Diagrammatics for $SU(2)$ invariant matrix product states

Andreas Fledderjohann, Andreas Klümper and Karl-Heinz Mütter

Fachbereich C Physik, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

E-mail: kluemper@uni-wuppertal.de

Received 26 July 2011, in final form 30 September 2011
Published 3 November 2011
Online at stacks.iop.org/JPhysA/44/475302

Abstract

We report on a systematic implementation of $su(2)$ invariance for matrix product states (MPS) with concrete computations cast in a diagrammatic language. As an application we present a variational MPS study of a spin-1/2 quantum chain. For efficient computations, we make systematic use of the $su(2)$ symmetry at all steps of the calculations: (i) the matrix space is set up as a direct sum of irreducible representations, (ii) the local matrices with state-valued entries are set up as superposition of $su(2)$ singlet operators, (iii) products of operators are evaluated algebraically by making use of identities for $3j$ and $6j$ symbols. The remaining numerical computations like the diagonalization of the associated transfer matrix and the minimization of the energy expectation value are done in spaces free of symmetry degeneracies. The energy expectation value is a strict upper bound of the true ground-state energy and yields definite conclusions about the accuracy of density-matrix renormalization group results reported in the literature. Furthermore, we present explicit results with accuracy better than $10^{-4}$ for nearest- and next-nearest-neighbour spin correlators and for general dimer–dimer correlators in the thermodynamical limit of the spin-$1/2$ Heisenberg chain with frustration.

PACS numbers: 03.67.-a, 05.30.-d, 75.10.Jm, 75.10.Pq

(Some figures may appear in colour only in the online journal)

1. Introduction

Interacting quantum many-body systems are a dynamical field of research. On one hand, quantum systems with many degrees of freedom show interesting cooperative phenomena that often elude simple physical intuition. On the other hand, the necessary calculations are computationally hard as the underlying Hilbert space grows exponentially with system size. From a pragmatical point of view, it is very important to identify low-dimensional manifolds of physically relevant and computationally tractable states. A very attractive class
of states is realized by the matrix-product states (MPS) which yield excellent results even when working with a reduced set. The computational efforts can be further minimized in the case of quantum systems with symmetries. Here, we present a variational MPS study for the frustrated antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain by use of a systematic implementation of $su(2)$ invariance paralleling the treatments in [1, 2].

MPS appear in different, but closely related ways. Historically, products of matrices with entries from a local Hilbert space first appeared as exact ground states (matrix-product ground states, MPG) for Hamiltonians with a special local ground-state structure, see [3, 4] and developments [5–13]. Second, in the literature on integrable systems, vertex operators [21–23] were introduced for a transfer matrix like construction of ground states of lattice systems. Third, the density-matrix renormalization group (DMRG) [14–18] algorithms were shown [19, 20] to result in states of MPS type. The MPG, vertex operators and DMRG are all realizations of MPS. Consequently, this important class of states attracted strong interest in the quantum computation community [24–30].

In applications of MPS, details may differ strongly. For instance, in MPG and DMRG realizations, the matrix index space is finite dimensional, whereas in the vertex-operator case, this space is mostly infinite dimensional. In MPG, the MPS are used as an ansatz for an ‘exact state’ for which a ‘parental Hamiltonian’ is to be found in subsequent investigations. In DMRG, the MPS appear as variational states for the Hamiltonian. In the case of the vertex operator, the full ground-state structure is captured at the expense of infinite-dimensional matrices.

Our investigation is motivated by the need for a computationally most efficient scheme for general $su(2)$ singlet states of MPS type. The local implementation of Lie group invariance has been used before in DMRG studies [31–34] and related MPS studies [35–37]. In [38, 39], $su(2)$ invariant MPGs and their parental Hamiltonians were constructed. A variational analysis of $su(2)$ invariant MPS for quantum chains and ladders was already presented in the early work [1, 2]. The paper [1] is well known for the insight that the finite-system DMRG leads to quantum states in MPS form, over which it variationally optimizes. To our knowledge, the computational scheme of $su(2)$ invariant MPS with arbitrary matrix space did not attract the attention the papers [1, 2] deserve.

Here we use a variational computation scheme very similar to [1, 2] based on $su(2)$ invariant MPS. However, we reduce the necessary constructions to a minimum without making any reference to DMRG algorithms. Also, we use a diagrammatic representation of some of the key objects and relations occurring in the process of the evaluation of the norm and the energy expectation value of the MPS. We hope that this approach will make the subject as accessible as possible. Our main application will be the study of ground-state energies, spin–spin and dimer–dimer correlations of the (frustrated) antiferromagnetic spin-$\frac{1}{2}$ Heisenberg chain with nearest- and next-nearest-neighbour interactions. For not too strong frustration, this system shows critical behaviour. Still, the variational $su(2)$ invariant MPS give excellent results even for the correlation functions. Probably, and in contrast to the expectation expressed in [2], the approach is applicable even to odd-legged spin-$\frac{1}{2}$ ladders that are not finitely correlated.

Obviously, and following scientific lore, it is important to use all available symmetries to find invariant blocks of the transfer matrix as low dimensional as possible in order to reduce the computational work involved with the diagonalization procedure. Even more important than the economical treatment of the transfer matrix is the efficient, nonredundant parameterization of the local building elements, i.e. the matrices with entries from the local Hilbert space. It is essential to parameterize these objects with as few parameters as possible to reduce the computational time of the minimization of the energy expectation value.
The paper is organized as follows. In section 2, we present a fairly general derivation of equilibrium states in the form of MPS and shortly summarize the tensor calculus of MPS with emphasis on realizations of symmetries. In section 3, we introduce the $su(2)$ invariant local objects based on Wigner’s $3j$ symbols. Here we also introduce the transfer matrices and evaluate products of operators by making use of identities involving the $3j$ and $6j$ symbols. In section 4, we present explicit results from numerical evaluations of the basic formulas derived in the previous section. The results are compared with DMRG data of the literature [40] for the frustrated spin-$\frac{1}{2}$ Heisenberg chain and conclusions about the accuracy of the methods are drawn.

