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Equivalence of the variational matrix product method and the density matrix renormalization group applied to spin chains

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Abstract. – We study the relationship between the Density Matrix Renormalization Group (DMRG) and the variational matrix product method (MPM). In the latter method one can also define a density matrix whose eigenvalues turn out to be numerically close to those of the DMRG. We illustrate our ideas with the spin-1 Heisenberg chain, where we compute the ground-state energy and the spin correlation length. We also give a rotational invariant formulation of the MPM.

The density matrix renormalization group (DMRG), introduced by White [1] in 1992, is a powerful numerical method to study the ground-state and static properties of quantum lattice systems, as for example the Heisenberg, t-J, and Hubbard models defined on chains, ladders and clusters. The DMRG uses the Wilsonian scheme of adding one point at each RG step. After many iterations the DMRG reaches a fixed point, and the ground state exhibits a matrix product structure (MP), as was shown by Ostlund and Rommer [2]. These authors proposed to start from a MP ansatz for the ground state of the system, determining the variational parameters by the standard variational method, without resorting to the DMRG. The advantage of the MPM is that it is analytical and does not require big computational resources. However, it is not clear how to treat large values of the number of states m used in the minimization of the energy. On the other hand, the relation between the MPM and the DMRG is not clear, apart from sharing a MP structure in the thermodynamic limit.

In this letter we show i) how to treat numerically and analytically larger values of m than those considered by other authors, thanks to the reduction of the basis obtained by exploiting the rotational symmetry of the problem, and ii) exhibit the relation between the MPM and the DMRG. In particular we shall see that the MPM naturally leads to a density matrix whose eigenvalues appear as variational parameters together with those that generate the MP ansatz. In fact our formalism is closely connected to that developed in ref. [3] (see also [4,5]). We apply

the MPM and the DMRG to the spin-1 Heisenberg chain, and compare the results obtained with both methods. For the ground-state energy density, the MPM gives a better estimate for all values of $m > 1$, which we interpret as being caused by the existence of a bound state in the middle of the superblock in the DMRG method. In the MPM this bound state is absent by construction. For increasing values of m the discrepancy between the MPM and the DMRG tends to disappear. The numerical results for the eigenvalues of the density matrices in both methods are similar, and they seem to converge to a common value when increasing m. From these results we conclude the equivalence between the MPM and the DMRG methods in the thermodynamic limit for large values of m.

Before we explain our approach in detail, let us recall the basics of the DMRG. Let us consider a 1D lattice of length N, called B_N, which we describe by a collection of m states. The addition of one more point leads to a larger lattice, $B_N \bullet$ which is described by $m \times m^*$ states, where m^* is the number of states of a single site. The DMRG is an algorithm to truncate the $m \times m^*$ states, associated to $B_N\bullet$, down to m states associated to B_{N+1}. The states kept in the truncation are the eigenstates with largest eigenvalues of a density matrix. This density matrix is constructed from the GS of a larger system, called the superblock $B_N \bullet \bullet B_N^{\mathrm{R}}$, which contains the original block $B_N\bullet$ together with its reflection $\bullet B_N^{\mathrm{R}}$. The reflected block acts as environment for the original block [1].

Let us now present the MPM. We shall consider a spin chain with spin S at each site, where S is an integer. Let us denote the basis states of the MPM as $|a, JM\rangle_N$, where N is the length of the chain, $a = 1, \cdots, d_J$ denotes the multiplicity of the total spin J of the state and M is the third component of the spin. Counting the number of multiplets we have $m = \sum_J \ d_J$, which corresponds to a number $m_W = \sum_J (2J+1)\ d_J$ of states in the standard DMRG. At the fixed point of the DMRG one has the matrix product law [2]

$$|a_1, J_1 M_1\rangle_N = \sum_{a_2 J_2, M_2, M} A_{a_1 J_1, a_2 J_2} \times \\ \times |SM\rangle_N \ \otimes |a_2, J_2 M_2\rangle_{N-1} \ \langle SM, J_2 M_2 \, | J_1 M_1\rangle \ , \tag{1}$$

where $\langle SM, J_2 M_2 \, | J_1, M_1\rangle$ are Clebsch-Gordan coefficients and $A_{a_1 J_1, a_2 J_2}$ are variational parameters subject to the following conditions:

$$A_{a_1 J_1, a_2 J_2} = 0 \ \text{ unless } \ |J_2 - S| \leq J_1 \leq J_2 + S \, , \tag{2}$$

$$\sum_{a_2, J_2} A^*_{a_1 J_1, a_2 J_2} \ A_{a_1' J_1, a_2 J_2} = \delta_{a_1 a_1'} \, . \tag{3}$$

Equation (2) follows from the CG decomposition $S \otimes J_2 \to J_1$ in (1), while condition (3) guarantees that the states $|a, JM\rangle_N$ constitute an orthonormal basis for all values of N. The initial data of the recurrence relation (1) is given by choosing a spin $S/2$ irrep at the end of the chain. This choice eliminates the multiplicity associated to the effective spins $S/2$ at the ends of the chain. The sum in J's in eq. (1) is of course restricted to a finite set of spins.

