Matrix product states approach to the Heisenberg ferrimagnetic spin chains

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We present a new method of constructing the matrix product (MP) states and apply it to the ground state of the Heisenberg spin chain with alternating spins $1$ and $\frac{1}{2}$ and antiferromagnetic exchange interactions between nearest neighbors (the simplest example of a quantum ferrimagnet). The elementary matrix state is constructed in a way which ensures given transformational properties under rotations, which allows one to fix the total spin and its $z$-projection of the entire MP wavefunction. We compare the variational MP results with the numerical results obtained through a Quantum Monte Carlo method; the agreement is found to be within 0.4% for the ground state energy and 5% for the correlation functions.

Recently, there has been a considerable progress in the study of one-dimensional (1d) quantum spin chains by means of the so-called matrix product (MP) states technique. For the first time, they were introduced as a convenient representation of the valence bond states (VBS) for integer-spin chains. In terms of the original spin states, VBS wavefunctions are highly non-local, but they factorize in terms of matrix states which considerably simplifies all calculations. Shortly after that, MP states have proved to be a useful tool for constructing new classes of spin Hamiltonians with exactly known ground states for variational study of the ground state properties of spin chains and spin ladders, and also for the study of elementary excitations which are solitons in the string order.

In this paper, we present a new method of constructing the matrix product (MP) states with fixed quantum numbers, namely the total spin and its $z$-projection, and demonstrate its use on the example of the Heisenberg spin chain with antiferromagnetic nearest neighbor interaction and alternating spins $1$ and $\frac{1}{2}$. This system, according to the Lieb-Mattis theorem, has a degenerate multiplet of ground states with the total spin $S_{tot} = L/2$; here $L$ is the number of unit cells, each cell consisting of spins $1$ and $\frac{1}{2}$. In each of the ground states the rotational symmetry is spontaneously broken, and the long-range magnetic order exists thus, one may consider this model as the simplest example of a quantum ferrimagnet. It should be mentioned that there exist real magnetic materials belonging to the family of Cu(II)Ni(II) complexes, which are well described by the above model, see Ref. 13 and references therein. For this model, we construct a MP wavefunction which has only two variational parameters, and show that our variational results for the ground state properties are in a very good agreement with the numerical data obtained by means of the Quantum Monte Carlo (QMC) technique.

Matrix states with given quantum numbers. First, let us recall some basic facts about the MP states. A matrix product state is defined as

$$|\Omega\rangle = \text{Tr} (g_1 g_2 \cdots g_L),$$

(1)

where the elementary matrix states $g_i$ are matrices composed from the spin states of the $i$-th magnetic elementary cell. The dimension of the elementary matrix depends on the problem: for example, translationally invariant VBS state for spin-$S$ chain can be represented with the help of $(S+1) \times (S+1)$ matrices. In the following, we will assume that $g_i$ is a square matrix. It is worthwhile to note that since the definition of (1) involves the trace sign, the MP state does not depend on the representation of the elementary matrices, i.e., any global unitary transformation $g_i \mapsto U g_i U^\dagger$ keeps $|\Omega\rangle$ invariant.

Let us demand that the elementary matrix $g$ has certain transformational properties. Namely, we would like to construct a multiplet of matrices $g^{im}$ transforming according to the $D^j$ representation of the rotation group under rotations $\hat{T}_R$:

$$\hat{T}_R g^{im} \simeq \sum_{m'} D^j_{m'm}(R) g^{im'},$$

(2)

