AN EFFICIENT ALGORITHM OF PARITY, TRANSLATIONAL AND SPIN-ROTATIONAL SYMMETRY FOR CHAINS

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The formalism for an efficient scheme for spin-rotational symmetric matrix-product states (MPSs), also known as tensor trains (TTs), is presented. The methodology is applied for the study of ground-state energy and correlation properties of the isotropic spin-1 bilinear-biquadratic quantum Heisenberg chain with nearest-neighbor interactions and periodic boundary conditions as an example. The mathematical framework can be used for arbitrary spin-rotational invariant spin-S chains.

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1. Introduction

Various studies are focusing on quantum systems on lattices as well as their ground-state phase transitions and are motivated by realizations of quantum chains/lattices as well as the relation of classical spin chains in $1 + d$ dimensions to d-dimensional quantum systems. General concepts of critical systems such as scaling, critical exponents and universality of quantum mechanical systems are gaining interest. Historically, research on classical phase transitions was performed by use of models such as Ising and Potts. Nowadays, understanding critical properties of especially low-dimensional systems is a driving force for the establishment of fundamental mathematical concepts [1, 2].

Modern approaches are of analytical or numerical type [3] and may be considered exact for special integrable cases or approximate for generic systems. The famous Bethe ansatz [4] is applicable for the eigenstates of the Hamiltonian and the corresponding transfer matrix of integrable systems with infinitely many conserved currents. In principle, integrable systems allow the analytical treatment of all eigenstates of the Hamiltonian [5].

Slightly distinct are exactly solvable systems with analytically tractable ground states but inaccessible higher-lying spectrum. Analytically, there are mappings of arbitrary systems to free bosonic systems. Quite general are maps of spin systems to bosonic systems on the basis of spin waves with an approximate treatment of boson–boson interactions. Especially for $1+1$ dimensional systems, mappings that allow to ignore certain irrelevant interactions and to obtain quite non-trivial results for spin–spin correlators in terms of vertex-operator correlators with non-trivial algebraic asymptotic decay exist.

Integrable systems in $1+1$ dimensions are very particular. Exact treatment of spectrum and correlation functions is achieved by a concerted combination of algebraic and analytic means of analysis. Such calculations yield valuable cornerstones for quantum many-body systems, but rely on rather special consistency properties of scattering events like Yang–Baxter equations [6]. Generic but approximate means involve numerical diagonalizations of Hamiltonians or transfer matrices on finite chains. Note that techniques for the complete diagonalization of an entire Hamiltonian defined on chains are typically restricted to 20 sites or to the determination of just the leading eigenstates up to 30 sites since the complexity of such calculations is high and involves Hilbert spaces of dimension 2^{20} or 2^{30} for spin-$\frac{1}{2}$ objects on 20 or 30 sites, respectively. Remarkably, such calculations are based on matrix-like operations.

An indirect analysis of the ground state of large system sizes makes use of a map to classical systems and a subsequent application of Monte Carlo simulations of the classical model [7]. Accessible system sizes are large, but accessible low temperatures are restricted by the so-called minus-sign problem: Boltzmann weights of spin-configurations may acquire minus signs that spoil the numerical accuracy of the calculations severely.

The focus of this work lies on intrinsically quantum-mechanical techniques like the variational approach to the ground-state computation based on MPS [8] that lead to highly efficient density matrix renormalization group (DMRG) techniques [9]. Note that there are many realizations of variational techniques in the literature [10–12]. Practically, the ground state of any gapped quantum spin chain can be described by MPSs [13]. Inversely, any MPS is the ground state of a local gapped Hamiltonian [14, 15].

Of particular importance is the treatment of quantum systems with symmetries either of discrete or continuous nature: They result from parity or SU(2)-invariant interactions. Here, we like to apply a modern ansatz of variational states of matrix product type with built-in SU(2) symmetry. Note that in this way many calculations can be done efficiently [16]. The local objects are degree-3 tensors with SU(2) invariance. The foundation of the formalism for a general computational scheme is given in this manuscript

and all calculations for $S = 1$ with the potential of generalization to arbitrary spin-S and in the higher-dimensional case to tensor network states with Abelian [17] and non-Abelian symmetries [18] are presented. Remarkably, implementation of non-Abelian symmetries is quite involved. Nevertheless, a guide for implementing a global SU(2) symmetry to tensor networks is well-known [19]. Within the framework of this study, calculations can be performed by use of Wigner 3-j symbols for the transfer matrix and eigenstate as well as Wigner 6-j symbols for the eigenvalues. This is caused by the decomposition of local matrix tensors into degeneracy and a structural part [20] ruled by the symmetry and given by the Clebsch–Gordan coefficients. Hence, in comparison with non-symmetric theories, the number of parameters is reduced.

