A simple way to avoid metastable configurations in the density-matrix renormalization-group algorithms

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We use the spin-1 Heisenberg chain with periodic boundary conditions to ilustrate that the systems get stuck in metastable configurations only when the density-matrix renormalization-group algorithm start with small number of states m. We also show that the convergence of the energies have a huge improvement if we start the algorithm with a large number of states m.

Keywords: spin model, DMRG, spin-1

The density-matrix renormalization-group [1, 2] (DMRG) is one of the most appropriate techniques to study static properties of the one-dimensional systems at zero temperature (for a review see, for example, Refs. 3 and 4). It is also possible to calculate dynamic properties [3–7] and work at finite-temperature through the DMRG [8–10]. The main advantage of DMRG, compared with the Lanczos exact diagonalization [11], is its capability to obtain the ground-state properties of *very large* systems in *a well controlled way*. Note that it is also possible to investigate large systems by Monte Carlo methods. However, the Monte Carlo technique is not appropriated to study frustrated/fermionic systems due to the "sign" problem.

Although the DMRG algorithm was developed for one-dimensional systems, it has been used to treat two-dimensional systems [12–17]. The procedure consists in mapping the low-dimensional model on an one-dimensional model with long range interactions. As first point out by Liang and Pang [12], the energies of two-dimensional systems, converge slower than the ones of one-dimensional systems with short range interactions. The number of states needed to keep a fixed accuracy seems to increase exponentially with the width of the system.

A similar effect also appears when we study one-dimensional systems with periodic boundary condition (PBC) [1, 2]. Since the DMRG was developed, it was observed that the ground state energy (as a function of the number of states m kept in the truncation process) converge faster for the system with open boundary condition (OBC) than the one with PBC. Although it is not completely understood, it seems that everytime that an operator that acts in the *left block* is directly connected with an operator that acts in the *right block* (see Fig. 1), the ground state energy convergence is slower. This has been observed for one-dimensional systems as well for the two-dimensional systems.

Another difficulty also appears when the left and right blocks are directly connected. Some times, in the simulations, the system gets stuck in some local minimum of energy (see Fig. 3(a)), even working with large values of m [18, 19]. This is a serious problem. If the energies do not change increasing m, we may think naively that the true ground state energy was reached. But in fact, the energy found is far from the true ground state.

Few years ago [19], White proposed a variation of the density-matrix renormalization-group algorithm with a single center site. This new algorithm has the advantage of (i) decreasing the computation time as well as the memory used, and more important, (ii) to avoid that the system gets stuck in metastable configurations. As discussed by White [19], the main reason that the simulations get stuck in metastable configurations is due to the fact that some important fluctuations between the system and environment are absent. This happens because the environment blocks lost some relevant states in the truncation process [20]. In order to incorporate the missing states for those fluctuations, White suggests that we have to add in the density-matrix ρ small terms like [19]

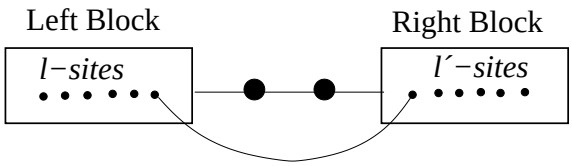

FIG. 1: A schematic representation of a system with size $L = l + l' + 2$ sites for the standard DMRG method with two center sites. The left (right) block contain $l(l')$sites. The solid lines represent the interactions.

$$\Delta\rho = a\sum_i A_i^+ \rho A_i + h.c. \qquad (1)$$

for each operator A_i that is connected directly with the environment. The constant a is a small free parameter, the magnitude of a is chosen to vary from $a \sim 10^{-2} - 10^{-4}$ [19].

In fact, using the one-dimensional spin-1 Heisenberg model with PBC as a test, White found that single-site DMRG method with the correction to the density-matrix, gets lower energy than the standard two-sites DMRG method [19].

