Exact results for SU(3) spin chains: Trimer states, valence bond solids, and their parent Hamiltonians

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We introduce several exact models for SU(3) spin chains: (1) a translationally invariant parent Hamiltonian involving four-site interactions for the trimer chain, with a threefold degenerate ground state. We provide numerical evidence that the elementary excitations of this model transform under representation $\overline{3}$ of SU(3) if the original spins of the model transform under representation 3. (2) a family of parent Hamiltonians for valence bond solids of SU(3) chains with spin representations 6, 10, and 8 on each lattice site. We argue that of these three models, only the latter two exhibit spinon confinement, and a Haldane gap in the excitation spectrum.

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Beginning with the invention of the Bethe ansatz in 1931^1 as a method to solve the $S=\frac{1}{2}$ Heisenberg chain with nearest neighbor interactions, a significant share of the entire effort in condensed matter physics has been devoted to the study of quantum spin chains. Faddeev and Takhtajan² discovered in 1981 that the elementary excitations (now called spinons) of the spin-1/2 Heisenberg chain carry spin 1/2 while the Hilbert space is spanned by spin flips, which carry spin 1. The fractional quantization of spin in spin chains is comparable to the fractional quantization of charge in quantized Hall liquids.³ In 1982, Haldane⁴ identified the O(3) nonlinear sigma model as the effective low-energy field theory of SU(2) spin chains, and argued that chains with integer spin possess a gap in the excitation spectrum, while a topological term renders half-integer spin chains gapless.

The general methods—the Bethe ansatz and the use of effective field theories including bosonization—are complemented by a number of exactly solvable models, most prominently among them the Majumdar-Ghosh (MG) Hamiltonian⁵ for the $S=\frac{1}{2}$ dimer chain, the AKLT model⁶ as a paradigm of the gapped S=1 chain, and the Haldane-Shastry model (HSM).^{7–9} In the HSM the wave functions for the ground state and single-spinon excitations are of a simple Jastrow form, elevating the conceptual similarity to quantized Hall states to a formal equivalence. One of the unique features of the HSM is that the spinons are free in the sense that they only interact through their half-Fermi statistics.^{10–12} The HSM has been generalized from SU(2) to SU(*n*).^{13–16}

For the MG and the AKLT model, only the ground states are known exactly. Nonetheless, these models have amply contributed to our understanding of many aspects of spin chains, each of them through the specific concepts captured in its ground state.^{17–24}

In the past, the motivation to study SU(n) spin systems with n > 2 has been mainly formal. The Bethe ansatz has been generalized to multiple component systems by Sutherland,²⁵ which has been applied to the SU(n) HSM (Refs. 13 and 14) and an SU(4) spin chain used for the description of transition-metal oxides.^{26–28} The effective field theory description of Haldane yielding the distinction between gapless half-integer spin chains and gapped integer spin chains, however, cannot be directly generalized to SU(n) chains, as there is no direct equivalent of the CP¹ representation used in Haldane's analysis.

In recent years, ultracold atoms in optical lattices have provided a framework for model realizations of various problems of condensed matter physics, including the phase transition from a superfluid to a Mott insulator,^{29,30} the fermionic Hubbard model,^{31,32} and SU(2) spin chains.^{33,34} In particular, the Hamiltonians for spin lattice models may be engineered with polar molecules stored in optical lattices, where the spin is represented by a single-valence electron of a heteronuclear molecule.³⁵ Systems of ultracold atoms in optical lattices may further provide an experimantal realization of SU(3) spin systems, and in particular antiferromagnetic SU(3) spin chains, in due course. A simple and intriguing possibility is to manipulate an atomic system with total angular momentum $F = \frac{3}{2}$ such that it simulates an SU(3) spin. For such atoms, one effectively suppresses the occupation of one of the middle states, say the $F^{z}=-\frac{1}{2}$ state, by shifting it to a higher energy while keeping the other states approximately degenerate. At sufficiently low temperatures, one is left with three internal states $F^{z} = -\frac{3}{2}, +\frac{1}{2}, +\frac{3}{2}$, which one identifies with the colors blue, red, and green of an SU(3) spin. In leading order, the number of particles of each color is now conserved, as required by the SU(3) symmetry. If one places one of these atoms at each site of an optical lattice and allows for a weak hopping, one obtains an SU(3)antiferromagnet for sufficiently large on-site repulsions U.

Motivated by both this prospect as well as the mathematical challenges inherent to the problem, we propose several exact models for SU(3) spin chains in this paper. The models are similar in spirit to the MG or the AKLT model for SU(2), and consist of parent Hamiltonians and their exact ground states. There is no reason to expect any of these models to be integrable, and none of the excited states are known exactly.

