Exact models for trimerization and tetramerization in spin chains

Stephan Rachel and Martin Greiter
Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, Postfach 6980, 76128 Karlsruhe, Germany
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We present exact models for an antiferromagnetic $S=1$ spin chain describing trimerization as well as for an antiferromagnetic $S=3/2$ spin chain describing tetramerization. These models can be seen as generalizations of the Majumdar-Ghosh model. For both models, we provide a local Hamiltonian and its exact threefold or fourfold degenerate ground state wave functions, respectively. We numerically confirm the validity of both models using exact diagonalization and discuss the low-lying excitations.

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I. INTRODUCTION

Spin 1 antiferromagnetic chains have been the subject of extensive study in the 1980s and 1990s. Many studies were motivated by Haldane's identification of the O(3) nonlinear sigma model as the effective low-energy theory for spin chains.[1] He pointed out that antiferromagnetic spin chains with integer spin representations possess a finite energy gap in the excitation spectrum and that the ground state correlations exhibit an exponential decay. Haldane's conjecture was substantiated through a rigorous theorem by Affleck and Lieb[2] and through the AKLT model[3–5] on theoretical site, and through the observation of the Haldane gap in spin 1 chains on experimental site.[6–10] Haldane's prediction has also been confirmed in detail by numerical studies.[11–13]

Recently, spin 1 chains have seen a considerable renewal of interest. Experimental realizations using polar molecules stored in optical lattices have been proposed,[14] with the spin represented by a single valence electron of a heteronuclear molecule. Moreover, it appears possible that the one-parameter family of Hamiltonians

$$\mathcal{H}_\theta = \sum_{i=1}^{N} \cos\theta\ \boldsymbol{S}_i\boldsymbol{S}_{i+1} + \sin\theta\ (\boldsymbol{S}_i\boldsymbol{S}_{i+1})^2 \qquad (1)$$

can be engineered in optical lattices using cold spin 1 bosonic particles with antiferromagnetic interactions, such as ^{23}Na, for arbitrary values of θ.[15,16]

The phase diagram of model (1) as a function of θ has been investigated by numerous authors (e.g., Refs. 17–32, and references therein) and is by now well understood. The point $\theta=0$ on the circle shown in Fig. 1, the antiferromagnetic Heisenberg point, is embedded in the so-called Haldane phase $(-\pi/4<\theta<\pi/4)$ which is characterized by a unique ground state, exponentially decaying correlations, and a gap between the ground state and the excited states. The Haldane phase includes at $\theta_{\mathrm{VBS}}=\arctan(1/3)$ the valence bond solid (VBS) or AKLT model. The AKLT Hamiltonian shares the most properties of the isotropic Heisenberg Hamiltonian but, in contrast to the isotropic Heisenberg model, possesses a ground state which can be written out explicitly.

Above the Haldane phase in Fig. 1, there is a critical phase $(\pi/4<\theta<\pi/2)$ with spin nematic correlations.[31] The phase transition at $\theta_{\mathrm{ULS}}=\pi/4$ was proposed to be of Kosterlitz-Thouless type.[24,30] At the transition point, Hamiltonian (1) reduces to the Uimin-Lai-Sutherland (ULS) model[33–35] which exhibits explicit SU(3) symmetry. The ULS model is a sum of permutation operators and exactly solvable via the nested Bethe ansatz.

At $\theta=\pi/2$, Hamiltonian (1) becomes ferromagnetic with gapless excitations. It reaches the ferromagnetic Heisenberg point at $\theta=\pm\pi$ and undergoes a first-order phase transition to a dimerized phase at $\theta=-3\pi/4$ where Eq. (1) is again SU(3) symmetric and has a highly degenerate ground state.[36] Close to this point there was a long-standing discussion regarding the possible existence of a small spin nematic phase. Recently, this was ruled out by numerical and analytical arguments.[31,37] In the dimerized phase $(-3\pi/4<\theta<-\pi/4)$, the excitations are gapped. At the Takhtajan-Babudjan point $\theta_{\mathrm{TB}}=-\pi/4$, the gap closes and the model is again exactly solvable via the nested Bethe ansatz,[38,39] has gapless excitations, and a unique ground state. Finally, the phase transition to the Haldane phase at $\theta=-\pi/4$ is of second order.[17,40]

Fath and Sólyom[22,24] observed in 1991 a *period tripling* in the spectrum of Eq. (1) in the critical phase $(\pi/4<\theta<\pi/2)$. The observation of *three soft modes* in their numerical studies caused a controversy whether or not it is a trimer phase.[41–43] Subsequent numerical studies concluded that there is no trimer phase.[44] Recently, it was found that the dominant correlations in this phase are not of singlet but of spin nematic (quadrupolar) character.[31]

