# Density Matrix Renormalization Group and Periodic Boundary Conditions: A Quantum Information Perspective

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We introduce a picture to analyze the density matrix renormalization group (DMRG) numerical method from a quantum information perspective. This leads to a variational formulation of DMRG which allows for dramatic improvements in the case of problems with periodic boundary conditions. The picture also explains some features of the method in terms of entanglement and teleportation.

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The discovery and development of the density matrix renormalization group (DMRG) method [1,2] to treat quantum many-body systems has enabled us to analyze and understand the physical properties of certain condensed matter systems with unprecedented precision [3]. Originally envisioned for 1D systems with short-range interactions at zero temperatures, during the last few years this method has been successfully extended to other situations [3]. Its mathematical foundations have been established [4,5] in terms of the so-called matrix product states (MPS) [6] and by now there exists a coherent theoretical picture of DMRG.

At the same time, the field of quantum information theory (QIT) has emerged to describe the properties of quantum many-body systems from a different point of view. A theory of entanglement has been established and has allowed us to describe and understand phenomena like teleportation [7] and to use them in the fields of communication and computation [8]. Recently it has been shown that QIT may also shed some new light on our understanding of condensed matter systems [9–11] and, in particular, on the DMRG method [12,13].

In this work we analyze the standard DMRG method using a physical picture which underlies QIT concepts. The picture has its roots in the AKLT (Affleck, Kennedy, Lieb, and Tasaki) model [14] and allows us to understand why DMRG offers much poorer results for problems with periodic boundary conditions (PBC) than for those with open boundary conditions (OBC), something which was realized at the origin of DMRG [2]. It also gives a natural way of improving the method for problems with PBC, in which several orders of magnitude in accuracy can be gained. The importance of this result lies in the fact that physically PBC are strongly preferable over OBC as boundary effects are eliminated and finite size extrapolations can be performed for much smaller system sizes.

Let us start by reviewing the simplest version of the DMRG method for 1D spin chains with OBC, involving a left block spin, a single physical spin, and a right block spin, typically represented as $B \bullet B$ [2,15]. We denote by $d$ the dimension of the Hilbert space corresponding to each spin, and by $D$ the number of states kept by the DMRG method. We assume that the spins at the edges have dimension $d_0 \geq D$ [16]. At some particular step the chain is split into two blocks and one spin in between. The left block ($L$) contains spins $1, \ldots, M-1$, and the right one ($R$) spins $M+1, \ldots, N$. Then a set of $D \times D$ matrices $A^s$ are determined such that the state

$$|\Psi\rangle = \sum_{s=1}^{d} \sum_{\alpha,\beta=1}^{D} A^s_{\alpha,\beta} |\alpha\rangle_L \otimes |s\rangle_M \otimes |\beta\rangle_R, \tag{1}$$

minimizes the energy. The states $|\alpha\rangle_{L,R}$ are orthonormal and have been obtained in previous steps. They can be constructed using the recurrence relations

$$|\alpha\rangle_L = \sum_{\alpha'=1}^{D} \sum_{s=1}^{d} U^{[M-1],s}_{\alpha,\alpha'} |s\rangle_{M-1} \otimes |\alpha'\rangle_{L'}, \tag{2}$$

where the block $L'$ contains the spins $1, \ldots, M-2$. The new matrices $U^{[M],s}$ are determined from $A^s$ and fulfill

$$\sum_{s=1}^{d} U^{[M],s} (U^{[M],s})^\dagger = \mathbf{1}. \tag{3}$$

For the blocks consisting of the edge spins alone, the $|\alpha\rangle$ are taken as the members of an orthonormal set.

In order to give a pictorial representation of the above procedure we introduce at site $M$ two auxiliary $D$-level systems, $a_M$ and $b_M$. The corresponding Hilbert spaces $H_{a,b}$ are spanned by two orthonormal bases $|\alpha\rangle_{a,b}$, respectively. We take $L$ and $a_M$ (and also $R$ and $b_M$) in the (unnormalized) maximally entangled state

$$|\phi\rangle := \sum_{\alpha=1}^{D} |\alpha\rangle \otimes |\alpha\rangle. \tag{4}$$