2. Derivation of MPS and realization of $SU(2)$ invariance

We study quantum spin systems with local interactions. It is well known that quantum systems in $d$ spatial dimensions can be mapped to classical systems in $d + 1$ dimensions. In this way, the ground-state properties of a quantum chain in the thermodynamical limit are encoded by a classical system on an unrestricted two-dimensional square lattice. Often, for numerical purposes, the quantum chain is mapped onto a kind of Ising model on a square lattice with a checkerboard structure; for analytical purposes, the mapping of quantum chains onto vertex models on periodic square lattices is more convenient. (The associated classical vertex model has nearest-neighbour couplings even for quantum spin chains with interactions ranging farther than nearest neighbours.) Here, the reasoning is based on equilibrium states, but obviously the derivation is more general and covers all steady-state systems with local interactions.

After mapping the quantum chain onto a vertex model, the correlation functions of the classical model on the full plane yield the correlations of the quantum chain, as is well known. It is less well known, but equally easy to understand that the partition function of a half-plane with arbitrary, but fixed, boundary spins yields the coefficients of the ground state of the quantum chain with respect to the standard basis. The evolution operator associated with a column of the full plane is known as the transfer matrix of the model. The corresponding objects of the half-plane are known as (lattice) vertex operators. As seen in figure 1, these objects carry spin variables on the left, on the right and one spin variable on the top. When considering these objects as matrices where the spin variables on the left play the role of the row index, and the spin variables on the right play the role of the column index, vertex operators are matrices with (local) spin state-valued entries. The goal of the DMRG procedure may be understood as the computation of the optimal truncation of the infinite-dimensional vertex operator to a finite-dimensional matrix space. In this section, we present the algebraic background for the construction of general $su(2)$ invariant MPS.

We first summarize the basic algebraic constructions needed for our investigation of many-body quantum spin systems. We place particular emphasis on the compatibility with symmetry groups, notably Lie groups. Eventually, we will be interested in the Lie group $SU(2)$ which is the reason for being specific from the beginning.

We consider the class of MPS

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

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

$SU(2)$-invariance of $|\psi\rangle$ is guaranteed if for the representation $U_s$ of $SU(2)$ in $\mathbb{C}^{2s+1}$, there is a representation $U_V$ in $V$ such that $U_s$ applied to any element of the matrix $g_i$, denoted by $U_s g_i$, yields a matrix identical to $U_V^{-1} \cdot g_i \cdot U_V$ where the dots refer to matrix multiplication.
Figure 1. (a) Illustration of the relation of quantum spin chains and classical models on square lattices. The rows and columns of the square lattice define the action of the row-to-row and the column-to-column transfer matrix. (b) The coordinates \( \langle \ldots \sigma_i \sigma_{i+1} \ldots | \psi \rangle \) of the ground state of the quantum system correspond to the partition functions of the classical model on the half-plane with fixed boundary spins \( \ldots \sigma_i \sigma_{i+1} \ldots \). The column of the half-plane with fixed boundary defines the vertex operator.

Obviously we obtain with (1)

\[
U_\nu \otimes U_\nu \otimes \ldots \otimes U_\nu |\psi\rangle = \text{Tr}(U_\nu g_1 \cdot U_\nu g_2 \cdot \ldots \cdot U_\nu g_L)
= \text{Tr} \left( U_\nu^{-1} \cdot g_1 \cdot U_\nu \cdot U_\nu^{-1} \cdot g_2 \cdot U_\nu \cdot \ldots \cdot U_\nu^{-1} \cdot g_L \cdot U_\nu \right)
= |\psi\rangle.
\]

(2)

The local condition for \( SU(2) \)-invariance can be written as

\[
U_\nu \otimes U_\nu g U_\nu^{-1} = g.
\]

(3)

with \( U_\nu \) and \( U_\nu \) acting from the left and \( U_\nu^{-1} \) from the right. The object \( g \) may be regarded as a tensor of the space \( V \otimes \mathbb{C}^{2s+1} \otimes V^* \) where \( V^* \) is the dual space to \( V \). (Note that the product \( A \cdot B \) of two linear maps \( A \) and \( B \) of the space \( V \) corresponds to the tensor product followed by a contraction of \( A \) and \( B \) viewed as tensors in \( V \otimes V^* \).)
For the purpose of imposing discrete lattice symmetries like parity, i.e. invariance with respect to reflections, we adopt a different point of view. Let us consider tensors $G$ from $V \otimes \mathbb{C}^{2k+1} \otimes V$. As a local condition for $SU(2)$-invariance, we demand

$$U_V \otimes U_\epsilon \otimes U_\epsilon^* G = G,$$

and as a local condition for parity invariance, we demand—as a sufficient condition—that $G$ be symmetric with respect to the exchange of ‘the first and the third index’ when written in a canonical basis.

The relation between $g$ and $G$ is realized by a $SU(2)$-invariant tensor $S$ from $V \otimes V$ (and by the invariant dual tensor $S^*$ from $V^* \otimes V^*$). Concrete candidates for $S$ (and $S^*$) will be given shortly.

