Spin 3/2 dimer model

S. Rachel\textsuperscript{(a)}

Institut für Theorie der Kondensierten Materie, Universität Karlsruhe
Postfach 6980, 76128 Karlsruhe, Germany, EU

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Abstract – We present a parent Hamiltonian for weakly dimerized valence bond solid states for arbitrary half-integral $S$. While the model reduces for $S = 1/2$ to the Majumdar-Ghosh Hamiltonian, we discuss this model and its properties for $S = 3/2$. Its degenerate ground state is the most popular toy model state for discussing dimerization in spin 3/2 chains. In particular, it describes the impurity-induced dimer phase in Cr8Ni as proposed recently. We point out that the explicit construction of the Hamiltonian and its main features apply to arbitrary half-integral spin $S$.

Introduction. – Valence bond solid (VBS) states played an important role for the understanding of quantum spin chains. Originally introduced as exact ground states of the integral spin $S$ Affleck-Kennedy-Lieb-Tasaki (AKLT) models \cite{1,2}, VBS states meanwhile refer to all spin $S$ states consisting of nearest neighbor singlet bonds. Amongst them, the spin 1/2 Majumdar-Ghosh (MG) states \cite{3,4} are the most important examples as their parent Hamiltonian corresponds to a certain point in the parameter space of the spin 1/2 $J_1$-$J_2$ model with antiferromagnetic $J_1$. As such, the MG model links dimerized VBS states and dimerized spin chains where the frustration is forced by next-nearest neighbor interactions. For $S > 1/2$, however, this exact link is not given anymore. The VBS states seem not to belong to the phase diagrams of the frustrated Heisenberg chains. Nonetheless, VBS states are often used as toy model states in order to discuss frustration in quantum spin chains, see for the spin 3/2 case refs. \cite{5–13} and references therein. Parent Hamiltonians, however, are only known for the Majumdar-Ghosh states \cite{3}, for the translational invariant AKLT states \cite{1}, and for the spin 1 dimer states \cite{5}. For spin 3/2 and larger $S$, no exact and translational invariant Hamiltonians are known having dimerized VBS states as their unique ground states. Most recently, valence bond solid states have attracted renewed interest. VBS states have been generalized to special unitary SU($n$) symmetry \cite{14–18}, to special orthogonal symmetry SO($n$) \cite{19,20}, and to symplectic symmetry $SP(n)$ \cite{21}. A supersymmetric extension of VBS states has been proposed recently \cite{22}.

In this letter, we present a parent Hamiltonian for the partially or weakly dimerized VBS states (see fig. 1 for the illustration of the spin 3/2 case). For spin 1/2, this Hamiltonian reduces to the MG Hamiltonian. The particular importance of the spin 3/2 Hamiltonian is given by its possible realization in the impurity-induced dimer phase in Cr8Ni as proposed recently \cite{12}. This molecular nanomagnet comprises eight chromium(III) ions with spin 3/2 and one nickel(II) ion with spin 1. The ground state of this Cr8Ni ring was shown to be well understood in the VBS picture \cite{12} by means of numerical simulations. Likewise, the Hamiltonian can be implemented within DMRG, as only standard spin interaction terms are

\begin{itemize}
  \item \textsuperscript{(a)}E-mail: rachel@tkm.uni-karlsruhe.de
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Fig. 1: Illustration of the spin 3/2 dimer states. (a) and (b) are the twofold degenerate partially dimerized VBS states. Each state can be seen as the covering of the AKLT state with one of the Majumdar-Ghosh states. The large gray-shaded circles are the lattice sites, while the small black dots denote a spin 1/2. The spins 1/2 on a lattice site will be projected onto the totally symmetric subspace, i.e., $S = 3/2$. The lines between two spins 1/2 denote a singlet bond.
present. This will allow for extensive numerical studies complementary to known results for the spin 3/2 $J_1$-$J_2$ model with antiferromagnetic $J_2$.

This letter is organized as follows: we start with a brief discussion of general properties of VBS states. Then we introduce the $S=3/2$ dimer Hamiltonian which has the weakly dimerized VBS states shown in fig. 1 as ground states and show that these are the unique ground states. We show that the lowest-lying excitations are fractionally quantized spin 1/2 spinons. Then we discuss the connection to the dimerized phase in the frustrated spin 3/2 Heisenberg model and static spin-spin correlations. Finally, we show that the explicit construction of the Hamiltonian as well as all qualitative results generalize to the case of arbitrary half-integral spin $S$.