The article is organized as follows. In Sect. 2, the mathematical framework for the implementation of su(2)-invariant MPSs is presented. Moreover, mathematical objects that are necessary for the application of the methodology on spin chains are introduced. In Sect. 3, explicit results from variational computations are given. In Sect. 4, conclusions are presented.

2. MPSs

2.1. Construction of su(2)-invariant MPSs

A class of MPSs is given by

$$|\psi\rangle = \mathrm{tr}_{\mathrm{aux}} \left(\boldsymbol{g}_1 \otimes \boldsymbol{g}_2 \otimes \ldots \otimes \boldsymbol{g}_L\right) \tag{1}$$

with $D \times D$ square matrices $\boldsymbol{g}_k$ as well as some corresponding auxiliary finite dimensional index space $V = \mathbb{C}^D$ and dual space V^*, where V is expressed by a direct sum over irreducable spin-j representations with each j appearing an arbitrary number of times n_j, which is denoted by an integer $i \in \{1, \ldots, n_j\}$. The trace is taken over the auxiliary matrix space. Dimensions of matrices $\boldsymbol{g}_k$ can be taken as arbitrary, but may be constrained by symmetry considerations and details of the model. Furthermore, the k^{th} copy of an su(2) Lie algebra spin-j space $\mathbb{C}^{1+2j}$ is taken as local quantum space V_k. Matrix entries of $\boldsymbol{g}_k$ are elements of V_k. The assumption of $\boldsymbol{g}_k$ as su(2)-invariant tensors in $V \otimes \mathbb{C}^{1+2j} \otimes V^*$ leads trivially to su(2)-invariant $|\psi\rangle$. The density matrix of the whole state is $\boldsymbol{\rho} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$.

Due to the construction orthogonal states labeled $|(j,i),m\rangle$ span V, where the magnetic quantum number is $m = -j, 1-j, \ldots, j$. As a result of translational invariance and for the sake of simplicity, site label k is dropped whenever possible. In $V \otimes \mathbb{C}^{1+2j} \otimes V^*$, any spin multiplet (j_1, i_1) from the first factor space, the only spin multiplet j_2 of the second space $(i_2 = 1)$, and any spin multiplet (j_3, i_3) from the third factor space are coupled to a

singlet state

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

where the coupling coefficient is given by a Wigner 3-j symbol and Einstein convention is used for m_1, m_2, m_3.

Obviously, su(2)-invariant tensors $\boldsymbol{g}_k$ can be expressed by use of site independent coefficients $A^{j_1,j_3}_{i_1,i_3}$ and a superposition of elementary singlet states

$$\boldsymbol{g}_k = \sum_{j_1,j_3} \sum_{i_1=1}^{n_1} \sum_{i_3=1}^{n_3} A^{j_1,j_3}_{i_1,i_3} \, |(j_1,i_1),j_2,(j_3,i_3)\rangle_k \, , \tag{2}$$

where $|(j_1,i_1),j_2,(j_3,i_3)\rangle_k$ is a complete orthonormal basis for the Hilbert space at site k.

Note that an odd permutation of the columns in Wigner 3-j symbols leads to a phase factor which results in $A^{j_3,j_1}_{i_3,i_1} = (-1)^{j_1+j_2+j_3} A^{j_1,j_3}_{i_1,i_3}$ as condition for parity invariance. $j_1 \leq j_3$ is assumed without loss of generality. Selection rules for non-zero Wigner 3-j symbols lead to integer $j_1+j_2+j_3$ and especially the combination with the noteworthy case $j_2 = 1$ yields only $\{j_1,j_3\} = \{0,1\}$ for $j_1 = 0$ and $\{j_1,j_3\} = \{j_1,j_1\},\{j_1,1+j_1\}$ for integer or half-integer j_1. On this condition, all possible coefficients $A^{j_1,j_3}_{i_1,i_3}$ reduce to a set of $n_{j_1} \times n_{j_1}$ matrices $\boldsymbol{A}^{j_1,j_1}$ and $n_{j_1} \times n_{1+j_1}$ matrices $\boldsymbol{A}^{j_1,1+j_1}$ with elements $(\boldsymbol{A}^{j_1,j_3})_{i_1,i_3} = A^{j_1,j_3}_{i_1,i_3}$.

