

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

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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 DMRG 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- $\frac{1}{2}$ Heisenberg chain with frustration.

1. Introduction

We use a systematic implementation of $su(2)$ invariance for matrix-product states (MPS), which parallels [1, 2], and perform a variational $su(2)$ -MPS study for the frustrated antiferromagnetic spin- $\frac{1}{2}$ Heisenberg chain.

The class of MPS is of particular importance for the study of quantum spin chains. The 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 special local ground-state structure, see [3, 4] and developments [5]-[13]. Second, in the literature on integrable systems, vertex-operators [20]-[22] were introduced for a transfer-matrix like construction of ground-states of lattice systems. Third, the density-matrix renormalization group (DMRG) [14]-[17] algorithms were shown [18, 19] 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 [23]-[29].

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 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 studied in for instance [33] where $su(2)$ invariant MPG and parental Hamiltonians were investigated, and particularly in the early work [1, 2] where also the variational analysis of $su(2)$ invariant MPS for quantum chains and ladders was introduced. 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. Non-Abelian symmetries were implemented in DMRG studies in for instance [30, 31].

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 taking any reference to DMRG algorithms. Also, we are going to 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, 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-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-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 Sect. 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 Sect. 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 $3j$ and $6j$ symbols. In Sect. 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 [32] for the frustrated spin- $\frac{1}{2}$ Heisenberg chain and conclusions about the accuracy of the methods are drawn.

2. Derivation of matrix product states and realization of $SU(2)$ invariance

We are going to study quantum spin systems with local interactions. It is well-known that quantum system 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 2-dimensional square lattice. Often, for numerical purposes, the quantum chain is mapped onto a kind of Ising model on a square lattice with 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