We can always write $|\Psi\rangle = P_M |\phi\rangle_{L,a_M} |\phi\rangle_{R,b_M}$, where $P_M$ maps $H_a \otimes H_b \rightarrow H_M$, with $H_M$ the space corresponding to the $M$th spin and [cf. (1)]

$$P_M = \sum_{s=1}^{d} \sum_{\alpha,\beta=1}^{D} A^s_{\alpha,\beta} |s\rangle\langle\alpha, \beta|. \tag{5}$$

 

In fact, we can proceed in the same way at any other site $k \neq 1, M, N$ by defining two auxiliary systems $a_k$ and $b_k$ and a map $Q_k$ defined as in (5) but with the matrices $U$ instead of the $A$. For the edge spins one and $N$ we define a single auxiliary system $b_1$ and $a_N$, respectively, and define accordingly the operators $Q_{1,N}$ which now map $H_{b,a} \rightarrow H_{1,N}$. Thus, the state $\Psi$ is then obtained by applying the operators $Q_1, \ldots, P_M, \ldots, Q_N$ to the set of maximally entangled states $\phi$ between the auxiliary systems $b_k$ and $a_{k+1}$ $(k = 1, \ldots, N-1)$ [see Fig. 1(a)].

The DMRG procedure can be now represented as follows. For fixed projectors $Q_{i\neq M}$, the energy is a quadratic function in the variables $P_M$ and hence the optimal $P_M$ (given fixed $Q_{i\neq M}$) can be found by solving an eigenvalue equation. From $P_M$, one obtains the operator $Q_M$ and goes to the next step at location $M+1$. One proceeds in the same way, moving to the right, until one reaches the location $N$. At that point, one starts moving to the left until one reaches location 1 at which point it moves again to the right. The procedure is continued until a fixed point for the energy is reached, something which always occurs since the energy is a monotonically decreasing function of the step number. This proves that DMRG with the $B \bullet B$ is a *variational method which always converges*: the variational class of states over which is optimized is the class of MPS with open boundary conditions.

The more standard scenario ($B \bullet \bullet B$) is represented in Fig. 1(b). The operator $P_M$ acts on the auxiliary subsystems $a_M$ and $b_{M+1}$ and maps $H_a \otimes H_b \rightarrow H_M \otimes H_{M+1}$. In this picture [for both configurations, Figs. 1(a) and 1(b)] it is very clear that the two edge spins are treated on a very different footing since they are represented by a single auxiliary system which are not entangled to any other.

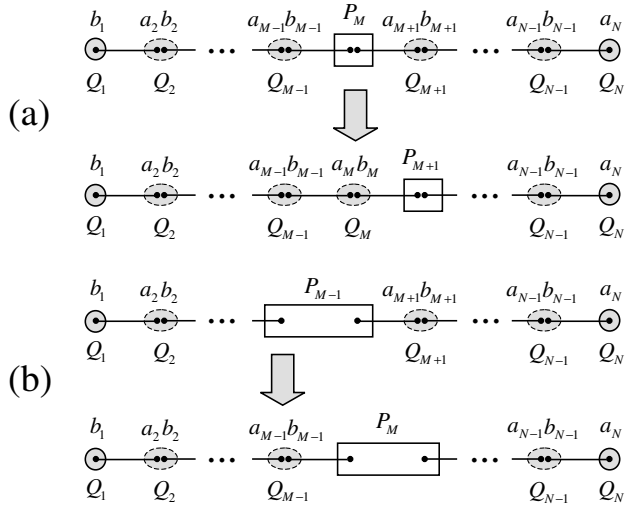


FIG. 1. Schematic picture of the DMRG method for the $B \bullet B$ (a) and the $B \bullet \bullet B$ (b) configurations. Horizontal lines represent maximally entangled states $|\phi\rangle$, the ellipses and circles (squares) the operators $Q$ ($P$) which map the auxiliary system into the physical ones.

In the case of a problem with PBC a slight modification of the scheme is used [2]. The idea is to still separate the system into two blocks and two spins as before but now with the configuration $B \bullet B \bullet$ . This ensures the sparseness of the matrices one has to diagonalize and thus it increases the speed of the algorithm [2]. One can draw the diagram corresponding to this procedure in a similar way as in Fig. 1. The important point is, however, that the variational class of states over which is optimized is still the class of MPS with open boundary conditions. In our opinion, this is the reason of the poor performance of the DMRG method for problems with PBC.

