use this family as a building block to construct out more complex models with a similar ground state. In particular, we show that the ground state of a family of frustrated four-leg spin tubes is also a product state of singlets. Besides, we analyze the relationship between these exactly solvable models and the case of frustrated spin tubes, which has been recently proposed as a model for the magnetic behavior of the compound Cu$_2$Cl$_4$D$_8$C$_4$SO$_2$. This compound seems to present frustrating anti-ferromagnetic next-nearest-neighbor exchange$^{10,11}$ and inelastic neutron scattering experiments reveal that it presents gapped and strongly one-dimensional excitations$^{12}$. So far, there are very few theoretical studies of this frustrated model. By means of numerical analysis we show in this work that the ground state of this model presents similar features that those found for the exactly solvable case.

The paper is organized as follows. In Section II we present the family of anti-ferromagnetic frustrated ladders and show that its ground state is a fully dimerized state. A discussion about the spectrum of these systems and the magnetic behavior is presented. In Section III the properties of the ground state in the vicinity of the exact dimerizing condition are discussed in terms of some quantum information measures of correlations. Afterward, we show that the exactly solvable model is representative of an extended manifold. In Section IV the previous model is used as a building block for more complex systems which also have a fully dimerized ground state. For the particular case of frustrated spin tubes, the manifold in the phase space with partially dimerized GS is explored.
by means of numerical analysis. In Section IV.A we perform a numerical study of the ground state corresponding to the effective model of the compound Cu$_2$Cl$_3$D$_8$C$_6$SO$_2$ and a comparison with the exact ground state of a very similar model belonging to the family where the ground state can be analytically determined is performed. Finally, in Section IV.B the conclusions and some perspectives are presented.

II. EXACT GROUND STATE IN SPIN-S LADDERS

A. Exact manifold

We consider the following Heisenberg model on a two legs spin-S ladder

\[
H = \sum_{i=1}^{N} J(i) \vec{S}_{2i-1} \cdot \vec{S}_{2i} + J'(i) \vec{S}_{2i} \cdot \vec{S}_{2(i+1)-1} + J''(i) \vec{S}_{2i-1} \cdot \vec{S}_{2(i+1)-1} + J_2(i) \vec{S}_{2i} \cdot \vec{S}_{2(i+1)}
\]

(1)

where \( \vec{S}_k \) represents the local spin on the site \( k \) and \( \vec{S}_k = \vec{S}_{k+2N} \), with \( N \) being the number of rungs. This ladder is represented in Figure 1A. Let us consider the case where all the couplings are positive (all the interactions are antiferromagnetic). Starting from the general spin-S model without translational invariance in Eq. (4) we can show that, imposing a simple constraint on the couplings on each square plaquette defined by the sites \( \{2i-1, 2i, 2(i+1)-1, 2(i+1)\} \), the ground state of the system is the fully dimerized state \( |\psi\rangle = \bigotimes_{i=1}^{N} |0\rangle_i \), with

\[
|0\rangle_i = \frac{1}{\sqrt{2S+1}} \sum_{m=-S}^{S} (-1)^{m+S}|m,-m\rangle_i,
\]

(2)

where index \( i \) labels the rung in the ladder and \(|m,-m\rangle_i\) are product states such that \( S_{2i-1}^+ |m,-m\rangle_i = -S_{2i}^- |m,-m\rangle_i = m|m,-m\rangle_i \) on the rung \( i \). In order to show that \(|\psi\rangle\) results an eigenstate of \( H \) with energy \( E_0 = -JNS(S+1) \), we rewrite the Hamiltonian in terms of local operators on each rung

\[
\vec{L}_i = \vec{S}_{2i} + \vec{S}_{2i-1}
\]

(3)

\[
\vec{K}_i = \vec{S}_{2i} - \vec{S}_{2i-1}.
\]

(4)

Here, \( \vec{L}_i \) is the total angular momentum of the rung \( i \), and \( \vec{K}_i \) is a set of local observables which completes the full local Lie algebra of observables:

\[
[L_{\mu}, L_{\nu}] = i\epsilon_{\mu\nu\lambda} L_{\lambda}
\]