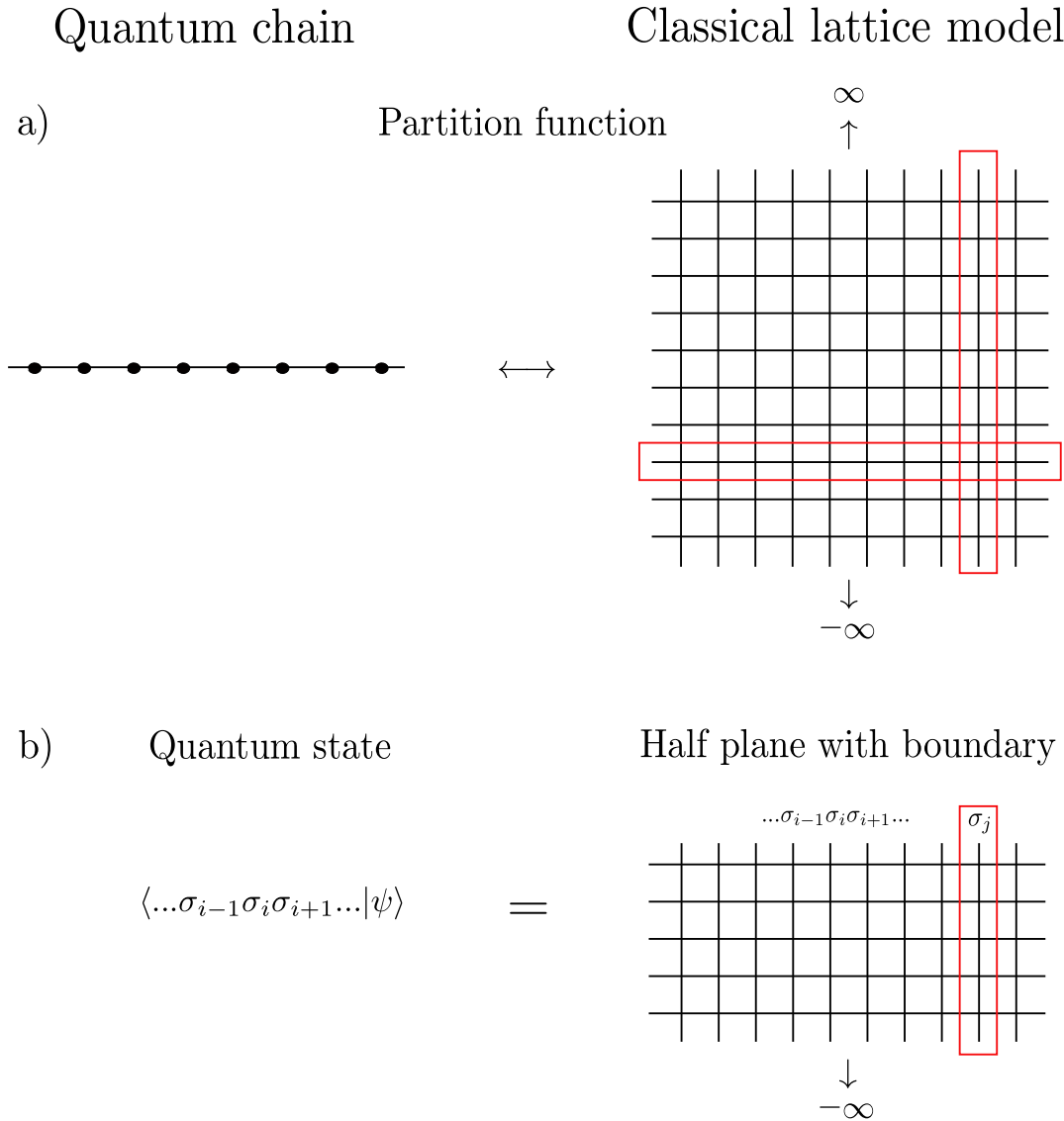


Figure 1. a) Illustration of the relation of quantum spin chains and classical models on square lattices. The rows and columns of the square lattice define the action of the row-to-row and the column-to-column transfer matrix. b) The coordinates $\langle \dots \sigma_{i-1} \sigma_i \sigma_{i+1} \dots | \psi \rangle$ 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 $\dots \sigma_{i-1} \sigma_i \sigma_{i+1} \dots$. The column of the half-plane with fixed boundary defines the vertex operator.

operators. With view to Fig. 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 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 matrix-product states

$$|\psi\rangle = \text{Tr}(g_1 \cdot g_2 \cdot \dots \cdot g_L) \quad (1)$$

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 a $su(2)$ 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 dots refer to matrix multiplication. Obviously we obtain with (1)

$$\begin{aligned} U_s \otimes U_s \otimes \dots \otimes U_s |\psi\rangle &= \text{Tr}(U_s g_1 \cdot U_s g_2 \cdot \dots \cdot U_s g_L) \\ &= \text{Tr}(U_V^{-1} \cdot g_1 \cdot U_V \cdot U_V^{-1} \cdot g_2 \cdot U_V \cdot \dots \cdot U_V^{-1} \cdot g_L \cdot U_V) \\ &= |\psi\rangle \end{aligned} \quad (2)$$

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

$$U_V \otimes U_s g U_V^{-1} = g, \quad (3)$$

meaning that 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 $V \otimes \mathbb{C}^{2s+1} \otimes V$. As a local condition for $SU(2)$ -invariance we demand

$$U_V \otimes U_s \otimes U_V G = G, \quad (4)$$

and as a local condition for parity invariance we demand – as a sufficient condition – that G be symmetric with respect to 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 $V^* \rightarrow V$. The $SU(2)$ -invariance of S as a tensor in $V \otimes V$ is written as $U_V \otimes U_V S = S$ from which we find

$$S(\tilde{v} U_V^{-1}) = U_V v = U_V S(\tilde{v}). \quad (5)$$

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

$$G = \text{id} \otimes \text{id} \otimes S g \quad (6)$$

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

Conversely, we establish S^* as a linear map $V \rightarrow V^*$ 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 $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$. 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. $SU(2)$ singlet states in $V \otimes V$ and $V^* \otimes V^*$ are given by

$$\begin{aligned} S &:= \sum_{j,i} \sum_{m=-j}^j (-1)^{j-m} |(j, i), m\rangle \otimes |(j, i), -m\rangle, \\ S^* &:= \sum_{j,i} \sum_{m=-j}^j (-1)^{j-m} \langle(j, i), m| \otimes \langle(j, i), -m|. \end{aligned} \quad (7)$$

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

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

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

Having spelled out the fundamental objects appearing as factors in $SU(2)$ -invariant matrix-product states, the concrete calculations are straightforward. We want to use $SU(2)$ singlets G in $V \otimes \mathbb{C}^{2s+1} \otimes V$. Having already allowed for reducible representations in V , we like to stress that for our applications we *must* deal with V as 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 '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 $3j$ symbols and the desired singlet is