2.2. Transfer matrix, norm, and projector

The transfer matrix

$$\boldsymbol{t} = \boldsymbol{g}^\dagger \otimes \boldsymbol{g} \tag{3}$$

is defined as a linear map $V \otimes V^* \to V \otimes V^*$ with dimension $(\sum_j (1+2j)\, n_j)^2$, where $\boldsymbol{g}^\dagger$ is the dual of $\boldsymbol{g}$. The norm of the MPS is thus given by

$$\langle\psi|\psi\rangle = \operatorname{tr} \boldsymbol{t}^L = \sum_n \Lambda_n^L \, . \tag{4}$$

Note that the eigenvalues are sorted in such a way that the absolute value decreases with increasing index n. In the thermodynamic limit $L \to \infty$ only the largest eigenvalues with corresponding right normalized eigenstate $|0\rangle$ contribute. For the diagonalisation of $\boldsymbol{t}$, numerics must be used. However, the fact that the leading eigenstate $|0\rangle$ is a singlet and the singlet subspace has dimension $\sum_j n_j^2$ in contrast to the total dimension, $(\sum_j (1+2j) n_j)^2$

simplifies the evaluation significantly. Moreover, note that the in this approach required explicit calculation of the transfer matrix is simplified by use of all available symmetries for the purpose of finding invariant blocks of the transfer matrix which are as low dimensional as achievable since decreasing the computational time with regard to the diagonalization is aimed for.

The projection operator on two spin-j_1 spaces onto the total spin-j subspace with Einstein convention for m_1, m_3, m_1', m_3' can be expressed as

$$\begin{aligned}\boldsymbol{P}_j \;=\; & (1+2j)\sum_{i_1=1}^{n_1}\sum_{m=-j}^{j}\begin{pmatrix} j_1 & j & j_1 \\ m_1 & m & m_3\end{pmatrix}\begin{pmatrix} j_1 & j & j_1 \\ m_1' & m & m_3'\end{pmatrix} \\ & \times\left(\left|\left(j_1,i_1\right),m_1\right\rangle\otimes\left|j,m\right\rangle\otimes\left|\left(j_1,i_1\right),m_3\right\rangle\right) \\ & \times\left(\left\langle\left(j_1,i_1\right),m_1'\right|\otimes\left\langle j,m\right|\otimes\left\langle\left(j_1,i_1\right),m_3'\right|\right)\,. \end{aligned} \tag{5}$$

The prefactor is caused by defining relations of projection operators, *i.e.* $\boldsymbol{P}_j^\dagger = \boldsymbol{P}_j$ and $\boldsymbol{P}_j^2 = \boldsymbol{P}_j$.

The expectation value $\frac{\langle\psi|\boldsymbol{P}_j|\psi\rangle}{\langle\psi|\psi\rangle}$ in the thermodynamic limit $L\to\infty$ can be calculated by use of the largest eigenvalue of $\boldsymbol{t}$ and Eq. (7). Due to the translational invariance, the calculation of this expectation value with site j is sufficient since

$$\frac{\langle\psi\left|\boldsymbol{P}_j\right|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\mathrm{tr}\,\left(\boldsymbol{t}_j\boldsymbol{t}^{L-2}\right)}{\mathrm{tr}\,\boldsymbol{t}^L} = \frac{\langle 0\left|\boldsymbol{t}_j\right|0\rangle}{\Lambda_0^2}\,, \tag{6}$$

where $\boldsymbol{t}_j$ is a modified transfer matrix in $V\otimes V^*$. It can be expressed as