(5a)

\[
[L_{\mu}, K_{\nu}] = i\epsilon_{\mu\nu\lambda} K_{\lambda}
\]

(5b)

\[
[K_{\mu}, K_{\nu}] = i\epsilon_{\mu\nu\lambda} L_{\lambda}
\]

(5c)

where \( \epsilon_{\mu\nu\lambda} \) is the fully antisymmetric Levi-Civita symbol and \( i \) is the imaginary unit (\( i^2 = -1 \)). In terms of this rung operators the Hamiltonian reads

\[
H = \sum_{i=1}^{N} J(i) \left( \frac{\vec{L}_i^2}{2} - SS\right) + \sum_{i=1}^{N} J'(i) \left( \frac{\vec{K}_i^2 + \vec{L}_i \cdot \vec{L}_{i+1}}{4} \right) + \sum_{i=1}^{N} \left( \frac{-J'(i) + J''(i)}{4} \right) \left( \vec{K}_i \cdot \vec{K}_{i+1} - \vec{L}_i \cdot \vec{K}_{i+1} \right) + \sum_{i=1}^{N} \left( \frac{-J'(i) - J''(i)}{4} \right) \left( \vec{L}_i \cdot \vec{K}_{i+1} - \vec{K}_i \cdot \vec{L}_{i+1} \right).
\]

(6)

If \( J'(i) + J''(i) = 2J_2(i) \), the last term in (6) vanishes and the state \(|\psi\rangle\) is an eigenstate of the Hamiltonian due to \( \vec{L}_i|0\rangle_i = 0 \). Noteworthy, this result is valid for any value of the local spin magnitude \( S \).

Now we are going to show that, provided the condition \( J(i) > \frac{(S+1)}{2}(J(i-1) + J'(i) + J''(i-1) + J''(i)) \), \(|\psi\rangle\) is the true ground state of the system. For this purpose, we rewrite the Hamiltonian in a convenient form (see Figure

![Figure 1](image-url)
\[ H = H_B + H_C + H_D + E_D \]  
\[ H_B = \frac{1}{4} \sum_{i=1}^{N} \left[ J' (i-1) \left( \vec{S}_{2i-2} + \vec{S}_{2i-1} + \vec{S}_{2i} \right)^2 + + J' (i) \left( \vec{S}_{2i-1} + \vec{S}_{2i} + \vec{S}_{2i+1} \right)^2 + + (J' (i-1) + J' (i)) S (\vec{S}_{2i-1} + \vec{S}_{2i})^2 - -(J' (i-1) + J' (i)) S (S + 1) \right] \]  
\[ H_C = \frac{1}{4} \sum_{i=1}^{N} \left[ J'' (i-1) \left( \vec{S}_{2i-3} + \vec{S}_{2i-1} + \vec{S}_{2i} \right)^2 + + J'' (i) \left( \vec{S}_{2i-1} + \vec{S}_{2i} + \vec{S}_{2i+2} \right)^2 + + (J'' (i-1) + J'' (i)) S (\vec{S}_{2i-1} + \vec{S}_{2i})^2 - -(J'' (i-1) + J'' (i)) S (S + 1) \right] \]  
\[ H_D = \sum_{i=1}^{N} \Delta (i) \left[ (\vec{S}_{2i-1} + \vec{S}_{2i})^2 \right] \]  

where \( E_D = -S (S + 1) \sum_i J (i) \) is the energy for the \( |\psi\rangle \) state and 
\[ \Delta (i) = J (i) - \frac{S + 1}{2} (J' (i-1) + J' (i) + J'' (i-1) + J'' (i)) \]

is an effective coupling constant associated to \( \mathbf{L}_i^2 \), the total angular momentum of the pair. \( H_{B,C} \) correspond, up to a constant, to the Hamiltonians of two zig-zag ladders (see Fig. 1B and 1C), while \( H_D \) is the Hamiltonian of a set of uncoupled pairs (Fig. 1D). Now we will show that \( H_B \) and \( H_C \) are semi-definite positive operators, being \( |\psi\rangle \) its ground state. To see it, we observe that the minimum eigenvalue of a sum of operators is bounded from below by the sum of the minimum eigenvalues of its terms:

\[ \min_{\lambda_i \in \Lambda} \lambda \geq \sum_i \min_{\lambda_i \in \Lambda} \lambda_i, \]

where \( \Lambda (O) = \{ \lambda_1, \lambda_2, \ldots \} \) denotes the spectrum of operator \( O \). Now, we notice that for \( J' (i-1), J' (i) > 0 \), due to the theorem of addition of angular momentum, each term in \( [8] \) and \( [9] \) is bounded from below by

\[ \lambda_i \geq \frac{J' (i-1) + J' (i)}{4} \min_{l_i \in \mathbb{Z}} | S - S_l | (| S - S_{l_i} | + 1) - S (S + 1) - S (l_i + 1) l_i = 0 \]

and hence, \( H_B, H_C \geq 0 \). Here, \( l_i \) is the total spin in rung \( i \).

On the other hand, is easy to verify that \( H_B |\psi\rangle = 0 \), from which it follows that \( |\psi\rangle \) is an eigenvector of \( H_{B,C} \) with minimum eigenvalue. Since for each \( i \), \( J (i) > \frac{S + 1}{2} (J' (i-1) + J' (i) + J'' (i-1) + J'' (i)) \), \( H_D \) also results positive, and hence, \( H \geq E_D \). But \( |\psi\rangle \) is an eigenstate of \( H \) which saturates that bound, so it is a ground state of \( H \).
For the $S = 1/2$ case the ground state of the system may correspond to $l_i = 0$ or $l_i = 1$, this is, the elementary excitations of the system can be seen as localized triplons. This is determined by the competition between the terms $J(i)\mathbf{L}_i^z$ and $J_2(i)\mathbf{L}_i \cdot \mathbf{L}_{i+1}$. By setting the condition $(S + 1)(\tilde{J}(i) + J'(i-1)) < J(i)$, $|\psi\rangle$ is the ground state, corresponding to $\{l_i = 0\}$. On the other hand, large values of $J_2$ favors larger values of $l_i$. In Figure 2 we show the energy per bond for a $S = 1/2$ ladder as a function of $J_2$ with $J' = J''$ (blue circles), calculated by means DMRG\cite{13}. Red circles corresponds to the energy of the GS in the sector $l_i = 1$. It is clear that for $J_2 > 0.7$ the spin ladder behaves like a $S = 1$ spin chain.

This result is important for two reasons. On the one hand, it gives us a picture about how the dimerization breaks when we cross the boundaries of the exact manifold: for large enough $J'$, the system suffers a level crossing to a higher value of the rung local spin $l_i$. On the other hand, we can take advantage of this result to gain information about the magnetic behavior of the system, as we will see in the next paragraphs.

C. Magnetic behavior

In order to discuss the magnetic behavior of the system, we introduce now a coupling term to an uniform external magnetic field $h$:

$$
H' = -h \sum_l L_{i,z} + H.
$$

The external magnetic field induces a competition between the one-site term and the magnetic field term. If all $J(i)$ are large, the GS remains being $|\psi\rangle$ up to a magnetic field value (lets say $h_1$) where there is a crossing level and the GS becomes the state with singlets in the even/odd rungs and fully polarized spin-1 states in the odd/even rungs. Notice that for these states the exchange interaction does not contributes.

Then, if we increase more the magnetic field, we obtain a second cross level with the state containing fully polarized spin-1 states in all the rungs. In the same way, we will find successive crossing levels with fully polarized states with spin total $l_{odd}$ and $l_{even}$ in odd and even rungs. Each one of these crossing levels result in a jump in the magnetization curve followed by a magnetization plateau. Hence, the magnetization process is given by successive jumps and plateaux. When we slightly move away from the condition $J'(i) = J''(i)$, these plateaux may remain present in the magnetization curve, whereas the jumps are smoothed. This frustration induced plateaux has been studied with DMRG for $S = 1/2$, $S = 1$ and $S = 3/2$ ladders\cite{14,15}. The present analysis provides a simple theoretical explanation for this behavior.