$$|(j_1, i_1), j_2, (j_3, i_3)\rangle :=$$

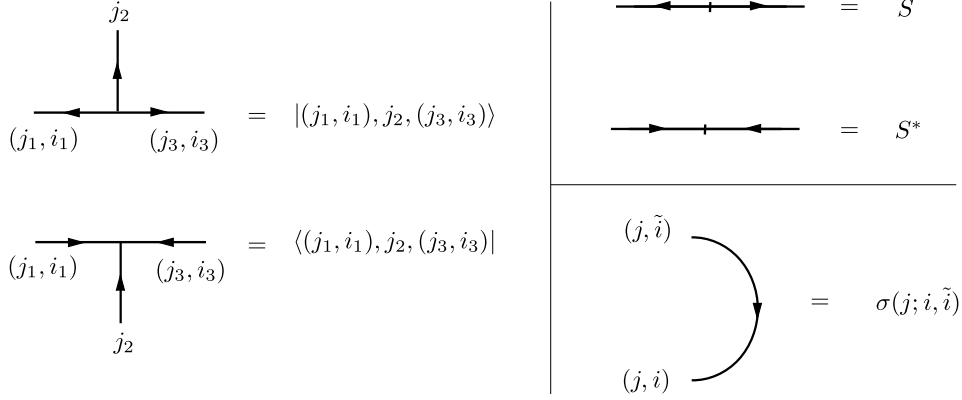


Figure 2. Introduction of the graphical notation for singlets appearing in product spaces. Three leg (vertex) symbols for $|(j_1, i_1), j_2, (j_3, i_3)\rangle$ and $\langle(j_1, i_1), j_2, (j_3, i_3)|$ appearing in products of three irreducible representations. Two leg (edge) symbols for the singlets S resp. S^* in $V \times V$ resp. $V^* \times V^*$, and arcs for singlets in $V \times V^*$ for the same spin j .

$$\begin{aligned}
 \begin{array}{c} \tilde{j}_2 \\ m_2 \\ | \\ \hline \begin{array}{cc} j_1 & j_3 \\ m_1 & m_3 \end{array} \end{array} &= \begin{array}{c} \begin{array}{cc} j_1 & j_3 \\ m_1 & m_3 \end{array} \\ \hline j_2 \\ m_2 \end{array} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\
 \\ \\
 \begin{array}{c} j \\ m \end{array} \text{ --- } \begin{array}{c} \tilde{j} \\ \tilde{m} \end{array} &= \begin{array}{c} \tilde{j} \\ \tilde{m} \\ \text{---} \\ j \\ m \end{array} = \delta_{\tilde{j}, j} \delta_{\tilde{m}, m} \\
 \\ \\
 \begin{array}{c} j \\ m \end{array} \text{ --- } \begin{array}{c} \tilde{j} \\ \tilde{m} \end{array} &= \delta_{\tilde{j}, j} \delta_{\tilde{m}, -m} (-1)^{j-m}
 \end{aligned}$$

Figure 3. Graphical notation for key arithmetic objects like Kronecker symbol and $3j$ symbol.

$$\sum_{m_1, m_2, m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} |(j_1, i_1), m_1\rangle \otimes |j_2, m_2\rangle \otimes |(j_3, i_3), m_3\rangle. \quad (8)$$

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

The singlet G can be written as superposition of these elementary singlets

$$G = \sum_{(j_1, i_1), (j_3, i_3)} A_{i_1, i_3}^{j_1, j_3} |(j_1, i_1), j_2, (j_3, i_3)\rangle \quad (9)$$

with suitable coefficients $A_{i_1, i_3}^{j_1, j_3}$. Note that j_2 has been suppressed as 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 $3j$ symbols with respect to exchange of two columns

$$\begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} = (-1)^{j_1 + j_2 + j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \quad (10)$$

we conclude that

$$A_{i_3, i_1}^{j_3, j_1} = (-1)^{j_1 + j_2 + j_3} A_{i_1, i_3}^{j_1, j_3}. \quad (11)$$

is a sufficient condition for parity invariance. Note that $j_1 + j_2 + j_3$ is always 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 is violated, the three multiplets can not couple to a singlet. Since $j_2 = \frac{1}{2}$, we are left with the combinations $\{j_1, j_3\} = \{0, \frac{1}{2}\}, \{\frac{1}{2}, 1\}, \{1, \frac{3}{2}\}, \dots$. 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 the symmetry (11) we may reduce all possible coefficients A to a set of $n_j \times n_{j+1/2}$ matrices $A^{j, j+1/2}$ with matrix elements

$$\left(A^{j, j+1/2} \right)_{i_l, i_r} := A_{i_l, i_r}^{j, j+1/2}. \quad (12)$$

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

$$\langle \psi | \psi \rangle = \text{Tr}(g_1^+ g_1 \cdot g_2^+ g_2 \cdot \dots \cdot g_L^+ g_L), \quad (13)$$