$$\begin{aligned}\frac{\boldsymbol{t}_j}{1+2j} \;=\; & \sum_{\{j_l,j_l'\}_{l=1}^3}(-1)^{j_1+j_3+j_1'+j_3'+2j+2s}A_{i_1,i_2}^{j_1,j_2}A_{i_2,i_3}^{j_2,j_3}\left(A_{i_1',i_2'}^{j_1',j_2'}\right)^*\left(A_{i_2',i_3'}^{j_2',j_3'}\right)^* \\ & \times\begin{pmatrix} j_1 & j & j_3 \\ m_1 & m_2 & m_3\end{pmatrix}\begin{pmatrix} j_1' & j & j_3' \\ m_1' & m_2 & m_3'\end{pmatrix}\begin{Bmatrix} s & j & s \\ j_1 & j_2 & j_3\end{Bmatrix} \\ & \times\begin{Bmatrix} s & j & s \\ j_1' & j_2' & j_3'\end{Bmatrix}\left|\left(j_1,i_1\right),m_1\right\rangle\left\langle\left(j_1',i_1'\right),m_1'\right| \\ & \otimes\left|\left(j_3,i_3\right),m_3\right\rangle\left\langle\left(j_3',i_3'\right),m_3'\right| \end{aligned} \tag{7}$$

by use of Einstein convention for $i_1, i_3, i_1', i_3', m_1, m_2, m_3, m_1', m_3'$ since $4(j_1+j_2+j_3)$ is even because the sum is an integer or a half-integer. Moreover, m_3 is a summation index in Eq. (5). Therefore, its sign can be changed.

On the other hand, Wigner 3-j symbols in Eq. (5) are 0 if $m_1 + m + m_3 = m_1' + m + m_3' = 0$ is not satisfied. $\boldsymbol{P}_j$ is multiplied with two tensors $\boldsymbol{g}$ and two tensors $\boldsymbol{g}^\dagger$. Furthermore, a sum over products of four Wigner 3-j symbols leads to Wigner 6-j symbols. Use of these relations yields Eq. (7) after a lengthy, but straightforward calculation.

3. Application

As an application of the mathematical framework, the physically rather complex isotropic spin-1 bilinear-biquadratic quantum Heisenberg chain with nearest-neighbor interactions and periodic boundary conditions on L sites written as a polynomial of nearest-neighbor spin vectors or as a superposition of projection operators

$$\begin{aligned} \boldsymbol{H} &= \sum_{k=1}^{L} \boldsymbol{h}_k \\ &= J \sum_{k=1}^{L} \left(\vec{\boldsymbol{S}}_k \vec{\boldsymbol{S}}_{1+k} + \alpha \left(\vec{\boldsymbol{S}}_k \vec{\boldsymbol{S}}_{1+k} \right)^2 \right) \\ &= J \sum_{k=1}^{L} \left(1 + \alpha + 3\left(\alpha - 1\right) \boldsymbol{P}_0\left(k\right) - 2\boldsymbol{P}_1\left(k\right) \right) \end{aligned} \tag{8}$$

is considered, where $\alpha \in \mathbb{R}$ is an arbitrary number in our calculations and $\vec{\boldsymbol{S}}_k$ are spin-S SU(2) matrix representations. For practical purposes, we take J to be 1 or -1. This Hamiltonian describes the most general SU(2)-invariant three-state-model with nearest-neighbor interactions. Due to the su(2)-invariant $|\psi\rangle$, the Lie algebra symmetry is a built-in property of the MPS representation of this chain with L many identical spins. Moreover, spin-j is arbitrary in our construction. Hence, $j = 1$ is chosen as the application. However, the presented framework is applicable to any spin-j Heisenberg chain with nearest-neighbor interaction of the form of $\sum_{k=1}^{L} Q(\vec{\boldsymbol{S}}_k \vec{\boldsymbol{S}}_{1+k})$, where $Q(x)$ is a polynomial with degree $2j$ in x. The reason is that every such Hamiltonian can be written as a superposition of projectors, *i.e.* $\sum_{k=1}^{L} \sum_{j'=0}^{2j-1} a_{j'} \boldsymbol{P}_{j'}(k)$. This fact is used in Eq. (8).

3.1. Review

Realizations of the isotropic spin-1 bilinear-biquadratic quantum Heisenberg chain are well-known [21]. Moreover, this model was used extensively for tensor network algorithms [22]. Its SU(2) symmetry is fixed due to the Mermin–Wagner–Coleman theorem [23]. Eigenstates can be described by the total angular momentum quantum number S. Note the discrete translational symmetry and SU(3) symmetry for $\alpha = 1, \pm\infty$ [24].