The tensor $S$ can equivalently be understood as a linear map from $V^*$ to $V$ as the multiplication of an arbitrary element $\tilde{v}$ of $V^*$ with $S$ yields an object in $V^* \otimes V \otimes V$; the subsequent contraction over the first and second space yields an element $v$ of $V$. Denoting $S(\tilde{v}) := v$, we establish $S$ as a map $V^* \to V$. The $SU(2)$ invariance of $S$ as a tensor in $V \otimes V$ is written as $U_V \otimes U_\epsilon S = \tilde{S}$ from which we find

$$S(\tilde{v} U_V^{-1} ) = U_V v = U_V S(\tilde{v}).$$

The object $G$ is obtained by the action of $S$ on the third space of $g$,

$$G = \text{id} \otimes \text{id} \otimes S \ g,$$

which takes (3) into (4) thanks to (5).

Conversely, we establish $S^*$ as a linear map $V \to V^*$ with $SU(2)$-invariance $S^*(U_V v) = S^*(v) U_V^{-1}$ and for the concrete realizations of $S$ and $S^*$, we find $S \cdot S^* = (-1)^{2j}$ and $S^* \cdot S = (-1)^{2j}$ in spin-$j$ subspaces. Hence, $S$ and $S^*$ are invertible and $g = \text{id} \otimes \text{id} \otimes S^{-1} G$.

Finally, we have to give explicit constructions for $S$ (and $S^*$) as $SU(2)$-invariant states in $V \otimes V$. This is the only place where we make explicit use of the fact that our Lie symmetry group is $SU(2)$. We take the space $V$ as a direct sum of some 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, in which case we label the different orthogonal multiplets by an integer $i$. The space $V$ is spanned by orthogonal states $| (j, i, m) \rangle$ where the magnetic quantum number $m$ varies from $-j$ to $+j$ in integer steps.

The $SU(2)$ singlet states in $V \otimes V$ and $V^* \otimes V^*$ are given by

$$S := \sum_{j,i} \sum_{m=-j}^j (-1)^{j+m} | (j, i, m) \rangle \otimes | (j, i, -m) \rangle,$$

$$S^* := \sum_{j,i} \sum_{m=-j}^j (-1)^{j+m} | (j, i, m) \rangle \otimes | (j, i, -m) \rangle,$$

where $S^*$ is related to $S$ by replacing the ket-states by the dual bra-states.

Applying our above-formulated definitions, we find for $v = | (j, i, m) \rangle$ that $S(\tilde{v}) = (-1)^{j+m} | (j, i, -m) \rangle$. Conversely, for $v = | (j, i, m) \rangle$ we have $S^*(v) = (-1)^{j-m} | (j, i, -m) \rangle$. Hence, the successive action of $S$ and $S^*$ yields $(-1)^{2j} \text{id}$.

3. Basic representation theoretical settings: 3$j$ and 6$j$ symbols

Having spelled out the fundamental objects appearing as factors in $SU(2)$-invariant MPS, the concrete calculations are straightforward. We use $SU(2)$ singlets $G$ in $V \otimes \mathbb{C}^{2k+1} \otimes V$. Having already allowed for reducible representations in $V$, we like to stress that for our applications, we must deal with $V$ as a direct sum of more than one irreducible representation. This is so as
for the most interesting case of \( s = \frac{1}{2} \), no singlet \( G \) exists if \( V \) is identical to just one spin-\( j \) multiplet. There is no half-integer spin in the tensor product decomposition of two spin-\( j \) for the most interesting case of \( s \).

Let us consider in \( V \otimes \mathbb{C}^{2s+1} \otimes V \) any spin multiplet \( (j_1, i_1) \) from the first factor space, the (only) spin multiplet \( j_2 = s \) of the second space and again any spin multiplet \( (j_3, i_3) \) from the third factor space. Disregarding scalar factors, there is at most one way of coupling these multiplets to a singlet state. The coupling coefficients are known as 3\( j \) symbols and the desired singlet is

\[
|\{j_1, i_1, j_2, j_3, i_3\}\rangle = \sum_{m_1, m_2, m_3} \left( \begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right) |(j_1, i_1) \rangle \otimes |j_2, m_2 \rangle \otimes |j_3, i_3, m_3 \rangle.
\]

(8)

Further below we will be using a graphical language for constructions and actual calculations. For instance, singlet (8) and its dual are depicted by three straight lines carrying arrows, see figure 2. The coupling coefficients of the singlets shown in figure 2 are given in figure 3. More precisely, the objects shown figure 2 are obtained by multiplying the objects in figure 3 by the states \( |\{j, i, m\}\rangle \) (or the dual) and summing over all magnetic quantum numbers \( m \).

The singlet \( G \) can be written as a superposition of these elementary singlets,

\[
G = \sum_{\{j_1, i_1, j_2, i_2, j_3, i_3\}} A^{j_1, j_2, j_3}_{i_1, i_2, i_3} |\{j_1, i_1, j_2, i_2, j_3, i_3\}\rangle,
\]

(9)

with suitable coefficients \( A^{j_1, j_2, j_3}_{i_1, i_2, i_3} \). Note that \( j_2 \) has been suppressed as an index-like argument of \( A \) as \( j_2 \) is always identical to \( \frac{1}{2} \) and unique (for this reason, no \( i_2 \) has been introduced above).

Due to the symmetry of 3\( j \) symbols with respect to the exchange of two columns,

\[
\left( \begin{array}{ccc} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{array} \right) = (-1)^{j_1 + j_2 + j_3} \left( \begin{array}{ccc} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{array} \right),
\]

(10)

we conclude that

\[
A^{j_1, j_2, j_3}_{i_1, i_2, i_3} = (-1)^{j_1 + j_2 + j_3} A^{j_3, j_1, j_2}_{i_3, i_1, i_2}
\]

(11)

is a sufficient condition for parity invariance. Note that \( j_1 + j_2 + j_3 \) is always an integer.