where $g^+ \in V^* \otimes (\mathbb{C}^{2s+1})^* \otimes V$ is the dual of $g \in V \otimes \mathbb{C}^{2s+1} \otimes V^*$ 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 r.h.s. of (13)

$$\langle \psi | \psi \rangle = \text{Tr}(\underbrace{T \cdot \dots \cdot T}_{L \text{ times}}) = \sum_{\Lambda} \Lambda^L, \quad (14)$$

where the sum is over all eigenvalues Λ 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 a (\tilde{j}, \tilde{i}) multiplet in V^* couple to a singlet iff $j = \tilde{j}$ (with arbitrary i and \tilde{i}). The (normalized) singlet is given by

$$\sigma(j; i, \tilde{i}) := \frac{1}{\sqrt{2j+1}} \sum_{m=-j}^j |j, i, m\rangle \otimes \langle j, \tilde{i}, m|. \quad (15)$$

Figure 4. Illustration of identity (18): The summation over two internal magnetic quantum numbers leads to an “arc”-singlet.

Graphically, this singlet is depicted by a link carrying an arrow pointing from the V^* to the V space.

The action of the transfer matrix T onto a singlet $\sigma(j; i, \tilde{i})$ produces similar singlets where j is changed by $\pm\frac{1}{2}$. The $\sigma(j_l; i_l, \tilde{i}_l) - \sigma(j_r; i_r, \tilde{i}_r)$ matrix element of T is

$$\langle j_l; i_l, \tilde{i}_l | T | j_r; i_r, \tilde{i}_r \rangle = \frac{1}{\sqrt{(2j_l + 1)(2j_r + 1)}} A_{i_l, i_r}^{j_l, j_r} \left(A_{\tilde{i}_l, \tilde{i}_r}^{j_l, j_r} \right)^*, \quad (16)$$

where $j_l = j_r \pm \frac{1}{2}$. (Expression (16) is the analogue of eq. (6) in [2], but here we do not impose condition (10) of [2].) The matrix T has a simple block structure with zero diagonal blocks and non-zero secondary diagonal blocks. From (11) we conclude that the matrix is symmetric. The defining blocks are

$$\langle j; i_l, \tilde{i}_l | T | j + 1/2; i_r, \tilde{i}_r \rangle = \frac{1}{\sqrt{(2j + 1)(2j + 2)}} A_{i_l, i_r}^{j, j+1/2} \left(A_{\tilde{i}_l, \tilde{i}_r}^{j, j+1/2} \right)^*. \quad (17)$$

In expression (16) the coefficients A and the complex conjugate A^* derive from the explicit appearance in (9) and the prefactor is obtained from the identity of $3j$ symbols (if j_1 is found in the product of j_2 and j_3)

$$\sum_{m_2, m_3} \begin{pmatrix} j'_1 & j_2 & j_3 \\ m'_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{1}{2j_1 + 1} \delta_{j_1, j'_1} \delta_{m_1, m'_1}, \quad (18)$$

illustrated in Fig. 4. The computation of the matrix elements of T is graphically presented in Fig. 5.

For a given space V with a certain number of spin-0, $\frac{1}{2}$, 1, $\frac{3}{2}$... multiplets and a certain set of parameters $A(j_l, i_l; j_r, i_r)$, the transfer matrix has to be diagonalized in the singlet space. The total number of non-zero coefficients $A(j_l, i_l; j_r, i_r)$ is $\sum_j n_j n_{j+1/2}$ (with sum over $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$ and n_j denoting the number of spin- j multiplets). The total dimension of $V \otimes V^*$ is $(\sum_j n_j (2j + 1))^2$, 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. The eigenvalues come in pairs $\pm\Lambda$. The two largest eigenvalues and the corresponding eigenstates determine the physics in the thermodynamic limit.

$$\begin{aligned}
 T = & \begin{array}{c} \xrightarrow{(\tilde{j}_1, \tilde{i}_1)} \quad \xleftarrow{(\tilde{j}_3, \tilde{i}_3)} \\ | \\ \xleftarrow{(j_1, i_1)} \quad \xrightarrow{(j_3, i_3)} \end{array} \times \begin{array}{c} (j, \tilde{i}) \\ \curvearrowright \\ (j, i) \end{array} \\
 \mapsto & \delta_{\tilde{j}_3, j} \delta_{j_3, j} \delta_{\tilde{i}_3, \tilde{i}} \delta_{i_3, i} \delta_{\tilde{j}_1, j_1} \cdot \frac{1}{2j_1+1} \cdot \begin{array}{c} (j_1, \tilde{i}_1) \\ \curvearrowright \\ (j_1, i_1) \end{array}
 \end{aligned}$$

Figure 5. Depiction of the transfer matrix T in terms of local vertices and the action onto singlet states.