Regardless of the spin nematic phase, $S=1$ models yielding trimerization can be constructed with a spin interaction beyond the nearest-neighbor case. Sólyom and Zittartz[45] presented such a model with four-site interaction. In this model,

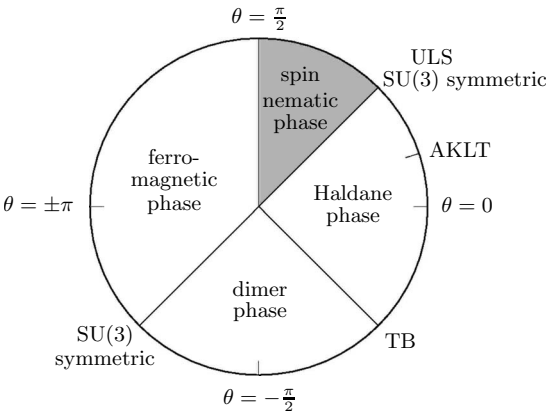

FIG. 1. Phase diagram of Hamiltonian (1) as a function of θ.

the trimer singlets are nested and each trimer singlet is placed on three non-neighboring sites, say on sites $3i-2$, $3i$, and $3i+2$ $(i=1,\ldots,N/3)$. Most recently, Corboz *et al.*[46] investigated numerically the bilinear-biquadratic Heisenberg model with nearest- and next-nearest-neighbor interactions:

$$\mathcal{H} = J_1 \sum_{i=1}^{N} \cos\theta\ \boldsymbol{S}_i\boldsymbol{S}_{i+1} + \sin\theta\ (\boldsymbol{S}_i\boldsymbol{S}_{i+1})^2 + J_2 \sum_{i=1}^{N} \cos\theta\ \boldsymbol{S}_i\boldsymbol{S}_{i+2} + \sin\theta\ (\boldsymbol{S}_i\boldsymbol{S}_{i+2})^2. \quad (2)$$

For certain values of the ratio J_2/J_1, they found in a small region around θ_{ULS} a trimerized phase in which the ground state becomes threefold degenerate as they approach the thermodynamic limit. This can be seen as the analogy of the dimer phase in the $S=1/2$ J_1-J_2 model for $J_2/J_1 \gtrsim 0.2411$.[47–49] Recently, trimerization and tetramerization were also discussed by Lecheminant and Totsuka[50,51] within a field theoretical approach where they considered a self-dual SU(n) Sine-Gordon model.

In Sec. II of this paper, we discuss an exact model for trimerization in an $S=1$ antiferromagnet. The model is exact for finite (and hence trivially also for infinite) chains. The ground state consists of simple trimer singlets (each of which is placed on three consecutive sites) and is threefold degenerate. Since the three ground states can be written as valence bond solids, the model is in the spirit of the Majumdar-Ghosh (MG) model[52,53] for $S=1/2$, where dimers occupy pairs of neighboring sites. We present a local Hamiltonian for which the trimer states are the exact zero-energy ground states, and identify numerically the elementary triplet excitation. It is a soliton consisting of two antisymmetrically coupled spins on adjacent sites. In Sec. III, we discuss the possible generalization to higher spin and introduce an exact model for the tetramerized (or, alternatively, quadrumerized) phase in a spin $S=3/2$ antiferromagnet. We numerically confirm the validity of the model using exact diagonalization. We further discuss low-lying excitations and give an outlook for tetramerization in other models.

II. MODEL FOR TRIMERIZATION

We consider a chain with $N=3\mu$ sites (μ integer) and impose periodic boundary conditions (PBCs). To write the trimer ground states as products of trimer singlets, we define an operator $T[i,j,k]$ which creates a trimer singlet on sites i, j, and k as follows:

$$T[i,j,k]|0\rangle = \frac{1}{\sqrt{6}}(|+,0,-\rangle + |0,-,+\rangle + |-,+,0\rangle - |+,-,0\rangle - |-,0,+\rangle - |0,+,-\rangle), \quad (3)$$

where $|+,0,-\rangle = c^\dagger_{i,+}c^\dagger_{j,0}c^\dagger_{k,-}|0\rangle$, etc., with the usual fermionic creation operators $c^\dagger_{i,\alpha}, \alpha=+,0,-$. Using Eq. (3) the three trimer ground states are given by

$$|\psi_1\rangle = \prod_{i=0}^{\mu-1} T[3i+1,3i+2,3i+3]|0\rangle,$$

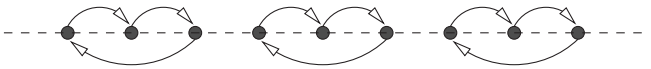

FIG. 2. Illustration of one of the trimer ground states on a chain with $N=3\mu$ sites, where three neighboring spins are antisymmetrically coupled.