Also note that only few combinations \( j_1, j_2, j_3 \) need to be considered: if the triangle condition \( |j_1 - j_2| \leq j_3 \leq |j_1 + j_2| \) or any condition obtained by permutations of the indices
Figure 3. Graphical notation for key arithmetic objects like the Kronecker symbol and the 3j symbol.

is violated, the three multiplets cannot couple to a singlet. Since \( j_2 = \frac{1}{2} \), we are left with the combinations \( \{ j_1, j_1 \} = \{0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \} \). This is a natural result, since \( j_1 \) and \( j_2 = \frac{1}{2} \) only couple to \( j_1 \pm \frac{1}{2} \). Let us denote by \( n_j \) the number of spin-\( j \) multiplets. By use of symmetry (11), we may reduce all possible coefficients \( A \) to a set of \( n_j \times n_j + \frac{1}{2} \) matrices \( A_{j, j + \frac{1}{2}} \) with matrix elements

\[
(A_{j, j + \frac{1}{2}})_{i, i'} := A_{j, j + \frac{1}{2}}^{i, i'}.
\]  

3.1. 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

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

where \( g^* \in V^* \otimes (\mathbb{C}^{2r+1})^* \otimes V^* \) is the dual of \( g \in V \otimes \mathbb{C}^{2r+1} \otimes V^* \) and the contraction over the second space is implicitly understood in \( g^* g \). Hence \( T := g^* g \) is a linear map \( V \otimes V^* \rightarrow V \otimes V^* \). For the computation of the norm, we employ the transfer matrix trick yielding for the rhs of (13)

\[
\langle \psi | \psi \rangle = \text{Tr}(T \cdot \ldots \cdot T) = \sum L \Lambda^L,
\]  

where the sum is over all eigenvalues \( \Lambda \) of \( T \). Obviously, in the thermodynamic limit, only the largest eigenvalue(s) contribute.

The computation of the leading eigenvalue is facilitated by the singlet nature of the leading eigenstate. There are not many independent singlet states in \( V \otimes V^* \). A \( (j, i) \) multiplet in \( V \) and
Figure 4. Illustration of identity (18): the summation over two internal magnetic quantum numbers leads to an 'arc'-singlet.

\[ j_1 \quad \begin{array}{c} j_2 \\ \end{array} \quad \begin{array}{c} j_3 \\ \end{array} = \delta_{j_1,j_1} \delta_{m_1,m_1} \cdot \frac{1}{2j_1+1} = \frac{1}{2j_1+1}. \]

8
3.2. Nearest-neighbour couplings

We are interested in the spin-\(\frac{1}{2}\) Heisenberg chain with nearest-neighbour interaction with the Hamiltonian

\[
H = \sum_{l=1}^{L} \vec{S}_l \vec{S}_{l+1}.
\]

The local Hamiltonian is \(h_l = \vec{S}_l \vec{S}_{l+1} = 1/4 - P_{0}^{nm}\) where \(P_{0}^{nm}\) is the projector onto the nearest-neighbour singlet space. We want to determine the MPS with minimal expectation value of the total Hamiltonian \(H = \sum_{l} h_l\). Due to translational invariance, this is achieved by minimizing the expectation value of a single local interaction. In analogy to (14), we obtain

\[
\langle \psi | P_{0}^{nm} | \psi \rangle = \text{Tr}(\bar{T} T \cdots T) = \Lambda_0^{L-2} \langle 0 | T_2 | 0 \rangle,
\]

where we assumed \(P_{0}^{nm}\) to act on sites 1 and 2. \(T_2\) is a modified transfer matrix acting in \(V \otimes V^*\), \(|0\rangle\) is the (normalized) leading eigenstate of the transfer matrix \(T\) and we kept the only term dominating in the thermodynamical limit. Hence,

\[
\frac{\langle \psi | P_{0}^{nm} | \psi \rangle}{\langle \psi | \psi \rangle} = \Lambda_0^{-2} \langle 0 | T_2 | 0 \rangle.
\]

The computation of the matrix elements of \(T_2\) is described graphically in figures 6 and 7. In contrast to the transfer matrix \(T\), the modified matrix \(T_2\) is block diagonal with the \(\sigma(j; i_l, \tilde{i}_l) = \sigma(j; i, \tilde{i})\) matrix element,

\[
\langle j; i_l, \tilde{i}_l | T_2 | j; i, \tilde{i} \rangle = \frac{1}{(2j+1)^2} B^{j,l}_{i_l, \tilde{i}_l} (B^{j,l}_{i, \tilde{i}})^*.
\]

The matrices \(B\) are given by

\[
B^{j,l}_{i,j} = \sum_{\tilde{j}} (-1)^{\frac{j+j'+j''}{2}} A^{j,l}_{j'} A^{j,l}_{j'}.\]
Figure 6. Depiction of the modified matrix $T_2$ in terms of local vertices.

$$T_2 = \begin{pmatrix} \langle \tilde{j}_1, \tilde{i}_1 \rangle & \langle \tilde{j}_1, \tilde{i}_1 \rangle & \langle \tilde{j}_2, \tilde{i}_2 \rangle \\ \tilde{j}_2 & \tilde{j}_2 & j_2 \\ \langle j_1, i_1 \rangle & \langle j_1, i_1 \rangle & \langle j_r, i_r \rangle \end{pmatrix}$$

Figure 7. The summation over two internal magnetic quantum numbers leads to an ‘edge’-singlet.

$$\frac{1}{2j_1+1} \left( \frac{(-1)^{j_1+j_2+j}}{j_1 m_1 j_3 m_3} \right) \left( \begin{array}{c} j_1 m_1 \\ j \end{array} \right) \left( \begin{array}{c} j_3 m_3 \\ j_1 m_1 j_3 m_3 \end{array} \right)$$