3.2. Nearest-neighbour couplings

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

$$H = \sum_{l=1}^L \vec{S}_l \vec{S}_{l+1}. \quad (19)$$

The local Hamiltonian is $h_{l,l+1} = \vec{S}_l \vec{S}_{l+1} = 1/4 - P_0^{nn}$ where P_0^{nn} is the projector onto the nearest-neighbour singlet space. 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 this is achieved by minimizing the expectation value of a single local interaction. In analogy to (14) we obtain

$$\langle \psi | P_0^{nn} | \psi \rangle = \text{Tr}(\tilde{T} \underbrace{T \cdot \dots \cdot T}_{L-2 \text{ times}}) = \Lambda_0^{L-2} \langle 0 | T_2 | 0 \rangle, \quad (20)$$

where we assumed P_0^{nn} 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

$$\frac{\langle \psi | P_0^{nn} | \psi \rangle}{\langle \psi | \psi \rangle} = \Lambda_0^{-2} \langle 0 | T_2 | 0 \rangle. \quad (21)$$

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

$$\langle j; i_l, \tilde{i}_l | T_2 | j; i_r, \tilde{i}_r \rangle = \frac{1}{(2j+1)^2} B_{i_l, i_r}^{j, j} \left(B_{i_l, \tilde{i}_r}^{j, j} \right)^*. \quad (22)$$

The matrices B are given by

$$B^{j, j} = \sum_{j_1} (-1)^{1/2+j+j_1} A^{j, j_1} A^{j_1, j}, \quad (23)$$

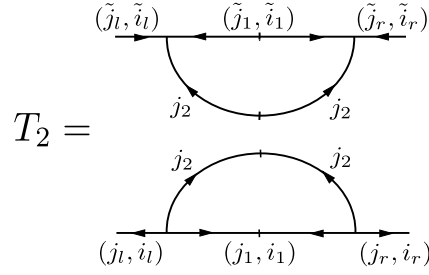


Figure 6. Depiction of the modified matrix T_2 in terms of local vertices.

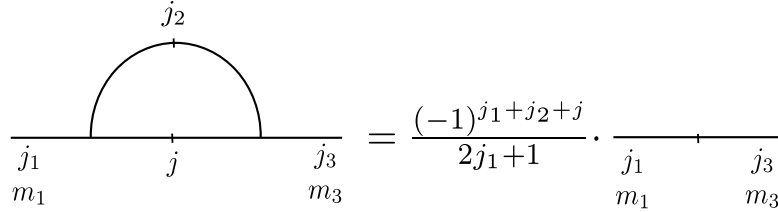


Figure 7. The summation over two internal magnetic quantum numbers leads to an “edge”-singlet.

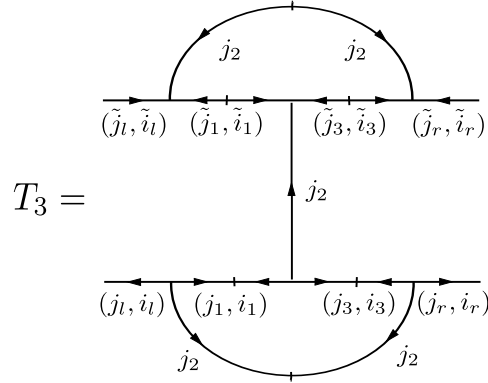


Figure 8. Depiction of the modified matrix T_3 in terms of local vertices.

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

$$B^{j,j} = \left[A^{j-1/2,j} \right]^T A^{j-1/2,j} + A^{j,j+1/2} \left[A^{j,j+1/2} \right]^T. \quad (24)$$

3.3. Next-Nearest-neighbour couplings

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

$$\frac{\langle \psi | P_0^{nnn} | \psi \rangle}{\langle \psi | \psi \rangle} = \Lambda_0^{-3} \langle 0 | T_3 | 0 \rangle. \quad (25)$$

$$\begin{aligned}
 &= (-1)^{2j_5+j_2+j_4+j_6} \left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} \cdot \left(\begin{matrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{matrix} \right) \\
 &= -(-1)^{1/2+j_4+j_6} \left\{ \begin{matrix} j_1 & 1/2 & j_3 \\ j_4 & 1/2 & j_6 \end{matrix} \right\} \cdot \begin{matrix} j_2 \\ m_2 \\ \hline j_1 & j_3 \\ m_1 & m_3 \end{matrix}
 \end{aligned}$$

Figure 9. The summation over three internal magnetic quantum numbers leads to a $6j$ symbol times an elementary vertex.