Known results for this model include the gapped Haldane phase with hidden topological order for $J = 1$ and $-1 < \alpha < 1$ [25], which contains the simple Heisenberg antiferromagnet for $\alpha = 0$ and the Affleck–Kennedy–Lieb–Tasaki (AKLT) case for $\alpha = \frac{1}{3}$ as well as a phase transition to the dimerized phase for $J = 1$ and $\alpha \leq -1$ or $J = -1$ and $\alpha \geq 1$, which contains the exactly solvable spin-$\frac{1}{2}$ XXZ model [26]. Discussions about a possible existence of a gapped nematic phase are ongoing [27]. The gapless ferromagnetic phase for $J = -1$ and $\alpha < 1$ is followed by a gapless phase with dominating quadrupolar spin correlations for $J = 1$ and $\alpha > 1$ [28]. Furthermore, note the Kosterlitz–Thouless phase transition for $J = 1$ and $\alpha = 1$ [29].

3.2. AKLT model

The AKLT model, *i.e.* the case of $\alpha = \frac{1}{3}$, can be dealt with by exactly using the presented method [8]. For the purpose of demonstrating the approach, the matrix

$$\boldsymbol{g} = \begin{pmatrix} |0'\rangle & -\sqrt{2}\,|+\rangle \\ \sqrt{2}\,|-\rangle & -\,|0'\rangle \end{pmatrix}$$

is considered, where the vector elements $|\pm\rangle$ and $|0'\rangle$ are eigenstates of $\boldsymbol{S}^z$. This matrix is determined by use of the fact that $\boldsymbol{h}$ annihilates matrix elements of $\boldsymbol{g} \otimes \boldsymbol{g}$. The transfer matrix $\boldsymbol{t}$

$$\boldsymbol{t} = \begin{pmatrix} 1 & & & 2 \\ & -1 & & \\ & & -1 & \\ 2 & & & 1 \end{pmatrix}$$

has eigenvalues -1 and 3. The density matrix is given by $\boldsymbol{\rho} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$, whereas the reduced density matrix $\boldsymbol{\rho}_l$ can be expressed by use of Einstein's summation convention for $\alpha, \alpha', \beta, \beta'$ with

$$\boldsymbol{\rho}_l = \frac{(\boldsymbol{g}_1 \otimes \ldots \otimes \boldsymbol{g}_l)_{\alpha\alpha'} \left(\boldsymbol{t}^{L-l}\right)_{\alpha'\beta',\alpha\beta} \left(\boldsymbol{g}_1^\dagger \otimes \ldots \otimes \boldsymbol{g}_l^\dagger\right)_{\beta'\beta}}{\operatorname{tr} \boldsymbol{t}^L},$$

which yields

$$\boldsymbol{\rho}_l = \frac{\boldsymbol{K}\,(L-l)\,\boldsymbol{K}\,(l)}{3^L + 3\,(-1)^L},$$

$$\boldsymbol{K}(l) = \begin{pmatrix} \frac{3^l+(-1)^l}{2} & & & (-1)^l \\ & \frac{3^l+(-1)^{1+l}}{2} & & \\ & & \frac{3^l+(-1)^{1+l}}{2} & \\ (-1)^l & & & \frac{3^l+(-1)^l}{2} \end{pmatrix} .$$

Eigenvalues of the reduced density matrix $\boldsymbol{\rho}_l$ are

$$\begin{aligned} \frac{1+3(-3)^{-l}}{4} &= \frac{1}{4}\left(1+3(-1)^{-l}\,\mathrm{e}^{-l\ln 3}\right) , \\ \frac{1-(-3)^{-l}}{4} &= \frac{1}{4}\left(1-(-1)^{-l}\,\mathrm{e}^{-l\ln 3}\right) . \end{aligned}$$

Thus, the well-known [8] correlation length $\xi = \frac{1}{\ln 3}$ of the AKLT model is reproduced, whereas the ground-state energy $e_0 = \frac{t\langle\psi|\boldsymbol{H}|\psi\rangle}{\langle\psi|\psi\rangle} = -\frac{2}{3}$ follows by use of Eq. (1).