**VBS states.** – In 1987, Affleck, Kennedy, Lieb and Tasaki (AKLT) introduced a spin 1 Hamiltonian which was constructed as a sum over a local projection operator. Its unique ground state can be understood as follows: on each lattice site are two spins 1/2 symmetrically coupled into an effective spin 1, while each of the spins 1/2 is antisymmetrically coupled to a spin 1/2 on its neighboring lattice sites, either to the right or to the left. For an illustration, see fig. 2(a). This state was called a valence bond solid. We wish to understand as a VBS all states consisting of local singlet bonds. In particular, we call the MG states and the spin 1 dimer states (see fig. 2(b)) also VBS states even though they break translational invariance spontaneously.

One of the main features of VBS states is that we are able to write down their wave functions explicitly as easily as we illustrate them. Schwinger bosons [23–25] constitute a convenient way to formulate spin $S$ representations. Arovas et al. [26] applied for the first time Schwinger bosons to the AKLT model and to VBS states in general. The spin $S$ operators

$$S^+ = a^\dagger b, \quad S^- = b^\dagger a, \quad S^z = (a^\dagger a - b^\dagger b)/2$$

(1)

are expressed by bosonic creation and annihilation operators which obey the standard commutation relations $[a, a^\dagger] = [b, b^\dagger] = 1$ while all other commutators vanish. The spin quantum number $S$ is given by $2S = a^\dagger a + b^\dagger b$ and the general spin $S$ state is defined as

$$|S, s_z\rangle = \frac{(a^\dagger)^{S+s_z}(b^\dagger)^{S-s_z}}{\sqrt{(S+s_z)! (S-s_z)!}} |0\rangle.$$

(2)

The spin 1/2 states are thus given by $c_{i\uparrow}^\dagger |0\rangle = a_{i\uparrow}^\dagger |0\rangle$ and $c_{i\downarrow}^\dagger |0\rangle = b_{i\downarrow}^\dagger |0\rangle$, respectively. The difference between the fermionic operators and Schwinger bosons shows up only when two or more creation operators act on the same site. While fermion operators create a singlet configuration $c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger |0\rangle$, Schwinger bosons create a totally symmetric representation.

The elegance of Schwinger bosons comes to light when defining the general spin $S$ VBS state:

$$|\psi_{(m,n)}\rangle = \prod_i (B_{2i})^m (B_{2i-1})^n |0\rangle,$$

(3)

where $B_i = a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger$ creates on sites $i$ and $i+1$ a singlet bond. We recover for $(m=1, n=0)$ and $(0,1)$, respectively, the MG states. The $S=1$ AKLT state can thus be written as $|\psi_{(1,1)}\rangle$ and the spin 1 dimer state (fig. 2(b)) as $|\psi_{(2,0)}\rangle$. Obviously, $m+n = 2S$ and there are always $2S+1$ VBS states. For half-integer $S$, there are always $S+\frac{1}{2}$ pairs of dimerized states with different strengths of dimerization. For integer $S$, there are $2S$ pairs of dimerized states and one additional AKLT state $|\psi_{(S,S)}\rangle$. Note that there is always a pair of completely dimerized VBS states regardless of $S$. We stress again that the Schwinger bosons ensure the symmetric projection on every lattice site.

In this letter, we are mainly interested in $S=3/2$ VBS states. There are four of them: completely dimerized states $|\psi_{(3,0)}\rangle$ and $|\psi_{(0,3)}\rangle$ (the latter is shown in fig. 3) and weakly dimerized states $|\psi_{(2,1)}\rangle$ and $|\psi_{(1,2)}\rangle$ (both are shown in fig. 1). For the weakly dimerized VBS states, we present in the next paragraph a parent Hamiltonian. We wish to mention that one can easily define a spin $S$ Hamiltonian in terms of local projection operators annihilating all $2S+1$ VBS states. It involves three-site interactions and reduces for $S=1/2$ to the well-known MG Hamiltonian. For $S>1/2$, however, this is not a parent Hamiltonian anymore as it has all spin $S$ VBS states as ground states. The Hamiltonian is given by