where the sign $\simeq$ means unitary equivalence. Further, assume that the desired dimension of the elementary matrix is $(N+1) \times (N+1)$ and that we know the complete set of wavefunctions of the elementary cell $\{|\psi_{\lambda\mu}\rangle\}$, $\lambda$ being the total spin and $\mu$ its $z$-projection. One can choose a basis in the matrix space consisting of the matrices $X^{kq} = (T^{kq})^\dagger$, $k = 0 \ldots N$, $q = -k \ldots k$. Here $T^{kq}$ are the $(N+1) \times (N+1)$ matrix representations of irreducible tensor operators transforming according to the $D^k$ representation of the rotation group; defining
$X^{kj} = (T^{kj})^\dagger$ just ensures that $X^{kj}$ transform according to the conjugate representation $\bar{D}^k$, like usual wavefunctions. In the simplest case $N=1$ (2×2 matrix space) the $T^{kj}$ matrices are just the identity matrix $\mathbb{I}$ and the Pauli matrices $\sigma^0 = \mathbb{I}$, $\sigma^\pm = \mp i/\sqrt{2}(\sigma_x \pm i\sigma_y)$:

$$T^{00} = \mathbb{I}, \quad T^{10} = \sigma^0, \quad T^{1,\pm 1} = \sigma^\pm;$$

(3)

explicit expressions for $T^{kj}$ in 3×3 space are given below. Then, our basis transforms as

$$\hat{T}_R X^{kj} = \sum_{q'} d_{q'q}^{k}(R) X^{kj},$$

(4)

which on the other hand amounts to a unitary transformation $\hat{T}_R X^{kj} = U(R) X^{kj} U^\dagger(R)$ and does not have any effect on the MP wavefunction.

It is easy to show that the following construction satisfies our requirement (3):

$$g^m = \sum_{k\lambda} c^{kj}_{\lambda} \sum_{\mu} \langle jm| kq, \lambda \mu \rangle X^{kj}|\psi_{\lambda \mu}\rangle.$$ 

(5)

Here $\langle jm| kq, \lambda \mu \rangle$ are the Clebsch-Gordan coefficients, and $c^{kj}_{\lambda}$ are arbitrary constants. In fact, we used the usual quantum mechanical addition rules for angular momenta, demanding that $g^m$ has certain quantum numbers $j, m$ characterizing the “hyperspin” defined in an extended space which is a direct product of $(N+1)\times(N+1)$ matrix space and the Hilbert space of the cell.

Then, we can construct a translational invariant matrix state with given hyperspin $J = L j$ and its $z$-projection $M = J$:

$$G^{JJ} = g_1^{jj} g_2^{jj} \cdots g_L^{jj}.$$ 

(6)

The matrix state $G^{JJ}$ belongs to the multiplet transforming according to $D^J$ and thus has the same structure as $g^J$, but now $|\psi_{\lambda \mu}\rangle$ have the meaning of many-body wavefunctions of an open spin chain (their total spin $\lambda = |J - N|, \ldots, |J + N|$ can differ from $J$ because of the edge effects). Taking the trace $|\Omega\rangle = \text{Tr}(G^{JJ})$, we pick up only the $M^{00}$ component, i.e. the state $|\psi_{J, J}\rangle$ describing a chain with periodic boundary conditions. Other states of the multiplet with $M < J$ can be obtained from $|\psi_{J, J}\rangle$ by applying $\hat{S}^{-}_\text{tot}$. It should be mentioned that the construction (3) allows several different values of $j$ even for the same size of the magnetic elementary cell; the number of possibilities grows fast with increasing the cell size, when more and more complicated magnetic structures with longer period are allowed. One can also construct various translationally non-invariant ‘excited’ MP states, but this goes beyond the scope of the present paper.

One can see that known MP states for VBS models and spin-1/2 ladder indeed follow the general structure described above. For example, the elementary matrix for the spin-1 AKLT state can be written in the form $g_{\text{AKLT}} = 1/\sqrt{3} \left\{ (\sigma^+)^4 |\beta\rangle + (\sigma^-)^4 |\alpha\rangle - (\sigma^0)^4 |\gamma\rangle \right\}$, which is exactly $g^{00}$ in our notation, and four components of the matrix $G^{00}$ defined by (3) describe a singlet and the Kennedy triplet states of the open spin-1 chain.