$$|\psi_2\rangle = \prod_{i=0}^{\mu-1} T[3i+2,3i+3,3i+4]|0\rangle,$$

$$|\psi_3\rangle = \prod_{i=0}^{\mu-1} T[3i+3,3i+4,3i+5]|0\rangle. \quad (4)$$

Note that the trimer ground states (4) break translational symmetry spontaneously, while they are invariant under translations by three lattice spacings. To illustrate the states, we show one of them in Fig. 2 by connecting the sites belonging to the trimer singlets by arrows.

To find an exact parent Hamiltonian for the trimer states, interactions including first-, second-, and third-nearest neighbors are required. More generally speaking, we conjecture that for the construction of an exact Hamiltonian for "n-merization" consisting of local projection operators, interactions involving $n+1$ neighboring sites are required. Assuming interactions involving less than $n+1$ sites, additional non-n-merized states might occur which will be annihilated by the Hamiltonian. We further stress that SU($3n$) symmetry is a crucial requirement for trimerization (even though we are unable to prove this statement rigorously).

For convenience we introduce the auxiliary operator $\mathcal{X}^{(4)}$. It acts on four consecutive sites,

$$\mathcal{X}^{(4)}_i = \sum_{\substack{j,j'=i \\ j<j'}}^{i+3} \boldsymbol{S}_j\boldsymbol{S}_{j'} + (\boldsymbol{S}_j\boldsymbol{S}_{j'})^2, \quad (5)$$

where $\boldsymbol{S}_j$ is the usual spin 1 operator. In terms of these the Hamiltonian we propose is given by

$$\mathcal{H} = \sum_{i=1}^{N} (\mathcal{X}^{(4)}_i - 6)(\mathcal{X}^{(4)}_i - 4). \quad (6)$$

As in the case of the MG Hamiltonian, Eq. (6) is a sum over projection operators. The trimer ground states (4) will be annihilated by these operators,

$$(\mathcal{X}^{(4)}_i - 6)(\mathcal{X}^{(4)}_i - 4)|\psi_\nu\rangle = 0,$$

for $\nu=1$, 2, or 3, and thus $\mathcal{H}|\psi_\nu\rangle=0$.

The key to the trimer phase is the explicit SU(3) symmetry at the ULS point in Fig. 1. The symmetry emerges because the bilinear-biquadratic $S=1$ Heisenberg interaction becomes proportional to the SU(3) symmetric permutation operator if the bilinear and the biquadratic term appear with the same coefficients (as it happens at the ULS point). The SU(3) symmetric permutation operator $\mathcal{P}^{(3)}_{\alpha\beta}$ fulfils

$$\mathcal{P}^{(3)}_{12}|+,0\rangle = |0,+\rangle, \quad \mathcal{P}^{(3)}_{12}|+,-\rangle = |-,+\rangle,$$

$$\mathcal{P}_{12}^{(3)}|0,-\rangle = |-,0\rangle, \quad \mathcal{P}_{12}^{(3)}|+,+\rangle = |+,+\rangle, \ldots,$$

i.e., $\mathcal{P}_{\alpha\beta}^{(3)}$ permutes the spins on site α and β. The permutation operator and the spin 1 operators are related by

$$\mathcal{P}_{\alpha\beta}^{(3)} = \boldsymbol{S}_\alpha \boldsymbol{S}_\beta + (\boldsymbol{S}_\alpha \boldsymbol{S}_\beta)^2 - 1. \tag{7}$$

On the other hand, the permutation operator is related to the SU(3) spin operators $\boldsymbol{J}_\alpha$ by

$$\mathcal{P}_{\alpha\beta}^{(3)} = 2\boldsymbol{J}_\alpha \boldsymbol{J}_\beta + \frac{1}{3}. \tag{8}$$