III. VICINITY OF THE EXACT MANIFOLD

Although we have shown that the state $|\psi\rangle$ is the GS of the model\cite{8} just when the condition $J'(i) + J''(i) = 2J_2(i)$ is fulfilled, this state represents a region in the parameter space, where results an accurate approximation to the true ground state. In order to characterize this region, we consider both measures of similarity between $|\psi\rangle$ and the GS, as well as measures of entanglement, characterizing the structure of the state and its correlations.

the Uhlmann’s Quantum Fidelity\cite{22}, provides a measure of the similarity between two quantum states:

$$
F[\rho, \sigma] = \text{Tr} \sqrt{\sqrt{\sigma} \rho \sqrt{\sigma}} = F[\sigma, \rho]
$$

where $\rho$ and $\sigma$ are two quantum states of the same system. If $\sigma$ corresponds to a pure state $|\alpha\rangle$, this quantity reduces to $F[\rho, |\alpha\rangle] = \sqrt{\langle \alpha | \rho | \alpha \rangle}$.

We start considering the fidelity between $|\psi\rangle$ and the true GS in a region close enough to the exact manifold such that a first order perturbative treatment would be feasible. Starting from the Hamiltonian\cite{8}, and using the algebraic properties of $L_{i,\mu}$ and $K_{i,\mu}$ the canonical first order perturbation theory leads to

$$
|\text{GS}\rangle \approx (1 - \frac{3}{64} N \gamma^2)^{1/2} |\psi\rangle + \frac{1}{4} \sum_i \frac{\sqrt{3}}{4} \gamma_i |i, i+1\rangle,
$$

(14)

where $|i, j\rangle = \frac{3/4}{\sqrt{S(S+1)}} \mathbf{K}_i \cdot \mathbf{K}_j |\psi\rangle$, $\gamma_i = \frac{S(S+1) J'(i) + J''(i) - 2J_2(i)}{3/4 (J'(i) + J''(i) + 1)/2}$ and $\gamma^2 = \frac{1}{N} \sum_i \gamma_i^2$. Notice the explicit SU(2) invariance of the approximation, as well as its translational invariance for the homogeneous case. In this way, the global fidelity is given by $(1 - \frac{3}{64} N \gamma^2)^{1/2}$, which is valid for $\frac{1}{N} \sum_i \gamma_i^2 \ll 1$. From now on, we are going to restrict to this last case and hence, $\gamma_i = \pm \gamma$. In this case, the previous result seems suggest that for large systems the dimerization is constrained just over the exact manifold. However, to look for high values of the fidelity in a large system is a very demanding condition. Due to its definition, for product states $F[|\alpha\rangle \otimes N, |\alpha'\rangle \otimes N] = (F[|\alpha\rangle, |\alpha'\rangle])^N$ and hence, for very similar states, the fidelity vanishes in the large $N$ limit. On the other hand, from (14) we can estimate the fidelity of a single rung with the singlet state $F_0[|\rho_{12}\rangle = F[|\rho_{12}\rangle, \text{singlet}] \approx (1 - 16 \tau^2^{1/2})^{1/2}$. When this approximation is valid, we can see that $F[|\text{GS}\rangle, |\psi\rangle] \approx F_0[|\rho_{12}\rangle^N$, which is just what we expect if the global states behaves like a product of the local states of the rungs, which is an important feature of the dimerized phase. A similar result can be obtained by the method of variational cluster mean field + RPA discussed in\cite{16}. This treatment predicts that the GS is well approximate by $|\psi\rangle$ plus small Gaussian correlations for $|\gamma| < 1$.