The computation of the matrix elements of T_3 is described graphically in Fig. 8 and Fig. 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 $\sigma(j_l; i_l, \tilde{i}_l) - \sigma(j_r; i_r, \tilde{i}_r)$ matrix element of T_3 is

$$\langle j_l; i_l, \tilde{i}_l | T_3 | j_r; i_r, \tilde{i}_r \rangle = \frac{1}{\sqrt{(2j_l+1)(2j_r+1)}} C_{i_l, \tilde{i}_l}^{j, j+1/2} \left(C_{\tilde{i}_l, \tilde{i}_r}^{j, j+1/2} \right)^*. \quad (26)$$

where $j_l = j_r \pm \frac{1}{2}$ and C^{j_l, j_r} is given by

$$C^{j_l, j_r} = \sum_{j_1, j_3} (-1)^{1/2+j_1+j_3} \left\{ \begin{matrix} j_l & 1/2 & j_r \\ j_3 & 1/2 & j_1 \end{matrix} \right\} A^{j_l, j_1} A^{j_1, j_3} A^{j_3, j_r}. \quad (27)$$

(There is no analogue to eqs. (26,27) in [1, 2].) Only three combinations of j_1, j_3 yield non-vanishing contributions. For $j_r = j_l + 1/2$ only $(j_1, j_3) = (j_l - 1/2, j_l), (j_l + 1/2, j_l), (j_l + 1/2, j_l + 1)$ are relevant. From this and the (sufficient) condition (11) for parity invariance we find

$$\begin{aligned}
 C^{j, j+1/2} &= \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j & 1/2 & j-1/2 \end{matrix} \right\} \left(A^{j-1/2, j} \right)^T A^{j-1/2, j} A^{j, j+1/2} \\
 &+ \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j & 1/2 & j+1/2 \end{matrix} \right\} A^{j, j+1/2} \left(A^{j, j+1/2} \right)^T A^{j, j+1/2} \\
 &+ \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j+1 & 1/2 & j+1/2 \end{matrix} \right\} A^{j, j+1/2} A^{j+1/2, j+1} \left(A^{j+1/2, j+1} \right)^T, \quad (28)
 \end{aligned}$$

where the $6j$ symbols evaluate to

$$\begin{aligned}
 \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j & 1/2 & j-1/2 \end{matrix} \right\} &= \frac{(-1)^{2j+1}}{2j+1}, \\
 \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j & 1/2 & j+1/2 \end{matrix} \right\} &= \frac{(-1)^{2j+1}}{(2j+1)(2j+2)}, \\
 \left\{ \begin{matrix} j & 1/2 & j+1/2 \\ j+1 & 1/2 & j+1/2 \end{matrix} \right\} &= \frac{(-1)^{2j}}{2j+2}, \quad (29)
 \end{aligned}$$

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

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 $5 \cdot 10^{-5}$ and dimer correlations are off the exact results by about 10^{-4} . This is achieved with $n_0 = 4$, $n_{1/2} = 4$, $n_1 = 3$, $n_{3/2} = 2$, $n_2 = 1$ ($n_s=0$ 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

$$\begin{aligned}
 A^{0,1/2} &= \begin{bmatrix} 1.0 & 0 & 0 & 0 \\ 0 & -0.283412 & 0 & 0 \\ 0 & 0 & 0.183208 & 0 \\ 0 & 0 & 0 & 0.679798 \end{bmatrix}, \\
 A^{1/2,1} &= \begin{bmatrix} 0.737765 & 0 & 0 \\ 0.257549 & -0.860519 & 0 \\ 0.610288 & -0.093768 & 0.050733 \\ 0.191246 & -0.631258 & 0.181757 \end{bmatrix} \\
 A^{1,3/2} &= \begin{bmatrix} 0.510676 & 0 \\ -0.5075510 & 0.714082 \\ -0.292858 & 0.712182 \end{bmatrix}, \quad A^{3/2,2} = \begin{bmatrix} 0.265736 \\ -0.607939 \end{bmatrix} \quad (30)
 \end{aligned}$$

and a value of the ground-state energy which compares well with the exact value [34]

$$e_0^{\text{num}} = -0.443\,092\,175\dots, \quad e_0^{\text{exact}} = -0.443\,147\,180\dots \quad (31)$$