The SU(3) generators at each lattice site α are defined as

$$\boldsymbol{J}_\alpha^a = \frac{1}{2} \sum_{\sigma,\sigma'=+,0,-} c_{\alpha\sigma}^\dagger \lambda_{\sigma\sigma'}^a c_{\alpha\sigma'}, \quad a = 1, \ldots, 8,$$

where λ^a are the SU(3) Gell-Mann matrices (see, e.g., Ref. 54). Equations (7) and (8) allow us to define a spin $S=1$ model which is simultaneously an SU(3) model. The ground states of the model are given by the trimer products (4). Note that Eq. (5) is up to an additive and multiplicative constant equal to the Casimir of the total SU(3) spin on four consecutive sites; Hamiltonian (6) corresponds to Eq. (12) in Ref. 54. We now explain the explicit construction for the SU(3) Hamiltonian which is equivalent to Eq. (6) and which describes trimerization. [A detailed discussion of this Hamiltonian for the SU(3) system can be found in Ref. 54.]

We consider a spin chain with a fundamental representation (1,0) of SU(3) on each lattice site. As mentioned above, for exact trimerization interactions involving four neighboring sites are required. To find the relevant SU(3) representations appearing on four consecutive sites, we couple four fundamental representations, $(1,0)\otimes(1,0)\otimes(1,0)\otimes(1,0) = 3\cdot(1,0)\oplus 2\cdot(0,2)\oplus 3\cdot(2,1)\oplus(4,0)$. In the ground state, only the representations (1,0) and (0,2) are present. This can be seen by considering four neighboring sites in the ground state configuration (see Fig. 2): either three spins are antisymmetrically coupled to a singlet (i.e., $\mathcal{A}[(1,0)\otimes(1,0)\otimes(1,0)]\otimes(1,0)=(1,0)$) or pairs of spins are antisymmetrically coupled to antifundamental representations (0,1) (i.e., $\mathcal{A}[(1,0)\otimes(1,0)]\otimes\mathcal{A}[(1,0)\otimes(1,0)]=(0,1)\otimes(0,1)=(1,0)\oplus(0,2)$). Hence, the projection operator onto the subspace (2,1) and (4,0) applied to one of the trimer ground states must be zero,

$$P_{\square\square\square\square}\,(i,j,k,l)\;|\psi_\nu\rangle = P_{\square\square\square\atop\square}\,(i,j,k,l)\;|\psi_\nu\rangle = 0 \tag{9}$$

for $\nu=1$, 2, or 3 if i, j, k, and l label four consecutive sites. The Young tableaux $\square\square\square\square$ corresponds to the representation (4,0) and $\square\square\square\atop\square$ to the representation (2,1). The conditions (9) single out states (4) uniquely as ground states, which enables us to write the parent Hamiltonian as

$$\mathcal{H} = \sum_{\langle ijkl\rangle} \left(P_{\square\square\square\square}\,(i,j,k,l) + P_{\square\square\square\atop\square}\,(i,j,k,l) \right). \tag{10}$$

The brackets $\langle\cdot\rangle$ indicate summation over four neighboring sites along the chain. We can rewrite this Hamiltonian in terms of SU(3) spin operators, such that it annihilates the states which carry exclusively the representation (1,0) or (0,2) on four consecutive sites:

$$\mathcal{H} = \sum_{i=1}^{N} \left[(\boldsymbol{J}_i + \boldsymbol{J}_{i+1} + \boldsymbol{J}_{i+2} + \boldsymbol{J}_{i+3})^2 - \frac{4}{3} \right] \times \left[(\boldsymbol{J}_i + \boldsymbol{J}_{i+1} + \boldsymbol{J}_{i+2} + \boldsymbol{J}_{i+3})^2 - \frac{10}{3} \right], \tag{11}$$

where we have used that the eigenvalues of the squared total spin on four neighboring sites, $\boldsymbol{J}_{4\ \text{sites}}^2$, is $\frac{4}{3}$ in case of the representation (1,0) and $\frac{10}{3}$ in case of the representation (0,2). The eigenvalues of the Casimir operators for the representations (2,1) or (4,0) are both larger than $\frac{10}{3}$. Hamiltonian (11) annihilates ground states (4) while the other states end up with a positive energy. Finally, we replace the SU(3) spin operators via Eqs. (7) and (8) by spin $S=1$ operators to obtain Eq. (6).

We have confirmed our predictions with exact diagonalization (ED) for chains with $N=9$ and $N=12$ sites. In both cases we found precisely three zero-energy ground states. These ground states are in the Brillouin zone located at $k=0, \frac{2\pi}{3}, \frac{4\pi}{3}$, reflecting the fact that the system is translationally invariant under translations by three lattice spacings. We have plotted the spectrum $E(k)$ in Fig. 3 for $N=18$ sites where we used Lanczos routine for diagonalization.