Now, we will see that for the $S = 1/2$ case, the value of $F_0[|\rho_{12}\rangle$ determines most of the features of the
dimerized phase. To see this, we observe that due to the $SU(2)$ symmetry, for the $S = 1/2$ case the local state of a rung is completely determined by $F_0[\rho]$:

$$\rho_{12} = \frac{1 - F_0^2[\rho_{12}]}{3} |0\rangle\langle 0| + \frac{4F_0^2[\rho_{12}] - 1}{3}|0\rangle\langle 1|.$$  

(15)

Since $\rho_{12}$ is the state of a subsystem associated to pure global state, a measure of the correlations between a rung and the rest of the system is given by its entanglement entropy\textsuperscript{2}. For the state (15) it is reduced to

$$S(\rho_{12}) = h\left(\frac{F_0^2[\rho_{12}]}{3}\right) + 3h\left(\frac{1 - F_0^2[\rho_{12}]}{3}\right)$$

where $h(x) = -x \log_2(x)$. For the dimerized phase, where the global state is well approximated by the fully dimerized state, which is a product state, $S(\rho_{12})$ should remain small. However, in order to give a more accurate idea about the limit value of $F_0[\rho_{12}]$ for which to speak of dimerization makes sense, is better to analyze the internal degree of entanglement of the rung. A measure of the degree of pairwise entanglement for mixed states is provided by the logarithmic negativity\textsuperscript{17,18}

$$\mathcal{E}^N[\rho] = \log_2 |\rho^{\dagger}|_1$$

where $|A|_1 = \text{tr} \sqrt{A^\dagger A}$ is the $L_1$ norm of the matrix $A$, and $\rho^{\dagger A}$ represents the partial transpose of $\rho$ with respect to the subsystem $A$, i.e. the linear map defined by $(|\alpha\rangle_A|\beta\rangle_B)(|\alpha'\rangle_A|\beta'\rangle_B)^{\dagger} = (|\alpha'\rangle_A|\beta\rangle_B)^{\dagger} (|\alpha\rangle_A|\beta'\rangle_B)$. This quantity is saturated by $\mathcal{E}^N[|\text{singlet}\rangle] = \log_2(1 + 2S)$ and vanishes for every separable state. For the rung state, and $S = 1/2$,

$$\mathcal{E}^N[\rho_{12}] = \log_2(1 + \max(0, 2F_0^2[\rho_{12}] - 1)).$$

As we can appreciate in Figure 3 for $F_0[\rho_{12}] \leq \frac{1}{\sqrt{2}} < 1/\sqrt{2}$, the local state is a classical state, and the correspondent global state is not dimerized anymore.

In Figure 4 a landscape of $F_0[\rho_{12}]$ (A) and $F_0[\rho_{23}]$ (B), obtained by numerical evaluation is shown, for the case of the symmetric ladder ($J'' = J'$). The presented results were evaluated by means of the Lanczos sparsedig code from\textsuperscript{19}. The red line indicates the intersection with the exactly dimerized manifold where the fully dimerized state is the ground state of the system. For the strong pair (A), the fidelity is symmetric with respect to the interchange between $J'$ and $J_2$, presenting a wide dimerized region ($F_0[\rho_{12}] > 0.95$) around the exact line $J' = J_2$. As we cross the critical value $J' = 0.6J$, $F_0[\rho_{12}]$ is suddenly reduced, due to the GS is now orthogonal to the dimerized one. For contiguous weakly coupled spins (B), we observe that near the exact line $F_0[\rho_{23}] \approx 1/2$, which is consistent with a fully mixed state. Then, for larger $J'$
these pairs become more entangled, at the expense of the entanglement in the rung (1 – 2). On the other hand, increasing $J_2$ the spins on the pair 1 – 3 tends to align, which reduces its fidelity to the singlet below $1/2$.

The present analysis seems to indicate that, in the region near to the exact manifold, the properties of the ground state can be studied perturbatively starting from the full dimerized state. Further improvements can be obtained by mean of a cluster mean field + RPA expansion as we have shown in a previous work. This opens a way to solve some effective models associated to certain quasi-one dimensional materials like KCuCl$_3$.

