Phase diagram of fragmented SU(2)-invariant spin ladders

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A two-parameter family of quantum spin ladders with local bilinear and biquadratic interactions, solvable by mapping onto fragments of integrable spin 1 chains, is studied. Phase diagram, consisting of four phases, ground state properties, and some excitations are discussed. Modulated structures of different periodicity, in particular a trimerized phase, are shown to appear. Some results are extended to the ladder associated to the most general spin 1 chain.

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I. INTRODUCTION

Integrable models have provided extremely valuable insight into the physics of one-dimensional quantum spin chains. There is a substantial lack of exact results for analogous two-dimensional systems and the solution of quantum spin ladders might provide a first step in that direction. Besides, spin ladders are currently experimentally accessible, interesting in their own and possibly related to high-T_c superconductivity.[1]

It has been established that the basic n-leg Heisenberg ladders, with bilinear exchange interactions along rungs and legs, are gapful (spin-liquid state) for n even and gapless for n odd.[1] These ladders do not seem to be integrable. On the other hand, examples of integrable ladders, containing additional biquadratic interactions, have been found and solved by some form of Bethe ansatz (BA).[2,3] Luckily, biquadratic interactions do arise in physically realizable systems, and a large class of these generalized, but still SU(2)-invariant ladders, have been proven to have a matrix-product (MP) ground state.[4] Still, the MP approach determines the ground state but, with the exception of few lucky cases, the whole set of excitations remains unknown.

In this paper, the following two-parameter family of SU(2)-invariant ladder Hamiltonians $H=\Sigma_{k=1}^{N}H_{k,k+1}$ will be studied

$$\begin{aligned}H_{k,k+1}(\tilde{\mu}_1,\tilde{\mu}_2)=&\ \tfrac{1}{2}(\mathbf{s}_k\cdot\mathbf{s}_{k+1}+\mathbf{t}_k\cdot\mathbf{t}_{k+1}+\mathbf{s}_k\cdot\mathbf{t}_{k+1}+\mathbf{s}_{k+1}\cdot\mathbf{t}_k)\\&-2((\mathbf{s}_k\cdot\mathbf{s}_{k+1})(\mathbf{t}_k\cdot\mathbf{t}_{k+1})+(\mathbf{s}_k\cdot\mathbf{t}_{k+1})\\&\times(\mathbf{s}_{k+1}\cdot\mathbf{t}_k))+\tilde{\mu}_1(\mathbf{s}_k\cdot\mathbf{t}_k+\mathbf{s}_{k+1}\cdot\mathbf{t}_{k+1})\\&+\tilde{\mu}_2(\mathbf{s}_k\cdot\mathbf{t}_k)(\mathbf{s}_{k+1}\cdot\mathbf{t}_{k+1})\end{aligned} \tag{1}$$

and the eigenvalue problem solved for any $\tilde{\mu}_1$, $\tilde{\mu}_2$. Here $\mathbf{s}_k$ and $\mathbf{t}_k$ are spin-1/2 matrices sitting on the first and the second leg, respectively. Hamiltonian (1) is actually a special point in a wider three-parameter class for which the relative strength of the first two terms is left arbitrary [see Eq. (11)]. All points in this manifold have the property of being reducible, through the introduction of the composite rung spin

$$\mathbf{S}_k=\mathbf{s}_k+\mathbf{t}_k \tag{2}$$

to the general spin-1 chain

$$H_0(\theta)=\sum_{k=1}^{N}(\cos\theta\mathbf{S}_k\cdot\mathbf{S}_{k+1}+\sin\theta(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^2). \tag{3}$$

In particular Eq. (1) corresponds to the BA solvable purely biquadratic spin-1 chain, $\theta=-\pi/2$. Selecting $\theta=0$, the Heisenberg spin-1 chain, would remove the second brackets in Eq. (1).[5] This seems physically more appealing but prevents the detailed analysis allowed by BA, since such a chain is not integrable. Choosing $\theta=\pi/2$ would yield the case considered by Wang.[6] Details about definitions and exact diagonalization are the subject of Secs. II and III.

The system defined by Eq. (1) has four phases, denoted $\langle 0\rangle$, $\langle 1\rangle$, $\langle 2\rangle$, and $\langle\infty\rangle$ in the following, connected by first order transition lines, namely discontinuities in some first order derivative of the ground state energy per site. Phases $\langle 1\rangle$ and $\langle 2\rangle$ are examples of modulated structures, called "mixed state" (MS) in Ref. 6, that is phases where triplets and singlets of Eq. (2) alternate with some kind of periodicity. In $\langle 2\rangle$ (three-rung periodicity), the ground state is a threefold degenerate global singlet where two rung triplets, locked into a singlet, alternate with isolated rung singlets. Such phase could be called trimerized. A trimerized ground state has been shown to occur in a generalized spin-1 chain,[7] not of the form (3), but, as will be discussed in Sec. VII, the two states are not quite the same. Phase $\langle 1\rangle$ has two-rung periodicity and a huge ($\sim 3^{N/2}$) ground state degeneracy. These results are proven in Sec. IV.

In Sec. V, exact elementary excitations are examined in the phase whose ground state is, effectively, that of the biquadratic chain, also a global singlet but made up of rung triplets. The simplest ones are created by introducing one rung singlet and leaving the remaining $N-1$ triplets locked into the ground state of the biquadratic chain with free ends. If $N-1$ is odd, such a ground state is presumably an SU(2) triplet containing one dynamical kink and one finds a band of singlet-triplet excitations, depending on two degrees of freedom, whose energy is degenerate in the singlet position. Such excitations had been found in a related ladder,[5] but their dependence on two degrees of freedom had not been discussed. On the other hand, similar ladders including biquadratic interactions are known to have two-parameter singlet-triplet excitations,[8,4] but their nature is different, being a pair of kink-antikink over a dimerized ground state, which is not what happens here.

In Sec. VI it is shown that phases $\langle 0\rangle$, $\langle 1\rangle$, and $\langle\infty\rangle$ are ubiquitous, i.e., they appear for each member of the wider three parameter family of spin ladders associated to the general spin-1 chain (3). Section VII presents a discussion and comparison with related works.

For the sake of completeness, the Appendix contains a review of known results on the biquadratic chain.

II. DEFINITION OF BASIC INVARIANTS

Each elementary plaquette involves four spins, say $(\mathbf{s}_1,\mathbf{t}_1,\mathbf{s}_2,\mathbf{t}_2)$. If only SU(2) invariance is required, the most general Hermitian plaquette Hamiltonian $H_{1,2}$ is a linear combination with real coefficients of 14 Hermitian invariants. If, beside SU(2) invariance, one requires symmetry under the exchange of the two legs and symmetry under the exchange of the two rungs, symmetries implemented by operators C and P

$$C\mathbf{s}_i C=\mathbf{t}_i,\quad (i=1,2),\quad C^2=1,$$

$$P\mathbf{s}_1 P=\mathbf{s}_2,\quad P\mathbf{t}_1 P=\mathbf{t}_2,\quad P^2=1,$$

then $H_{1,2}$ is a linear combination with real coefficients of 8 Hermitian invariants.

The proof goes as follows. The local plaquette Hilbert space is $\mathcal{H}_{1,2}\simeq V_1^{(s)}\otimes V_1^{(t)}\otimes V_2^{(s)}\otimes V_2^{(t)}\simeq C^{16}$. It breaks into the orthogonal sum of SU(2) multiplets: one quintuplet (dim $=5$), three triplets (dim$=9$) and two singlets (dim$=2$). Within each multiplet, all states are obtained by application of the lowering operator $\mathbf{S}_{1,2}^-$ to the highest weight vector (h.w.v.) $v^{(s)}$, where

$$\mathbf{S}_{1,2}=\mathbf{s}_1+\mathbf{s}_2+\mathbf{t}_1+\mathbf{t}_2,\quad \mathbf{S}_{1,2}^{\pm}=\mathbf{S}_{1,2}^x\pm i\mathbf{S}_{1,2}^y,$$

$$\mathbf{S}_{1,2}^+v^{(s)}=0,\quad \mathbf{S}_{1,2}^2v^{(s)}=s(s+1)v^{(s)},\quad v^{(s)}\in\mathcal{H}_{1,2}.$$