In the spin-2 case one possibility is to construct $T^{1m}$ as the matrix representations of $S=1$ spin operators, and $T^{2m}$ can be expressed as bilinear forms of $T^{1m}$. This yields the following expressions for $T^{kj}$ in 3×3 space:

$$T^{10} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad T^{1,\pm 1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$T^{20} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad T^{2,\pm 1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$T^{2,\pm 2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$ 

(7)

The matrix $T^{00}$ is proportional to the identity matrix $\mathbb{I}$, and the relationship $T^{j=\pm m} = (-1)^m (T^{jm})^\dagger$ holds. If the elementary cell consists of a single $S=2$ spin, then the elementary matrix $g^{00}$ constructed according to (3) is $g_{S=2} = \sum_m c^{(2m)}_0 |\psi_{2m}\rangle$, which coincides with the $S=2$ VBS matrix $c^{(2)}_0$ components of $G^{00}$ describe degenerate ground states of the open spin-2 VBS chain.

In case of a spin-$\frac{1}{2}$ ladder the elementary cell consists of two spins, and according to (3) one gets the ansatz used in Ref. (3)

$$g_{\text{ladder}} = c^{00}_0 \cdot \mathbb{I} \cdot |s\rangle + c^{11}_0 g_{\text{AKLT}}.$$ 

Here $|s\rangle$ denotes the singlet state, and the states $|\mu\rangle$ in $g_{\text{AKLT}}, \mu = 0, \pm 1$ now should be interpreted as the triplet states of two $S=\frac{1}{2}$ spins.

Our ansatz (3) allows one to construct MP states with spontaneously broken rotational symmetry (nonzero total spin $J$), which is practically important for the case of ferrimagnets. In the next Section we apply our formalism to the simplest model of a quantum ferrimagnet and argue that it really provides a good description of its ground state properties.

Application to the Heisenberg model with alternating spins 1 and $\frac{1}{2}$. We consider the model described by the Hamiltonian

$$\hat{H} = \sum_n (S_n \tau_n + \tau_n S_{n+1})$$ 

(8)

where $S_n$ and $\tau_n$ are respectively spin-1 and spin-$\frac{1}{2}$ operators at the $n$-th elementary magnetic cell (with $S^z$ eigenstates denoted as $(+, 0, -)$ and $(\uparrow, \downarrow)$, respectively). The elementary cell consists of spins 1 and $\frac{1}{2}$, the exchange interaction exists only between nearest neighbors, and all bonds are antiferromagnetic and of the same strength which is set to unity (see Fig. 1).
According to the Lieb-Mattis theorem\[1\] the ground state of this model has total spin $S_{\text{tot}} = L/2$, where $L$ is the number of elementary cells. The rotational symmetry is spontaneously broken in the ground state, which leads to a ferromagnetic long-range order. Thus, we have to construct the elementary matrix $g$ with $j = m = 1/2$. The complete set of cell wavefunctions $\psi_{\text{cell}}$ contains one doublet ($\lambda = 1/2$) and one quartet ($\lambda = 3/2$):

\[
\begin{align*}
|\psi_{1/2,1/2}\rangle &= \sqrt{2/3}|\uparrow\rangle - 1/\sqrt{3}|\downarrow\rangle, \\
|\psi_{1/2,-1/2}\rangle &= -\sqrt{2/3}|\uparrow\rangle + 1/\sqrt{3}|\downarrow\rangle, \\
|\psi_{3/2,3/2}\rangle &= |\uparrow\rangle, \\
|\psi_{3/2,-3/2}\rangle &= |\downarrow\rangle, \\
|\psi_{3/2,1/2}\rangle &= \sqrt{2/3}|\uparrow\rangle + 1/\sqrt{3}|\downarrow\rangle, \\
|\psi_{3/2,-1/2}\rangle &= \sqrt{2/3}|\downarrow\rangle + 1/\sqrt{3}|\uparrow\rangle.
\end{align*}
\]