IV. Frustrated Four-Leg Spin Tubes.

The family of ladders presented above can be used as a “building block” to obtain more complex models with a product state as its ground state. It is straightforward to show that there is a family of Hamiltonians corresponding to four-leg spin tubes that present also a dimerized ground state. These Hamiltonians can be written as a sum of two ladders whose Hamiltonians are given by Eq. and $N$ square plaquettes as represented in Figure 5.

$$H_{tube} = H_{ladder1} + H_{ladder2} + \sum_{j=1}^{N} H_{square,j}$$ (16)

Where $N$ is the number of rungs in the ladders. $H_{ladder1}$ and $H_{ladder2}$ are Hamiltonians corresponding to the upper and lower ladders in Fig. 5 and $H_{square,j}$ is the Hamiltonian of the $j$-th square plaquette in the figure. These square plaquettes have also a dimerized ground state corresponding to dimers in the strongest bonds, as can be easily seen since the square is a special case of ladders discussed previously with 2 rungs. Let us concentrate in the homogeneous case $J(i) = J$, $J'(i) = J'$ and $J''(i) = J''$, $\forall i$, keeping in mind that all the conclusions can be easily generalized for the inhomogeneous case. Different combinations of couplings $J'$, $J''$ and $J_2$ preserving the constraint $J' + J'' = 2J_2$ gives different geometries of four-leg spin tubes with a fully dimerized ground state that can be written as $|\psi_{tube}⟩ = |\psi⟩_{ladder1} \times |\psi⟩_{ladder2}$. Then, following the same steps as in the previous section is easy to show that the state $|\psi_{tube}⟩$ is an eigenstate of the system and there is a range of couplings where this state is the ground state of the system. Besides, as in the ladder case, we can expect this exact GS to be representative of a finite region around the exact manifold of the parameter space.

We will consider now the particular cases of tubes with $J' = J''$ and $J'' = 0$. For these two cases, the fully dimerized state $|\psi_{tube}⟩$ is the ground state of the system if the following condition is satisfied

$$J' < \left\{ \begin{array}{ll} \frac{\xi J}{S(S+1)} & S = \frac{1}{2} \geq 1 \end{array} \right.$$

(17)

where $\xi = 1/3$ for $J' = J''$ and $\xi = 2/3$ for $J'' = 0$. In Figure 5 we show the energy per rung in units of $S(S+1)$ as a function of the coupling $J_2$ corresponding to the case $J' = 0$ and $J'(i) = 2J_2$ for different values of the spin. The range of values where the ground state is the product singlet state (i.e. $E/N_{rungs} = -1$) is bigger than that found analytically. The reason is that Eq. 17 represents just a sufficient condition, being the real range larger in general.

As we have seen for the ladders, the symmetrical case $J' = J''$ is special. The excited states correspond to localized triplons and the eigenvalues of the Hamiltonian can be labeled by the set of values of the total momentum in the rungs $\{t_i\}$. This situation gives a rich magnetization profile, containing a sequence of jumps and plateaux. Such rich scenario is due by the competition between the terms in the Hamiltonian that favors states with minimal total momentum in each rung, spin-exchange terms and the magnetic field contribution. The crossing levels between the ground state $|\psi_{tube}⟩$ and the state with alternation of one singlet and one triplet in each rung determines the jump in the magnetization curve between the plateaux at $m = 0$ and $m = \frac{1}{12}$. In this case, system frustration promotes the magnetization plateaux and the jumps in the magnetization profile, containing a sequence of jumps and plateaux. Such rich scenario is due by the competition between the terms in the Hamiltonian that favors states with minimal total momentum in each rung, spin-exchange terms and the magnetic field contribution. The crossing levels between the ground state $|\psi_{tube}⟩$ and the state with alternation of one singlet and one triplet in each rung determines the jump in the magnetization curve between the plateaux at $m = 0$ and $m = \frac{1}{12}$. In this case, system frustration promotes the magnetization plateaux and the jumps in the magnetization curve.
curve but also makes the ground state simpler (in each magnetization sector the ground state is a direct product of rung-states).

