Matrix product states for $su(2)$ invariant quantum spin chains

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Abstract. A systematic and compact treatment of arbitrary $su(2)$ invariant spin-$s$ quantum chains with nearest-neighbour interactions is presented. The ground-state is derived in terms of matrix product states (MPS). The fundamental MPS calculations consist of taking products of basic tensors of rank 3 and contractions thereof. The algebraic $su(2)$ calculations are carried out completely by making use of Wigner calculus. As an example of application, the spin-1 bilinear-biquadratic quantum chain is investigated. Various physical quantities are calculated with high numerical accuracy of up to 8 digits. We obtain explicit results for the ground-state energy, entanglement entropy, singlet operator correlations and the string order parameter. We find an interesting crossover phenomenon in the correlation lengths.

Keywords: density matrix renormalisation group, tensor network simulations, entanglement entropies, spin chains, ladders and planes
1. Introduction

Matrix product states (MPS) continue to attract scientific attention either as a subject in its own right, or as realizations [1, 2] in density matrix renormalization group (DMRG) studies [3–6]. In the condensed matter community, the interest in such states developed with the discovery of AKLT models with exact ground-states of the type of MPS with finite dimensional auxiliary space [7, 8], also called valence bond solids. Generalizations including anisotropic models followed in [9–15], where especially in [11–13] the formulation as matrix product states was used. The models [7, 8], despite their fine-tuned interactions, were found to be representatives of ‘typical’ systems. The naturally appearing boundary degrees of freedom added even more interest to the MPS states as they realize symmetry protected topological order [16, 17]. On the practical side, the MPS allowed for a variational treatment of the ground-state of a given Hamiltonian [1, 2, 18–21] resulting in the current understanding of DMRG techniques, see e.g. [6]. Finally, in the literature on integrable lattice systems MPS states appear where the local tensor is called vertex operator [22–24].

In this paper we are interested in the fundamental implementation of Lie algebra symmetries in MPS with su(2) as a most important example, however with arbitrary spin-\(s\) in the quantum space. By doing this, we are convinced that many calculations can be performed more efficiently than without use of the symmetry. To give an example of this reasoning we like to remind again of the AKLT model [7, 8]. By use of a transfer matrix formalism, all correlation functions of the state can be calculated from the eigenstates and eigenvalues of the transfer matrix. In the case of AKLT, the transfer matrix is nothing but a product of two \(3j\) symbols. The eigenstates themselves are nothing but \(3j\) symbols, and the eigenvalues are \(6j\) symbols. All of these objects
are ‘tabulated’ and no actual calculation is needed, just the right identification is necessary.

The use of Lie algebra symmetries in DMRG calculations has some history \[25–30\]. For an introduction to the DMRG algorithm from the perspective of the MPS formulation with particular emphasis on Abelian and non-Abelian symmetries we like to refer to \[31\]. This non-Abelian MPS-algorithm based on recoupling coefficients and the Wigner-Eckart theorem found many applications \[32, 33\]. Similar applications of non-Abelian symmetries as su(2) in MERA and TEBD algorithms can be found in \[34, 35\], as well as use of anyonic symmetries in \[36\].

In the paper \[29\] two of the current authors have started to formulate the local tensors of MPS and various associated objects like transfer matrices in a su(2) invariant manner by use of Wigner calculus. The aim was the formulation of a variational MPS calculus with an energy function(al) that is set up by use of su(2) tensor product decompositions and recoupling coefficients, and in the numerical part allows for an evaluation without representation theoretical means. The work \[29\] was restricted to spin-1/2 in the quantum space. In this paper we present the generalization to arbitrary spin-s and report on concrete applications to the spin-1 bilinear-biquadratic quantum chain which we investigate in a large part of the Haldane phase. In addition to the generalization over \[29\] we managed to formulate less intricate graphical rules for the construction of the basic components of MPS calculations. We believe that such transparent rules are also essential for calculations in the higher dimensional case of tensor network states, see for instance \[37–41\] and especially for variational treatments \[42–47\].