Figure 8. Depiction of the modified matrix $T_3$ in terms of local vertices.

$$T_3 = \begin{pmatrix} \langle \tilde{j}_1, \tilde{i}_1 \rangle & \langle \tilde{j}_1, \tilde{i}_1 \rangle & \langle \tilde{j}_2, \tilde{i}_2 \rangle \\ \tilde{j}_2 & \tilde{j}_2 & j_2 \\ \langle j_1, i_1 \rangle & \langle j_1, i_1 \rangle & \langle j_r, i_r \rangle \end{pmatrix}$$

where only the values $j_1 = j \pm \frac{1}{2}$ lead to non-zero terms. (Equations (22) and (23) are the analogue of equation (26) in [2].) Using this and the (sufficient) condition (11) for parity invariance, we find

$$B^{i,j} = [A^{j-i+j} T A^{j-i-j} + A^{j-i+j}] T.$$

(24)

3.3. Next-nearest-neighbour couplings

The next-nearest-neighbour interactions are manageable, too. In the thermodynamical limit, we find

$$\frac{\langle \psi \mid P_{0}^{\text{nnn}} \mid \psi \rangle}{\langle \psi \mid \psi \rangle} = \Lambda_0^{-3} \langle 0 \mid T_3 \mid 0 \rangle.$$

(25)

The computation of the matrix elements of $T_3$ is described graphically in figures 8 and 9. In contrast to the modified transfer matrix $T_2$, but like $T$, the matrix $T_3$ has zero diagonal
blocks and non-zero secondary diagonal blocks. The \( \sigma(j_i; i_i, \tilde{i}_i) - \sigma(j_r; i_r, \tilde{i}_r) \) matrix element of \( T_3 \) is

\[
\langle j_i; i_i, \tilde{i}_i | T_3 | j_r; i_r, \tilde{i}_r \rangle = \frac{1}{\sqrt{(2j_i + 1)(2j_r + 1)}} C^{b; j}_{b; \tilde{b}} (C^{b; j}_{b; \tilde{b}})^*.
\]

(26)

where \( j_i = j_r \pm \frac{1}{2} \) and \( C^{b; j}_{b; \tilde{b}} \) is given by

\[
C^{b; j}_{b; \tilde{b}} = \sum_{j_{i-h}} (-1)^{j_i+j_r+j_{i-h}} \left\{ \begin{array}{ccc}
\tilde{j}_i & \frac{1}{2} & j_r \\
\tilde{j}_3 & \frac{1}{2} & \tilde{j}_1
\end{array} \right\} A^{b; \tilde{i}_i} A^{b; \tilde{i}_r} A^{b; j_{i-h}}.
\]

(27)

Only three combinations of \( j_i, j_3 \) yield non-vanishing contributions. For \( j_r = j_i + 1/2 \), only \( (j_i, j_3) = (j_i - 1/2, j_i), (j_i + 1/2, j_i) \) and \( (j_i + 1/2, j_i + 1) \) are relevant. From this and the (sufficient) condition (11) for parity invariance, we find

\[
C^{\tilde{i}_i; j_{i-h}} = \sum_{j_{i-h}} (-1)^{\tilde{j}_i+j_{i-h}+j_{i-h}} \left\{ \begin{array}{ccc}
\tilde{j}_i & \frac{1}{2} & j_{i-h} \\
\tilde{j}_3 & \frac{1}{2} & \tilde{j}_1
\end{array} \right\} A^{\tilde{i}_i; j_{i-h}} A^{\tilde{i}_i; j_{i-h}} A^{\tilde{i}_i; j_{i-h}}.
\]

(28)

where the \( 6j \) symbols evaluate to

\[
\left\{ \begin{array}{ccc}
j & \frac{1}{2} & j + \frac{1}{2} \\
j & \frac{1}{2} & j - \frac{1}{2}
\end{array} \right\} = (-1)^{2j+1} 2j + 1,
\]

\[
\left\{ \begin{array}{ccc}
j & \frac{1}{2} & j + \frac{1}{2} \\
j & \frac{1}{2} & j - \frac{1}{2}
\end{array} \right\} = (-1)^{2j+1} 2j + 1,
\]

\[
\left\{ \begin{array}{ccc}
j & \frac{1}{2} & j + \frac{1}{2} \\
j & \frac{1}{2} & j + \frac{1}{2}
\end{array} \right\} = \frac{(2j + 1)(2j + 2)}{2j + 2},
\]

\[
\left\{ \begin{array}{ccc}
j & \frac{1}{2} & j + \frac{1}{2} \\
j & \frac{1}{2} & j + \frac{1}{2}
\end{array} \right\} = \frac{(2j + 1)(2j + 2)}{2j + 2}.
\]

(29)

with an exception for \( j = 0 \) where the first listed \( 6j \) symbol has to be taken as 0.

The reader is referred to [35] and especially to [1, 2] for \( su(2) \) tensor algebra and the use of \( 3j, 6j \) and also \( 9j \) symbols. Some of the above-presented relations appeared already in [1, 2], but no analogue to equations (26) and (27).
4. Results

For the nearest-neighbour spin-\(\frac{1}{2}\) Heisenberg chain, we found that already a few low-dimensional multiplets in the matrix space \(V\) yield excellent results, e.g. the ground-state energy differs from the exact result \(e_0 = 1/4 - \ln 2\) by about \(5 \times 10^{-5}\) and dimer correlations are off the exact results by about \(10^{-4}\). This is achieved with \(n_0 = 4, n_2 = 4, n_1 = 3, n_3 = 2, n_2 = 1\) for all \(s\) (\(n_s = 0\) for \(s > 2\)). Note that the attempt to include higher spin multiplets at the expense of reducing the low-spin multiplets is not successful as for instance \(n_s = 1\) for all \(s\) leads to the simple dimer (Majumdar–Ghosh) state.