The parameters $A_{a_1 J_1, a_2 J_2}$ are determined by minimizing the energy of the states $|a, JM\rangle_N$ in the limit where $N \to \infty$. For this purpose let us define the following quantity:

$$E^{(N)}_{aa'J} = {}_N \langle a, JM| \, H_N \, |a', JM\rangle_N \ , \tag{4}$$

where H_N is the Hamiltonian acting on the chain with N sites. From eq. (1) one can derive a recursion formula for $E^{(N)}_{aa'J}$,

$$E^{(N)}_{aa'J} = V_{aa'J} + \sum_{bb'J'} T_{aa'J, bb'J'} \ E^{(N-1)}_{bb'J'} \qquad (N \geq 3) \, , \tag{5}$$

where $\mathbf{T}$ is a matrix with entries (from now on we assume the reality of $A_{a_1 J_1, a_2 J_2}$)

$$T_{aa'J,bb'J'} = A_{aJ,bJ'}\ A_{a'J,b'J'} \tag{6}$$

and $V_{aa'J}$ is the matrix element of the piece of the Hamiltonian which couples the sites N and $N-1$, which does not depend on N,

$$V_{aa'J} =_N \langle a, JM|\, H_{N-1,N}\, |a', JM\rangle_N\ . \tag{7}$$

For the Heisenberg model, $H_{N-1,N} = \mathbf{S}_{N-1}\cdot\mathbf{S}_N$, and applying the Wigner-Eckart theorem, we find the following expression for W in terms of 6-j symbols:

$$V_{a_1 a_2 J_1} = \sum_{a_3 J_2, a_4 J_3, a_5 J_4} \mathcal{H}_{J_1 J_2 J_3 J_4}\quad A_{a_1 J_1, a_3 J_2} A_{a_2 J_1, a_4 J_3}\ A_{a_3 J_2, a_5 J_4} A_{a_4 J_3, a_5 J_4}\,, \tag{8}$$

$$\begin{aligned}\mathcal{H}_{J_1,J_2,J_3,J_4} = (-)^{2S+J_1+J_2+J_3+J_4+1}\, S\,(S+1)\,(2S+1)\,\times \\ \times\sqrt{(2J_2+1)\,(2J_3+1)}\begin{Bmatrix} 1 & S & S \\ J_1 & J_2 & J_3 \end{Bmatrix}\begin{Bmatrix} 1 & S & S \\ J_4 & J_2 & J_3 \end{Bmatrix}.\end{aligned} \tag{9}$$

The solution of (5) can be expressed in matrix notation as

$$|E^{(N)}\rangle = \left(1 + \mathbf{T} + \mathbf{T}^2 + \ldots + \mathbf{T}^{N-3}\right)\ |V\rangle + \mathbf{T}^{N-2}\,|E^{(2)}\rangle\,, \tag{10}$$

where $|E^{(N)}\rangle$ is regarded in (10) as a vector whose components are labeled by $(aa'J)$. The entries of $\mathbf{T}$ are given by eq. (6).

In the limit $N\to\infty$ the contribution from $|E^{(2)}\rangle$ drops off and we shall show below that $E^{(N)}_{aa'J}$ behaves as

$$\lim_{N\to\infty}\frac{1}{N}\,E^{(N)}_{aa'J} = \ \delta_{aa'}\ \ e_\infty\,, \tag{11}$$

where e_∞ can be identified with the ground-state energy density and reads

$$e_\infty = \sum_{aa'J}\ \rho_{aa'J}\ V_{aa'J}\,. \tag{12}$$

In eq. (12) $\rho_{aa'J}$ is the right eigenvector of the matrix $\mathbf{T}$ with eigenvalue 1, and plays the role of a density matrix in the MPM. The proof of eqs. (11) and (12) follows from the existence of an eigenvalue of the matrix $\mathbf{T}$ equal to 1 [3, 2]. This property can be deduced from the normalization condition (3). Let us call $|v\rangle$ and $\langle\rho|$ the right and left eigenvectors associated to the eigenvalue 1 of $\mathbf{T}$, which we shall assume to be unique,