The method we propose for the case of PBC is very clear in terms of this picture (Fig. 2): we replace the variational class of states to the MPS with periodic boundary conditions. One has to substitute *at all sites k* the spin by *two* auxiliary systems $a_k$ and $b_k$ of dimension $D$, with $b_k$ and $a_{k+1}$ (with $a_{N+1} := a_1$) in a maximally entangled state and find the maps $P_k$: $H_a \otimes H_b \rightarrow H_k$ which lead to a state

$$|\Psi\rangle = P_1 \otimes P_2 \cdots P_{N-1} \otimes P_N |\phi\rangle^{\otimes N}, \tag{6}$$

with the minimal energy. This minimization can be performed in a similar way to the one used in the standard DMRG method: for fixed $Q_{i\neq M}$, the energy and the normalization of the state are a quadratic function of $P_M$, and hence the optimal $P_M$ can be determined through solving a generalized eigenvalue problem. Before showing how to do this in practice, we derive some formulas in terms of these operators. We write

$$P_k = \sum_{s=1}^{d} |s\rangle\langle\varphi_s^{[k]}|, \qquad \langle\varphi_s^{[k]}| = \sum_{\alpha,\beta} B_{\alpha,\beta}^{[k],s} \langle\alpha, \beta|. \tag{7}$$

Thus, the problem is solved once the states $\varphi$ (or equivalently, the matrices $B$) are determined. Note that starting from these states, it is possible to calculate expectation values of products of local observables [4], since

$$\langle\Psi|O_1 \cdots O_N|\Psi\rangle = \mathrm{Tr}(E_{O_1}^{[1]} \cdots E_{O_N}^{[N]}), \tag{8}$$

where

$$E_O^{[k]} = \sum_{s,s'=1}^{d} \langle s|O|s'\rangle B^{[k],s} \otimes (B^{[k],s})^*. \tag{9}$$

Thus, the main idea to perform the minimization is very simple. Given the Hamiltonian $H$ describing the system,

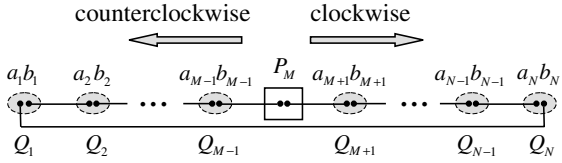


FIG. 2. Proposed configurations for the case of PBC. One may also use two spins instead of one.

one chooses one site $M$ and writes the energy as

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\psi^{[M]}|H_M|\psi^{[M]}\rangle}{\langle\psi^{[M]}|N_M|\psi^{[M]}\rangle}, \tag{10}$$

where $|\psi^{[M]}\rangle = \oplus_s|\psi_s^{[M]}\rangle$ is a vector built by concatenating the $\psi_s^{[M]}$, and $N_M$ and $H_M$ are $d \times D^2$ Hermitian square matrices which are built using the vectors $\psi_s^{[k]}$ at $k \neq M$. For example, $N_M = \oplus_s N_0$ is a block diagonal matrix with identical blocks $N_0$ which has matrix elements $(N_0)_{(\alpha,\alpha'),(\beta,\beta')} = (\tilde{N}_0)_{(\alpha,\beta),(\alpha',\beta')}$, with

$$\tilde{N}_0 = E_{\mathbf{1}}^{[M+1]} \cdots E_{\mathbf{1}}^{[N]} E_{\mathbf{1}}^{[1]} \cdots E_{\mathbf{1}}^{[M-1]}. \tag{11}$$

Thus, at this step the operator $P_M$ is found by solving the generalized eigenvalue problem

$$H_M|\psi^{[M]}\rangle = \lambda N_M|\psi^{[M]}\rangle, \tag{12}$$

with $\lambda$ minimum, which in turn gives the energy at this step. Then one chooses another site and proceeds in the same way until the energy converges. At the end we have all the $P_k$ and can evaluate all expectation values.

Let us now explain how one can make the method efficient. Let assume that we have a set of spins in a ring. The idea is to determine operators $P_k$ in a clockwise order (first $P_1$, then $P_2$, until $P_{N-1}$), then improve them following a counterclockwise ordering (from $P_N$ to $P_2$), then again clockwise, until the fixed point is reached. At each step, a normalization condition similar to (3) is imposed, depending on whether we are in a clockwise or counterclockwise cycle, which makes the matrix $N_M$ well behaved. On the other hand, at each step only the operators which are strictly needed in later steps are calculated in an efficient way and stored.