The paper is organized as follows. In section 2 we shortly summarize the tensor calculus of MPS and introduce the su(2) invariant local objects based on Wigner’s 3j symbols. Many objects are presented in diagrammatical manner and are based on graphs with three-pointed vertices. The graphical rules are formulated and explicit formulas for various kinds of transfer matrices are given. We treat general nearest-neighbour couplings, entanglement entropy and string order. Also some details on our optimization technique and its comparison to infinite and finite size DMRG algorithms are given. In section 3 we present explicit results from numerical variational calculations for the spin-1 bilinear-biquadratic chain. The results are compared with numerical data of the literature. In section 4 we present our conclusions.

2. Realization of su(2) invariance

We consider the class of matrix-product states

\[ |\psi\rangle = \text{Tr}(g_1 \cdot g_2 \cdot \ldots \cdot g_L), \]

where \( g_i \) is a square matrix with some auxiliary (index) space \( V \). The matrix entries of \( g_i \) are elements of a local quantum space \( V_i \) which we take as the \( i \)th copy of a \( su(2) \) spin-s space \( \mathbb{C}^{2s+1} \).

The \( su(2) \)-invariance of \( |\psi\rangle \) is guaranteed if the objects \( g_i \) are \( su(2) \) invariant tensors in \( V \otimes V^* \otimes \mathbb{C}^{2s+1} \), where \( V^* \) is the dual space to \( V \). We treat the case of a finite dimensional \( V \), however with arbitrary dimensionality. This space will consist of a direct sum over irreducible spin-\( j \) representations where \( j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \). Each \( j \) may appear an
arbitrary number of times \( n_j \), in which case we label the different orthogonal multiplets by an integer \( i \in \{1, ..., n_j\} \). The space \( V \) is spanned by orthogonal states \( |(j, i), m) \) where the magnetic quantum number \( m \) varies from \( -j \) to \( +j \) in integer steps.

Let us consider in \( V \otimes V^* \otimes \mathbb{C}^{2k+1} \) any spin multiplet \( |j_1, i_1) \) from the first factor space, any spin multiplet \( |j_2, i_2) \) from the second factor space, and the (only) spin multiplet \( s \) of the third space. Disregarding scalar factors, there is at most one way of coupling these multiplets to a singlet state. The coupling coefficients are known as \( 3j \) symbols and the desired singlet is

\[
g_{(j_1, i_1), (j_2, i_2)}^s := \sum_{m_1, m_2, m} (-1)^{j_1 - m_1} \left( \begin{array}{ccc} j_1 & j_2 & j \\ m_1 & -m_2 & m \end{array} \right) |(j_1, i_1), m_1) \otimes |(j_2, i_2), m_2) \otimes |s, m). \tag{2}\]

We are going to use graphical rules for the construction of \( su(2) \) invariant tensors like \( g \). We associate with any graph consisting of three-pointed stars (vertices) and closed or open directed lines (bonds) an \( su(2) \)-invariant tensor:

- Bonds carry an angular momentum label \( j \) and a label \( m \in \{-j, ..., +j\} \) where summation over \( m \) is implied. The label \( j \) is usually explicitly shown, \( m \) is not. (In case we are dealing with several multiplets of type \( j \) we number those with an integer \( i \) and label the bond with \((j, i)\).)
- Bonds evaluate to factors

\[
(-1)^{j - m} \text{ in case of a closed bond},
\]

\[
|j, m) \text{ in case of an open bond with outgoing arrow},
\]

\[
(-1)^{-m} |j, m| \text{ in case of an open bond with ingoing arrow}.
\]

- Vertices evaluate to a factor

\[
\left( \begin{array}{ccc} j_1 & j_2 & j_3 \\ \pm m_1 & \pm m_2 & \pm m_3 \end{array} \right) \text{ where } (j_1, m_1), (j_2, m_2), (j_3, m_3)
\]

are read off from the bonds of the vertex in anti-clockwise manner. The sign of each entry \( m_i \) in the \( 3j \) symbol is determined by the arrow direction: \(+\) and \(-\) for ‘out’ and ‘in’.

The number of open bonds is equal to the rank of the tensor. Note that due to the symmetries of the \( 3j \) symbols an arrow on a closed bond with associated label \( j \) may be reverted resulting in a factor\(^3 (-1)^j \).