Let us choose the simplest case of $2 \times 2$ matrix space, then the basis is $X^{00} = 1$, $X^{10} = -\sigma^0$ and $X^{1,1} = -\sigma^+$ (cf. Eq. (3)), and, according to (4), the most general form of the elementary matrix with $j = m = 1/2$ is

\[
g = c_1M_{0,1/2} + c_2M_{1,1/2} + c_3M_{1,3/2},
\]

\[
M_{0,1/2} = |\psi_{1/2,1/2}\rangle \langle \psi_{1/2,1/2}|,
\]

\[
M_{1,1/2} = -1/\sqrt{3}\sigma^0|\psi_{1/2,1/2}\rangle - \sqrt{2/3}\sigma^{-1}|\psi_{1/2,-1/2}\rangle,
\]

\[
M_{1,3/2} = -1/\sqrt{3}\sigma^0|\psi_{3/2,1/2}\rangle - 1/\sqrt{6}\sigma^{-1}|\psi_{3/2,-1/2}\rangle - 1/\sqrt{2}\sigma^+|\psi_{3/2,3/2}\rangle.
\]

Thus, $g$ contains two independent variational parameters $u = c_1/c_2$ and $v = c_2/c_3$, which are assumed to be the same throughout the chain. By the construction, the variational MP state $|\Omega\rangle = \text{Tr}(g_1g_2 \cdots g_L)$ has total spin $S_{\text{tot}} = L/2$, i.e., the same as the true ground state.

The quantum averages can be calculated using the transfer matrix technique; for example, for any operator $\hat{F}$ acting on the states of only one unit cell one has $\langle \Omega | \hat{F} | \Omega \rangle = \text{Tr}(G^{\ell-1} \hat{F} G) / \text{Tr}(G^\ell)$, where $G = g^* \otimes g$ is the transfer matrix, $\hat{F} = g^* \otimes (\hat{F}g)$, and the sign $\otimes$ means an outer matrix product; further details can be found in Refs. 3, 4. The resulting expression for the ground state energy per unit cell is rather lengthy but still manageable,

\[
E_{\text{var}} = (1/18Q)(A + B/Z),
\]

\[
Z = [12v^2(u^2 + 1) + 3(1/2), 
Q = (3a^2 + v^2 + 1 + Z)^2,
A = -180a^2 - 360uv^2 - 20v^4 - 180\sqrt{2}u^3 + 36\sqrt{6}uv^2 - 40\sqrt{2}v^3 - 108u^3 + 36\sqrt{7}uv - 96v^2 + 27\sqrt{6}u - 29\sqrt{2}v + 4,
B = -1440u^4v^2 - 480uv^4 - 180\sqrt{2}u^3v + 108\sqrt{6}uv^2 - 540\sqrt{7}uv^3 + 36\sqrt{6}uv^4 - 1404u^2v^2 + 288\sqrt{3}uv^3 - 108v^4 + 210uv^2 + 324\sqrt{6}uv^2 - 72\sqrt{2}v^3 - 144u^2 + 108\sqrt{3}uv - 108v^2 + 81\sqrt{6}u - 27\sqrt{2}v + 18.
\]

Its numerical minimization gives $E_{\text{var}}^{\text{min}} = E_{\text{MP}} = -1.449$ (at $u = -1.303, v = 1.079$). Using this solution, one can also calculate average spin values $\langle s_i^2 \rangle$ and spin correlation functions $\langle s_i^z s_{i+n}^z \rangle$, where $s, s' \in \{S, \tau\}$. Correlation functions behave as $a + be^{-n/\xi}$, the correlation length $\xi$ being extremely short, $\xi = 0.365$ in the unit cell lengths. In the regular spin wave (SW) theory the decay is exponential only asymptotically, and $\xi \approx 0.7$. The spin wave theory is predicted by the spin wave theory.\[10\] The QMC data were obtained at $L = 32$. The numerical uncertainty is less than 0.002, which is much smaller than the symbol size.