It is very important to note that, in the standard DMRG algorithms, White shown [1, 2] that the new blocks built in the renormalization process are *better represented* by the following transformation: $H_{sis}^{new} = OH_{sis}^{old}O^\dagger$. Where the rows of O are the m eigenvectors of the density-matrix ρ that are associated with the largest eigenvalues. So, if we add in the density matrix the term $\Delta\rho$, the matrix O will not have anymore all the *optimal states*. Actually, it is quite surprising that the DMRG with the correction in the density matrix gets a lower energy.

In this article, we present a simple procedure to avoid that the system gets stuck in metastable configurations using the standard DMRG algorithm with two center sites. Note that

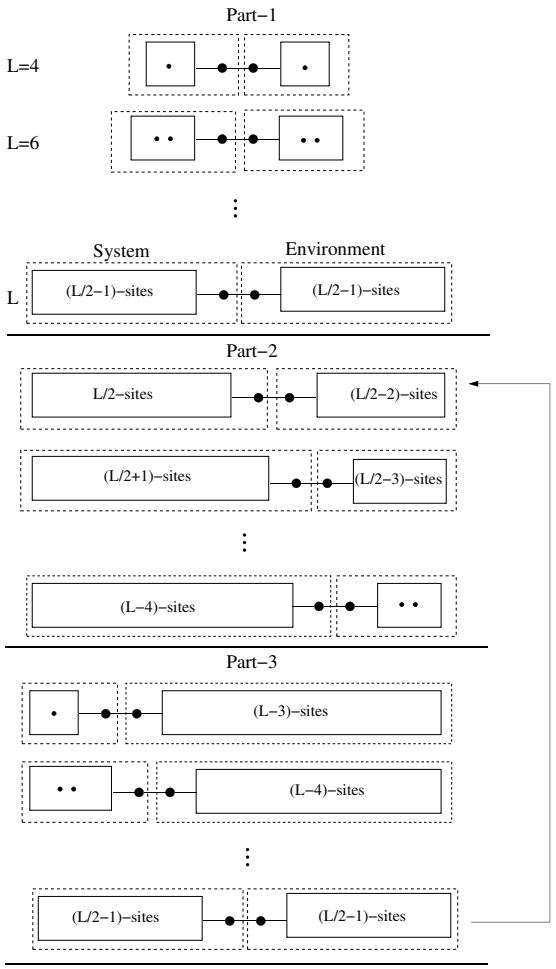

FIG. 2: A schematic representation of the DMRG algorithm with two center sites for a finite system with size L. The right and left blocks are represented by solid line rectangles, while the system and environment by the dotted line rectangles. In the first part of the algorithm, we add two new center sites at each interaction until reach the desized size.

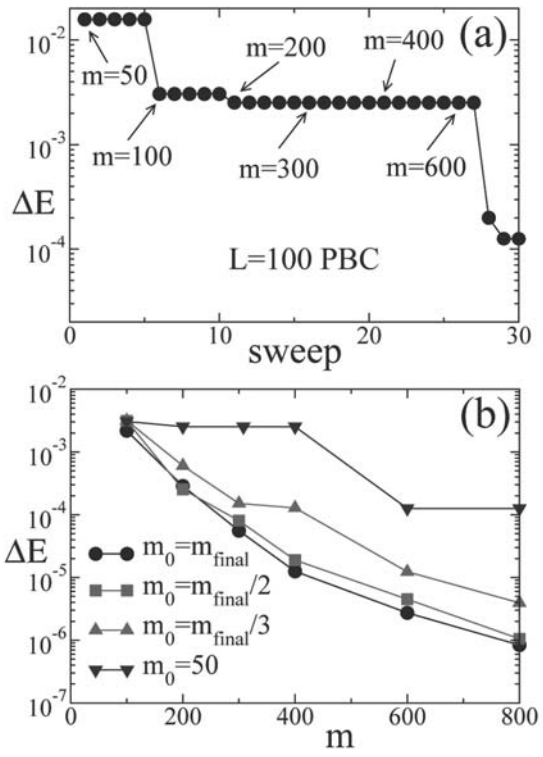

FIG. 3: The error in the energy ΔE for the one-dimensional spin-1 Heisenberg model with size $L = 100$ and PBC. (a) ΔE as function of the sweeps. The arrows indicate the value of m in that sweep. (b) ΔE vs. m for some values of m_0 (see text).

the DMRG method with two center sites demand more CPU time and memory. But as we see, it has the advantage of obtaining lower energy than the single-site DMRG method with correction in the density-matrix. Besides that, it is free of non-controlled parameters, and more important, the transformation matrix O is built considering only the optimal states.