In figure 1 we show the graphical depiction of \( g_{(j_1, i_1), (j_2, i_2)}^s \) and its dual which is obtained by changing ket-vectors into bra-vectors and vice versa. A general \( su(2) \) invariant tensor \( g \) can be written as superposition of these elementary singlets

\[
g = \sum_{(j_1, i_1), (j_2, i_2)} A_{(j_1, i_1), (j_2, i_2)} \cdot g_{(j_1, i_1), (j_2, i_2)}^s \tag{3}\]

with suitable coefficients \( A_{(j_1, i_1), (j_2, i_2)} \). Note that \( s \) does not appear as index of \( A \) as \( s \) is always fixed and unique (for this reason no \( i_3 \) has been introduced either). Due to the symmetry of \( 3j \) symbols with respect to exchange of two columns

\(^3\)Reverting the arrow on a closed bond leads to an exchange \( m \leftrightarrow \pm m \) (only) in the \( 3j \) symbols at the ends of the bond, keeping the factor \((-1)^{j - m} \) on the bond. Replacing \( m \leftrightarrow -m \) everywhere restores the original distribution of \( \pm m \) at the ends, but turns the sign factor associated with the bond to \((-1)^{j - m} = (-1)^{j - m} \cdot (-1)^{j - m} = (-1)^{j - m} \cdot (-1)^{j - m} \).
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\[
g^{s}_{j_1, j_2} = \frac{s}{j_1 - j_2} , \quad g^{s}_{(j_1, i_1), (j_2, i_2)} = \frac{s}{(j_1, i_1) - (j_2, i_2)}
\]

\[
(g^{s}_{j_1, j_2})^+ = (-1)^{j_1 - j_2 + s}.
\]

**Figure 1.** Graphical depiction of the $\text{su}(2)$ invariant basic tensor $g^{s}_{j_1, j_2}$ and its dual $(g^{s}_{j_1, j_2})^+$. Note that the sign factor $(-1)^{j_1 - j_2 + s}$ appearing in the graphical depiction of the dual can be dropped as it disappears in the products along the quantum chain. In our applications there may be different copies of multiplets of the same type $j_1$ and $j_2$ associated with the bonds which will be explicitly noted like $g^{s}_{(j_1, i_1), (j_2, i_2)^{\ast}}$.

\[
\begin{pmatrix}
  j_3 & j_2 & j_1 \\
  m_3 & m_2 & m_1
\end{pmatrix} = (-1)^{j_1 + j_2 + s} \begin{pmatrix}
  j_1 & j_2 & j_3 \\
  m_1 & m_2 & m_3
\end{pmatrix},
\]

we conclude that

\[A_{(j_1, i_1), (j_2, i_2)} = \pm (-1)^{j_1 + j_2 + s} A_{(j_2, i_2), (j_1, i_1)}^{\ast}\]

with globally fixed $\pm$, is a sufficient condition for parity invariance. Note that $j_1 + j_2 + s$ is always integer.

Also note that only few combinations $j_1, j_2, s$ need to be considered: if the triangle condition $|j_1 - j_2| \leq s \leq |j_1 + j_2|$ is violated, the three multiplets can not couple to a singlet.

### 2.1. Norm and transfer matrix

Next, we want to calculate the norm $\langle \psi | \psi \rangle$ and the expectation value of the Hamiltonian $\langle \psi | H | \psi \rangle$ in the thermodynamic limit. The computation leads to

\[
\langle \psi | \psi \rangle = \text{Tr}(g^{s_1}_{1} g^{s_1}_{1} \cdot g^{s_2}_{2} g^{s_2}_{2} \cdot \ldots \cdot g^{s_L}_{L} g^{s_L}_{L}),
\]

where $g^{\ast} \in V^{\ast} \otimes V \otimes (\mathbb{C}^{2^{s+1}})^{\ast}$ is the dual of $g \in V \otimes V^{\ast} \otimes \mathbb{C}^{2^{s+1}}$ and the contraction over the third space is implicitly understood in $g^{\ast}$. Hence $T = g^{\ast}$, $g$ is a linear map $V \otimes V^{\ast} \rightarrow V \otimes V^{\ast}$. A quite explicit expression for $T$ is given in a mixed algebraic and graphical manner in figure 2.

For the computation of the norm we employ the transfer matrix trick yielding for the rhs of (6)

\[
\langle \psi | \psi \rangle = \text{Tr} T^L = \sum_{\Lambda} \Lambda^L,
\]

where the sum is over all eigenvalues $\Lambda$ of $T$. Obviously, in the thermodynamic limit only the largest eigenvalue(s) $\Lambda_0$ contribute. The corresponding left and right eigenstates are denoted by $\langle 0 |$ and $| 0 \rangle$.