$$H_S = \sum_{i=1}^{3S} \sum_{\mu=S+1} A_{\mu} P_{i,\mu} P_{i+1,\mu+2}.$$

(4)
Spin 3/2 dimer Hamiltonian. – Now we present the Hamiltonian which uniquely singles out the weakly dimerized VBS states $|\psi_{(2,1)}\rangle$ and $|\psi_{(1,2)}\rangle$ as shown in fig. 1. This Hamiltonian is a sum of projection operators $P_i^{(S)}$, which project onto the spin $S$ subspace on $\mu + 1$ neighboring sites:

$$\mathcal{H}^{\text{dimer}} = \sum_i \left( A_2^{i} P_{i,i+1,i+2}^{(\frac{3}{2})} + A_2^{i} P_{i,i+1,i+2}^{(\frac{3}{2})} \right)$$

Consequently, the additive term $\beta \mathcal{H}_2$ in (7) does not affect the weakly dimerized VBS state while the fully dimerized state will be lifted to higher energy. This lifting is controlled by the parameter $\beta > 0$ and can be tuned continuously.

The auxiliary Hamiltonian $\mathcal{H}_1$ has the four $S = 3/2$ VBS states as exact zero-energy ground states, $\mathcal{H}_1|\psi_{(2,0)}\rangle = \mathcal{H}_1|\psi_{(2,1)}\rangle = \mathcal{H}_1|\psi_{(1,2)}\rangle = \mathcal{H}_1|\psi_{(1,3)}\rangle = 0$. This can be seen as follows: Consider three neighboring sites of one of the four VBS states (no matter which of the VBS states, completely or partially dimerized ones): there are always three singlet bonds and three individual spin 1/2 representations, $0 \otimes 0 \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = 2 \cdot \frac{1}{2} \otimes \frac{3}{2}$. In general, the tensor product between three spins 3/2 is given by $\frac{3}{2} \otimes \frac{3}{2} \otimes \frac{3}{2} = 2 \cdot \frac{1}{2} \otimes \frac{3}{2} \otimes \frac{3}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{3}{2}$. The projection onto the subspace with representation $S = 5/2$, $S = 7/2$, and $S = 9/2$ singles out the four VBS states as ground states. We can express the local projection operator in terms of spin operators as done in eq. (5). Now we consider the nearest neighbor projection operator $P_i^{(3)}$. The Hamiltonian $\mathcal{H}_2 = \sum_i P_i^{(3)}$ has an infinite ground-state degeneracy. This can be seen as every state is a ground state where two spins 1/2 per site are in the AKLT configuration and the third spin 1/2 is “free”. The partially dimerized states obviously belong to this set of ground states while the completely dimerized states are not ground states of $\mathcal{H}_2$. Consequently, the term $\beta \mathcal{H}_2$ in (7) lifts the completely dimerized states continuously to higher energy as $\beta$ is increased. The partially dimerized states remain as unique ground states. This scenario is shown in fig. 4 for a chain with $N = 12$ sites and periodic boundary conditions where the data was obtained by means of exact diagonalization.

For open boundary conditions the situation changes: the dimer states are no global singlets anymore, edge states emerge, and the dimer states are fourfold (singlet and triplet) and ninefold (singlet, triplet, and quintuplet) degenerate. When cutting the dimer states, either one individual spin 1/2 or two symmetrically coupled spins 1/2 remain which are not coupled in local singlet bonds (the two different cuts correspond to the two ground states in case of periodic boundary conditions). The dangling spins at the edges cause the degeneracy of the dimer ground states. For the first situation (N even) the two edge spins couple into a singlet and a triplet, $1/2 \otimes 1/2 = 0 \oplus 1$, yielding a fourfold degenerate dimer state. For the second situation (N even), the two spins 1/2 at each edge are symmetrically coupled into a triplet, $S_1 \otimes S_2 = 1$. Hence, the two edge spins carry spin 1 and will be coupled into singlet, triplet, and quintuplet, $1 \oplus 1 = 0 \oplus 1 \oplus 2$, yielding a ninefold degenerate ground state. This manifold degeneracy of the ground state in case of open boundary conditions can be nicely observed numerically, when looking at the different $S^z$-subspaces.