Even while respecting the constraint \( J' + J'' = 2J_2 \), for \( J'' \neq J' \) this is not true any more. Terms like \( \vec{L}_i \cdot \vec{L}_{i+1} \) appears and gives a non trivial triplon dispersion. Changing the value of \( J''/J' \) the magnetization plateaux reduce its widths and jumps between plateaux transform into a smooth piece of the magnetization curve.

The existence of the exact result for tubes also leads us to ask in which conditions, two ladders which present dimer order in its ground state, conserve it when they become weakly coupled, assembling a tube. From a perturbative argument, for small enough interladder couplings, we expect that the global state stays dimerized. However, due to the exact result Eq. (17), despite it becomes more frustrated, for larger couplings the system approach to another exact dimerized configuration. As a result, the region presenting dimer order would be enlarged. As an example, we will consider the case in which the interaction between ladders are given between correspondent spins on each ladder and on one of the diagonals of each plaquette (see the inset of Figure 7), calling \( J_\perp \) and \( J_d \) the respective coupling constants. This case is interesting since recently, a similar topology was proposed (but for \( J_d = 0 \)) as the appropriate model describing the compound \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \). Despite this case does not satisfy the exact dimerization condition for tubes, it is interesting to find out if it could support dimer order. In Figure 7 the behavior of the fidelity between the state of a rung and the singlet state, as well the entanglement entropy of this subsystem with the rest of the tube is depicted, for weakly coupled zig-zag ladders, as a function of the inter-chain couplings. Notice that the dimerization over the lateral ladders is not broken for quite large values of \( J_\perp \) and \( J_d \) near the exact dimerization condition. It would suggest that we can expect the presence of dimer order in the model proposed for \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \).

In the next sections we extend this result for a more realistic case, when the ladders does not satisfies the exact dimerizing condition. For it, we take advantage of the exact result for the four legs frustrated tube discussed above starting from a highly frustrated system but with a separable GS.

A. Effective Hamiltonian of the four-leg spin tube material \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \)

In a Recent experiment, inelastic neutron scattering has been used to investigate the magnetic excitations in the quantum spin-liquid system \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \). In that work, it was suggested that the appropriate Heisenberg Hamiltonian is a \( S = 1/2 \) four-leg spin-tube with no bond alternation as the showed in Figure 8a). There are a scarce number of theoretical results on this kind of prototypical models on the spin tubes. We study numerically the frustrated four leg spin tube model proposed to describe the compound \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \).

The proposed model is closely related to the family of spin tubes presented in the previous sections. Consider the member of the family of spin tubes with a fully dimerized ground state schematized in Figure 8b). This model can be obtained from the Hamiltonian proposed for the material adding an extra diagonal coupling in each square. This modified Hamiltonian belongs to the family of spin tubes presenting a dimer product ground state. If the ground state properties of these two models are similar, the effective model for \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \) may be studied starting from the exactly known ground state, taking the diagonal couplings in the squares as a perturbation. Although this perturbative study is out of the scope of the present paper we can see that the dimerized state is robust in the exact model. This robustness suggest to make an expansion around the dimer ground and incorporating triplon excitations. In the rest of this section, we are going to analyze numerically the proposed model for the material \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \), looking for fingerprints on the properties predicted for the exactly solvable case, leaving the analytical study of the corrections for a future work.

B. The model for the material and the exactly solvable model

Above we have analyzed the behavior of the ground state in tubes near the dimerization condition. Now, we are going to discuss which are the common features between these results and the behavior of a more realistic family of tubes. In particular, we consider the model proposed by Garlea et al. for the \( \text{Cu}_2\text{Cl}_4\text{D}_8\text{C}_4\text{SO}_4 \) compound. In order to see what features are shared between our exactly solvable model and the model proposed in 10,11, we explore numerically the ground state of Hamiltonians on the family \( J > J_2, J' \), corresponding to the

FIG. 6. (Color On-line) Ground state energy per bond in units of \( S(S+1) \) as a function of \( J_2 \) calculated with DMRG for a four-leg spin tube with 160 spins, \( J'' = 0 \) and \( J' = 2J_2 \). Blue circles, red squares and yellow rhombi correspond to \( S = 1/2, S = 1 \) and \( S = 3/2 \) respectively.
FIG. 7. (Color On-line) Dimerization in the case of weakly coupled ladders as a function of inter-ladder couplings calculated by using the Lanczos method with \( L = 4, J_2 = 0.5J' \) and \( J' = 0.95J \) (see the inset). (A) Entanglement entropy of a strong coupled pair with the rest of the tube. (B) Fidelity of the local state with the singlet state. The region in which the fidelity is over 0.99 matches with such that the entanglement entropy is lower than 0.2.