$H_{1,2}$ is SU(2)-invariant, i.e., $[H_{1,2},\mathbf{S}_{1,2}]=0$, therefore it maps h.w.v. into h.w.v. of the same spin. So, spin-2 h.w.v. must be mapped into itself, each spin-1 h.w.v. will in general be mapped into a linear combination of all three spin-1 h.w.v. and the same happens for the two spin-0 h.w.v.. Altogether, imposing hermiticity, 6 real parameters plus 4 complex (hence 8 real) ones. The total spin $\mathbf{S}_{1,2}$ commutes with C and P, so h.w.v. can be labeled by C and P eigenvalues. Define, with self-explanatory notation,

$$e_0=|\uparrow\uparrow\rangle_s,\quad f_0=|\uparrow\uparrow\rangle_t,\quad \overline{e_0}=|\downarrow\downarrow\rangle_s,\quad \overline{f_0}=|\downarrow\downarrow\rangle_t,$$

$$e_1=|\downarrow\uparrow\rangle_s,\quad f_1=|\downarrow\uparrow\rangle_t,\quad e_2=|\uparrow\downarrow\rangle_s,\quad f_2=|\uparrow\downarrow\rangle_t.$$

The 6 h.w.v. $v^{(s)}$ will be chosen to be

$$\begin{aligned}
&v^{(2)}=e_0f_0 && (2,1,1),\\
&v_1^{(1)}=e_0f_1-e_0f_2+e_1f_0-e_2f_0 && (1,1,-1),\\
&v_2^{(1)}=e_0f_1+e_0f_2-e_1f_0-e_2f_0 && (1,-1,1),\\
&v_3^{(1)}=e_0f_1-e_0f_2-e_1f_0+e_2f_0 && (1,-1,-1),\\
&v_1^{(0)}=e_1f_1+e_2f_2-e_1f_2-e_2f_1 && (0,1,1),\\
&v_2^{(0)}=e_1f_1+e_1f_2+e_2f_1+e_2f_2-2e_0\overline{f_0}-2\overline{e_0}f_0 && (0,1,1).
\end{aligned}$$

The three numbers in the right column are eigenvalues of $S_{1,2}$, C, P. If C and P symmetries are imposed, $H_{1,2}$ maps $v^{(2)}$ into itself and each $v_i^{(1)}$ $(i=1,2,3)$ into itself, while its action on the span of $\{v_i^{(0)};i=1,2\}$ is determined by 4 real numbers

$$H_{1,2}v^{(2)}=m^{(2)}v^{(2)},\quad H_{1,2}v_i^{(1)}=m_i^{(1)}v_i^{(1)},\quad i=1,2,3,$$

$$H_{1,2}v_i^{(0)}=\sum_{j=1}^{2}m_{ji}^{(0)}v_j^{(0)},\quad i=1,2.$$

This proves that the general $H_{1,2}$ is a linear combination with real coefficients of 8 linearly independent invariants (notice incidentally that h.w.v. $v_i^{(0)}$ are orthogonal but unnormalized, $\|v_2^{(0)}\|^2=3\|v_1^{(0)}\|^2$, so $m_{12}^{(0)}=3m_{21}^{(0)*}$). One can choose 7 of them to be three bilinear (Heisenberg) terms

$$I_{1,2}^{(1)}=\mathbf{s}_1\cdot\mathbf{s}_2+\mathbf{t}_1\cdot\mathbf{t}_2,\tag{4}$$

$$I_{1,2}^{(2)}=\mathbf{s}_1\cdot\mathbf{t}_1+\mathbf{s}_2\cdot\mathbf{t}_2,\tag{5}$$

$$I_{1,2}^{(3)}=\mathbf{s}_1\cdot\mathbf{t}_2+\mathbf{s}_2\cdot\mathbf{t}_1,\tag{6}$$

three biquadratic (plaquette) terms

$$I_{1,2}^{(4)}=(\mathbf{s}_1\cdot\mathbf{s}_2)(\mathbf{t}_1\cdot\mathbf{t}_2),\tag{7}$$

$$I_{1,2}^{(5)}=(\mathbf{s}_1\cdot\mathbf{t}_1)(\mathbf{s}_2\cdot\mathbf{t}_2),\tag{8}$$

$$I_{1,2}^{(6)}=(\mathbf{s}_1\cdot\mathbf{t}_2)(\mathbf{s}_2\cdot\mathbf{t}_1),\tag{9}$$

and the identity $\mathcal{I}$. An eighth one is necessary to have a complete set, but it involves more complicated combinations of the basic spins and it will not be needed in the following. To show that the six in Eqs. (4)–(9) plus the identity are indeed linearly independent, write

$$H_{1,2}=c_0\mathcal{I}+\sum_{k=1}^{6}c_kI_{1,2}^{(k)}.$$

It is a matter of easy algebra to find the action of the basic invariants (4)–(9) on the h.w.v., resulting in

$$m^{(2)}=c_0+\frac{c_1+c_2+c_3}{2}+\frac{c_4+c_5+c_6}{16},$$

$$m_1^{(1)}=c_0+\frac{-c_1+c_2-c_3}{2}+\frac{-3c_4+c_5-3c_6}{16},$$

$$m_2^{(1)}=c_0+\frac{c_1-c_2-c_3}{2}+\frac{c_4-3c_5-3c_6}{16},$$

$$m_3^{(1)}=c_0+\frac{-c_1-c_2+c_3}{2}+\frac{-3c_4-3c_5+c_6}{16}, \qquad (10)$$

$$m_{11}^{(0)}=c_0+\frac{-3c_1}{2}+\frac{9c_4+3c_5+3c_6}{16},$$

$$m_{22}^{(0)}=c_0+\frac{c_1-2c_2-2c_3}{2}+\frac{c_4+7c_5+7c_6}{16}$$

$$m_{21}^{(0)}=\frac{c_2-c_3}{2}+\frac{-c_5+c_6}{8},$$

and $m_{12}^{(0)}=3m_{21}^{(0)}$. The vanishing of all $\{m_i^{(s)}\}$ implies the vanishing of all $\{c_i\}$, proving linear independence of the invariants chosen.

Scalar products of the rung spin will now be expressed in terms of these invariants. Clearly

$$\mathbf{S}_1\cdot\mathbf{S}_2=I_{1,2}^{(1)}+I_{1,2}^{(3)},$$

while the biquadratic term $(\mathbf{S}_1\cdot\mathbf{S}_2)^2$ seems to involve more complicated invariants. But since it is invariant under C and P, it must be a linear combination of the 8 basic ones. Actually, the six (4)–(9) and the identity are sufficient: from Eq. (10)

$$(\mathbf{S}_1\cdot\mathbf{S}_2)^2=\frac{3\mathcal{I}}{4}-\frac{I_{1,2}^{(1)}}{2}+I_{1,2}^{(2)}-\frac{I_{1,2}^{(3)}}{2}+2I_{1,2}^{(4)}+2I_{1,2}^{(6)}.$$

Consider now the one-parameter spin ladder Hamiltonian (3) where each spin $\mathbf{S}$ is the composite object defined in Eq. (2). Two parameters can be added after noticing that the charges

$$Q_1=\sum_{k=1}^{N}\mathbf{S}_k^2,\qquad Q_2=\sum_{k=1}^{N}\mathbf{S}_k^2\mathbf{S}_{k+1}^2$$

commute with $H_0(\theta)$ for any θ. This can easily be checked by a direct calculation. Finally, the Hamiltonian to be studied is

$$\begin{aligned}H(\theta,\mu_1,\mu_2)&=H_0(\theta)+\mu_1Q_1+\mu_2Q_2\\&=\sum_{k=1}^{N}\Bigg[\left(\cos\theta-\frac{\sin\theta}{2}\right)(I_{k,k+1}^{(1)}+I_{k,k+1}^{(3)})\\&\quad+2\sin\theta(I_{k,k+1}^{(4)}+I_{k,k+1}^{(6)})\\&\quad+(\sin\theta+\mu_1+3\mu_2)I_{k,k+1}^{(2)}+4\mu_2I_{k,k+1}^{(5)}\Bigg]\\&\quad+N\left(\frac{3\sin\theta}{4}+\frac{3\mu_1}{2}+\frac{9\mu_2}{4}\right).\end{aligned} \qquad (11)$$

Equation (1) is Eq. (11), up to a constant shift, if one takes $\theta=-\pi/2$ and

$$\tilde{\mu}_1=-1+\mu_1+3\mu_2,\qquad \tilde{\mu}_2=4\mu_2. \qquad (12)$$

In the following, parameters (μ_1,μ_2) will be adopted to describe the model. It is always possible, through Eq. (12), to revert to the original ones $(\tilde{\mu}_1,\tilde{\mu}_2)$.