The minimization of the energy expectation value yields the following list of coefficients:

\[
A^{0,1}_0 = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & -0.283412 & 0 & 0 \\
0 & 0 & 0.183208 & 0 \\
0 & 0 & 0 & 0.679798
\end{bmatrix},
A^{1,1} = \begin{bmatrix}
0.737765 & 0 & 0 & 0 \\
0.257549 & -0.860519 & 0 & 0 \\
0.610288 & -0.093768 & 0.050733 & 0 \\
0.191246 & -0.631258 & 0.181757 & 0
\end{bmatrix},
A^{1,2} = \begin{bmatrix}
0.510676 & 0 & 0 & 0 \\
-0.5075510 & 0.714082 & 0 & 0 \\
-0.292858 & -0.712182 & 0 & 0
\end{bmatrix},
A^{3,2} = \begin{bmatrix}
0.265736 & 0 & 0 & 0 \\
0 & 0.607939 & 0 & 0
\end{bmatrix}
\]

and a value of the ground-state energy which compares well with the exact value \(e_0 = -0.443147180\ldots\)

Note that \(A^{0,1}_0\) is strictly diagonal, and the other matrices have strictly zero entries above the diagonal due to a ‘gauge’ freedom. The MPS is invariant under a transformation \(A^{i,j}_l \to O^{-1}_i A^{i,j}_l O_j\) where \(O_j\) are arbitrary orthogonal \(n_j \times n_j\) matrices. Also note that the entries of the matrices are strictly real.

Next we give numerical results for the dimer–dimer correlation function

\[
\tilde{D}_n := \langle \vec{S}_1 \cdot \vec{S}_2 (\vec{S}_{n+1} \cdot \vec{S}_{n+2}) \rangle.
\]

For \(n \to \infty\), this converges to \(e_0^2\); hence, it is more instructive to study the connected dimer correlations

\[D_n := \tilde{D}_n - \tilde{D}_\infty.\]

For \(n = 2, 3, 4\), the values are known exactly [42] which we use for comparison with our MPS calculations

\[
D_2^{\text{num}} = +0.060639 \ldots, \quad D_2^{\text{exact}} = +0.060824 \ldots,
D_3^{\text{num}} = -0.027838 \ldots, \quad D_3^{\text{exact}} = -0.027737 \ldots,
D_4^{\text{num}} = +0.018986 \ldots, \quad D_4^{\text{exact}} = +0.018928 \ldots.
\]

We expect that the absolute numerical accuracy is similar also for larger distances \(n\) of the local dimer operators. These results are plotted in figure 10 as \((-1)^n D_n\) versus \(n\). Note that all \((-1)^n D_n\) are positive which implies a sublattice structure with sign alternation of the correlations. There is no long-range order for the spin-\(\frac{1}{2}\) Heisenberg chain with nearest-neighbour interactions.

Next we are interested in the frustrated spin-\(\frac{1}{2}\) Heisenberg chain with the Hamiltonian

\[
H = \sum_{j=1}^L (\vec{S}_j \cdot \vec{S}_{j+1} + \alpha \vec{S}_j \cdot \vec{S}_{j+2}).
\]
The system shows algebraically decaying dimer–dimer correlations for $\alpha \leq 0.2411 \ldots$, see figure 11, and long-range dimer order for $\alpha > 0.2411 \ldots$, see figure 10(b). The critical value $\alpha_c = 0.2411$ was established in [43, 44]. The dimer–dimer correlations are fitted well by algebraic curves for all $\alpha \leq 0.2411 \ldots$ with an $\alpha$-dependent exponent. From field theoretical considerations, the exponent is expected to be identical to 1. We attribute the deviations to logarithmic corrections for $\alpha < 0.2411 \ldots$ which apparently vanish at $\alpha_c$.

As an illustration of spin–spin-correlation functions, we present results for the nearest- and next-nearest-neighbour cases in table 1. For $\alpha = 0$, the exact values are known [41] $C_2^{\text{exact}} = e_0^{\text{exact}}$, see (32), and [42] $C_3^{\text{exact}} = 0.182039 \ldots$. Even for $C_3$, our numerical value deviates from the exact value less than $10^{-4}$. Due to the variational nature of our calculations, the expectation values of the energy are strict upper bounds for the ground-state energy. Note that for the cases $\alpha = 0.1, 0.2411, 0.3, 0.4$, our results are lower than those given in [40] with small differences ranging from $10^{-4}$ to $10^{-3}$. Hence, the deviation of these DMRG results from
Figure 11. Dimer–dimer correlations of the spin-$\frac{1}{2}$ Heisenberg chain with the frustration parameter $\alpha \leq 0.2411$: double log plot of $(-1)^n D_n \alpha$ versus distance $n$ and algebraic lines $c/n^b$ from fits to the data for $n$ in the range $[10, 25]$.