3.3. Results for the ground state with $-1 \leq \alpha \leq \frac{1}{3}$

Numerical results obtained by a program written in Maple are presented in this subsection. For $\boldsymbol{P}_0$ and $\boldsymbol{P}_1$ in the Hamiltonian given in Eq. (8), Eq. (5) is used. Calculations were performed for $-1 \leq \alpha \leq \frac{1}{3}$ and $J = 1$.

For the algorithm, the transfer matrix $\boldsymbol{t}$ is given explicitly by Eqs. (2) and (3), while the Hamiltonian can be written down by use of Eqs. (5) and (8). Wigner 3-j and 6-j symbols are evaluated explicitly during this calculation. Eigenvalues and right as well as left eigenvectors of the explicitly determined $\boldsymbol{t}$ are computed. The analysis of the expectation value in $|\psi\rangle$ of $\boldsymbol{H}$ is performed by use of the relation

$$\frac{\langle\psi\,|\boldsymbol{h}|\,\psi\rangle}{\langle\psi|\psi\rangle} = J\Lambda_0^{L-2}\,\langle 0\,|(3(\alpha-1)\,\boldsymbol{t}_0 - 2\boldsymbol{t}_1)|\,0\rangle ,$$

which follows from Eqs. (6) and (8), where $|n\rangle$ are the corresponding right orthonormalized eigenvectors to the eigenvalues Λ_n of the transfer matrix $\boldsymbol{t}$ in the spin-1 subspace. The gradient of the energy with respect to $A^{j_1,j_2}_{i_1,i_2}$, *i.e.* $\boldsymbol{\nabla} = \boldsymbol{\partial_A}$, can be computed due to the fact that $\boldsymbol{t}$ and $J(3(\alpha-1)\boldsymbol{t}_0 - 2\boldsymbol{t}_1)$ are polynomials in $A^{j_1,j_2}_{i_1,i_2}$. Moreover, Λ_0 and $|0\rangle$ also depend on these parameters. Hence, gradients of Λ_0 and $|0\rangle$ are calculated by use of the gradient of the transfer matrix and the leading eigenstate

$$\boldsymbol{\nabla}\Lambda_0 = \langle 0\,|\boldsymbol{\nabla t}|\,0\rangle , \qquad \boldsymbol{\nabla}\,|0\rangle = -\sum_n \frac{\langle n\,|\boldsymbol{\nabla t}|\,0\rangle}{\Lambda_n - \Lambda_0}\,|n\rangle$$

in analogy to the quantum mechanical perturbation theory. Hence, the energy is minimized with respect to $A^{j_1,j_2}_{i_1,i_2}$ under the constraint that $|0\rangle$ is the leading eigenstate of $\boldsymbol{t}$. An optimization routine of Maple was used for this analysis. Remarkably, this described approach for the minimization leads to an efficient and stable numerical analysis, since $J(3(\alpha-1)\boldsymbol{\nabla}\boldsymbol{t}_0 - 2\boldsymbol{\nabla}\boldsymbol{t}_1)$ and $\boldsymbol{\nabla}|0\rangle$ are used for the computation of all tensors and the infinite product, respectively, that result from the infinite sized MPS.

Purely integer of half-odd integer spin multiplets is considered for the sake of simplicity. Results for $n_{\frac{1}{2}} = 3$, $n_{\frac{3}{2}} = 2$, and $n_{\frac{5}{2}} = 2$ are presented. The ground-state energy per site for $\alpha = -1$ is found to be $e_0 = -3.991$, which deviates only by the order of 10^{-3} from the exactly known value $e_0 = -4$ [30]. Note that for this point, the model is critical which decreases the accuracy. Correspondingly, $e_0 = -1.4014849$ is found for $\alpha = 0$, which is off by the order of 10^{-7} from the best-known numerical value [31]. The exact result $e_0 = -\frac{2}{3}$ for the AKLT case of $\alpha = \frac{1}{3}$ is reproduced by the presented method.

By increasing the numbers of copies of spin multiplets in the auxiliary space to $n_{\frac{1}{2}} = 6$, $n_{\frac{3}{2}} = 6$, $n_{\frac{5}{2}} = 4$, and $n_{\frac{7}{2}} = 1$, $e_0 = -3.9995$ for $\alpha = -1$ is obtained, which deviates by the order of 10^{-4} from the exact value in contrast to the previous 10^{-3} precision. Thus, the accuracy of the analysis can be enhanced by such a scheme. Moreover, these results proof the stability of the presented approach.