The computation of the leading eigenvalue is facilitated by the singlet nature of the leading eigenstate. There are not many independent singlet states in $V \otimes V^{\ast}$. A $(j, i)$
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$$T = \sum_{\{j, i\}} A_{(j_1, i_1), (j_2, i_2)} A^*_{(j'_1, i'_1), (j'_2, i'_2)}.$$  

Figure 2. Definition of the transfer matrix $T$. The graph appearing in the definition evaluates according to the given rules to a $su(2)$ invariant tensor. The sum extends over all four pairs of labels $(j_1, i_1), (j_2, i_2), (j'_1, i'_1), (j'_2, i'_2)$.

Figure 3. Multiplication of fundamental tensor with unnormalized singlet states.

The action of the transfer matrix $T$ onto singlets produces singlets with matrix elements

$$\langle j; i, i' | T | j'; i_r, i'_r \rangle = \frac{(-1)^{h-h+s}}{\sqrt{(2h+1)(2h_r+1)}} A_{(j, i), (j', i')} A^*_{(j, i), (j', i')}.$$  

For this calculation the identity depicted in figure 3 has been used (where for the derivation of (9) $j = s$ is to be used). The total dimension of $V \otimes V^*$ is $\left[ \sum_j n_j (2j + 1) \right]^2$, but the singlet subspace is much lower dimensional: $\sum_j n_j^2$. Due to the still high dimensionality, the diagonalisation in the singlet space has to be done numerically.

In order to give full meaning to the graphical operations in figure 3 we complement our rules by

- Isolated (directed) bonds carry an angular momentum label $j$ and evaluate to a product of the factors $|j, m\rangle$ for the end with outgoing arrow, $(-1)^m |j, m\rangle$ for the end with ingoing arrow.
- Concatenations of two or more graphs correspond to contractions over pairs of open bonds and naturally lead to identifications of the labels that are carried by the joined bonds. 

Graphically, this singlet is depicted by a link carrying an arrow pointing from the $V^*$ to the $V$ space, a label $j$ in the middle and $i, i'$ at the respective ends.

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- Concatenations of two or more graphs correspond to contractions over pairs of open bonds and naturally lead to identifications of the labels that are carried by the joined bonds. 

Note that these rules are consistent with the above rule for the factor contributed by a closed bond. Also note that indices $i$ identifying different multiplets of the same type $j$ appear on the bonds and usually pertain to the entire bond. The only exception are the singlet states represented by arcs with possibly different labels $i$ and $i'$ at the ends.

### 2.2. Nearest-neighbour couplings

We are interested in the spin-$s$ Heisenberg chain with most general nearest-neighbour interaction. The corresponding Hamiltonian can be written in two alternative ways

$$H = \sum_{l=1}^{L} Q(S_{l} S_{l+1}) = \sum_{l=1}^{L} \sum_{j=0}^{2s-1} a_{j} P_{j} \quad (+\text{const.})$$

either with a polynomial $Q$ of degree $2s$ applied to the scalar product of the nearest-neighbour spin vectors, or as a superposition of $2s$ many projection operators $P_{j}$ onto nearest-neighbour spin multiplets $[j]$. The operator $P_{j}$ is given in terms of $3j$ symbols like

$$P_{j} = (2j + 1) \sum_{m_{1}, m_{2}, m_{1}', m_{2}'} \left[ \begin{array}{ccc} s & s & j \\ m_{1} & m_{2} & m_{1}' & m_{2}' \end{array} \right] \cdot |s, m_{1}'\rangle \otimes |s, m_{2}'\rangle,$$

and is graphically depicted in figure 4. We want to determine the matrix-product state with minimal expectation value of the total Hamiltonian $H = \sum_{l} h_{l}$. Due to translational invariance the expectation value of a single projector $P_{j}$ acting on sites 1 and 2 needs to be calculated leading to

$$\langle \psi | P_{j} | \psi \rangle = \text{Tr}(T_{j} T_{1} \cdots \cdot T_{L-2}) = \Lambda_{0}^{L-2} \langle 0 | T_{j} | 0 \rangle.$$

$T_{j}$ is a modified transfer matrix acting in $V \otimes V^{\ast}$, $|0\rangle$ is the (normalized) leading eigenstate of the transfer matrix $T$ and we kept the only term that dominates in the thermodynamical limit. Hence

$$\frac{\langle \psi | P_{j} | \psi \rangle}{\langle \psi | \psi \rangle} = \Lambda_{0}^{2} \langle 0 | T_{j} | 0 \rangle.$$
the ‘magnetic’ quantum numbers. In this way, triangles are reduced to vertices times $6j$ symbols. Details of these calculations are shown in figure 5. The final result of these calculations is given in figure 6.