Fractionally quantized excitations. – As already discussed, we are able to define the model Hamiltonian...
tary excitations of (7) are also spin-1/2 spinons. This is not the Majumdar-Ghosh Hamiltonian, for $S_N$ is expected, but the value

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states. As the Hilbert space of spin $S$ as domain walls interpolating between different ground states. In fact, the left spinon in the cartoon constitutes a domain wall between the ground states $\langle \psi_{(2,1)} \rangle$ and $\langle \psi_{(3,0)} \rangle$ while the right spinon constitutes a domain wall between $\langle \psi_{(3,0)} \rangle$ and $\langle \psi_{(2,1)} \rangle$.

(c) For clarity we have fixed the left spinon. From the sequence (a), (b), and (c) we note that the spinons can occupy only half the number of sites (see the explanation in the text). The reader should notice that the “states” shown in (a), (b), and (c) are not exact eigenstates of $H_1$ but the cartoons provide a good intuitive picture of the low-lying excitations.

$H_1(S)$ (see eq. (4)) acting on three neighboring sites for arbitrary spin $S$ exhibiting a $(2S + 1)$-fold degenerate ground state, i.e., the $2S + 1$ possible spin $S$ VBS states [10,32]. For $S = 1/2$, this model corresponds to the MG Hamiltonian, for $S = 1$ to the Hamiltonian proposed by Sen and Surendran [32], and for $S = 3/2$ to $H_1$ of eq. (5). In all of these Hamiltonians, the lowest-lying excitation will be a pair of deconfined $S = 1/2$ spinons. This is easy to understand as the spinons emerge in these models as domain walls interpolating between different ground states. As the Hilbert space of spin $S$ antiferromagnets is spanned by spin flips which carry spin 1, the spin 1/2 excitation has to be seen as a fractionally quantized excitation. We illustrate this situation for the Hamiltonian $H_1$ in fig. 5. In the cartoon fig. 5, we notice another interesting point: even though the spinons are free they can only occupy every second lattice site. If there are only a few spinons in a chain, the number of orbitals available to them is roughly half the number of sites reflecting their fractionally quantized character.

Now the question remains whether this picture of free spinon excitations holds for the Hamiltonian $H_{\text{dimer}}$ considered in this paper. As we mentioned above, relevant in our cartoons is only the number of singlet bonds between neighboring sites while the order of singlet bonds is irrelevant and, hence, a VBS state is identified uniquely by $m$ and $n$. The cartoon in fig. 6 suggests that elementary excitations of (7) are also spin 1/2 spinons. This is not unexpected as the Hamiltonian (7) is the Hamiltonian $H_1$ plus an additional term $H_2$ which lifts up the fully dimerized states out of the ground-state manifold. In conclusion, the whole consideration of deconfined spinon excitations in the spin 3/2 dimer model is consistent with the picture that the origin of the Haldane gap [33] is a confinement force between spinons [16,34]. The generic $S = 3/2$ spin chain, the nearest neighbor Heisenberg model, is known not to exhibit a Haldane gap and, hence, the spinons cannot be confined. While the generic spin 3/2 chain has a gapless excitation spectrum, the Hamiltonians $H_{\text{dimer}}$ and $H_1$ as well as all spin $S$ Hamiltonians mentioned at the beginning of this section exhibit a gapped excitation spectrum as it costs a finite energy to break a singlet bond. This energy cost survives in the thermodynamic limit but it is not the Haldane gap.

**Discussion.** - The Hamiltonian (7) has the weakly dimerized states $\langle \psi_{(2,1)} \rangle$ and $\langle \psi_{(1,2)} \rangle$, respectively, as exact ground states. Dimerization is usually caused by frustration. In one spatial dimension this is realized in a next-nearest-neighbor Heisenberg model, $\mathcal{H} = \sum_i S_i S_{i+1} + \alpha S_i S_{i+2}$, when the next-nearest-neighbor coupling $\alpha$ exceeds a critical value $\alpha_c$.

The spin 1/2 Heisenberg model is characterized by a critical phase for $\alpha < \alpha_c = 0.2411$ [35-37]. The system undergoes a second-order phase transition to a dimerized phase for $\alpha > \alpha_c$. For $\alpha_{MG}$, the Hamiltonian corresponds to the Majumdar-Ghosh model exhibiting the exact dimer states $\langle \psi_{(1,0)} \rangle$ and $\langle \psi_{(0,1)} \rangle$ as ground states. Notice that the dimerization becomes exact in the thermodynamic limit only. That is, the ground state becomes perfectly degenerate due to the broken translation symmetry. One ground state has total momentum $k = 0$ while the other has $k = \pi$. Except for $\alpha_{MG}$, the ground-state degeneracy is
not in the finite system. Nevertheless, ground states in the dimer phase are known to exhibit a good overlap with the MG ground states.