$$\mathbf{T}\,|v\rangle = |v\rangle\,, \tag{13}$$

$$\langle\rho|\,\mathbf{T} = \langle\rho|\,. \tag{14}$$

Then eq. (3) implies that $|v\rangle$ is given in components by $v_{aa'J} = \delta_{aa'}$. On the other hand the quantities $\rho_{aa'J}$ that appear in (12) are nothing but the components of $\langle\rho|$, and they are found by solving the eigenvalue problem (14). In eq. (12) we have normalized $\langle\rho|$ according to

$$\langle\rho|v\rangle = 1\ \to\ \sum_{aa'J}\ \rho_{aa'J} = 1\,. \tag{15}$$

In a field-theoretical language $|v\rangle$ and $\langle\rho|$ play the role, respectively, of incoming $|0\rangle$ and outgoing vacua $\langle 0|$, which are left invariant by the transfer matrix operator $\mathbf{T}$, that shifts by one lattice space the spin chain. On the other hand, $\rho_{aa'J}$ has the properties of a density matrix, and it corresponds precisely to the reduced density matrix of the blocks in the DMRG formalism, as we shall show below. It is remarkable that the MP ansatz (1) leads in a natural way to a density matrix formalism. This suggest that a rigorous mathematical formulation of the DMRG could perhaps be achieved within the MPM.

By analogy with the DMRG we may choose a basis where the density matrix becomes diagonal, *i.e.* $\rho_{aa'J} = w^2_{aJ}\,\delta_{aa'}$. Under this assumption eq. (14) reads

$$\sum_{a_1 J_1} w^2_{a_1 J_1}\; A_{a_1 J_1, a_2 J_2}\; A_{a_1 J_1, a'_2 J_2} = \; w^2_{a_2 J_2}\;\delta_{a_2 a'_2}\,. \tag{16}$$

A solution of eqs. (16) is obtained using eq. (3) and assuming the following "detailed balanced" condition [6]:

$$w_{a_1 J_1}\; A_{a_1 J_1, a_2 J_2} \;=\; w_{a_2 J_2}\; A_{a_2 J_2, a_1 J_1}\,. \tag{17}$$

This equation is very useful since we can eliminate almost a half of the A's in terms of the other half, and use the w's as independent variationally parameters. Hence the problem reduces to the minimization of the GS energy (12) with respect to the variational parameters w_{aJ} and $A_{a_1 J_1, a_2 J_2}$ subject to the constraints (2), (3) and (17). For a MP ansatz with no multiplicities, *i.e.* $d_J = 1$, one can solve all the constraints in terms of an independent set of parameters, however when $d_J > 1$ it is more efficient to use a numerical program of minimization with constraints.

Taking into account all the variables and constraints one sees that the total number of independent variational parameters, N_A, is given by

$$N_A = \frac{1}{2}\sum_{J_1 \neq J_2} \Lambda_{J_1 J_2}\;\; d_{J_1}\; d_{J_2}\;\; + \sum_J\; d_J - 1\,, \tag{18}$$

where $\Lambda_{J_1 J_2}$ is 1 if J_1 and J_2 satisfy eq. (2) and zero otherwise.

TABLE I. – *m is total the number of multiplets, N_A is the number of independent variational parameters, d_J is the number of multiplets with spin J, $e_\infty^{\mathrm{MP,DMRG}}$ is the* GS *energy density of the* MPM (DMRG), *$1 - P_m$ is the probability of the states truncated out in the* DMRG *and ξ^{MP} is the spin correlation length of the* MP *state. The exact results are given by $e_\infty = 1.4014845$ and $\xi = 6.03$* [7].

m	N_A	$d_{1/2}$	$d_{3/2}$	$d_{5/2}$	$-e_\infty^{\mathrm{MP}}$	$-e_\infty^{\mathrm{DMRG}}$	$1 - P_m$	ξ^{MP}
1	0	1	0	0	1.333333	1.333333	1.6×10^{-2}	0.910
2	2	1	1	0	1.399659	1.369077	1.4×10^{-3}	2.600
3	4	2	1	0	1.401093	1.392515	1.3×10^{-5}	3.338
4	7	2	2	0	1.401380	1.401380	1.6×10^{-5}	3.937
5	10	2	2	1	1.401443	1.401436	7.6×10^{-6}	4.085
6	13	2	3	1	1.401474	1.401468	1.3×10^{-6}	4.453