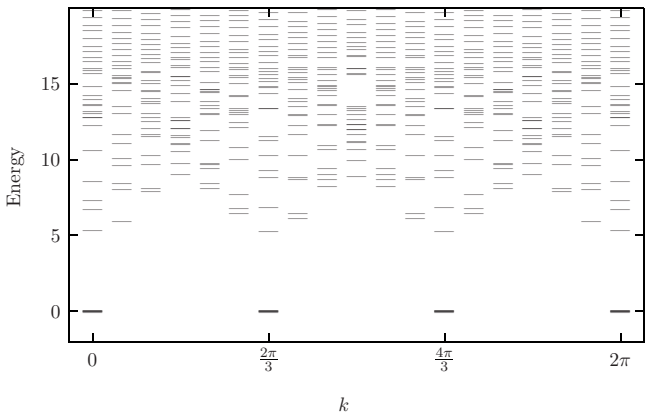

FIG. 3. Spectrum of the spin 1 model (6) for trimerization on a chain with $N=18$ sites. The zero-energy ground states (labeled by thick lines in the spectrum) are at $k=0, \frac{2\pi}{3}, \frac{4\pi}{3}$ in the Brillouin zone.

Even though we cannot write down any of the excited states exactly, we are able to elaborate on key properties like the quantum numbers involved. To create an excitation, we inevitably have to break a trimer, i.e., create a domain wall between the degenerate ground states. There are, however, two different types of domain walls [see Figs. 4(a) and 4(b)] which correspond to different excitations.

As explained above, our model exhibits an SU(3) symmetry, and we may view the trimer singlets (4) as SU(3) singlets. Breaking such an SU(3) singlet yields either an individual SU(3) spin with fundamental representation (1,0) or two antisymmetrically coupled spins on adjacent sites with the resulting antifundamental representation (0,1), i.e.,

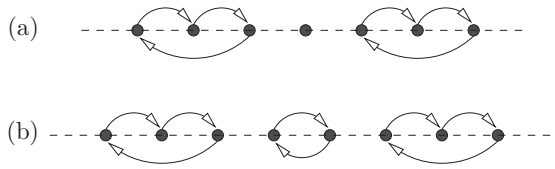

FIG. 4. (a) Possible triplet excitation as a domain wall on a chain with $3\mu+1$ sites. (b) Possible triplet excitation as a domain wall on a chain with $3\mu+2$ sites. The excitations consist of two antisymmetrically coupled spins on adjacent sites.

$\mathcal{A}[(1,0)\otimes(1,0)]=(0,1)$. Note that both (1,0) and (0,1) are three-dimensional representations. Since the only three-dimensional representation of SU(2) is the triplet, the excitation has to be a triplet regardless of which type it corresponds to.

The first type consists of an individual spin $S=1$, playing the role of a domain wall between two different trimer ground states, e.g., between $|\psi_1\rangle$ and $|\psi_2\rangle$ [see Fig. 4(a)]. The second type consists of two spins $S=1$ on adjacent sites. They are coupled such that the internal Hilbert space spanned by this excitation is three dimensional, i.e., $|e_+\rangle=\frac{1}{\sqrt{2}}(|+,0\rangle-|0,+\rangle)$, $|e_0\rangle=\frac{1}{\sqrt{2}}(|+,-\rangle-|-,+\rangle)$, and $|e_-\rangle=\frac{1}{\sqrt{2}}(|0,-\rangle-|-,0\rangle)$. This second type of triplet excitation is also as a domain wall between two different ground states, e.g., between $|\psi_1\rangle$ and $|\psi_3\rangle$ [see Fig. 4(b)]. Since either type of domain wall could in principle decay into two domain walls of the other type, only one type can be an eigenstate of Hamiltonian (6) above.

In Ref. 54 we have this question numerically investigated for the corresponding SU(3) model. We have found evidence that the domain wall placed on adjacent sites as shown in Fig. 4(b) is the elementary excitation. As pointed out above, this domain wall corresponds to an excitation transforming according to the antifundamental representation (0,1) of the SU(3) model. This is what we expect as the spinon excitations for antiferromagnetic SU(3) spin chains generally transform according to the representation (0,1). For the Haldane-Shastry model (HSM), this was shown by explicit construction of the exact one spinon eigenstates.[55,56] On more general grounds, the low-energy behavior of an SU(3) spin chain with fundamental representation is described by the $SU(3)_{k=1}$ Wess-Zumino-Novikov-Witten (WZNW) model. The elementary excitations in this model transform likewise according to the representation (0,1) under SU(3) rotations.[57,58]