The normalization condition is based on the following fact. Given the state $\Psi$, characterized by matrices $B$, if we substitute $B^{[M],s} \to B^{[M],s}X := U^{[M],s}$ and $B^{[M+1],s} \to X^{-1}B^{[M+1],s}$, where $X$ is a nonsingular matrix, we obtain the same state. Analogously, we can substitute $B^{[M],s} \to YB^{[M],s} := V^{[M]}$ and $B^{[M-1],s} \to B^{[M-1],s}Y^{-1}$. We choose $X$ in the clockwise cycles to impose (3) and $Y$ in the counterclockwise ones to impose

$$\sum_{s=1}^{d} (V^{[M],s})^\dagger (V^{[M],s}) = \mathbf{1}. \tag{13}$$

Thus, at the point of determining the operator $P_M$,

$$|\Psi\rangle = Q_1 \otimes \cdots Q_{M-1} \otimes P_M \otimes \tilde{Q}_{M+1} \cdots \otimes \tilde{Q}_N |\phi\rangle^{\otimes N}, \tag{14}$$

where $Q_k$ and $\tilde{Q}_k$ are defined as in (7) but with $U$ and $V$ instead of $B$, respectively. Thus, the operators $X$ and $Y$ are all of them moved over, such that they are now included in those corresponding to $P_M$. It can be easily shown that these conditions on the operator $U$ ($V$) are equivalent to imposing that $E_{\mathbf{1}}$ has the maximally entangled state $|\phi\rangle$ as right (left) eigenvector with eigenvalue 1. This is immediately reflected in the fact that the matrix $N_M$ is better behaved, which makes the problem numerically stable.

Let us now illustrate how the procedure works with simplest nearest-neighbor Hamiltonian $\sigma_z^{[k]}\sigma_z^{[k+1]}$, namely, the Ising model. Let us assume that we are running the optimization of the operators clockwise and that we want to determine $P_M$. So far, in previous steps, apart from the matrices $U$ and $V$, we have stored (i) for each $k < M$, the following four operators:

$$r_k := E_{\mathbf{1}}^{[1]} E_{\mathbf{1}}^{[2]} \cdots E_{\mathbf{1}}^{[k-2]} E_{\mathbf{1}}^{[k-1]}, \tag{15a}$$

$$s_k := E_{\sigma_z}^{[1]} E_{\mathbf{1}}^{[2]} \cdots E_{\mathbf{1}}^{[k-2]} E_{\mathbf{1}}^{[k-1]}, \tag{15b}$$

$$t_k := E_{\mathbf{1}}^{[1]} E_{\mathbf{1}}^{[2]} \cdots E_{\mathbf{1}}^{[k-2]} E_{\sigma_z}^{[k-1]}, \tag{15c}$$

$$h_k := \sum_{n=1}^{k-2} E_{\mathbf{1}}^{[1]} E_{\mathbf{1}}^{[2]} \cdots E_{\sigma_z}^{[n]} E_{\sigma_z}^{[n+1]} \cdots E_{\mathbf{1}}^{[k-2]} E_{\mathbf{1}}^{[k-1]}, \tag{15d}$$

and (ii) for each $k > M$ other four similar operators which contain products from $E^{[k]}$ to $E^{[N]}$. With them, one can build $H_M$ and $N_0$ by few matrix multiplications and thus determine $P_M$ by solving (12). From it, $Q_M$ is determined. Then, we construct $r_{M+1}$, $s_{M+1}$, $t_{M+1}$, and $h_{M+1}$ starting from $r_M$, $s_M$, $t_M$, and $h_M$. We continue in the same vein, finding four matrices at each step, and storing them, until we reach $N$. Then we start moving counterclockwise and start constructing the corresponding four matrices at each step. Notice that in order to construct the matrices $H_M$ and $N_0$ we have to use the stored matrices (15) which were determined when we were moving clockwise. Thus, with this procedure we have to store of the order of $4N$ matrices of dimension $D^2$. Using sparse matrix multiplications to solve the eigenvalue problem [17] and to update the matrices $r_M$, $s_M$, $t_M$, $h_M$, the number of operations per step scales as $D^5$ and is independent of $N$. At the end, when we have reached the fixed point, we can determine the expectation value of any operator by using (8)