As a benchmark test, in this work, we consider the one-dimensional spin-1 Heisenberg model

$$H = J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1},$$

where the coupling J was set to unity to fix the energy scale. We investigated the model above with DMRG technique with OBC and PBC. We use the finite-size algorithm for sizes up to $L = 100$ and keeping up to $m = 4000$ states per block in the final sweep. The discarded weight, $1 - P_m$, was typically about $10^{-6} - 10^{-13}$ in the final sweep (see Fig. 4(b)).

Before presenting the results, let us first briefly describe the DMRG algorithm for finite-size systems, which is crucial in our discussion. We can divide the finite-size DMRG algorithm in three parts, as illustrated in Fig. 2. In the first part, we use the standard infinite system density-matrix algorithm until reach the desired lattice size. This first part of the algorithm is used only once to obtain the environment blocks that will be used in the second part of the algorithm. As we see later, the fact that the system gets stuck in some metastable configurations is related with this part of the algorithm. Once we reach the desired size we start to sweep, as illustrated in Fig. 2. Note that in the third part of the algorithm the environment blocks are those blocks built in the second part of the algorithm. Usually, all the measurements are done in last iteration of the third part of the algorithm (the symmetric configuration).

In general, if we want the ground state energy $E_0(L,m)$ of a system with lattice size L and $m = m_{final}$ states per block, we start the first part of the algorithm with $m_0 < m_{final}$ (typically is used $m_0 \sim 50 - 100$). We increase at each sweep the states kept in the truncation process until we reach the final value m_{final}.

In Fig. 3(a), we present the error in the energy, defined as $\Delta E = E_0(L,4000) - E_0(L,m)$ [21], as function of the number of sweeps for the one-dimensional spin-1 Heisenberg model with size $L = 100$ under PBC. We have done for each value of m five sweeps [22]. As we can see in this figure, for the sweeps with m between 100-400, there is no improvement in the convergence [23]. This is a serious problem. For instance, if we had defined the error in the energy as $\Delta E = E_0(L,400) - E_0(L,m)$, we could be thought that we had reached the ground states energy with high accuracy. But

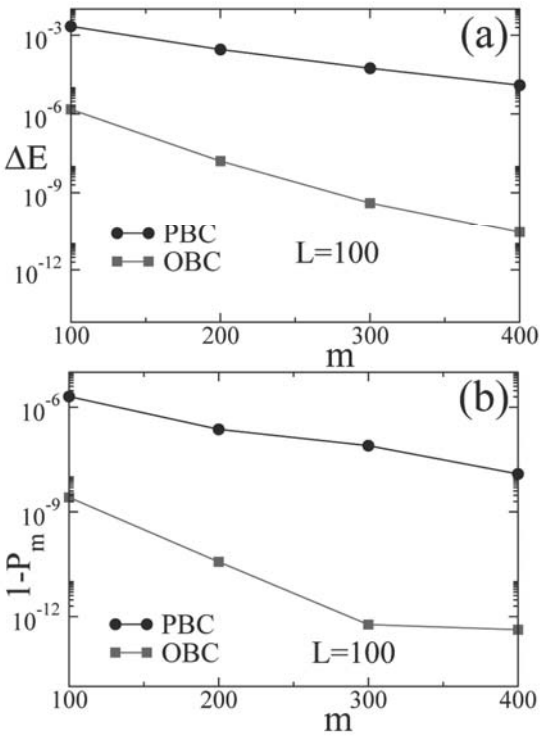

FIG. 4: (a) ΔE vs. m for the one-dimensional spin-1 Heisenberg model with lattice size $L = 100$ under PBC (filled cicles) and OBC (filled squares). (b) The truncation error $1 - P_m$ vs. m.

in fact, the energy is still far from the true ground state. In order to avoid this serious problem, as we mentioned before, White proposed to add in the density-matrix the small term $\Delta\rho$ defined in Eq. 1. By using this new approach, White was able to improve the convergence up to two orders of magnitude [19].