Note that the triplet excitations are gapped, as it costs a finite energy to break a trimer. In Fig. 5 we have plotted the gap size for the finite chains versus the inverse system length. Fitting data points for $N=6$, 9, 12, 15, and 18 yields a huge gap $\Delta=4.56\pm0.04$ for the thermodynamic limit. This gap, however, is not the Haldane gap exhibited by the antiferromagnetic $S=1$ Heisenberg chain or the AKLT model, which we understand as due to a confinement force between spinons. This is consistent, as the SU(3) Heisenberg model does not display a Haldane gap.[2,54] The static spin-spin correlations of our model (6) decay abruptly, as adjacent trimer singlets are uncorrelated.

So far, we have used mappings (7) and (8) to construct a model of an antiferromagnetic $S=1$ spin chain with an SU(3)

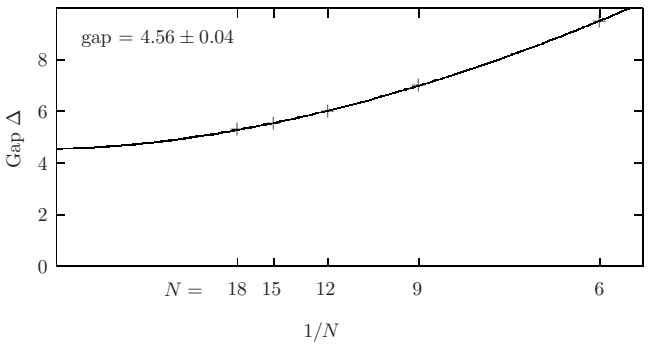

FIG. 5. The gap size of a chain with certain length N is plotted vs the inverse chain length. Data points for $N=6$, 9, 12, 15, and 18 yield the fitted value of $\Delta=4.56\pm0.04$.

symmetry. As a possible generalization, we might look for models of spin S antiferromagnets with an $SU(2S+1)$ symmetry, i.e., models in which $n=2S+1$ spins might form an n-mer rather than three neighboring spins a trimer. Corboz *et al.*[46] advocated that such an n-merized phase should appear in an appropriate J_1-J_2 model provided the ratio J_1/J_2 exceeds a certain critical value. Note that this is not in contradiction to our previous statement that $n+1$-site interactions are required for tetramerization. Corboz *et al.* proposed an n-merized phase which becomes exact in the thermodynamic limit only. Our statement is restricted to models describing exact n-merization.

The generalization of our construction is based on the mapping

$$\mathcal{P}^{(n)}_{\alpha\beta}=\sum_{\rho=0}^{n-1}a^{(n)}_{\rho}(\boldsymbol{S}_{\alpha}\boldsymbol{S}_{\beta})^{\rho}, \tag{12}$$

where the $\boldsymbol{S}_{\alpha}$ are spin S operators and $\mathcal{P}^{(n)}_{\alpha\beta}$ with $n=2S+1$ is the SU(n) symmetric permutation operator, exists in general. A method to determine the constants $a^{(n)}_{\rho}$ has been developed by Kennedy;[59] Itoi and Kato[30] obtained them explicitly up to $S=2$. We now use these results to introduce a spin 3/2 parent Hamiltonian which describes tetramerization.

III. MODEL FOR TETRAMERIZATION

We consider a spin $S=3/2$ antiferromagnetic chain with $N=4\mu$ sites (μ integer) and PBCs. The operator $Q[i,j,k,l]$ creates a tetramer singlet on sites i, j, k, and l,

$$Q[i,j,k,l]|0\rangle = \frac{1}{\sqrt{4!}}\sum_{\alpha,\beta,\gamma,\delta=\pi(3/2,1/2,-1/2,-3/2)}c^{\dagger}_{i,\alpha}c^{\dagger}_{i+1,\beta}c^{\dagger}_{i+2,\gamma}c^{\dagger}_{i+3,\delta}|0\rangle. \tag{13}$$

The sum in Eq. (13) extends over all 24 permutations π of the four states $|\frac{3}{2}\rangle_i=c^{\dagger}_{i,\frac{3}{2}}|0\rangle$, $|\frac{1}{2}\rangle_i=c^{\dagger}_{i,\frac{1}{2}}|0\rangle$, $|-\frac{1}{2}\rangle_i=c^{\dagger}_{i,-\frac{1}{2}}|0\rangle$, and $|-\frac{3}{2}\rangle_i=c^{\dagger}_{i,-\frac{3}{2}}|0\rangle$. The four tetramer ground states are given by

FIG. 6. Illustration of a tetramer state on a chain with $N=4\mu$ sites, where four neighboring spins are antisymmetrically coupled.

$$|\phi_\nu\rangle = \prod_{i=0}^{\mu-1} Q[4i+\nu, 4i+1+\nu, 4i+2+\nu, 4i+3+\nu]|0\rangle, \tag{14}$$

with $\nu=1$, 2, 3, or 4. One of these ground states is illustrated in Fig. 6.