One further remark. Since each rung space $V_k^{(s)}\otimes V_k^{(t)}$ carries a spin $1\oplus 0$ representation, not just spin 1, $(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^3$ is linearly independent from $\mathbf{S}_k\cdot\mathbf{S}_{k+1}$ and $(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^2$. But, from Eq. (10), it can be seen that $(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^3$ is a linear combination of the first two powers, $\mathcal{I}$, $I_{k,k+1}^{(2)}$ and $I_{k,k+1}^{(5)}$, that is why adding a cubic term to $H_0(\theta)$ does not generalize Eq. (11).

The composite rung spin has, of course, been introduced in several previous works. It lies behind the physical idea that even-legged and odd-legged Heisenberg ladders should be in different phases.[1] More closely to this work, it has been used[4] to map two-leg ladders into the AKLT chain[10] [Eq. (3) at $\tan\theta=1/3$]. Earlier, Xian and then Kitakani and Oguchi[5] had studied Eq. (11) at $\theta=0$, but without the rung-rung interaction $I_{k,k+1}^{(5)}$ which is actually responsible for the rise of two new phases. More recently, the full spin ladder (11) has been related to Eq. (3) and studied for $\theta=\pi/4$.[6]

III. FRAGMENTATION AND BETHE ANSATZ

Charges Q_1 and Q_2 have a simple physical meaning. In each four dimensional rung space $V_k=V_k^{(s)}\otimes V_k^{(t)}\simeq C^4$ one introduces the singlet-triplet basis $\{|s\rangle_k;|t\rangle_k,t=-1,0,1\}$ consisting of the singlet and the triplet of the rung spin (2), i.e.,

$$\mathbf{S}_k^2|s\rangle_k=0,\qquad \mathbf{S}_k^2|t\rangle_k=2|t\rangle_k,\qquad S_k^z|t\rangle_k=t|t\rangle_k.$$

Then $Q_1/2$ counts the number of triplets and $Q_2/4$ counts the number of pairs of neighboring triplets.

Now consider the 3^N dimensional subspace (of the total 4^N- dimensional Hilbert space of the ladder) spanned by $|t_1,t_2,\ldots t_N\rangle$, $(t_k=-1,0,1)$. In this sector Q_1 and Q_2 are constant, at $2N$ and $4N$ respectively, and H_0 acts effectively as a spin-1 chain with periodic boundary conditions (p.b.c.). Such chain is Bethe ansatz solvable in three cases:[22] (a) $\theta=\pi/4$, (b) $\theta=-\pi/4$ and (c) $\theta=-\pi/2$ In case (a) it is the SU(3)-invariant Sutherland-Uimin chain,[11] in case (b) the Babujian-Takthajian chain[12] and in case (c) the purely biquadratic chain.[13]

Next, consider states containing one singlet and $N-1$ triplets. Eigenvalues of the two conserved charges are fixed at

$$Q_1=2(N-1),\qquad Q_2=4(N-2)$$

regardless of triplet's position. If the singlet is, say, on the Nth rung (due to p.b.c. the singlet's position is actually immaterial), H_0 acts on these vectors like

$$H_0\simeq\sum_{k=1}^{N-2}[\cos\theta\mathbf{S}_k\cdot\mathbf{S}_{k+1}+\sin\theta(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^2] \qquad (13)$$

that is exactly like a spin-1 chain of length $N-1$ and free boundary conditions (f.b.c.). The singlet can be positioned anywhere, it just opens a fracture in a ring of spins; consequently each eigenvalue of Eq. (13) appears with an N-fold degeneracy in the ladder spectrum. More importantly, the spectrum of Eq. (13) can be found exactly by Bethe ansatz, at least in cases (a), (b), and (c) which have been more or less extensively studied for f.b.c.[9,14,15] The opposite situation arises when all rungs are singlets. There is only one such state and its eigenvalue is trivially zero.

Between these extreme cases, and orthogonal to them, there is all possible intermediate situations, characterized by alternating fragments of triplets and singlets. Sectors are labeled by a sequence of positive integers, the lengths of fragments, $\{N_1^{(0)},N_1^{(1)},N_2^{(0)},N_2^{(1)},\dots,N_n^{(0)},N_n^{(1)}\}$, with $\Sigma_{j=1}^n N_j^{(0)}=N^{(0)}$, $\Sigma_{j=1}^n N_j^{(1)}=N^{(1)}$ and $N^{(0)}+N^{(1)}=N$. Each sector is spanned by the $3^{N^{(1)}}$ vectors

$$|\phi\rangle=|\underbrace{s,s,\dots,s}_{N_1^{(0)}};\underbrace{t_1^{(1)},t_2^{(1)},\dots,t_{N_1^{(1)}}^{(1)}}_{N_1^{(1)}};\underbrace{s,s,\dots,s}_{N_2^{(0)}};\underbrace{t_1^{(2)},t_2^{(2)},\dots,t_{N_2^{(1)}}^{(2)}}_{N_2^{(1)}};\dots\rangle.$$

On all these basis vectors

$$H_0|\phi\rangle=\sum_{j=1}^n H_0^{(j)}|\phi\rangle,$$

$$\begin{aligned}H_0^{(j)}|\phi\rangle&=|s,s,\dots,s\rangle_{N_1^{(0)}}\otimes|t_1^{(1)},t_2^{(1)},\dots,t_{N_1^{(1)}}^{(1)}\rangle_{N_1^{(1)}}\otimes\dots\\&\otimes H_0^{(j)}|t_1^{(j)},\dots,t_{N_j^{(1)}}^{(j)}\rangle_{N_j^{(1)}}\\&\otimes|s,s,\dots,s\rangle_{N_{j+1}^{(0)}}\otimes\dots,\end{aligned}$$

where $H_0^{(j)}$ acts on the string of triplets like a spin-1 chain of length $N_j^{(1)}$ and f.b.c. Call $|\psi\rangle_{N_j^{(1)}}$ any of its eigenvectors and $E_j(N_j^{(1)})$ the relevant eigenvalue. Then

$$\begin{aligned}|\psi\rangle=|s,s,\dots,s\rangle_{N_1^{(0)}}\otimes|\psi_1\rangle_{N_1^{(1)}}\otimes|s,s,\dots,s\rangle_{N_2^{(0)}}\otimes\dots\\\otimes|\psi_n\rangle_{N_n^{(1)}}\end{aligned}\tag{14}$$

is an eigenvector of H_0 with eigenvalue

$$E=\sum_{j=1}^n E_j(N_j^{(1)}).\tag{15}$$

Vectors in Eq. (14) provide a complete set for the whole ladder to the extent the vectors $|\psi_j\rangle_{N_j}$ provide a complete set of eigenvectors for the spin-1 chain of length N_j, so diagonalization of the spin-1 chain with p.b.c. and f.b.c. provides a complete solution to the diagonalization problem of the spin ladder (11). In general this is only a partial simplification. Instead, in cases (a), (b), and (c) eigenvalues can in principle be found, for all fragments, by the suitable Bethe ansatz, see Ref. 6 for case (a). What happens here is very similar, actually almost identical, to what happens in the mixed Heisenberg chains studied by Niggemann *et al.*[16] There, composite rung spins alternate with single spins and, very much like it happens here, fragmentation takes place when one rung spin is in a singlet state. In the following I will partly adopt notation and methods introduced in their work.

IV. THE GROUND STATE PROBLEM

To identify the ladder ground state one must minimize Eq. (15). An easy first step is to choose, in Eq. (15), the lowest eigenvalue for each fragment. To fix the notation, denote with $E_0^{(p)}(N;1)$ the lowest eigenvalue of the N-site spin-1 chain with p.b.c. and with $E_0^{(f)}(N';1)$ the lowest one for the N'-site chain with f.b.c. Then, in a sector $\{N_j^{(0)},N_j^{(1)}\}_{j=1}^n$ the lowest eigenvalue is

$$E=\begin{cases}\sum_{j=1}^n (E_0^{(f)}(N_j^{(1)};1)+(2\mu_1+4\mu_2)N_j^{(1)}-4\mu_2), \\ \qquad N^{(1)}\neq 0,N,\\ E_0^{(p)}+(2\mu_1+4\mu_2)N,\quad N^{(1)}=N,\\ 0,\quad N^{(1)}=0.\end{cases}\tag{16}$$