Note that the dimension of the auxiliary space for $n_{\frac{1}{2}} = 3$, $n_{\frac{3}{2}} = 2$, and $n_{\frac{5}{2}} = 2$ is 26. In contrast, MPSs without built-in SU(2) symmetry that lead to equivalent results would have dimension 90, which is rather large for calculations with periodic boundary conditions. Furthermore, it is also remarkable that the total dimension of $V \otimes V^*$ is $(\sum_{j=\frac{1}{2}}^{\frac{5}{2}}(1+2j)n_j)^2 = 676$, while the singlet subspace has dimension $\sum_{j=\frac{1}{2}}^{\frac{5}{2}} n_j^2 = 17$, which demonstrates that the presented approach simplifies the mathematical evaluation of the transfer matrix $\boldsymbol{t}$ significantly.

3.4. Correlation functions

Calculation of all correlation functions of the state can be done by use of the representation of the transfer matrix in Eq. (4). As an example, the two-point spin–spin correlation function $\langle \boldsymbol{S}^z_0 \boldsymbol{S}^z_r \rangle = \frac{\langle\psi|\boldsymbol{S}^z_0 \boldsymbol{S}^z_r|\psi\rangle}{\langle\psi|\psi\rangle}$ is considered, whereas this correlator is connected to the ground-state two-point function ω_r of $\boldsymbol{H}$ in Eq. (8) by $\langle \boldsymbol{S}^z_0 \boldsymbol{S}^z_r \rangle = 2\omega_r$ [3] due to the fact that the ground state of the Hamiltonian is constructed by the MPS ansatz in Eq. (1). Nevertheless, it is possible to perform all calculations for other correlators.

The two-point spin–spin correlation function $\langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle$ in the thermodynamic limit $L \to \infty$ can be expressed as

$$\begin{aligned} \langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle &= \frac{\operatorname{tr}\left(\boldsymbol{t}^{L-r} \boldsymbol{S}_0^z \boldsymbol{t}^r \boldsymbol{S}_r^z\right)}{\operatorname{tr} \boldsymbol{t}^L} \\ &= \frac{\sum_{\beta,\gamma} \Lambda_\beta^{L-r} \Lambda_\gamma^r \left|\langle \beta \left| \boldsymbol{S}^z \right| \gamma \rangle\right|^2}{\sum_\alpha \Lambda_\alpha^L} \overset{L\to\infty}{\longrightarrow} \sum_n \left(\frac{\Lambda_n}{\Lambda_0}\right)^r \left|\langle 0 \left| \boldsymbol{S}^z \right| n \rangle\right|^2 , \end{aligned} \tag{9}$$

while $\langle 0|\boldsymbol{S}^z|n\rangle$ can be determined by use of

$$\langle 0 \left| \boldsymbol{S}^z \right| n \rangle = (-1)^{j_1+2j_2+j_3} \sqrt{\frac{2}{3}} A_{i_2,i_3}^{j_2,j_3} A_{i_3,i_1}^{j_3,j_1} \begin{Bmatrix} j_2 & 1 & j_1 \\ 1 & j_3 & 1 \end{Bmatrix} . \tag{10}$$

Equation (10) holds since j can be rewritten with Wigner 3-j symbols as

$$j = (-1)^{1+2j} \sqrt{j\,(1+j)\,(1+2j)} \begin{pmatrix} j & 1 & j \\ j & 0 & -j \end{pmatrix} .$$

Hence, $\boldsymbol{S}^z$ in a spin-j-multiplet transforms with respect to the upper index z as a spin-1 object and has matrix elements given by Wigner 3-j symbols. Moreover, the introduced methodology in Sect. 2 yields

$$\begin{aligned} \langle 0 \left| \boldsymbol{S}^z \right| n \rangle &= (-1)^{1+j+j_1+2j_2+j_3 \pm 2j+2(1+j_1+j_2)} \sqrt{j\,(1+j)\,(1+2j)} A_{i_2,i_3}^{j_2,j_3} A_{i_3,i_1}^{j_3,j_1} \\ &\quad \times \begin{Bmatrix} j_2 & 1 & j_1 \\ j & j_3 & j \end{Bmatrix} \begin{pmatrix} j_2 & j_1 & 1 \\ m_2 & m_1 & m \end{pmatrix} \begin{pmatrix} j_2 & j_1 & 1 \\ m_2 & m_1 & 0 \end{pmatrix} \\ &= \frac{(-1)^{1+j+j_1+2j_2+j_3 \pm 2j+2(1+j_1+j_2)}}{3} A_{i_2,i_3}^{j_2,j_3} A_{i_3,i_1}^{j_3,j_1} \begin{Bmatrix} j_2 & 1 & j_1 \\ j & j_3 & j \end{Bmatrix} . \end{aligned}$$