In analogy to the MG and the trimer model (6), a Hamiltonian which annihilates the tetramer states can be written as a sum over projection operators. For convenience we introduce an auxiliary operator $\tilde{\mathcal{X}}^{(5)}$ acting on five neighboring sites

$$\tilde{\mathcal{X}}_i^{(5)} = \sum_{\substack{j,j'=i \\ j<j'}}^{i+4} \mathcal{P}_{jj'}^{(4)} = \sum_{\substack{j,j'=i \\ j<j'}}^{i+4} \sum_{\rho=0}^{3} a_\rho^{(4)} (\boldsymbol{S}_j \boldsymbol{S}_{j'})^\rho,$$

with the constants[30,59]

$$a_0^{(4)} = -\frac{67}{32}, \quad a_1^{(4)} = -\frac{9}{8}, \quad a_2^{(4)} = \frac{11}{18}, \quad a_3^{(4)} = \frac{2}{9}. \tag{15}$$

Note that $\mathcal{P}_{jj'}^{(4)}$ is the SU(4) symmetric permutation operator whereas the $\boldsymbol{S}_j$ are spin 3/2 operators. In terms of the auxiliary operator the parent Hamiltonian is given by

$$\mathcal{H}^{\text{quadr}} = \sum_i (\tilde{\mathcal{X}}_i^{(5)} + 5)(\tilde{\mathcal{X}}_i^{(5)} + 2). \tag{16}$$

This Hamiltonian is positive semidefinite, exact by construction, and annihilates states (14):

$$(\tilde{\mathcal{X}}_i^{(5)} + 5)(\tilde{\mathcal{X}}_i^{(5)} + 2)|\phi_\nu\rangle = 0,$$

which implies $\mathcal{H}^{\text{quadr}}|\phi_\nu\rangle = 0$ for $\nu=1$, 2, 3, or 4. It represents an exact model for tetramerization in a spin 3/2 antiferromagnet.

We have confirmed our predictions with ED for chains with $N=8$ and $N=12$ sites. The spectrum of the 12-site chain is shown in Fig. 7, where the four zero-energy ground states are located at $k=0$, $\frac{\pi}{2}$, π, and $\frac{3\pi}{2}$, reflecting that the ground states are invariant under translations by four lattice spacings.

Since Hamiltonian (16) is similar to Eq. (6), we contend ourselves with a brief discussion. Interactions between five neighboring sites are required to ensure annihilation of each tetramer singlet and, hence, annihilation of states (14). In order to find the correct projection operators, we couple five SU(4) spins with fundamental representation:

$$\begin{aligned}(1,0,0) \otimes (1,0,0) \otimes (1,0,0) \otimes (1,0,0) \otimes (1,0,0) \\ = 4 \cdot (1,0,0) \oplus 5 \cdot (0,1,1) \oplus 6 \cdot (2,0,1) \\ \oplus 5 \cdot (1,2,0) \oplus 4 \cdot (3,1,0) \oplus (5,0,0).\end{aligned}$$

In the tetramer ground states, only the representations (1,0,0) and (0,1,1) are present. The projection operators onto the subspaces in which the representations (1,0,0) and (0,1,1) are absent hence annihilate states (14). Since these states are the only states which contain representations (1,0,0) and (0,1,1) on five consecutive sites, a Hamiltonian in terms of projection operators may be written as

$$\mathcal{H}^{\text{quadr.}} = \sum_{\langle ijklm \rangle} \Big(P_{\square\!\square\!\square\!\square} (i,j,k,l,m) + P_{\square\!\square\!\square\!\square} (i,j,k,l,m) + P_{\square\!\square\!\square\!\square} (i,j,k,l,m) + P_{\square\!\square\!\square\!\square} (i,j,k,l,m) \Big),$$

where $\langle\cdot\rangle$ indicates summation over five neighboring sites along the chain. We then replace the projection operators by SU(4) spin operators and rewrite the SU(4) spin operators by spin $S=3/2$ operators using mapping (12). This yields Hamiltonian (16).