Note that $A^{0,1/2}$ 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 $A^{j_l, j_r} \rightarrow \mathcal{O}_{j_l}^{-1} A^{j_l, j_r} \mathcal{O}_{j_r}$ where \mathcal{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

$$\tilde{D}_n := \langle (\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_{n+1} \cdot \vec{S}_{n+2}) \rangle. \quad (32)$$

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

$$D_n := \tilde{D}_n - \tilde{D}_\infty. \quad (33)$$

For $n = 2, 3, 4$ the values are known exactly [35] which we use for comparison with our MPS calculations

$$\begin{aligned} D_2^{\text{num}} &= +0.060\ 639\dots, & D_2^{\text{exact}} &= +0.060\ 824\dots, \\ D_3^{\text{num}} &= -0.027\ 838\dots, & D_3^{\text{exact}} &= -0.027\ 737\dots, \\ D_4^{\text{num}} &= +0.018\ 986\dots, & D_4^{\text{exact}} &= +0.018\ 928\dots \end{aligned} \quad (34)$$

We expect that the absolute numerical accuracy is similar also for larger distances n of the local dimer operators. These results are plotted in Fig. 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 Hamiltonian

$$H = \sum_{l=1}^L \left(\vec{S}_l \vec{S}_{l+1} + \alpha \vec{S}_l \vec{S}_{l+2} \right). \quad (35)$$

The system shows algebraically decaying dimer-dimer correlations for $\alpha \leq 0.2411\dots$, see Fig. 11, and long-range dimer order for $\alpha > 0.2411\dots$, see Fig. 10 b). The critical value $\alpha_c = 0.2411$ was established in [36, 37]. The dimer-dimer correlations are fitted well by algebraic curves for all $\alpha \leq 0.2411\dots$ with α -dependent exponent. From field theoretical considerations the exponent is expected to be identical to 1. We attribute the deviations to logarithmic corrections for $\alpha < 0.2411\dots$ which apparently vanish at α_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 [34] $C_2^{\text{exact}} = e_0^{\text{exact}}$, see (31), and [35] $C_3^{\text{exact}} = 0.182\ 039\dots$. 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 cases $\alpha = 0.1, 0.2411, 0.3, 0.4$ our results are lower than those given in [32] with small differences ranging from 10^{-4} to 10^{-3} . Hence, the deviation of these DMRG results from 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. In our approach we deal with the strictly infinitely long chain. The numerical computations of the data presented in this section were done by use of Maple 13 on a laptop computer. The total computation for the seven cases of the frustration parameter took about 1 hour.

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 (30) will contain intrinsically complex numbers.

5. Conclusion

We showed how to employ systematically $su(2)$ invariance for matrix product states and how to carry out the variational computation of the ground state energy in a numerically