Following Ref. 16, a spin 0 rung is joined to, say, the right of each triplets fragment, bringing its length to $j+1$. Set n_j to be the number of triplet fragments of length $j+1$ (i.e., j triplets plus one singlet at the edge). Consider, for the time being, only fragmented configurations, i.e., $N^{(0)}>0$, specified by $\{n_0,n_1,n_2,\dots\}$ which must satisfy

$$\sum_{j=0}^{N-1}(j+1)n_j=N.$$

Their energy is 0 for $n_0=N$, otherwise

$$\begin{aligned}E(n_0,n_1,\dots,n_N)\\=\sum_{j=1}^{N-1}(E_0^{(f)}(j;1)+j(2\mu_1+4\mu_2)-4\mu_2)n_j,\end{aligned}$$

where $E_0^{(f)}(1;1)=0$ by definition. In the limit $N\to\infty$ the densities $w_j=n_j/N$ must be chosen to minimize

$$\begin{aligned}\lim_{N\to\infty}\frac{E}{N}=\epsilon(w_0,w_1,w_2,\dots)\\=\sum_{j=0}^{+\infty}(E_0^{(f)}(j;1)+j(2\mu_1+4\mu_2)-4\mu_2)w_j,\end{aligned}\tag{17}$$

$$\sum_{j=0}^{+\infty}(j+1)w_j=1. \tag{18}$$

As observed in Ref. 16, the problem (17), (18) has arisen in classical statistical mechanics of systems with competing interactions.[17] Owing to the linearity of Eq. (17) in the parameters $\{w_j\}$, the extremum occurs when one $w_j\neq 0$ and all others are zero. Then

$$w_j=\frac{1}{j+1},\quad w_k=0\quad (k\neq j)$$

and the ground state energy per site is

$$\epsilon=\epsilon(j)=\frac{E_0^{(f)}(j;1)+j(2\mu_1+4\mu_2)-4\mu_2}{j+1}. \tag{19}$$

The relevant phase is denoted $\langle j\rangle$. One is left with the task of determining the minimum in the sequence of real quantities (19), $j\geqslant 0$ where it is understood that $\epsilon(0)=0$. The minimum might be reached at $j\to\infty$, or $\epsilon(\infty)=e_0+2\mu_1+4\mu_2$ where e_0 is the ground state energy per site of the spin chain, independent from boundary conditions. The thermodynamical analysis outlined above does not allow to distinguish between the periodically closed sector $N^{(1)}=N$ and the open sector where, for instance, one singlet is introduced. In Appendix B it is shown in detail that, when $\inf_{j\geqslant 0}\epsilon(j)=\lim_{j\to\infty}\epsilon(j)$, then the ground state indeed belongs to the sector $N^{(1)}=N$.

All said so far is true for any value of θ in Eq. (11). Yet, a comparison of $\epsilon(j)$ requires the knowledge of $E^{(f)}(j;1)$, in principle for any j. The BA solvable cases (a), (b), (c) are perhaps not the most physically relevant, but they allow an efficient computation of $E^{(f)}(j;1)$. In the following I will mostly concentrate on case (c), the purely biquadratic spin 1 chain. The information available for this chain is summarized in Appendix A. The relevant results on finite size ground state energies are gathered in Table I. Some considerations on models with arbitrary θ are postponed to Sec. VI.

It can be shown that the (μ_1,μ_2) plane is divided into four regions, corresponding to four different ground state energies per site, hence four different phases. Since μ_1 and μ_2 often appear in the combination $2\mu_1+4\mu_2$ define

$$\mu_3=2\mu_1+4\mu_2.$$

First, seek the (μ_2,μ_3) values for which $\epsilon(0)$ is lowest, that is $0<\epsilon(j)$, $j\geqslant 1$. It is convenient to rewrite this condition adding and subtracting a term containing e_0 [whose numerical value is reported in Eq. (A1)]

$$4\mu_2<s_0(j)+j(e_0+\mu_3),\quad j\geqslant 1,\quad s_0(j)\overset{def}{=}E_0^{(f)}(j;1)-je_0.$$

The sequence $s_0(j)$ is bounded, so a first necessary condition is $e_0+\mu_3>0$. Furthermore, from Table II, $s_0(j)$ is increasing in the range $2\leqslant j\leqslant 51$, with a minimum

$$s_0(2)=E_0^{(f)}(2;1)-2e_0=-4-2e_0\simeq 1.5937. \tag{20}$$

TABLE I. Ground state energies of the biquadratic chain.

N	$E_0^{(f)}(N;1)$
1	0
2	−4
3	−6
4	−9.561 552 81
5	−11.763 723 82
6	−15.143 256 69
7	−17.454 021 00
8	−20.731 010 75
9	−23.110 963 57
10	−26.321 314 67
11	−28.749 674 12
12	−31.912 900 40
13	−34.377 230 72
14	−37.505 205 73
15	−39.997 421 80
16	−43.097 947 02
17	−45.612 471 78
18	−48.690 967 68
19	−51.223 778 87
20	−54.284 175 20
21	−56.832 269 12
22	−59.877 512 03
23	−62.438 582 09
24	−65.470 940 86
25	−68.043 174 37
26	−71.064 436 65
27	−73.646 381 47
28	−76.657 982 12
29	−79.248 455 76
30	−82.251 565 07
31	−84.849 590 92
32	−87.845 176 69
33	−90.449 938 29
34	−93.438 810 50
35	−96.049 617 90
36	−99.032 461 69
37	−101.648 726 25
38	−104.626 126 62
39	−107.247 341 91
40	−110.219 802 50
41	−112.845 529 74
42	−115.813 487 17
43	−118.443 342 59
44	−121.407 178 95
45	−124.040 826 24
46	−127.000 876 53
47	−129.638 018 37
48	−132.594 578 84
49	−135.234 951 29
50	−138.188 285 05
51	−140.831 652 64

TABLE II. Sequences $s_0(n)$, $s_1(n)$, and $s_2(n)$ up to $n=51$.

n	$s_0(n)$	$s_1(n)$	$s_2(n)$
1	n.d	n.d.	n.d.
2	1.593 726 86	8	n.d.
3	2.390 590 29	6	2
4	1.625 900 91	6.374 368 54	4.342 329 22
5	2.220 593 33	5.881 861 91	3.763 723 82
6	1.637 923 89	6.057 302 68	4.357 442 52
7	2.124 023 01	5.818 007 00	4.072 412 60
8	1.643 896 69	5.923 145 93	4.365 505 38
9	2.060 807 30	5.777 740 89	4.190 412 96
10	1.647 319 63	5.849 181 04	4.370 493 00
11	2.015 823 61	5.749 934 82	4.249 891 37
12	1.649 460 76	5.802 345 53	4.373 870 12
13	1.981 993 87	5.729 538 45	4.284 699 29
14	1.650 882 29	5.770 031 65	4.376 301 43
15	1.955 529 65	5.713 917 40	4.307 097 34
16	1.651 867 86	5.746 392 94	4.378 131 50
17	1.934 206 53	5.701 558 97	4.322 494 36
18	1.652 574 06	5.728 349 14	4.379 556 44
19	1.916 626 30	5.691 530 99	4.333 608 04
20	1.653 093 40	5.714 123 71	4.380 695 87
21	1.901 862 91	5.683 226 91	4.341 937 23
22	1.653 483 43	5.702 620 19	4.381 626 80
23	1.889 276 80	5.676 234 74	4.348 368 87
24	1.653 781 46	5.693 125 29	4.382 401 03
25	1.878 411 38	5.670 264 53	4.353 457 53
26	1.654 012 53	5.685 154 93	4.383 054 58
27	1.868 931 14	5.665 106 27	4.357 565 78
28	1.654 193 92	5.678 369 05	4.383 613 32
29	1.860 583 71	5.660 603 98	4.360 939 53
30	1.654 337 83	5.672 521 73	4.384 096 26
31	1.853 175 41	5.656 639 39	4.363 750 78
32	1.654 453 07	5.667 430 75	4.384 517 67
33	1.846 554 90	5.653 121 14	4.366 123 06
34	1.654 546 12	5.662 958 21	4.384 888 48
35	1.840 602 15	5.649 977 52	4.368 147 08
36	1.654 621 79	5.658 997 81	4.385 217 21
37	1.835 220 66	5.647 151 46	4.369 890 82
38	1.654 683 72	5.655 466 30	4.385 510 55
39	1.830 331 86	5.644 596 94	4.371 406 10
40	1.654 734 70	5.652 297 56	4.385 773 88
41	1.825 870 89	5.642 276 49	4.372 733 06
42	1.654 776 89	5.649 438 40	4.386 011 54
43	1.821 784 90	5.640 159 17	4.373 903 12
44	1.654 811 97	5.646 845 53	4.386 227 07
45	1.818 028 11	5.638 219 37	4.374 941 37
46	1.654 841 25	5.644 483 40	4.386 423 40
47	1.814 562 84	5.636 435 58	4.375 867 89
48	1.654 865 80	5.642 322 50	4.386 602 97
49	1.811 356 78	5.634 789 64	4.376 699 02
50	1.654 886 45	5.640 338 17	4.386 767 82
51	1.808 382 29	5.633 266 11	4.377 448 12