2.2.1. Minimization of the expectation value of the Hamiltonian

By use of (10) and (12) we write the expectation value of the Hamiltonian in the MPS $|\psi\rangle$ as

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \Lambda_0^{L-2}\langle0|T_H|0\rangle,$$

where $|0\rangle$ is the leading eigenstate of the transfer matrix $T$. From here we assume that all eigenstates $|n\rangle$ of $T$ are orthonormalized. Note that $T$ and $T_H$ are polynomials (of degree 2 and 4) in the variational coefficients $A$ introduced in (3).

The goal is to minimize the energy with respect to the parameters $A$ under the condition that $|0\rangle$ be the leading eigenstate of $T$. We use the built-in optimization routine of Maple and use the following means for providing the gradient of the energy. First of all, the derivatives of $T$ and $T_H$ with respect to $A$ can be calculated easily as these objects are polynomials in $A$. Furthermore, also $\Lambda_0$ and $|0\rangle$ depend on $A$. Their
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Gradients \( \nabla = \frac{\partial}{\partial a} \) are computed from the gradient of \( T \) and from the eigenstates and eigenvalues of the 'unperturbed' \( T \) as

\[
\nabla \Lambda_0 = \langle 0 | \nabla T | 0 \rangle, \quad \nabla | 0 \rangle = - \sum_{n=0} \frac{\langle n | \nabla T | 0 \rangle}{\Lambda_n - \Lambda_0} | n \rangle,
\]

like in quantum mechanical perturbation theory. Lastly, we want to comment on the relation of our minimization scheme to the infinite and finite size MPS based DMRG algorithms. In iDMRG [48, 49] products of finitely many tensors are increased in order to reach as quickly as possible very large system sizes. In fDMRG a product of a fixed number of tensors, for fixed system size, is optimized. Usually, both iDMRG and fDMRG optimize one or two tensors at a time, in fDMRG this is successively applied in sweeps to all tensors. In our approach we account for a simultaneous optimization of all tensors in the infinite product as we compute the local contribution by two tensors (via \( \nabla T \)) and that by the infinite environment (via \( \nabla | 0 \rangle \)). Accounting for both contributions renders the optimization procedure efficient, consistent and of course numerically stable. The expression (15) has actually a correspondence in DMRG calculations. Usually, local updates of tensors are performed, the simultaneous derivative of all tensors is not done as it leads to a large sum over a long string of factors like \( \sum_n T^n \nabla T T^{L-n} | 0 \rangle \). Actually, this can be carried out by use of the eigenvalue spectrum of \( T \) and the geometric series and realizes an alternative derivation of (15) for \( \nabla | 0 \rangle \).

In practical calculations we keep the multiplet content of the auxiliary space fixed, i.e. we optimize with respect to the variational parameters \( A \) for a certain number of spin-\( j \) representations with certain \( j \) values. This yields the optimum in the given setting, but also allows for an adaptive extension. The entanglement spectrum of the reached state gives clear indications on which spin values \( j \) are relevant for introducing additional multiplets or for dropping multiplets. This can be done any time during the calculations: after enlarging the auxiliary space we take the previously obtained variational parameters \( A \) as initial values for the new setting.