In table I we present the results for the case of spin $S = 1$, obtained with the MPM and a version of the DMRG where the rotational symmetry has been used to eliminate the redundancy in the states kept [8]. The case $m = 1$ corresponds to the AKLT wave function [9,10], where e_∞ computed with the MPM and the DMRG coincide. This is because from eq. (18) there is no adjustable parameter in the ansatz. The case $m = 4$ is the one considered in [2]. The ground-state energy $e_\infty(m)$ obtained with the MPM is always lower than the DMRG energy; this is related to the fact that the wave function generated by the infinite system DMRG is not uniform. The DMRG optimizes the ground state of the superblock $[B] \bullet \bullet [B]$, where $[B]$ denotes the m-state block spin, while the block $[B \bullet]$ has $3m$ degrees of freedom. From the view point of the MPM, the block $[B \bullet]$ should be optimized with m degrees of freedom. As a result, a shallow bound state appears between the left-half of the system $[B] \bullet$ and the right-half $\bullet [B]$, and the numerical precision in the ground-state energy is spoiled in DMRG, especially when m is small. A way to improve the DMRG from this error is to consider a superblock $[B] \bullet [B]$ at the last several steps in the infinite system DMRG algorithm. By choosing this superblock configuration, the degree of freedom of the block $[B \bullet]$ is automatically restricted to m because the "reservoir" $[B]$ has only m degrees of freedom.

In order to compute the spin-spin correlation lengths ξ of the MP states (1), we have to find out a recursion formula for the reduced matrix elements of the spin operators $\mathbf{S}$, which is given by

$$
\begin{aligned}
&{}_N\langle a_1 J_1 || \mathbf{S}_1 || a_2 J_2 \rangle_N = \\
&= \textstyle\sum_{a_3 J_3 a_4 J_4} \; T^{(1)}_{a_1 J_1 a_2 J_2, a_3 J_3 a_4 J_4} \; {}_{N-1}\langle a_3 J_3 || \mathbf{S}_1 || a_4 J_4 \rangle_{N-1}
\end{aligned} \tag{19}
$$

with

$$
\begin{aligned}
T^{(1)}_{a_1 J_1 a_2 J_2, a_3 J_3 a_4 J_4} &= (-)^{J_2 + J_3 + S + 1} \, A_{a_1 J_1, a_3 J_3} A_{a_2 J_2, a_4 J_4} \times \\
&\times \sqrt{(2J_1 + 1)\,(2J_2 + 1)} \begin{Bmatrix} J_3 & J_1 & S \\ J_2 & J_4 & 1 \end{Bmatrix} .
\end{aligned} \tag{20}
$$

TABLE II. – *a and J are the labels of the irrep, w^2_{MP}, are the eigenvalues of the* MP *density matrix, and $\overline{w}^2_{\mathrm{DMRG}}$ are the corresponding* DMRG *eigenvalues kept in the* RG *process and normalized to* 1. *The data correspond to $m = 6$.*

a	J	w^2_{MP}	$\overline{w}^2_{\mathrm{DMRG}}$
1	1/2	0.9695581	0.9696232
2	1/2	0.0007662	0.0007599
1	3/2	0.0295443	0.0294877
2	3/2	0.0001119	0.0001089
3	3/2	0.0000078	0.0000085
1	5/2	0.0000118	0.0000118

The correlation length ξ is then given by the highest eigenvalue λ, in absolute value, of $\mathbf{T}^{(1)}$ by the formula

$$\xi = -1/\ln\lambda\,. \tag{21}$$

For the AKLT case (*i.e.* $d_J = \delta_{J,1/2}$), eqs. (19) and (20) reproduce the exact spin-spin correlator found in ref. [10]. To analyze the relation MPM *vs.* DMRG more in detail, we give in table II the eigenvalues of the matrix $\rho_{aa'J}$, and those of the DMRG reduced density matrix in the case where $m = 6$. The latter matrix has dimension $3m$ and the truncation DMRG method consists in choosing m states with highest eigenvalues w^2_{DMRG}, which add up to $1-P_m$ (see table I). For this reason we have to scale the DMRG weights of the states kept in order that they sum up to 1:

$$\overline{w}^2_{\mathrm{DMRG}} = w^2_{\mathrm{DMRG}}/P_m\,. \tag{22}$$

The results shown in tables I and II suggest that the predictions made by the MPM and the DMRG should become identical for large values of m.

In summary we have shown in this paper that the MPM leads in a natural way to the DMRG. Indeed the notion of a density matrix emerges in the MPM when trying to minimize the GS energy density. Moreover the eigenvalues of this density matrix are used in our method as variational parameters. We have also presented a rotational invariant formulation of the MPM method which uses all the power of group theory to reduce the computational complexity of the problem.

In a later publication we shall present the results for the spin gap and other observables for various spin chains and ladders using the MPM [11]. An interesting problem is the generalization of the MPM to the case of holes. The results of ref. [12] concerning the t-J ladder suggest that this generalization is possible and worthwhile studying it.

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