What can be said for $j>51$? From Appendix A, $s_0(j)$ has different limits at $j\to\infty$ for j even ($e^{(s,+)}$) and j odd ($e^{(s,-)}$) but they are both larger than $-4-2e_0$. It seems, from Table II, that $s_0(j)$ at $j\simeq 51$ is already rather close to the asymptotic regime, so one can safely, although not completely rigorously, conclude that $s_0(j)$, $j\geqslant 2$, is minimal at $j=2$ and that, since $e_0+\mu_3>0$

$$\inf_{j\geqslant 2}(s_0(j)+j(e_0+\mu_3))=s_0(2)+2(e_0+\mu_3)=-4+2\mu_3.$$

Hence, the three necessary *and* sufficient conditions for being in phase $\langle 0\rangle$ are

$$\begin{gathered} e_0+\mu_3>0 \\ 2\mu_3-4\mu_2>4 \quad (\text{phase } \langle 0\rangle) \\ \mu_3-4\mu_2>0. \end{gathered} \tag{21}$$

The third condition comes from $\epsilon(0)<\epsilon(1)$, considered separately.

Phase $\langle 1\rangle$. The conditions for its existence, $\epsilon(1)<\epsilon(0)$ and $\epsilon(1)<\epsilon(j)$, $j\geqslant 2$ are rewritten, from Eq. (19)

$$\mu_3-4\mu_2<0, \quad \mu_3+4\mu_2>s_1(j),$$

$$s_1(j)\overset{def}{=}-2E^{(f)}(j;1)/(j-1) \quad (j\geqslant 2),$$

where $s_1(j)$ is listed in Table II, up to $j=51$. It is decreasing in this range and it certainly is at large *j*. In fact, from the known numerical values (A1), (A8), and (A9), $2e_0+2e^{(s,\pm)}<0$; moreover

$$\begin{aligned} s_1(j)&=\frac{-2e_0j-2e^{(s,\pm)}}{j-1}+o(1/j) \\ &=-2e_0-\frac{2e_0+2e^{(s,\pm)}}{j}+o(1/j) \quad (j\to\infty). \end{aligned}$$

Hence one can conclude that $\sup_{j\geqslant 2}s_1(j)=s_1(2)=8$ and phase $\langle 1\rangle$ appears when

$$\mu_3-4\mu_2<0, \quad \mu_3+4\mu_2>8 \quad (\text{phase } \langle 1\rangle). \tag{22}$$

Phase $\langle 2\rangle$. The conditions for its existence are $\epsilon(2)<\epsilon(0)$, $\epsilon(2)<\epsilon(1)$ and $\epsilon(2)<\epsilon(j)$, $j\geqslant 3$, or, remembering that $E_0^{(f)}(2;1)=-4$

$$\mu_3-2\mu_2<2, \quad \mu_3+4\mu_2<8, \quad \mu_3+4\mu_2>s_2(j) \quad (j\geqslant 3),$$

$$s_2(j)\overset{def}{=}(3E_0^{(f)}(j;1)+4(j+1))/(-j+2) \quad (j\geqslant 3).$$

The sequence $s_2(j)$ is listed in Table II and it is increasing up to $j=51$. It certainly is for large *j* where

$$\begin{aligned} s_2(j)&=\frac{3e_0j+3e^{(s,\pm)}+4(j+1)}{-j+2}+o(1/j) \\ &=-3e_0-4+\frac{-6e_0-3e^{(s,\pm)}-12}{j}+o(1/j) \end{aligned}$$

because $-6e_0-3e^{(s,\pm)}-12<0$. This time, it is not so straightforward to guess the upper limit of $s_2(j)$. If $s_2(j)$ keeps increasing for $j>51$ up to the asymptotic regime where one can rely on the previous equation, then $\sup_{j\geqslant 3}s_2(j)=\lim_{j\to+\infty}s_2(j)=-3e_0-4\simeq 4.3906$ and phase $\langle 2\rangle$ appears for

$$\mu_3-2\mu_2<2,\quad -3e_0-4<\mu_3+4\mu_2<8\quad (\text{phase }\langle 2\rangle). \tag{23}$$

On the other hand, one cannot rule out the possibility that $\sup_{j\geqslant 3}s_2(j)$ lie slightly above and this would leave a tiny window for an additional phase. However, the existence of phase $\langle 2\rangle$ is unquestionable.

Finally, phase $\langle\infty\rangle$, whose ground state is that of the periodic spin 1 chain, shows up when, for each j, $\epsilon(j)<\epsilon(\infty)\overset{def}{=}\lim_{j\to\infty}\epsilon(j)$. Since $\epsilon(\infty)=e_0+\mu_3$, this means

$$e_0+\mu_3<0,\quad e_0+\mu_3<(\mu_3-4\mu_2)/2,$$

$$e_0+\mu_3<s_0(j)-4\mu_2\quad (j\geqslant 2).$$

We already know that $s_0(j)$ is minimal at $j=2$, so the third condition amounts to $e_0+\mu_3+4\mu_2<s_0(2)=-4-2e_0$ which, by itself, implies the second inequality. Hence

$$e_0+\mu_3<0,\quad \mu_3+4\mu_2<-4-3e_0\quad (\text{phase }\langle\infty\rangle) \tag{24}$$

are the necessary and sufficient conditions that guarantee the appearance of phase $\langle\infty\rangle$. Appendix B completes the proof: the ground state is that of the periodic spin 1 chain because, under conditions (24), local variations around the sector $N^{(1)}=N$ only lead to an increase in energy.

Under the foregoing assumption on the upper limit of sequence $s_2(j)$ there is no room for other phases because inequalities (21)–(24), with their separating lines, fill the whole (μ_2,μ_3) plane. The ground state energy per site is $\epsilon(0)=0$ (phase $\langle 0\rangle$), $\epsilon(1)=(\mu_3-4\mu_2)/2$ (phase $\langle 1\rangle$), $\epsilon(2)=(-4+2\mu_3-4\mu_2)/3$ (phase $\langle 2\rangle$) and $\epsilon(\infty)=e_0+\mu_3$ (phase $\langle\infty\rangle$). It shows first derivative discontinuities at the boundaries.

Here are some general features of the four phases. Define the total spin

$$\mathbf{S}_{\text{tot}}=\sum_{k=1}^{N}\mathbf{S}_k,\quad \mathbf{S}_{\text{tot}}^2=S_{\text{tot}}(S_{\text{tot}}+1).$$

In phase $\langle\infty\rangle$ the ground state is simply that of the periodic biquadratic spin-1 chain. Supposing N even, it is a global singlet and, it was conjectured in Ref. 13, its degeneracy should be 2. Phase $\langle 0\rangle$ has certainly a unique ground state and of course $S_{\text{tot}}=0$. As to phase $\langle 2\rangle$, the ground state is, again, a tensor product of local singlets, hence a global singlet, $S_{\text{tot}}=0$. In fact, it is represented by the sequence $|\ldots,s,t,t,s,t,t,s,t,t,s,\ldots\rangle$ where neighboring triplets $|t_k,t_{k+1}\rangle$ are locked into the singlet ground state of $-(\mathbf{S}_k\cdot\mathbf{S}_{k+1})^2$. Supposing $N=0$ (mod 3) to avoid problems with AFM seams, the ground state is threefold degenerate: rung singlets sit on rungs labeled k (mod 3), with the freedom of choice $k=0,1,2$. It clearly spontaneously breaks translational invariance. Finally, phase $\langle 1\rangle$, described by the sequence $|\ldots,t,s,t,s,t,s,\ldots\rangle$ is rather different because nothing fixes the state of each isolated triplet resulting in a huge degeneracy, $2\cdot 3^{N/2}$. Not only is translational invariance spontaneously broken, but one is dealing with $N/2$ effectively noninteracting triplets that can combine in a "ferrimagnetic" state $S_{\text{tot}}=N/2$, or combine in local pairs yielding $S_{\text{tot}}=0$ (these are only two of the many possibilities). In other words, the ground state is not necessarily an eigenstate of $\mathbf{S}_{\text{tot}}$.

Phases $\langle 1\rangle$ and $\langle 2\rangle$ are examples of what has been called mixed state (MS) in Ref. 6.