Note the Einstein convention for m_1, m_2. Furthermore, the knowledge that $1 + j_1 + j_2 \in \mathbb{N}_0$ and $j = 1$ yields the desired Eq. (10).

Use of Eqs. (9) and (10) together with the previously introduced transfer matrix algorithm yields the desired correlators. Exemplary results of this analysis are summarized in Table 1. The expected exponential decay is observed. Comparison [3] of the obtained values for the correlators yields good agreement with an order of at least 10^{-3} for precision even for the critical case. Note that the analysis can be performed for all positive r. Exemplary results are given in Fig. 1. However, only integer r is of physical relevance.

Note that remarkably, all of the presented results (the ground-state properties and correlation functions) for a certain α can be determined together within computation times lower than a minute by use of notebook computing.

Table 1. Results for the spin–spin correlator $\langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle$ for $J = 1$, $\alpha = 0$, and $\alpha = \sqrt{1 - \frac{2}{\sqrt{5}}} = \tan \frac{\pi}{10}$.

r	$\langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle\big\|_{\alpha=0}$	$\langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle\big\|_{\alpha=\sqrt{1-\frac{2}{\sqrt{5}}}}$
1	−1.401	−1.337
2	0.731	0.456
3	−0.525	−0.161
4	0.353	0.058
5	−0.262	−0.021
6	0.187	0.008

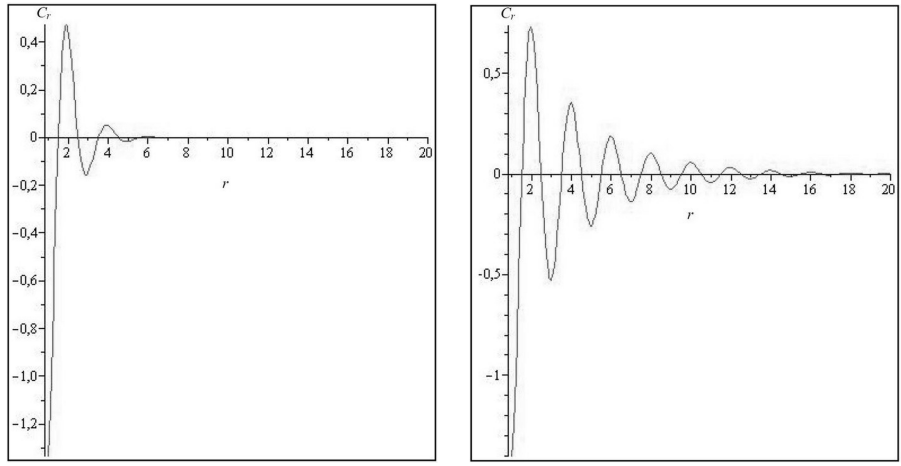

Fig. 1. Correlation function $C_r = \langle \boldsymbol{S}_0^z \boldsymbol{S}_r^z \rangle$ for $\alpha = \frac{1}{3}$ (left) and $\alpha = 0$ (right).

4. Conclusion

An efficient formulation of su(2)-invariant MPSs for arbitrary spin-S was presented. The goal of this manuscript was to calculate ground-state properties such as energy or two-point correlation functions for spin-S chains within this framework. Basic objects for the calculation are tensors of rank 3. The computation was done explicitly by use of Wigner 3-j and 6-j symbols. The usefulness of this mathematical scheme was proven by its application on the isotropic spin-1 bilinear-biquadratic quantum Heisenberg chain with nearest-neighbor interactions and periodic boundary conditions. Exemplary results for the ground-state energy and spin–spin correlators were presented.

The achieved accuracy is acceptable for practical purposes. Nevertheless, the precision can be enhanced quite easily for higher numbers of copies of spin multiplets in the auxiliary space.

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