\[\text{FIG. 1. The Heisenberg spin chain with alternating spins 1 (large circles) and } \tau \text{ (small circles); boxes show the unit cells.}\]

\[\text{FIG. 2. Longitudinal spin correlation functions } K_{zz}(l), \text{ where } s \text{ and } s' \text{ can be either } S = 1 \text{ or } \tau = 1/2, \text{ and } l \text{ is the distance between spins in unit cell lengths, so that for integer (half-integer) } l \text{ the correlation is measured between spins of same (different) type, respectively: (a) correlations between } S = 1 \text{ and any other spin; (b) correlations between } S = \tau \text{ and any other spin. The dashed line shows the asymptotic value predicted by the spin wave theory. The QMC data were obtained at } L = 32. \text{ The numerical uncertainty is less than 0.002, which is much smaller than the symbol size.}\]
reduction is also overestimated in the SW calculation.

The results were compared with the numerical data obtained with the quantum Monte Carlo (QMC) method based on the Trotter-Suzuki decomposition of checkerboard type. The raw data for a set of the Trotter numbers \( n \) were extrapolated into the \( n \to \infty \) limit with a parabolic fitting formula. We have calculated the chains of length \( L = 4, 8, 16, \) and 32 under the periodic boundary condition in the subspace with fixed total magnetization \( S^z = L/2 \). Though the \( L = 32 \) data are already close to the corresponding thermodynamic limit values, we have carried out the \( L \to \infty \) extrapolation. We have checked that almost the same results are obtained at two temperatures, \( T = 0.04 \) and 0.02, and thus we assume that \( T = 0.02 \) is low enough to describe the ground state properties successfully. Typically, about \( 10^6 \) MC steps were needed to reach the equilibrium. The ground state energy per unit cell was estimated to be \( E_{\text{QMC}} = -1.455 \pm 0.001 \) in the thermodynamic limit, which agrees very well with the MP variational result. The agreement is also good for the average spin values, the MP calculation gives \( \langle S_i^z \rangle = 0.779 \) and \( \langle \tau_i^z \rangle = -0.279 \), to be compared with the QMC results \( 0.793 \pm 0.002 \) and \( -0.293 \pm 0.002 \), respectively. In Fig. 1 we show the results for various spin-spin correlation functions obtained in the MP approach, together with the QMC data. The discrepancy never exceeds 5\% which is much better than the corresponding SW result.

Summary. To conclude, we propose a new version of the matrix product (MP) states approach to the description of quantum spin chains, which allows one to construct MP states with certain quantum numbers \( J \) (the total spin) and \( M \) (its \( z \)-projection). Known MP representations of VBS states for integer-spin antiferromagnetic chains and recently proposed MP ansatz for \( S = \frac{1}{2} \) ladders correspond to the particular case \( J = 0, M = 0 \) of our ansatz. The method can be useful for the variational description of quantum ferrimagnetic chains whose ground state has nonzero \( J \), and of higher-\( S \) spin ladders. We apply our approach to the isotropic ferrimagnetic Heisenberg chain with alternating spins 1 and \( \frac{3}{2} \); on the other hand, we study this system numerically using the quantum Monte Carlo (QMC) technique. For both ground state energy and the correlation functions we obtain very good agreement between the variational results and the QMC data. We think that the fundamental reason for the success of the MP approach to the ferrimagnetic chain is that in this model the correlations of fluctuations above the long-range order are very short-ranged. MP ansatzes generally yield short range correlations which is just appropriate here.

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FIG. 2. Longitudinal spin correlation functions $K_{ss'}^z(l)$, where $s$ and $s'$ can be either $S=1$ or $S=\frac{1}{2}$, and $l$ is the distance between spins in unit cell lengths, so that for integer (half-integer) $l$ the correlation is measured between spins of same (different) type, respectively; (a) correlations between $S=1$ and any other spin; (b) correlations between $S=\frac{1}{2}$ and any other spin. The dashed line shows the asymptotic value predicted by the spin wave theory. The QMC data were obtained at $L = 32$. The numerical uncertainty is less than 0.002, which is much smaller than the symbol size.