Consider a chain with N lattice sites, where N has to be divisible by three, and periodic boundary conditions (PBCs). On each lattice site we place an SU(3) spin which transforms under the fundamental representation $\mathbf{3}=(1,0)$, i.e., the spin can take the values (or colors) blue (b), red (r), or green (g). [We label the representations of SU(3) by their dimensions (the bold numbers) or their Dynkin coordinates (a pair of non-negative integers).³⁶] The trimer states are obtained by requiring the spins on each three neighboring sites to form an SU(3) singlet $\mathbf{1}=(0,0)$, which we call a trimer and sketch it by $\circ - \circ - \circ$. The three linearly independent trimer states are given by



FIG. 1. Dispersions of the representations 3 (left) and 3 trial states (right) in comparison to the exact excitation energies of Eq. (5). The lines are a guide to the eye.

and two more states obtained by shifting this one by one or two lattice sites, respectively. Introducing operators $c_{i\sigma}^{\dagger}$, which create a fermion of color σ (σ =b,r,g) at lattice site *i*, the trimer states can be written as

$$|\psi_{\text{trimer}}^{(\mu)}\rangle = \prod_{i} \left(\sum_{(\alpha,\beta,\gamma)=\pi(b,r,g)} \operatorname{sgn}(\pi) c_{i\alpha}^{\dagger} c_{i+1\beta}^{\dagger} c_{i+2\gamma}^{\dagger}\right)|0\rangle,$$
(2)

where $\mu = 1, 2, 3$ labels the three degenerate ground states, *i* runs over the lattice sites subject to the constraint that $\frac{i-\mu}{3}$ is integer, and the sum extends over all six permutations π of the three colors b, r, and g.

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

$$J_i^a = \frac{1}{2} \sum_{\sigma, \sigma' = b, r, g} c_{i\sigma}^{\dagger} \lambda_{\sigma\sigma'}^a c_{i\sigma'}, \quad a = 1, \dots, 8,$$
(3)

where the λ^a are the Gell-Mann matrices.³⁶ The operators (3) satisfy the commutation relations $[J_i^a, J_j^b] = \delta_{ij} f^{abc} J_i^c$, a, b, c = 1, ..., 8, with f^{abc} the structure constants of SU(3). We further introduce the total SU(3) spin of ν neighboring sites $i, ..., i + \nu - 1$,

$$J_{i}^{(\nu)} = \sum_{j=i}^{i+\nu-1} J_{j},$$
 (4)

where J_i is the eight-dimensional vector formed by its components (3). The parent Hamiltonian for the trimer states (2) is given by

$$H_{\text{trimer}} = \sum_{i=1}^{N} \left(\left(\boldsymbol{J}_{i}^{(4)} \right)^{4} - \frac{14}{3} \left(\boldsymbol{J}_{i}^{(4)} \right)^{2} + \frac{40}{9} \right).$$
(5)

To verify this Hamiltonian, note that since the spins on the individual sites transform under the fundamental representation 3, the SU(3) content of four sites is

PHYSICAL REVIEW B 75, 060401(R) (2007)

$$\mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} = 3 \cdot \mathbf{3} \oplus 2 \cdot \mathbf{\overline{6}} \oplus 3 \cdot \mathbf{15} \oplus \mathbf{15'}, \qquad (6)$$

i.e., we obtain representations 3, $\overline{6}=(0,2)$, and the two nonequivalent representations 15=(2,1) and 15'=(4,0). All these representations can be distinguished by their eigenvalues of the quadratic Casimir operator.³⁶

For the trimer states (1), the situation simplifies as we only have the two possibilities

$$\begin{array}{cccc} \circ & - \circ & \circ & \hat{=} & \mathbf{1} \otimes \mathbf{3} = \mathbf{3}, \\ \circ & - \circ & \circ & - \circ & \hat{=} & \mathbf{\overline{3}} \otimes \mathbf{\overline{3}} = \mathbf{3} \oplus \mathbf{\overline{6}}, \\ \end{array}$$

[where $\overline{\mathbf{3}} = (0, 1)$], i.e., the total SU(3) spin on four neighboring sites can only transform under representations **3** or $\overline{\mathbf{6}}$. The eigenvalues of the quadratic Casimir operator for these representations are $\frac{4}{3}$ and $\frac{10}{3}$, respectively. The auxiliary operators

$$H_i = \left(\left(\boldsymbol{J}_i^{(4)} \right)^2 - \frac{4}{3} \right) \left(\left(\boldsymbol{J}_i^{(4)} \right)^2 - \frac{10}{3} \right)$$
(7)

hence annihilate the trimer states for all values of i, while they yield positive eigenvalues for **15** or **15**', i.e., all other states. Summing H_i over all lattice sites i yields Eq. (5).