For the spin 3/2 Heisenberg model with next-nearest neighbor interaction $\alpha$, Roth and Schollwöck found the phase transition to the dimerized phase at $\alpha_{c,3/2} \approx 0.33$ [9]. They further computed the maximum dimerization for $\alpha_{\text{max}} = 0.415$. We expect that the ground states in the spin 3/2 dimer phase correspond to the weakly dimerized states rather than the completely dimerized states, i.e., our Hamiltonian (7) can be seen as the $S = 3/2$ analog of the MG model. We can further conjecture that the states $|\psi(2,1)\rangle$ and $|\psi(1,2)\rangle$ will have an excellent overlap with the ground states in the dimer phase investigated by Roth and Schollwöck for sufficiently large system lengths. Such system lengths are not computable within ED. Nevertheless, in principle the Hamiltonian (7) is implementable within DMRG as pointed out above and the calculation of overlaps might be feasible. Furthermore, it might be interesting to compute the static spin-spin correlations within DMRG. Correlations are known to decay quite fast in dimer phases, for the MG states, however, the correlations decay abruptly, i.e., $\langle S_i S_{i+2}\rangle = 0$. Hence, the question remains for the spin 3/2 dimer model whether the spin-spin correlations decay fast, say exponentially, or abruptly.

**Generalization to arbitrary half-integer $S$.** — We are able to formulate the generalized version of the Hamiltonian (7) to arbitrary half-integer $S$. It involves interactions between three neighboring sites and is formulated in terms of projection operators as follows:

$$\mathcal{H}^S = \sum_i \left( \sum_{\mu_1 = S+1}^{2S} A_{\mu_1} P^{(\mu_1)}_{i,i+1,i+2} + \beta \sum_{\mu_2 = S+\frac{1}{2}}^{2S} A_{\mu_2} P^{(\mu_2)}_{i,i+1} \right).$$

(9)

We have restricted $S$ to be half-integer and $\beta > 0$. The twofold degenerate ground state of $\mathcal{H}^S$ is explicitly given by $|\psi(S+\frac{1}{2},S+\frac{1}{2})\rangle$ by means of (3). For $S = 1/2$, the weakly dimerized states reduce to the well-known Majumdar-Ghosh (MG) states (in this case, the “weakly dimerized” states coincide with the completely dimerized states). Since the second sum in (9) does not contribute for $S = 1/2$, the Hamiltonian (9) reduces to the sum over the projection operator onto the $S = 3/2$ subspace on three-neighbor dimerization sites which is known to be the MG Hamiltonian. For $S = 3/2$, the Hamiltonian $\mathcal{H}^S$ is equivalent to (7). For larger $S$, e.g. $S = 5/2$, we find easily the Hamiltonian $\mathcal{H}_1 = \mathcal{H}_1(\frac{5}{2})$ which has a $(2S+1)$-fold degenerate-ground-state manifold consisting of all VBS states. Again the term $\mathcal{H}_2$ lifts up all VBS to higher energy except the weakly dimerized states. For $S = 5/2$, the Hamiltonian $\mathcal{H}_2$ is given by $\mathcal{H}_2 = \sum_i [13397 (S_i S_{i+1}) + 3582 (S_i S_{i+1})^2 + 400 (S_i S_{i+1})^3 + 16 (S_i S_{i+1})^4] + 274505/16$. Although one is restricted to small chain lengths when $S$ becomes 5/2 or larger, all these terms are implementable within ED and the $S = 5/2$ spin-dimer model $\mathcal{H}_1 + \beta \mathcal{H}_2$ might be verified numerically.

**Conclusion.** — In conclusion, we have presented a parent Hamiltonian for the weakly dimerized VBS states with arbitrary half-integer $S$. For spin 3/2, we have explained its construction explicitly and have discussed its main properties. These weakly dimerized spin 3/2 VBS states might be realized in the impurity-induced dimer phase of the ground state of the molecular nanomagnet Cr8Ni. The path for further numerical consideration has been pointed out. Finally, the generalization to spin $S$ has been explained.

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