In this article, we show another simple procedure to avoid that the system to get stuck in metastable configurations. Our main result is presented in Fig. 3(b). In this figure, we show the error in the energy as function of m for different values of m_0. We clearly see that if we start the first part of the DMRG algorithm with a small value of m_0 (filled triangles down), the convergence is much worse than the one that started with $m_0 = m_{final}$ (filled circles). From this observation, we conclude that a simple way to gain a huge improvement in the convergence is to start the algorithm with large values of m_0. And more important, if we start with $m_0 = m_{final}$ the system *does not get stuck* in metastable configurations. We emphasize that the system gets stuck in metastable configurations, as we observe in Fig. 3(b), due to the fact that some important states were missed in the truncation process *in the first part* of the algorithm.

It is also important to observe that the difference of the energies obtained with $m_0 = m_{final}$ and $m_0 = m_{final}/2$ is very small. In particular for $m = m_{final} = 800$ this difference is $2\text{x}10^{-7}$. So, we can save CPU time starting the DMRG algorithm with $m_0 = m_{final}/2$, and even so, we still obtain results with a very high accuracy.

In Table 1, we show some energies obtained using the standard DMRG algorithm with two center sites (standard two-sites) and $m_0 = m_{final}/2$ for two values of m_{final}. We also present the energies (taken from Ref. 19) obtained with the single-site DMRG method with the correction to the density-matrix (corrected single site). Note that the energies obtained by the standard DMRG with two center sites are slightly lower than the ones acquired by White in Ref. 19.

m_{final}	340	4000
standard two-sites	-140.148 370	-140.148 403 904 64
corrected single-site	-140.148 279	-140.148 403 903 92

TABLE I: The ground state energies of the spin-1 Heisenberg chain with lattice size $L = 100$ and PBC for two values of m_{final}. The energies for the single-site DMRG method with the correction was taken from Ref. 19. We use $m_0 = m_{final}/2$ in the standard DMRG with two center sites.

Finally, we point out that indeed the convergences of the energies have a significant improvement if we use $m_0 = m_{final}$ (or $m_0 = m_{final}/2$) instead of $m_0 = 50$ for the model under PBC. However, the energies obtained with PBC still converge much slower than the ones with OBC, as we can observed in Fig. 4(a). As we can see in this figure, if we use OBC and $m = 400$ we basically obtain the ground state energy with the precision of the computer. Similar behavior is also found in the truncation error $1 - P_m$, as presented in Fig. 4(b).

In conclusion, in this work we study the one-dimensional spin-1 Heisenberg model with periodic/free boundary conditions. We shown that the standard DMRG algorithm with two center sites gets stuck in metastable configurations only when few states are selected in the grow process (the first part of the algorithm, where is used the infinity size algorithm). A simple way to obtain a huge improvement in the convergence is to start the algorithm with the same numbers of states of the final sweep. Even using this procceding, we observe that the convergence of the ground state energy for the system under periodic boundary condition is slower than the one with open boundary condition. Finally, our results suggest that it may be possible also that a similar improvement can be reached with this approach if it is consider the single-site DMRG algorithm without the correction to the density-matrix.

Acknowledgments

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[20] Note that some trials, such as adding extra random states, were tested. However did not work very well (see Ref. 19).
[21] We use $m_0 = 2000$, in the first part of the algorithm, to obtain the energy $E(L, 4000)$.
[22] For $m > 2000$ we did two sweeps.
[23] Similar results were obtained by White in Ref. 19, although for $m = 600$ our error in the energy seems to be one order of the magnitude smaller than the one presented by White.