V. EXCITATIONS

The four phases display a rich variety of excitations. Most of them, especially in the fragmented phases $\langle 0\rangle$, $\langle 1\rangle$ and $\langle 2\rangle$ can easily be determined resorting to Eq. (16), therefore only phase $\langle\infty\rangle$ will be extensively treated in the following. Appendix B gives a complete discussion of how, in phase $\langle\infty\rangle$, "local" perturbations of the biquadratic ground state can only lead to an increase of energy.

A first kind of excitations, within the sector $N^{(1)}=N$, are those of the biquadratic chain itself. Supposing N even, they exist in even number and have a gap (see Appendix A for a more exhaustive discussion)

$$\Delta E_{\text{gap}}\simeq 0.173179.$$

A second kind of excitation, called TSST (triplet-to-singlet spin flip) in Ref. 5, is obtained by introducing one singlet, sector $N^{(1)}=N-1$. There is N ways to do so and the eigenvalue is N-fold degenerate. This implies that linear superpositions of such states produce eigenstates of the shift operator, all with the same energy. As a matter of fact, dispersionless excitations have already been found in akin ladders.[4] The energy difference is [see Eq. (16)]

$$\Delta E(N)=E_0^{(f)}(N-1;1)-E_0^{(p)}(N;1)-\mu_3-4\mu_2,$$

$$\Delta E=\lim_{N\to\infty}\Delta E(N)=e^{(s,-)}-e_0-\mu_3-4\mu_2.$$

From conditions (24) it follows that $\Delta E>2e_0+4+e^{(s,-)}\simeq 0.1479$ confirming that the energy can only be increased by fragmentation. At the same time, that numerical value shows that, at least near the boundary lines, the energy scale is comparable, actually slightly smaller, than ΔE_{gap}. Therefore fragmentation may be relevant to the low energy physics of the ladder. Despite what might seem, such excitations depend on two degrees of freedom. In fact, as discussed in Appendix A, the ground state of the fragment of triplets, i.e., the ground state of the open biquadratic chain with $N-1$ (odd) sites, is only the lowest in a continuous band. This adds a second degree of freedom to the singlet's position. Therefore, if n is the singlet position

$$\Delta E(\alpha,n)=\epsilon(\alpha)-\epsilon(\pi)+e^{(s,-)}-e_0-\mu_3-4\mu_2,$$

$$\alpha\in(0,\pi).$$

Here $\epsilon(\alpha)-\epsilon(\pi)$, always positive, measures the excitation energy of the single kink in the open spin chain and vanishes at $\alpha\to\pi$, see Eq. (A6). The n-dependence is, of course, trivial. Nonetheless, it is at least plausible that under a small variation of coupling constants in Eq. (1), for instance a different relative weight between $I^{(1)}$ and $I^{(3)}$, or $I^{(4)}$ and $I^{(6)}$ interactions, ΔE might acquire a genuine two-parameter form. Since the triplets fragment is presumably locked into a spin-1 state (see Appendix A), $S_{\rm tot}=1$ for such states. Triplet-singlet excitations have been found in similar ladders, but they arise through a different mechanism.[8,4]

When two rung singlets are introduced ($N^{(1)}=N-2$), their energy becomes position dependent. If they sit on rungs n_1,n_2 and $d=n_2-n_1\geqslant 1$, then from Eq. (16)

$$\Delta E(N;n_1,n_2)=E_0^{(f)}(d-1;1)+E_0^{(f)}(N-d-1;1)-E_0^{(p)}(N;1)-2\mu_3-8\mu_2+4\mu_2\delta_{d,1}.$$

If $N\to\infty$, keeping n_1, n_2 fixed [$p(d)$ is the parity of d]

$$\Delta E(d)=\begin{cases} s_0(d-1)-2e_0+e^{[s,p(d-1)]}-2\mu_3-8\mu_2 & (d>2),\\ -3e_0+e^{(s,-)}-2\mu_3-8\mu_2 & (d=2),\\ -2e_0+e^{(s,+)}-2\mu_3-4\mu_2 & (d=1).\end{cases}\tag{25}$$

Notice that all these excitation energies are exact. It is easy to see that $\Delta E(d)>0$ always. It represents a sort of "static interaction energy" between singlets, whose distance dependence is governed by $s_0(d)$. The open chain surface energy is different for even and odd lengths, so $s_0(d)$ has a uniform d-dependence only if the parity of d is fixed. When d is even, $\Delta E(d)$ uniformly decreases (see Table II) from a maximum $\Delta E(2)$ to a minimum $\lim_{d\to\infty}\Delta E(d)=-2e_0+2e^{(s,-)}-2\mu_3-8\mu_2$. When d is odd, the behavior is certainly uniform for $d\geqslant 3$, because $\Delta E(d)$ increases from $\Delta E(3)$ to a maximum $\lim_{d\to\infty}\Delta E(d)=2e^{(s,+)}-2e_0-2\mu_3-8\mu_2$. Still, $\Delta E(1)$ is not necessarily lower or higher than $\Delta E(3)$, since

$$\Delta E(3)-\Delta E(1)=-4-2e_0-4\mu_2$$

whose sign is left undetermined from conditions (24). The short range behavior can be either repulsive or attractive.

A third possible kind of excitation, named n-TSSF in Ref. 5, is produced by the insertion of a block of m singlets, represented by $|\ldots,t,t,t,s,s,s,s,t,t,t,t,\ldots\rangle$. Now, from (16), supposing N even as always

$$\Delta E(N;m)=E_0^{(f)}(N-m;1)-m\mu_3-4\mu_2-E_0^{(p)}(N;1),$$

$$\Delta E(m)=\lim_{N\to\infty}\Delta E(N;m)=-(m-1)(e_0+\mu_3)+e^{[s,p(m)]}-e_0-\mu_3-4\mu_2,$$

which is positive under conditions (24). At $e_0+\mu_3=0$ these perturbations determine the instability versus phase $\langle 0\rangle$.

VI. OTHER VALUES OF θ

It is easy to see that phases $\langle 0\rangle$, $\langle 1\rangle$ and $\langle\infty\rangle$ will be present no matter what value θ takes in Eq. (11). In this general situation, Eq. (16) will formally be the same but now with $E_0^{(f)}(N_j^{(1)};1;\theta)$ and $E_0^{(p)}(N;1;\theta)$, the energies of the spin-1 chain (3) with arbitrary θ. The proof of Sec. IV goes through unchanged. One has to find the minimum of

$$\epsilon(j;\theta)=\frac{E_0^{(f)}(j;1;\theta)+j\mu_3-4\mu_2}{j+1},\quad \epsilon(0;\theta)=0.$$

The conditions for phase $\langle 0\rangle$ amount to

$$4\mu_2<s_0(j)+j(e_0(\theta)+\mu_3)\quad (j\geqslant 1),$$

$$s_0(j)\overset{def}{=}E_0^{(f)}(j;1;\theta)-e_0(\theta)j.\tag{26}$$

Notice that $s_0(j)$ is bounded. Set

$$s_0(j_1)=\inf_{j\geqslant 1}s_0(j).$$

Of course j_1 might be $+\infty$. In this case, since $\lim_{j\to\infty}s_0(j)=e^{(s,\pm)}$, the two possible surface energies, one has $s_0(j_1)=\min\{e^{(s,+)},e^{(s,-)}\}$. At any rate, $s_0(j_1)$ is finite. A necessary condition required by Eq. (26) is $e_0(\theta)+\mu_3>0$, but since one does not know the exact value j_1 one can only give sufficient conditions for the existence of $\langle 0\rangle$, namely

$$e_0(\theta)+\mu_3>0\quad (\text{phase }\langle 0\rangle),$$

$$4\mu_2<\inf_{j\geqslant 1}s_0(j)+\inf_{j\geqslant 1}j(e_0(\theta)+\mu_3)=s_0(j_1)+e_0(\theta)+\mu_3,$$

which can always be simultaneously satisfied by suitable values of (μ_2,μ_3).

Likewise, for phase $\langle\infty\rangle$, the condition $\epsilon(j)>e_0(\theta)+\mu_3$, ($j\geqslant 0$), translates into $e_0(\theta)+\mu_3<0$ and $e_0(\theta)+\mu_3+4\mu_2<s_0(j)$, ($j\geqslant 1$), which can both be fulfilled taking

$$e_0(\theta)+\mu_3<0,\quad e_0(\theta)+\mu_3+4\mu_2<s_0(j_1)\quad (\text{phase }\langle\infty\rangle).$$

These conditions are necessary and sufficient, and are compatible.