2.3. Entanglement

Next, we consider a finite segment of length \( l \) inside a very long quantum chain. The reduced density matrix \( \rho_l \) is obtained from the total density matrix \( \rho \) by taking the trace over all local spaces except for those at sites 1, ..., \( l \)

\[
\rho_l := \text{Tr}_{\text{partial}} \rho.
\]

This object can be written in terms of basis states on the \( l \) sites

\[
|\alpha, \beta; l \rangle := (g_1 g_2 \cdots g_l)_{\alpha, \beta}, \quad \langle a, b; l | := (g_1^* g_2^* \cdots g_l^*)_{a, b}.
\]

Note that these states are usually not orthonormalized, but satisfy

\[
\langle a, b; l | \alpha, \beta; l \rangle \approx_{l \to \infty} \Lambda_0^l \langle \alpha, a | 0 \rangle \langle 0 | \beta, b \rangle, \quad := R_a^l \quad := t_b^l
\]

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where \( |0\rangle \) and \( |0\rangle \) are the left and right leading eigenstates of the transfer matrix \( T \), and we have defined the matrices \( R \) and \( L \).

The matrix elements of the reduced density matrix for a large block can then be given in the form
\[
\langle a, b; l | \rho_j | \alpha, \beta, l \rangle = (RL^T R)^a_j \cdot (LR^T L)^b_j.
\]

Hence, the reduced density matrix in an orthonormalized basis is isomorphic to \( RL^T \). Furthermore, the entanglement entropy for a large block is twice the entropy of the matrix \( RL^T \).

### 2.4. Hidden order

Next, we are interested in the computation of long-range string order \([16,17]\), i.e. ‘hidden order’. Due to symmetry, the standard two-point spin–spin-correlators decay to zero for large separations \( l \) of the operators \( S^{z}_0 \) and \( S^{z}_l \). However, the expectation value of the spin operators times \( \exp(i\pi \sum_{1 \leq j \leq l-1} S^{z}_j) \) does not necessarily vanish. It is known to be non-zero for the Haldane phase of the Heisenberg chain. By use of transfer matrices we find
\[
\langle S^{z}_0 \mathcal{O}_{1,l-1} S^{z}_l \rangle = \Lambda^{-l-1}_0 \langle 0 | T^z(T^z)^{-1} T^z | 0 \rangle,
\]
where the modified transfer matrices \( T^z \) and \( T^r \) are defined similar to the standard transfer matrix \( T \) with the additional action of the spin operators on the physical space: \( T^z := g^z S^z g \) and \( T^r := g^z \exp(\pi i S^z) g \). In case of \( T^r \) we may apply an important simplification rewriting the action of \( \exp(\pi i S^z) \) on the third component of \( g \) as the action of \( \exp(\pi i(-S^z_1 + S^z_2)) \) on the first two components of \( g \). This is due to \( su(2) \) (actually \( u(1) \)) invariance: on the rhs of (2) only terms with \( m_1 - m_2 + m = 0 \) contribute. Now these operators on the horizontal bonds cancel pairwise in the product of the \( l-1 \) many \( T^r \) transfer matrices, except for one factor on the left and one on the right end, see figure 7(a). These factors may then be associated in the general bookkeeping with the \( T^r \) resulting in
\[
\langle S^{z}_0 \mathcal{O}_{1,l-1} S^{z}_l \rangle = \Lambda^{-l-1}_0 \langle 0 | T^z_r T^{l-1}_r T^z_l | 0 \rangle,
\]
where \( T^z_{r,l} \) are identical to \( T^z \) with the additional action of \( \exp(-\pi i S^z_2) \) and \( \exp(\pi i S^z_1) \) in the \( r \) and \( l \) case. For large separation we find the leading contribution
\[
\mathcal{O}_2 := \lim_{l \to \infty} \langle S^{z}_0 \mathcal{O}_{1,l-1} S^{z}_l \rangle = \Lambda^{-2}_0 \langle 0 | T^z_{r} | 0 \rangle \langle 0 | T^z_{l} | 0 \rangle,
\]
just from knowing the leading eigenstate of \( T \).

Working with the modified transfer matrices leads to the insertion of a vertex (3j symbol) into the vertical line in the graphical depiction in figure 2, and used in figure 7(a), as well as associating minus signs with a right resp. left bond. The additional vertex has two bonds with spin-\( s \) and a third bond with spin-1 (and fixed \( m = 0 \) for dealing with the \( z \) component of the spin operator).