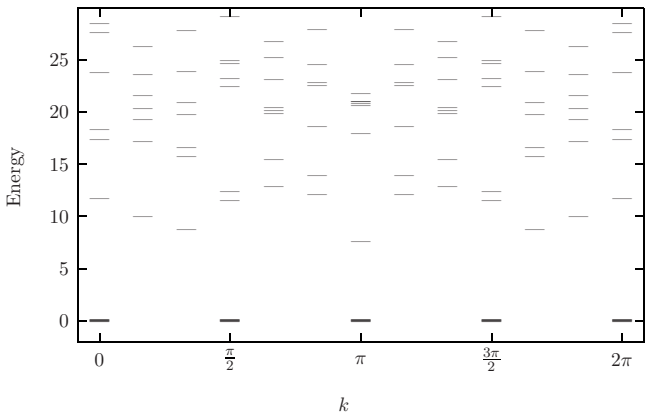

FIG. 7. Spectrum of the spin 3/2 model (16) for tetramerization on a chain with $N=12$ sites. The zero-energy ground states (labeled by thick lines in the spectrum) are at $k=0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ in the Brillouin zone.

Whereas the model for trimerization exhibited two possible candidates for the low-lying excitation, the model for tetramerization exhibits three candidates. When breaking a tetramer singlet which we might view as an SU(4) singlet, one obtains either an individual SU(4) spin with fundamental representation (1,0,0), or two antisymmetrically coupled spins on adjacent sites with representation (0,1,0), or three antisymmetrically coupled spins on consecutive sites with antifundamental representation (0,0,1). Whereas the representations (1,0,0) and (0,0,1) are four dimensional, the representation (0,1,0) is six dimensional. The excitations with fundamental and antifundamental representation correspond to the quadruplet excitation carrying spin $S=3/2$ in the SU(2) spin chain, while the six-dimensional representation (0,1,0) corresponds to the antisymmetric content of $\frac{3}{2} \otimes \frac{3}{2} = \mathbf{0} \oplus \mathbf{1} \oplus \mathbf{2} \oplus \mathbf{3}$, i.e., $\mathbf{0} \oplus \mathbf{2}$.

In order to motivate that the quadruplet excitation placed on three consecutive sites is the elementary excitation, we consider an SU(4) spin chain. For the SU(n) HSM (and particularly for the SU(4) HSM), the lowest lying excitation carries the antifundamental representation.[56] Moreover, the

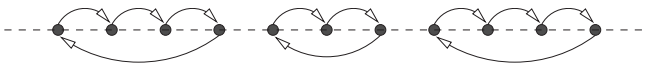

FIG. 8. Quadruplet excitation serving as a domain wall between two of the tetramer ground states on a spin $S=\frac{3}{2}$ chain with $4\mu+3$ sites.

low-energy behavior of SU(4) spin chains with fundamental representation is described by the $SU(4)_{k=1}$ WZNW model where the lowest lying excitation carries the quantum number (0,0,1); i.e., it transforms under the antifundamental representation under SU(4) rotations.[57,58] This representation can be realized by antisymmetrizing three SU(4) spins with fundamental representation (1,0,0). It corresponds in the spin $S=3/2$ model to the quadruplet excitation placed on three consecutive sites (see Fig. 8). This quadruplet excitation is gapped, as it costs a finite energy to break a tetramer singlet.

Most recently, the SU(4) J_1-J_2 model with fundamental representation was investigated both within a level spectroscopy analysis of the ED data[60] and within the density-matrix renormalization group (DMRG) analysis.[61] As proposed by Corboz *et al.*,[46] the existence of a tetramerized phase was verified for the regime $J_1 \approx J_2$.[60,61]

IV. CONCLUSION

In conclusion, we propose exact models for trimerization and tetramerization in antiferromagnetic spin 1 and spin 3/2 chains, respectively. They can be seen as generalizations of the Majumdar-Ghosh model. The models consist of a local Hamiltonian involving four-site or five-site interactions, respectively, with a threefold or fourfold degenerate ground state. The ground states are products of local trimer or tetramer singlets where each trimer or tetramer is placed on three or four consecutive sites. We have numerically investigated the excitation spectrum and verified the validity of both models using exact diagonalization on finite chains.

After this work was completed we became aware of another interesting generalization[62] of the Majumdar-Ghosh model where three-anion interactions in the context of a chain of Fibonacci anions are investigated.

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