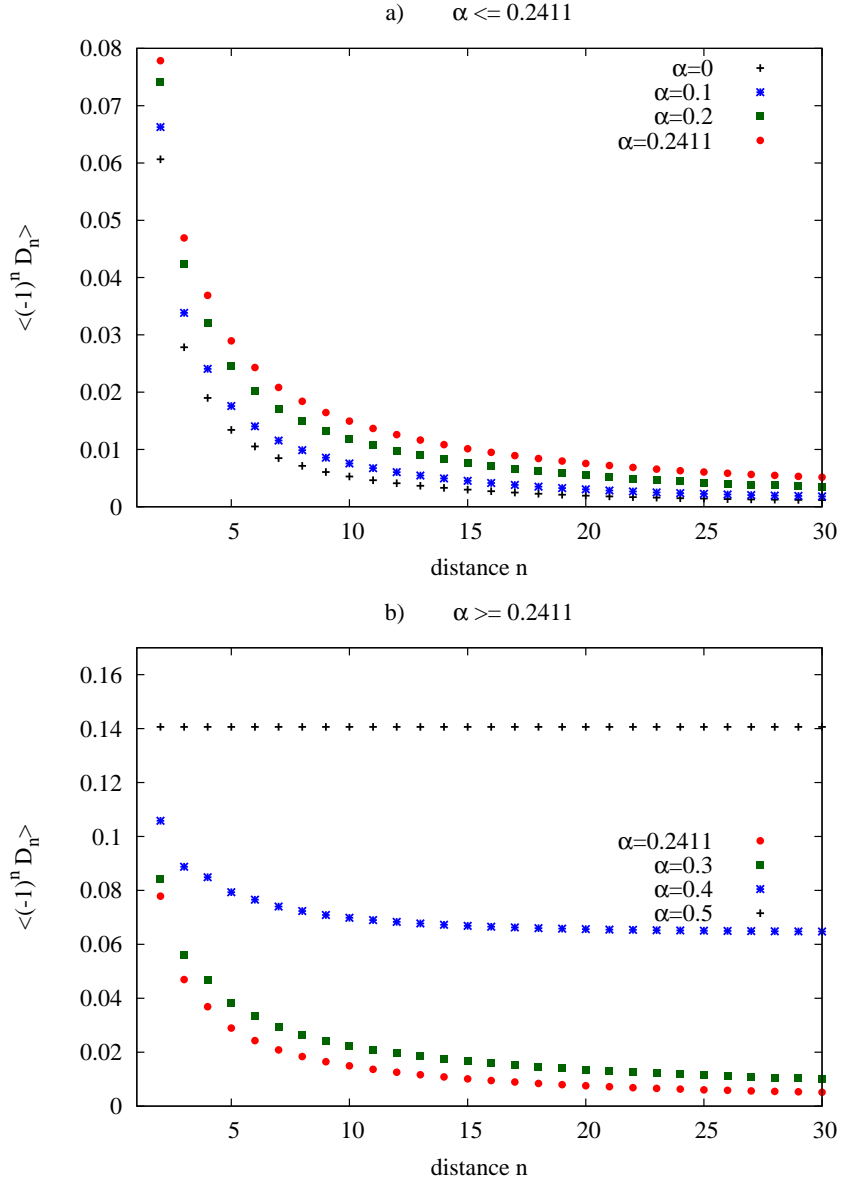


Figure 10. Dimer-dimer correlations of the spin- $\frac{1}{2}$ Heisenberg chain with frustration parameter α : Linear plots of $(-1)^n D_n$ for a) $\alpha = 0, 0.1, 0.2, 0.2411$ and b) $\alpha = 0.2411, 0.3, 0.4, 0.5$. Note the long-range order in plot b) for $\alpha > 0.2411$.

α	0.0	0.1	0.2	α_c	0.3	0.4	0.5
C_2	-0.443092	-0.442655	-0.440916	-0.439574	-0.436475	-0.420659	-0.375000
C_3	0.181942	0.173570	0.162233	0.156176	0.144794	0.100870	0.0
e_0	-0.443092	-0.425298	-0.408469	-0.401920	-0.393037	-0.380311	-0.375000

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 α . The ground-state energy $e_0 = C_1 + \alpha C_2$ is given in the last row.

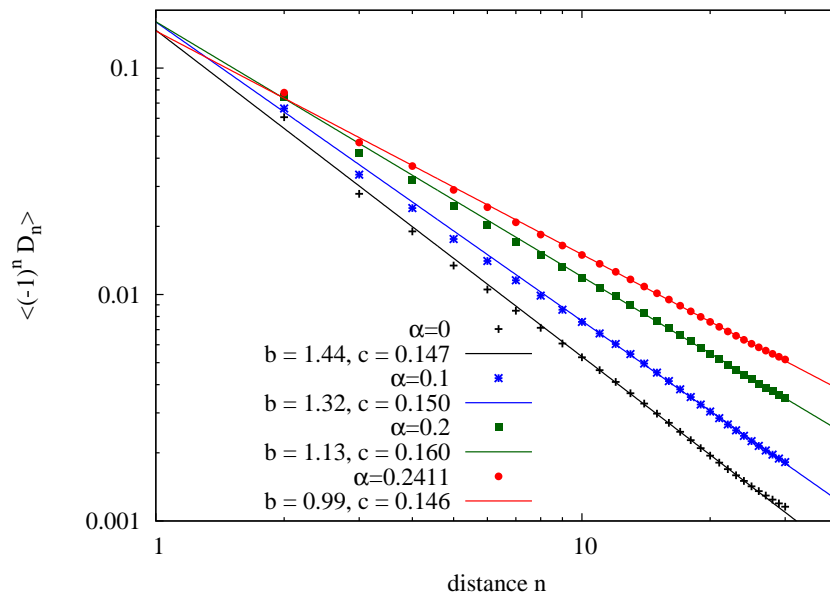


Figure 11. Dimer-dimer correlations of the spin- $\frac{1}{2}$ Heisenberg chain with frustration parameter $\alpha \leq 0.2411$: Double log plot of $(-1)^n D_n$ versus distance n and algebraic lines c/n^b from fits to the data for n in the range $[10, 25]$.

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 the 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 4 singlets, 4 doublets, 3 triplets, 2 quadruplets, and 1 quintuplets. 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 straight forward, 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.

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