We need matrix elements of \( T^{z}_{r,l} \) in the singlet subspace. This result looks like (9) with two additional factors on the rhs. A factor \( \sqrt{s(s+1)(2s+1)} \) stems from treating the spin operators by 3j symbols and takes care of the normalization \( (\hat{S})^2 = s(s+1) \).
The second factor originates from the summation over internal \( m \) variables of the graph in figure 7(b). On for instance the left side of the graph, the triangle is reduced to a star yielding a 6\( j \) symbol. Hence for \( T^z \) we obtain the factor

\[
(-1)^{j_r} \sum_m \begin{pmatrix} j_r & j_r & 1 \\ 1 & 1 & j_l \end{pmatrix} \begin{pmatrix} j_r & j_r & 1 \\ m & -m & 0 \end{pmatrix},
\]

where the last sum evaluates to \( \sqrt{(2j_r + 1)(4j_r(j_r + 1))} \) for half odd integer \( j_r \) and simply 0 for integer \( j_r \).

3. Results

For the nearest-neighbour spin-1 quantum chain with bilinear and biquadratic interaction

\[
H = \sum_{i=1}^{L} ((\hat{S}_i \cdot \hat{S}_{i+1}) + \alpha (\hat{S}_i \cdot \hat{S}_{i+1})^2)
\]
we performed calculations for $-1 \leq \alpha \leq 1/3$. In the auxiliary space we used alternatively purely integer spin multiplets and purely half-odd integer spin multiplets. In the diagrams we show results for $n_{1/2} = 6, n_{3/2} = 6, n_{5/2} = 4, n_{7/2} = 1 (n_s = 0$ for $s > 7/2$) where $n_s$ is the number of independent spin-$s$ multiplets. This corresponds to a 68-dimensional auxiliary space. Taking into account a gauge freedom already described in [29] we have to deal with 80 variational parameters. The actual calculations have been carried out in Maple 13. The minimum in energy was found by the built-in optimization routine and also—with similar results—by a simple gradient procedure.

For $\alpha = 0$ we found a ground-state energy per site of $e_0 = -1.40148401$ which is off by (only) $3 \cdot 10^{-8}$ from the best known numerical value of $-1.401484038971$ [50]. Our result for the string order parameter is $O_2 = 0.374327$ to be compared with $0.37432509$ by [50]. We obtain for the entanglement entropy $S = 2.7786$ and for the correlation length of singlet operators $\xi = 2.1102$. Our value for the entropy compares well with that reported in [51].

At $\alpha = -1$ the model is critical and the accuracy of the data in the above approximation is worse. Still the results for the ground-state energy $e_0 = -3.9995$, the expectation values of the projectors onto nearest-neighbour singlets and triplets $\langle P_0 \rangle = 0.5727$ and $\langle P_1 \rangle = 0.0939$ deviate only by $5 \cdot 10^{-4}$ from the exactly known values $e_0 = -4, \langle P_0 \rangle = 0.5732747261...$ and $\langle P_1 \rangle = 0.093391941...$ [52]. In figure 8 results for correlation functions of singlet operators, i.e. projectors $P_0$ and $P_1$ onto nearest-neighbour singlets and triplets, are shown. At large distances these correlators decay algebraically with exact exponent 1 [53], which is obscured at the accessible distances by subleading terms.

At $\alpha = 1/3$ our results reproduce the known analytical facts about the AKLT model [7, 8]. Here only a single $s = 1/2$ multiplet in the auxiliary space is enough to realize the
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The state with a single spin-$1/2$ multiplet on each bond is of course the VBS state where the $3j$ symbol at the vertex produces a spin-$1$ by symmetrization, and the product of two vertices in the auxiliary space (contraction) corresponds to antisymmetrization of two spin-$1/2$ objects.

In the course of our numerical experiments we found that the same state can be constructed also by integer spin multiplets in the auxiliary space. This can be understood analytically: One needs for instance one spin-$0$ and one spin-$1$ multiplet. The spin-$0$ and spin-$1$ couple with weight $1/\sqrt{6}$ and the spin-$1$ with itself with ‘weight’ $-1/3$. We like to note that effects of alternative choices of purely exact ground state with $e_0 = -2/3$, string order parameter $O_2 = 4/9$ and entanglement entropy $S = \log_2 4 = 2$. The state with a single spin-$1/2$ multiplet on each bond is of course the VBS state where the $3j$ symbol at the vertex produces a spin-$1$ by symmetrization, and the product of two vertices in the auxiliary space (contraction) corresponds to antisymmetrization of two spin-$1/2$ objects.