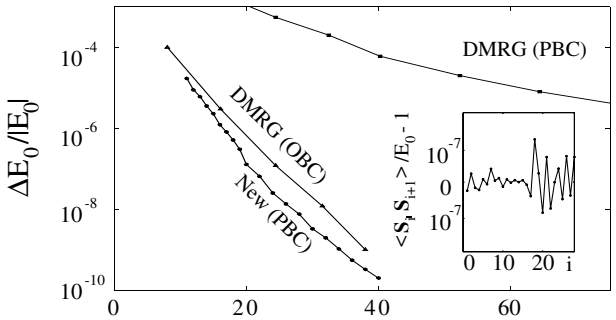


FIG. 3. Left: comparison between DMRG (squares) [2] and the new method (circles) for PBC, and $N = 28$. For reference the DMRG results [2] for the Heisenberg chain with OBC (triangles) are also shown. Inset: variation of the local bond strength from the average along the chain, calculated with the new method and $D = 40$.

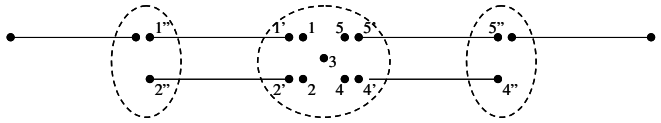


FIG. 4. Converting a general 5-qubit state into a MPS via teleportation (see the text).

and determining the required matrices using (9). Note that after convergence with $D$ fixed, $D$ can be increased by adding zeros to all projectors plus some additional noise term.

We have applied the above method to the spin 1/2 Heisenberg chain. We have plotted in Fig. 3 the energies obtained as a function of $D$ and compared them with those obtained by the standard DMRG method with OBC and PBC. From the figure it is clear that the accuracies we obtain are comparable with those obtained with DMRG for problems with OBC but much better than for PBC. We have determined the errors by comparing with the exact results [18]. In the inset of Fig. 3 we have plotted the local bond strength $\langle \mathbf{S}^{[k]}\mathbf{S}^{[k+1]}\rangle$ as a function of $k$. The result is practically independent of the position $k$, as opposed to what occurs with OBC.

Finally we show that the picture introduced here may be valuable to understand the properties of states $\Psi$ in terms of the language and tools developed in the field of QIT. First, one can easily see that the entropy of the block formed by systems $(k_0, k_0+1, \ldots, k_1)$ is bounded by $2\log_2(D)$, as this block is connected to the rest only via $a_{k_0}$ and $b_{k_1+1}$, and thus the rank of the reduced density operator for the block is bounded by the product of the dimensions of the corresponding Hilbert spaces. Second, the concept of teleportation allows us to show that any state can be written in the form (6) (MPS [4,6]) if we choose $D = d^{\lfloor N/2\rfloor}$. As an example, consider a general state $|\psi\rangle$ of five qubits and a MPS with bonds consisting of one or two maximally entangled states (Fig. 4). Assume the third particle consists of nine virtual particles [19], of which five are in the state $|\psi\rangle$ while the other ones are part of maximally entangled states with the virtual particles of the neighbors. Virtual measurements of the form $M = \langle 00| + \langle 11|$ on the pairs of qubits $(1, 1'; 2, 2'; 4, 4'; 5, 5')$ effectively teleport the virtual qubits 1, 2, 4, 5onto $1'', 2'', 4'', 5''$ of the neighboring particles. There a similar measurement can be done to teleport the qubits $1'', 5''$ to their final destination, hence creating the actual state $|\psi\rangle$ on the five remaining physical qubits. The actual projectors $P$ defining the MPS can immediately be read off from this picture, hence yielding a constructive way of representing any state as a MPS. Finally, we note that the usefulness of the MPS relies in the fact that, for translational invariant problems, the set of possible nearest-neighbor reduced density operators of MPS with small $D$ already gives a very good approximation to the convex set of all possible ones arising from general translational invariant states.

In summary, we have shown that DMRG can be formulated as a variational method for minimizing the energy over the set of matrix product states. We have given a pictorial view of the DMRG method and identified the reason of its poor performance for problems with PBC. Our picture immediately leads to a modified version of the DMRG method which dramatically improves the results. This is done at the expense of no longer using sparse matrices. We believe that the method may allow us to treat problems in condensed matter systems which so far have been difficult to tackle with the standard DMRG method. In any case, the present work illustrates how the developments made in QIT during the last few years may prove useful in other branches of physics.

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