There are two different kinds of domain walls between the degenerate ground states. The first kind consists of an individual SU(3) spin, which transforms under representation 3; the second kind consists of two antisymmetrically coupled spins on two neighboring sites, and hence transforms under representation $\overline{3}$. Since they can decay into each other, only one of these domain walls can constitute an approximate eigenstate of the trimer model. We have performed numerical studies on chains with N=13 and N=14, which clearly indicate that the elementary excitations of the trimer chain (5)transform under $\overline{3}$ (see Fig. 1). This result appears to be a general feature of representation 3 SU(3) spin chains, as it was recently shown explicitly to hold for the HSM as well.¹⁶ The elementary excitations of the trimer chain are deconfined, meaning that the energy of two localized representation 3 domain walls or colorons does not depend on the distance between them.

We now introduce a family of exactly soluble valence bond models for SU(3) chains of various spin representations of the SU(3) spins at each lattice site. To formulate these models, we will use SU(3) Schwinger bosons b, b^{\dagger} (blue), r, r^{\dagger} (red), and g, g^{\dagger} (green),³⁸ which are defined by $|b\rangle$ $=c_b^{\dagger}|0\rangle=b^{\dagger}|0\rangle$, $|r\rangle=c_r^{\dagger}|0\rangle=r^{\dagger}|0\rangle$, and $|g\rangle=c_g^{\dagger}|0\rangle=g^{\dagger}|0\rangle$, and satisfy $[b, b^{\dagger}]=[r, r^{\dagger}]=[g, g^{\dagger}]=1$ while all other commutators vanish. The Schwinger bosons can be used to combine spins transforming under the fundamental representation 3=(1,0)symmetrically, and hence to construct representations such as 6=(2,0) and 10=(3,0).

The trimer states (2) can be rewritten using SU(3) Schwinger bosons as $|\psi_{\text{trimer}}^{(\mu)}\rangle = \Psi^{\mu}[b^{\dagger}, r^{\dagger}, g^{\dagger}]|0\rangle$ with

EXACT RESULTS FOR SU(3) SPIN CHAINS: TRIMER...

$$\Psi^{\mu}[b^{\dagger}, r^{\dagger}, g^{\dagger}] = \prod_{\substack{i \\ \left(\frac{i-\mu}{3} \text{ integer}\right)}} \left(\sum_{(\alpha, \beta, \gamma) = \pi(b, r, g)} \operatorname{sgn}(\pi) \alpha_{i}^{\dagger} \beta_{i+1}^{\dagger} \gamma_{i+2}^{\dagger}\right).$$
(8)

We obtain a representations **6** VBS from two trimer states by projecting the tensor product of two fundamental representations **3** onto the symmetric subspace, i.e., onto the **6** in the tensor product $3 \otimes 3 = \overline{3} \oplus 6$. Graphically, we illustrate this as follows:

This construction yields three linearly independent 6 VBS states, which are readily written out using Eq. (8),

$$\left|\psi_{\text{6VBS}}^{(\mu)}\right\rangle = \Psi^{\mu}[b^{\dagger}, r^{\dagger}, g^{\dagger}] \cdot \Psi^{\mu+1}[b^{\dagger}, r^{\dagger}, g^{\dagger}] |0\rangle \tag{10}$$

for $\mu = 1, 2, \text{ or } 3$. These states are zero-energy ground states of the parent Hamiltonian $H_{6\text{VBS}} = \sum_{i=1}^{N} H_i$ with

$$H_i = \left(\left(\boldsymbol{J}_i^{(4)} \right)^2 - \frac{4}{3} \right) \left(\left(\boldsymbol{J}_i^{(4)} \right)^2 - \frac{10}{3} \right) \left(\left(\boldsymbol{J}_i^{(4)} \right)^2 - \frac{16}{3} \right) \quad (11)$$

(see Ref. 37). Note that the operators J_i^a , $a=1,\ldots,8$, are now given by 6×6 matrices, as the Gell-Mann matrices only provide the generators (3) of the fundamental representation **3**. As in the trimer model, two distinct types of domain walls exist, which transform according to representation **3** and $\overline{3}$. Since both excitations are merely domain walls between different ground states, there is no confinement between them.