Figure 9. (a) Plot of (minus) the ground-state energy $e_0$ and of the entanglement entropy $S$ versus the interaction parameter $\alpha$. Also shown are the expectation values of the projection operators $P_0$ and $P_1$ onto nearest-neighbour singlets and triplets. (b) Plot of the correlation lengths $\xi_{\pm}$ for singlet operators. Here $\xi_{+}$ describes the uniformly decaying exponential contribution, and $\xi_{-}$ describes the oscillating contribution. Note the crossover of the correlation lengths at $\alpha_c \approx -0.7$. Also shown is the string order parameter $O_2$ where the small finite result at $\alpha = -1$ is due to the finiteness of the number of multiplets in our MPS calculations.
half-integer or purely integer spin representations in the auxiliary space on the entanglement spectrum have been studied \[54\] for distinguishing topologically trivial and non-trivial phases \[55\].

The dependence of the ground-state energy \(e_0\) and of the expectation values of the projection operators \(P_0, P_1\) on \(\alpha\) is quite smooth—not to say boring—see figure 9(a). The true behaviour of the entanglement entropy would show a singularity at \(\alpha = -1\), but only rises to the finite value of \(S = 5.565\) in our treatment due to the finite number of multiplets. Likewise, the finite string order \(O_2\), see figure 9(b), decreases upon approaching \(\alpha = -1\), but does not drop to exactly 0.

We calculated the correlation lengths of singlet correlation functions from the next-leading eigenvalues of the transfer matrix \(T\). The next-leading positive and negative eigenvalues result in the correlation lengths \(\xi_+\) and \(\xi_-\). For approaching \(\alpha = -1\) both lengths increase, in an exact treatment they would diverge. At some \(\alpha_c \simeq -0.7\) the lengths show a crossover. Interestingly, for \(\alpha \simeq -0.6\) the papers \[1, 56\] reported a softening of an excitation gap at momentum \(\pi\). We believe, that this is not a coincidence. In any case, the implication of the crossover is that for \(\alpha < \alpha_c\).
singlet correlators will generically show oscillating asymptotics, see figure 10(a), and for \( \alpha > \alpha_c \) the asymptotics will be uniformly decaying. However, matrix elements may be of different orders of magnitude and may obscure this behaviour at finite distances, see figure 10(b) where only at sufficiently large distances the oscillations set in.

The dependence of \( \xi_\pm \) on \( \alpha \) is not very smooth for \( \alpha \) values above \( \simeq -0.1 \). Note that the leading correlation lengths describe the asymptotics of the correlations, but a finite dimensional auxiliary space allows only for a reliable computation of shorter ranged correlators. These values are smooth as functions of \( \alpha \) and actually are rather small. In fact, for \( \alpha = 1/3 \) all singlet correlators are zero.

4. Conclusion

In this paper we presented a most economical formulation of general \( su(2) \) invariant MPS with arbitrary spin-\( s \) in the quantum space. The basic objects for the calculation of expectation values of nearest-neighbour interactions and of correlation functions appear as contractions over products of fundamental tensors of rank 3. The contractions involve internal sums over ‘magnetic quantum numbers’ which were evaluated explicitly by use of Wigner calculus. The results of these algebraic calculations were presented in \( su(2) \) invariant manner in terms of \( 3j \) and \( 6j \) symbols.

The usefulness of the \( su(2) \) invariant formulation was demonstrated at the example of the spin-1 bilinear-biquadratic quantum chain directly in the thermodynamical limit. For a large part of the Haldane phase we determined by variational calculations the ground-state energy, the expectation values of projection operators on nearest-neighbour singlet and triplet spaces, the entanglement entropy, string order and singlet operator correlations as well as their leading correlation lengths.

The achieved accuracy is probably more than acceptable for practical purposes. Our numerical calculations were done in Maple 13 and resulted in an accuracy of \( 3 \cdot 10^{-8} \) for the ground-state energy of the strictly bilinear spin-1 Heisenberg chain. These results were obtained for 6, 6, 4, 1 copies of spin-\( 1/2 \), \( 3/2 \), \( 5/2 \), \( 7/2 \) multiplets in the auxiliary space which in total is 68-dimensional.

In future work we want to develop a ‘normal’ program code to do faster calculations and to deal with larger dimensional auxiliary spaces. Ultimately, and by making use of the gained experience with the \( su(2) \) calculus of MPS, we intend to tackle tensor-network calculations.

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