Table 1. Numerical values for the correlations $C_n := \langle \vec{S}_1 \vec{S}_{n+1} \rangle$ for $n = 1, 2$ and various values of the frustration parameter $\alpha$. The ground-state energy $e_0 = C_1 + \alpha C_2$ is given in the last row.

| $\alpha$ | 0.0  | 0.1  | 0.2  | $\alpha$ | 0.3  | 0.4  | 0.5  |
|----------|------|------|------|----------|------|------|------|
| $C_2$    | -0.443 092 | -0.442 655 | -0.440 916 | -0.439 574 | -0.436 475 | -0.420 659 | -0.375 000 |
| $C_1$    | 0.181 942  | 0.173 570  | 0.162 233  | 0.156 176  | 0.144 794  | 0.100 870  | 0.0   |
| $e_0$    | -0.443 092 | -0.425 298  | -0.408 469  | -0.401 920  | -0.393 037 | -0.380 311 | -0.375 000 |

the true ground-state energy must be of the same order or even larger. In DMRG calculations, there are two sources of errors: (i) truncation of the Hilbert space and (ii) finite-size effects due to the finite length of the considered chains. These errors were minimized considerably in the $su(2)$ invariant time-evolving block decimation (TEBD) algorithm [36] where for the unfrustrated case $\alpha = 0$, high numerical accuracy for the spin–spin correlation functions was achieved (e.g. nine significant digits for $C_2$ albeit with many more states than used in our analysis).

In our approach, we deal with the strictly infinitely long chain. As seen above, a low number of multiplets are sufficient for an accuracy of about four significant digits. The numerical computations of the data presented in this section were done by the use of Maple 13 on a laptop computer. The total computation for the seven cases of the frustration parameter took about 1 h. A curious question arises with respect to the systematic choice of multiplets for maximizing the accuracy by keeping fixed the number of variational parameters. We think that the number and spin of the relevant multiplets of the matrix index space $V$ are related to the number and spin of low-lying energy states of long chain segments. This will be investigated in future work.

A more complete study of the correlation functions and of the physics of frustrated systems with $\alpha > 0.5$ will be presented elsewhere. Here we like to note that for $\alpha > 0.5$, the matrices replacing (31) will contain intrinsically complex numbers.
5. Conclusion

We showed how to employ systematically $su(2)$ invariance for matrix product states (MPS) and how to carry out the variational computation of the ground-state energy in a numerically most efficient manner. The algebraic computations for the $su(2)$-invariant building blocks were put in diagrammatic formulation. As an example, we used the (frustrated) spin-$\frac{1}{2}$ Heisenberg chain with nearest- and next-nearest-neighbour interaction. Our algebraic constructions led to the main results (16) for the transfer matrix, and (22), (23) and (26), (27) for the modified transfer matrices, where the coefficient matrix has to satisfy relation (11) for parity invariance.

Our calculations are very similar to those of [1, 2] who applied the method to gapped spin-$1$ chains and spin ladders. The variational MPS calculations for the spin-$\frac{1}{2}$ Heisenberg chain are demanding on their own: the model shows algebraically decaying correlation functions and it is by no means clear if signatures of this decay can already be seen in variational MPS calculations with only few multiplets in the matrix space. Also, in contrast to [1, 2], the matrix space we had to deal with consists of all integer and half-odd integer spin multiplets. In our concrete calculation, we used a matrix space composed of four singlets, four doublets, three triplets, two quadruplets and one quintuplet. We managed to calculate the ground-state energy within a precision better than $10^{-4}$. Also, the correlation functions were computed within an accuracy of the order $10^{-4}$ and allowed for the identification of the scaling dimension in the case of critical frustration ($\alpha = 0.2411$).

The actual numerical calculations like matrix diagonalizations were reduced by the algebraic $su(2)$ implementation from a 1156-dimensional to a 46-dimensional space. The systematic inclusion of more and higher spin multiplets is obvious. Generalizations of these calculations are straightforward, e.g. to spin-$S$ Heisenberg chains with competing interactions.

We are convinced that a systematic application of symmetries to the MPS analysis of quantum spin chains will provide high-quality data with only small truncation errors.

Acknowledgments

The authors would like to thank F Göhmann, M Karbach and J Sirker for valuable discussions, and J Dukelsky and A Schadschneider for relevant information on related work. The authors gratefully acknowledge support by Deutsche Forschungsgemeinschaft under project Renormierungsgruppe KL 645/6-1.