Finally, the inequalities for $\langle 1\rangle$ are rewritten

$$\mu_3-4\mu_2<0,$$

$$\mu_3+4\mu_2>-\frac{2E_0^{(f)}(j;1;\theta)}{j-1}\overset{def}{=}s_1(j),\quad j\geqslant 2.$$

Sequence $s_1(j)$ is also bounded. Set $s_1(j_2)=\sup_{j\geqslant 2}s_1(j)$. The ensuing necessary and sufficient conditions are

$$\mu_3-4\mu_2<0,\quad \mu_3+4\mu_2>s_1(j_2)\quad (\text{phase }\langle 1\rangle).$$

On the contrary, it is in general impossible to draw conclusions on the existence of other phases. For example, phase $\langle 2\rangle$ would be present if it were possible to fulfill simultaneously

$$4\mu_2-2\mu_3>E_0^{(f)}(2;1;\theta),\quad \mu_3+4\mu_2<-2E_0^{(f)}(2;1;\theta),$$

$$\mu_3+4\mu_2>s_2(j), \tag{27}$$

$$s_2(j)\overset{def}{=}((j+1)E_0^{(f)}(2;1;\theta) \\ -3E_0^{(f)}(j;1;\theta))/(j-2)\quad (j\geqslant 3).$$

Notice that $s_2(j)$ is also bounded. If we set $s_2(j_3)=\sup_{j\geqslant 3}s_2(j)$, the second and the third inequality in Eq. (27) are compatible if and only if

$$s_2(j_2)<-2E_0^{(f)}(2;1;\theta). \tag{28}$$

At least for $\theta=0$, $e_0(\theta)$ has been determined to a great accuracy and one can attempt to estimate whether Eq. (28) holds. It is known that[18]

$$e_0(\theta=0)\simeq -1.401\,484.$$

On the other hand, not many data seem to have been published for $E_0^{(f)}(j;1;0)$ even at small j. Diagonalization of Eq. (3), with free boundaries, can easily be carried out numerically up to 7 sites (as a test, I diagonalized the periodic chain as well and compared the results with those published in Ref. 19). It is sufficient to examine the sector $S^z_{tot}=0$ because, owing to $SU(2)$ invariance, all possible eigenvalues are bound to appear there. Now, $E_0^{(f)}(2;1;0)=-2$, while the sequence $\{s_2(j)\}_{j=3}^{7}$ is found to have the approximate values $\{1,1.9606,1.8302,2.0277,1.9807\}$. Furthermore

$$\lim_{j\to\infty}s_2(j)=-2-3e_0\simeq 2.204\,46.$$

It is of course impossible to draw a rigorous conclusion from these results, but it looks extremely likely that inequality (28) is true and therefore phase $\langle 2\rangle$ is present also for $\theta=0$.

VII. DISCUSSION

It is useful to compare the ladders considered here with those studied in previous papers. To shorten notation, I will denote by $|\underline{0}\rangle_{\langle x\rangle}$ the ground state of phase $\langle x\rangle$, or one of them if it is degenerate. In the work of Niggeman *et al.* similar methods were employed but for different systems, namely the mixed Heisenberg chains. Perhaps the most closely related ladders are that of Xian,[5] which is Eq. (11) for $\theta=0$ and $\mu_2=0$ (perturbations of this ladder were considered in Refs. 20,21) and that of Wang.[6] Xian finds only two phases, $\langle 0\rangle$ and $\langle\infty\rangle$ in the present notation, but, since $\theta=0$, his ground state $|\underline{0}\rangle_{\langle\infty\rangle}$ is that of the spin 1 Heisenberg chain. The absence of phases $\langle 1\rangle$ and $\langle 2\rangle$ can be understood when one notices that even for the case considered in this paper, $\theta=-\pi/2$, phases $\langle 1\rangle$ and $\langle 2\rangle$ would be missing without the rung-rung interaction $I^{(5)}_{k,k+1}$, as can be seen by setting $\mu_2=0$ in Eqs. (22) and (23). Wang instead, considering the full ladder (11), points out the existence of MS phases.

The ground state of a wide class of SU(2)-invariant ladders has the matrix-product (MP) form.[4] Such states can be translationally invariant or dimerized

$$|\psi_0^{(\mathrm{inv})}(u)\rangle=\mathrm{Tr}\prod_{n=1}^{N}g_n(u),$$

$$|\psi_0^{(\mathrm{dim})}(u_1,u_2)\rangle=\mathrm{Tr}\prod_{n=1}^{N/2}g_{2n-1}(u_1)g_{2n}(u_2),$$

$$g_n(u)=\begin{bmatrix} u|s\rangle_n+|0\rangle_n & -\sqrt{2}|1\rangle_n \\ \sqrt{2}|-1\rangle_n & u|s\rangle_n-|0\rangle_n\end{bmatrix}.$$

For models with translationally invariant MP ground states, $u=0$ and $u=\infty$ are the only points which have a significant overlapping with the ladders presented here. At $u=0$ the MP state is made up of rung triplets and is, effectively, the ground state of the AKLT spin-1 chain. That is what one gets for Eq. (11) by setting $\tan\theta=1/3$ and keeping μ_1, μ_2 small enough. Now, $|\underline{0}\rangle_\infty$ is also made up of triplets, but it is that of the biquadratic spin 1 chain, hence a different kind. Furthermore, $|\underline{0}\rangle_{\langle 0\rangle}$, $|\underline{0}\rangle_{\langle 1\rangle}$ and $|\underline{0}\rangle_{\langle 2\rangle}$ all contain rung singlets and are certainly not $|\psi_0^{(\mathrm{inv})}(0)\rangle$. Conversely, after suitable normalization, the limit $|\psi_0^{(\mathrm{inv})}(\infty)\rangle$ is made up entirely of rung singlets. There is only one such state so it must coincide with $|\underline{0}\rangle_{\langle 0\rangle}$. Of course excitations may differ according to the detailed form of the Hamiltonian. At any rate, $|\underline{0}\rangle_{\langle 1\rangle}$ and $|\underline{0}\rangle_{\langle 2\rangle}$ break translational invariance so they can never be of the form $|\psi_0^{(\mathrm{inv})}(u)\rangle$ for any u. For the same reason, $|\underline{0}\rangle_{\langle 2\rangle}$, which is invariant under a three-rung translation, can never be of the form $|\psi_0^{(\mathrm{dim})}(u_1,u_2)\rangle$ either, since the latter is invariant under a two-rung translation. But, within the large lowest energy eigenspace of phase $\langle 1\rangle$, at least one vector is in MP form. To show it, notice that at finite, nonvanishing values of u_1, u_2, $|\psi_0^{(\mathrm{dim})}(u_1,u_2)\rangle$ is a linear combination necessarily containing kets with all triplets and the ket with all singlets. The only way to reproduce $|\underline{0}\rangle_{\langle 1\rangle}$ is to set $u_1=0$ and to take $u_2\to\infty$ after proper normalization of $g_{2n}(u_2)$. The outcome is a linear combination of kets which have singlets on even rungs and triplets on odd rungs, exactly like $|\underline{0}\rangle_{\langle 1\rangle}$. It should be observed though the MP approach only in a few cases allows us to find the whole spectrum, as it is instead possible from BA for Hamiltonian (1).

Finally, a trimerized ground state similar but not identical to $|\underline{0}\rangle_{\langle 2\rangle}$ has been found in Ref. 7 for a generalized spin-1 chain. It should be noted though that their chain contains interactions beyond nearest neighbors, so that the global singlet is obtained as a direct product of intertwined local singlets constructed out of three spin-1, a different configuration from what appears here.

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APPENDIX A: THE BIQUADRATIC SPIN-1 CHAIN

The purely biquadratic spin-1 chain is integrable for periodic[13] and free[15,23] boundary conditions. The definition of the relevant elliptic parameters differs in the two cases, as treated in the literature. For the sake of readability, a Landen transformation[24] has been applied to the results of Ref. 13, in order to make notations compatible.