Let us now turn to the **10** VBS chain. By combining the three different trimer states (8) symmetrically,

$$\psi_{10\text{VBS}}\rangle = \Psi^{1}[b^{\dagger}, r^{\dagger}, g^{\dagger}] \cdot \Psi^{2}[b^{\dagger}, r^{\dagger}, g^{\dagger}] \cdot \Psi^{3}[b^{\dagger}, r^{\dagger}, g^{\dagger}]|0\rangle,$$
(12)

we automatically project out the representation 10 in the tensor product $3 \otimes 3 \otimes 3 = 1 \oplus 2 \cdot 8 \oplus 10$ generated on each lattice site by the three trimer chains. This construction yields a unique state



The parent Hamiltonian acts on pairs of neighboring sites. It is constructed by noting that the only representations that are included in both $\mathbf{10} \otimes \mathbf{10}$ and $\mathbf{\overline{3}} \otimes \mathbf{\overline{3}} \otimes \mathbf{3} \otimes \mathbf{3}$ (which is the representation content of the total spin of two neighboring sites of the VBS state as indicated by the dashed box above) are the representations $\mathbf{\overline{10}} = (0,3)$ and $\mathbf{27} = (2,2)$. With the eigenvalues of the Casimir operator, which are 6 and 8, respectively, we obtain the parent Hamiltonian for Eq. (12) PHYSICAL REVIEW B 75, 060401(R) (2007)

$$H_{10VBS} = \sum_{i=1}^{N} \left((J_i J_{i+1})^2 + 5 J_i J_{i+1} + 6 \right).$$
(14)

The Hamiltonian (14) provides the equivalent of the AKLT model,⁶ whose unique ground state is constructed from dimer states by projection onto spin 1, for SU(3) spin chains.

Since the **10** VBS state (12) is unique, domain walls connecting different ground states do not exist. We hence expect the coloron and anti-coloron excitations to be confined in pairs, as illustrated below. The state between the excitations is no longer annihilated by Eq. (14), as there are pairs of neighboring sites containing representations different from $\overline{10}$ and **27**, as indicated by the dotted box below. As the number of such pairs increases linearly with the distance between the excitation, the confinement potential depends linearly on this distance.

coloron anti-coloron

$$\overline{3}$$
 $\overline{3}$
 $\overline{0}$ $\overline{0}$

The confinement force between the pair induces a linear oscillator potential for the relative motion of the constituents. The zero-point energy of this oscillator gives rise to a Haldane-type energy gap (see Ref. 39 for a similar discussion in the two-leg Heisenberg ladder). We expect this gap to be a generic feature of representation **10** spin chains with short-range antiferromagnetic interactions.

Finally, we construct a representation **8** VBS state, where **8**=(1,1) is the adjoint representation of SU(3). Consider first a chain with alternating representations **3** and $\overline{3}$ on neighboring sites, which we combine into singlets. This can be done in two ways, yielding the two states

We then combine one $3\overline{-3}$ state with the one shifted by one lattice spacing. This yields representations $3 \otimes \overline{3} = 1 \oplus 8$ at each site. The 8 VBS state is obtained by projecting onto the adjoint representations 8. Corresponding to the two $3\overline{-3}$ states illustrated above, we obtain two linearly independent 8 VBS states, Ψ^L and Ψ^R , which may be visualized as

These states transform into each other under parity or color conjugation (interchange of **3** and $\overline{3}$). The corresponding states may be formulated as a matrix product.³⁷

The parent Hamiltonian for these states is constructed along the same lines as above, yielding

$$H_{8\text{VBS}} = \sum_{i=1}^{N} \left((\boldsymbol{J}_i \boldsymbol{J}_{i+1})^2 + \frac{9}{2} \boldsymbol{J}_i \boldsymbol{J}_{i+1} + \frac{9}{2} \right).$$
(17)

 Ψ^L and Ψ^R are the only (zero-energy) ground states of Eq. (17) for $N \ge 3$.

The low-energy excitations of the **8** VBS model are given by coloron-anticoloron bound states

We find a linear confinement potential between the excitations, and hence a Haldane-type gap in the spectrum. Numerical studies on a chain with N=8 sites provide evidence in support of this conclusion.³⁷ In addition to the bound state (18), the model allows for domain wall between the two ground states Ψ^L and Ψ^R . They consist of bound states of either two colorons or two anticolorons, which are confined through the same mechanisms as the coloron-anticoloron

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PHYSICAL REVIEW B 75, 060401(R) (2007)

bound state (18), as one may easily infer from a cartoon similar to the one above. We hence expect a Haldane gap for each individual domain wall as well.

The results regarding confinement and deconfinement of the excitations of the **6**, **10**, and **8** VBS presented here are consistent with a rigorous theorem by Affleck and Lieb⁴⁰ on the existence of energy gaps in the spectrum of SU(n) nearest-neighbor Heisenberg spin chains.

In conclusion, we have formulated several exact models of SU(3) spin chains. We first introduced a trimer model and presented evidence that the elementary excitations of the model transform under the SU(3) representations conjugate to the representation of the original spin on the chain. We further introduced three SU(3) valence bond solid chains with representation **6**, **10**, and **8**, respectively, on each lattice site. The elementary excitations of the **10** and the **8** valence bond solid chain were found to be confined.

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