In Figure 7a, a landscape of several entanglement observables, corresponding to the ground state of a tube with couplings as in Figure 7a are depicted. In the top panels, the fidelity between the local state of a single rung and the singlet state (Panel A) and the entanglement entropy of a rung (Panel B) are shown. Due to the \( SU(2) \) symmetry, for local states of a single rung the entanglement entropy is a function of the fidelity to the singlet state. As we could expect from a composite mean field treatment, the local state of a single rung can be accurately approximated by a pure singlet state in a relatively wide region around the condition \( J' = 2J_2 \), even if \( J_2 \) is moderately large. On the bottom panels we can appreciate also the entanglement of a plaquette composed by two parallel rungs with the rest of the tube (Panel C) and the internal entanglement between two rungs in the same plaquette, measure by its logarithmic negativity (Panel D). We observe that the region in which the entanglement between a plaquette and the rest of the tube is weak, is a little larger than the dimerized region. As we approach to the point in which the dimerization is broken, the entanglement between rungs in the same plaquette grows, but it never reach saturation. It suggest that the system does not present a plaquette order but a \( SU(2) \) symmetry-broken phase with dimer order as the system becomes less frustrated.

For \( J' \) and \( J_2 \to 0 \), the global state reduces to a product state of singlets, and the entanglement entropy vanishes. However, this quantity is still small in a large region around the line \( J_2 = 2J' \), in a similar way that we would observe in our exactly solvable model. This result is compatible with what we obtain through a cluster mean field treatment based on rungs instead single spins.

FIG. 8. (Color On-line) Different spin tubes geometries.

V. DISCUSSION AND PERSPECTIVES

In the present paper, a general \( SU(2) \) invariant quantum spin-S Heisenberg ladder was investigated. A sufficient condition for the existence of a fully dimerized exact ground state was shown for a wide subfamily of such systems. Besides, by means of a combination of numerical
and analytical techniques, the existence of this phase for a general value of the local spin was proven, showing that the region in the parameter space corresponding to the dimerized phase is reduced as the magnitude of the local spin grows.

In the case of symmetrical frustration the excitations can be also determined exactly and the magnetization process was discussed.

The family of Hamiltonians with a fully dimerized ground state can be extended from the family of ladders into a more complex models. As an example we build a family of frustrated 4-leg spin tubes with a dimerized ground state. We study the common features between the results on the members of the family of spin tube Hamiltonians presenting a dimer product ground state and the behavior of a more realistic Hamiltonians. In particular, we have considered a model proposed for the Cu$_2$Cl$_4$D$_8$C$_4$SO$_2$ compound$^{10,11}$

We have studied numerically the ground state properties around the exact manifold in the parameter space showing that these remain close to the exact case over a finite region. Due to the large stability of this phase against external perturbations, a quantum simulator that could reproduce this kind of couplings would be able to prepare a large number of fully entangled pairs in a robust way. In the last years several proposals for the experimental simulations of spin systems in ion trap experiments$^{21,22}$ suggest that this kind of setup could be readily in a near future.

We hope this study can be taken as a starting point for a more systematic study of the ground state properties and excitations around the lines on the parameter space where the ground state was exactly determined.

As a perspective, the study of holes in this system can be a very interesting project. In 2D has been recently proved that the quantum statistics of holes in a dimer background can be changed without affect the energy dispersion$^{25}$ and the density of holes has an impact on the magnetization plateaux$^{26}$. As we start from these families of models where the ground state is a dimer covering, introducing holes in the system may result in a very interesting phase diagram.

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