Define an elliptic modulus from the relation

$$\frac{K'(k)}{K(k)}=\frac{1}{\pi}\ln(1/q),\quad q=\frac{3-\sqrt{5}}{2},$$

where $K(k)$ and $K'(k)$ are the elliptic integrals of first and second kind. The ground state energy, which is the same in the two cases, is then

$$e_0=-1-\frac{\sqrt{5}}{2}\left(1+4\sum_{n=1}^{+\infty}\frac{q^{2n}}{1+q^{2n}}\right)\simeq-2.796863\ldots. \tag{A1}$$

For the periodic case, energy and momentum of the excitations are given, in the limit $N\to\infty$, by

$$\Delta E=\sum_{i=1}^{2\nu}\tilde{\epsilon}(p_i),\quad \Delta P=\sum_{i=1}^{2\nu}p_i,$$

$$\tilde{\epsilon}(p)=\frac{\sqrt{5}}{\pi}K(k)\sqrt{k'^2+k^2\sin p},\quad k'^2+k^2=1. \tag{A2}$$

There is a gap in the spectrum

$$\begin{aligned}\Delta E_{\mathrm{gap}}&=2\tilde{\epsilon}(0)\\&=2\frac{\sqrt{5}}{\pi}K(k)k'\\&=\sqrt{5}\prod_{n=1}^{+\infty}\left(\frac{1-q^n}{1+q^n}\right)^2\simeq0.173178\ldots.\end{aligned} \tag{A3}$$

The free boundary case has been solved by noticing that the spectrum is the same, up to degeneracies, as that of the XXZ spin-1/2 chain with a boundary field[15]

$$\begin{aligned}H_{XXZ}=&-\frac{1}{2}\sum_{k=1}^{N-1}(\sigma_k^x\sigma_{k+1}^x+\sigma_k^y\sigma_{k+1}^y-\cosh\gamma\sigma_k^z\sigma_{k+1}^z)\\&+\frac{\sinh\gamma}{2}(\sigma_1^z-\sigma_N^z),\end{aligned} \tag{A4}$$

$$E_{\mathrm{bQ}}=E_{XXZ}-\frac{7}{4}(N-1),\quad q=e^{-\gamma}.$$

The mapping, valid for any N, works because both Hamiltonians can be written as sums over generators of the same Temperley-Lieb algebra.[15] Consequently, ground state energies of Eq. (A4) are for any N identical, up to a shift, to ground state energies of the biquadratic chain with free boundaries. In turn, Eq. (A4) has been solved by coordinate Bethe ansatz,[25] so eigenvalues are found from solutions of a set of coupled trascendental equations

$$\begin{aligned}&\frac{1}{\pi}\Theta\left(\alpha_j;\frac{\gamma}{2}\right)-\frac{1}{2\pi N}\sum_{k=1,k\neq j}^{n}(\Theta(\alpha_j-\alpha_k;\gamma)\\&\qquad+\Theta(\alpha_j+\alpha_k;\gamma))=\frac{I_j}{N},\quad j=1\ldots n,\end{aligned}$$

$$\Theta(\alpha;x)\overset{def}{=}-i\ln\left[\frac{\sinh\left(x+\frac{i\alpha}{2}\right)}{\sinh\left(x-\frac{i\alpha}{2}\right)}\right]=2\arctan\left(\tan\frac{\alpha}{2}\coth x\right), \tag{A5}$$

$$E=\frac{1}{2}(N-1)\cosh\gamma-2\sinh\gamma\sum_{j=1}^{n}\Theta'\left(\alpha_j;\frac{\gamma}{2}\right).$$

The function $\Theta(\alpha;x)$ is defined to be continuous for real α. The $\{I_j\}$ in Eq. (A5) are positive integers.[25,23] The ground state belongs to the sector $n=N/2$ (N even) or $n=(N-1)/2$ (N odd). In both cases, in Eq. (A5), $I_j=j$, $j=1,2\ldots n$. Data in Table I have been obtained by numerically solving Eq. (A5) with this choice of integers.

Excitations are, in general, gapful (no dispersion relation can be written here because linear momentum is not conserved):

$$\Delta E=\sum_{i=1}^{2\nu}\epsilon(\alpha_i),$$

$$\epsilon(\alpha)=2\sinh\gamma\frac{K(k)}{\pi}\mathrm{dn}\left(\frac{K(k)\alpha}{\pi};k\right),\quad \alpha\in(0,\pi),$$

$$\Delta E_{\mathrm{gap}}=2\epsilon(\pi)=\sqrt{5}\prod_{n=1}^{+\infty}\left(\frac{1-q^n}{1+q^n}\right)^2,$$

as in Eq. (A3). When N is odd, though, the ground state is at the bottom of a one-parameter, continuous, gapless (in the $N\to\infty$ limit) band of eigenvalues.[26] Within this band

$$\Delta E(\alpha)=\epsilon(\alpha)-\epsilon(\pi),\quad \alpha\in(0,\pi). \tag{A6}$$

This may be interpreted by saying that the ground state at N odd is not the "vacuum," but it contains one particle (kink) which can take up a whole band of dynamical states.

Surface energies for open antiferromagnetic chains differ, in general, when the limit $N\to\infty$ is taken for N even ($e^{(s,+)}$) or N odd ($e^{(s,-)}$). They are defined by

$$E_0(N)=e_0N+e^{(s,\pm)}+o(1)\quad(N\to\infty) \tag{A7}$$

and, for the case at hand, they can be computed exactly from Eq. (A5). For the biquadratic chain, one finds[23,26]

$$e^{(s,+)}=1+2\sqrt{5}\sum_{n=1}^{+\infty}\frac{q^{2n}-q^{4n}}{1+q^{4n}}\simeq1.655\,009\,2 \tag{A8}$$

$$e^{(s,-)}=1+\frac{\sqrt{5}}{2}\left(1+4\sum_{n=1}^{+\infty}\frac{q^{2n}-q^{4n}}{1+q^{4n}}-\sum_{n=0}^{+\infty}\frac{4q^{2n+1}}{1+q^{4n+2}}\right)$$
$$\simeq 1.741\,598\,6. \tag{A9}$$

APPENDIX B: GROUND STATE PROOF FOR PHASE $\langle\infty\rangle$

It has to be proven that, within the boundaries of region (24), the ladder ground state indeed belongs to the sector $N^{(1)}=N$, therefore it is just the ground state of Eq. (3) at $\theta=-\pi/2$. Here it will be shown that it is the lowest energy state within the class which encompasses the sectors $\{N_j^{(1)},N_j^{(0)}\}_{j=1}^n$ where $\{N_j^{(0)}\}_{j=1}^n$ and $\{N^{(1)}\}_{j=1}^{n-1}$ are arbitrarily large but kept finite as $N\to\infty$. In other words, only one triplet fragment, $N_n^{(1)}$, has a diverging size in the thermodynamic limit, as dictated by the analysis of Sec. IV. It will be assumed that $\inf_{j\geqslant 2}s_0(j)=s_0(2)$.

From Eq. (16)

$$\Delta E(N)=\sum_{j=1}^{n-1}E_0^{(f)}(N_j^{(1)};1)+E_0^{(f)}(N_n^{(1)};1)+\mu_3N^{(1)}-4n\mu_2$$
$$-[E_0^{(p)}(N;1)+\mu_3N].$$

When $N\to\infty$, setting $\Delta E=\lim_{N\to\infty}\Delta E(N)$

$$\Delta E=\sum_{j=1}^{n-1}E_0^{(f)}(N_j^{(1)};1)+e_0N_j^{(1)}+e^{[s,p(N_n^{(1)})]}-\mu_3N^{(0)}$$
$$-4n\mu_2-e_0N.$$

Since $N_n^{(1)}=N-N^{(0)}-\Sigma_{j=1}^{n-1}N_j^{(1)}$ and $e^{(s)}\geqslant e^{(s,+)}$

$$\Delta E\geqslant\sum_{j=1}^{n-1}\big(E_0^{(f)}(N_j^{(1)};1)-e_0N_j^{(1)}\big)-(e_0+\mu_3)N^{(0)}$$
$$+e^{(s,+)}-4n\mu_2. \tag{B1}$$

The bracketed term is $s_0(N_j^{(1)})$. Actually $s_0(j)$ has been defined for $j\geqslant 2$, whereas in Eq. (B1) $N_j^{(1)}$ can be 1 for some j. The definition of $s_0(j)$, though, makes sense for $j=1$, too. In that case $s_0(1)=-e_0>s_0(2)$, so it is also true that $\inf_{j\geqslant 1}s_0(j)=s_0(2)$. Then

$$\Delta E\geqslant(n-1)s_0(2)+e^{(s,+)}-(e_0+\mu_3)N^{(0)}-4n\mu_2>ns_0(2)$$
$$-(e_0+\mu_3)N^{(0)}-4n\mu_2$$

because $e^{(s,+)}>s_0(2)$. Next, notice that

$$N^{(0)}\geqslant n$$

because to create a new fragment at least one singlet must be added. So, setting $N^{(0)}=n+\Delta N^{(0)}$,

$$\Delta E>-(e_0+\mu_3)\Delta N^{(0)}+n\big(s_0(2)-e_0-\mu_3-4\mu_2\big),$$

which is positive due to inequalities (24).

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