References

[1] Dukelsky J, Martin-Delgado M A, Nishino T and Sierra G 1998 Equivalence of the variational matrix product method and the density matrix renormalization group applied to spin chains Europhys. Lett. 43 457
[2] Roman J M, Sierra G, Dukelsky J and Martin-Delgado M A 1998 The matrix product approach to quantum spin ladders J. Phys. A: Math. Gen. 31 9729
[3] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 Phys. Rev. Lett. 59 799
[4] Affleck I, Kennedy T, Lieb E H and Tasaki H 1988 Commun. Math. Phys. 115 477
[5] Fannes M, Nachtergaele B and Werner R F 1989 Exact antiferromagnetic ground states of quantum spin chains Europhys. Lett. 10 633
[6] Fannes M, Nachtergaele B and Werner R F 1992 Finitely correlated states on quantum spin chains Commun. Math. Phys. 144 443
[7] Klümper A, Schadschneider A and Zittartz J 1991 Equivalence and solution of anisotropic spin-1 models and generalized $t-J$ Fermion models in one dimension J. Phys. A: Math. Gen. 24 L955–9
[8] Klümper A, Schadschneider A and Zittartz J 1992 Groundstate properties of a generalized VBS-model Z. Phys. B 87 281–7
[9] Klöppers, A., Schadschneider, A. and Zittartz, J. 1993 Matrix-product-groundstates for one-dimensional spin-1 quantum antiferromagnets Europhys. Lett. 24 293
[10] Lange, C., Klöpper, A. and Zittartz, J. 1994 Exact groundstates for antiferromagnetic spin-one chains with nearest and next-nearest neighbour interactions Z. Phys. B 96 267
[11] Kolezhuk, A. K. and Mikeska, H. J. 1998 Finiteley correlated generalized spin ladders Int. J. Mod. Phys. B 12 2325–48
[12] Kolezhuk, A. K. and Mikeska, H. J. 1998 Mixed spin ladders with exotic ground states Eur. Phys. J. B 5 543
[13] Kolezhuk, A. K., Mikeska, H. J. and Yamamoto, S. 1997 Matrix product states approach to the Heisenberg ferrimagnetic spin chains Phys. Rev. B 55 R3336
[14] White, S. R. 1992 Density matrix formulation for quantum renormalization groups Phys. Rev. Lett. 69 2863
[15] White, S. R. and Nocqua, R. 1992 Real-space quantum renormalization groups Phys. Rev. Lett. 68 3487
[16] White, S. R. 1992 Density matrix formulation for quantum renormalization groups Phys. Rev. Lett. 69 2863
[17] White, S. R. 1993 Density-matrix algorithms for quantum renormalization groups Phys. Rev. B 48 10345–56
[18] Sierra, G. and Nishino, T. 1997 The density matrix renormalization group method applied to interaction round a face Hamiltonians Nucl. Phys. B 495 505–32
[19] Jeckelmann, E. 2002 Dynamical density-matrix renormalization-group method Phys. Rev. B 66 045114
[20] Schollwöck, U. 2005 The density-matrix renormalization group Rev. Mod. Phys. 77 259
[21] Ostlund, S. and Rommer, S. 1995 Thermodynamic limit of the density matrix renormalization for the spin-1 Heisenberg chain Phys. Rev. Lett. 75 3537
[22] Rommer, S. and Ostlund, S. 1997 A class of ansatz wavefunctions for 1D spin systems and their relation to DMRG Phys. Rev. B 55 2164–81
[23] Jimbo, M., Miki, K., Miwa, T. and Nakayashiki, A. 1992 Correlation functions of the XXZ model for $\Delta < -1$ Phys. Lett. A 168 256
[24] Jimbo, M. and Miwa, T. 1996 Quantum KZ equation with $|q| = 1$ and correlation functions of the XXZ model in the gapless regime J. Phys. A: Math. Gen. 29 2923
[25] Boos, H. E., Göhmann, F., Klöpper, A. and Suzuki, J. 2006 Factorization of multiple integrals representing the density matrix of a finite segment of the Heisenberg spin chain J. Stat. Mech. 2006 P04001
[26] Verstraete, F., Cirac, J. I., Latorre, J. I., Rico, E. and Wolf, M. M. 2005 Renormalization-group transformations on quantum states Phys. Rev. Lett. 94 140601
[27] Verstraete, F. and Cirac, J. I. 2006 Matrix product states represent ground states faithfully Phys. Rev. B 73 094423
[28] Verstraete, F., Wolf, M. M., Perez-Garcia, D. and Cirac, J. I. 2006 Criticality, the area law, and the computational power of projected entangled pair states Phys. Rev. Lett. 96 220601
[29] Wolf, M. M., Ortiz, G., Verstraete, F. and Ignacio, Cirac, J. I. 2006 Quantum phase transitions in matrix product systems Phys. Rev. Lett. 97 110403
[30] Schuch, N., Wolf, M. M., Verstraete, F. and Ignacio, Cirac, J. I. 2007 Computational complexity of projected entangled pair states Phys. Rev. Lett. 98 140506
[31] Bauer, B., Corboz, P., Orús, R. and Troyer, M. 2011 Implementing global Abelian symmetries in projected entangled-pair state algorithms Phys. Rev. B 83 125106
[32] Schuch, N., Wolf, M. M., Verstraete, F. and Ignacio, Cirac, J. I. 2008 Simulation of quantum many-body systems with strings of operators and Monte Carlo tensor contractions Phys. Rev. Lett. 100 040501
[33] Wada, T. 2000 Interaction round a face DMRG method applied to rotational invariant quantum spin chains Phys. Rev. E 61 1199–206
[34] Wada, T. and Nishino, T. 2001 Interaction-round-a-face density-matrix renormalization-group method Comput. Phys. Commun. 142 162–73
[35] McCulloch, I. P. and Galácsi, M. 2002 The non-Abelian density matrix renormalization group algorithm Europhys. Lett. 57 852
[36] Dukelsky, J. and Pittel, S. 2004 The density matrix renormalization group for finite Fermi systems Rep. Prog. Phys. 67 513–52
[37] McCulloch, I. 2007 From density-matrix renormalization group to matrix product states J. Stat. Mech. P10014
[38] Singh, S., Zhou, H-Q and Vidal, G. 2010 Matrix product decomposition and classical simulation of quantum dynamics in the presence of a symmetry New J. Phys. 12 033029
[39] Singh, S., Pfeifer, R. N. C. and Vidal, G. 2010 Tensor network decompositions in the presence of a global symmetry Phys. Rev. A 82 050301
[40] Sanz, M., Wolf, M. M., Perez-Garcia, D. and Cirac, J. I. 2008 Matrix product states: symmetries and two-body Hamiltonians Phys. Rev. A 79 042308
[41] Tu, H-H and Sanz, M. 2010 Exact renormalization in quantum spin chains Phys. Rev. B 82 104404
[42] Chitra, R., Puri, S., Krishnamurthy, H. R., Sen, D. and Ramasesha, S. 1995 Density-matrix renormalization-group studies of the spin-Heisenberg system with dimerization and frustration Phys. Rev. B 52 6581–7
[41] Hulthén L 1938 Über das austauschproblem eines kristalles. Ark. Mat. Astron. Fys. A 26 1–105
[42] Sato J, Shiroishi M and Takahashi M 2006 Exact evaluation of density matrix elements for the Heisenberg chain J. Stat. Mech. P12017
[43] Okamoto K and Nomura K 1992 Phys. Lett. A 169 433
[44] Eggert S 1996 Numerical evidence for multiplicative logarithmic corrections from marginal operators Phys. Rev. B 54 R9612–5