A simple detailed example of the Density Matrix Renormalization Group procedure applied to Heisenberg model

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Abstract

The Density Matrix Renormalization Group (DMRG) method is applied to a simple Heisenberg model to compute its low--lying eigensystem. The computational aspects of the procedure are given in details, where some system symmetries are considered. This permits us to reduce the computational effort provided in diagonalizing matrices. It shows also the relevance of symmetry concept in dealing with quantum systems.

Keywords: Density matrix renormalization group, Heisenberg model.

Resumen

El Grupo de Renormalización de la Matriz de Grupo (DMRG) es un método que se aplica a un simple modelo de Heisenberg para calcular its low--lying eigensystem. Los aspectos computacionales del procedimiento se dan en detalles, donde algunas simetrías de sistemas son consideradas. Esto nos permite reducir el esfuerzo computacional proporcionado en la diagonalización de matrices. Esto muestra también la relevancia del concepto de simetría en el trato con los sistemas cuánticos.

Palabras clave: Densidad de la matriz de grupo de renormalización, modelo de Heisenberg.

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I. INTRODUCTION

The present paper is to give a detailed example of the application of a numerical method (the Density Matrix renormalization Group, DMRG) to compute low lying eigenstates of a quantum system (the one dimensional Heisenberg model).

Before that, the reader needs to be informed about the essential features of the applied numerical method as well as the quantum system to be used. In fact, historically, the DMRG procedure, developed by S. R. White in 1992 [1] (see also: [2], [3] and [4]), has appeared as a remedy to the Wilson's renormalization approach failure [5] to reproduce accurate results for many strongly correlated systems. In fact, the criterion of keeping eigenstates with lowest energies introduced by Wilson was behind this failure. In order to fix the situation, S. White has considered that a system (block) must be connected to an other block (environment) to form a superblock, and therefore each part contributes to the ground state of the superblock through its own states. As a part of solution, he introduced a new criterion for selecting the eigenstates to be kept in the renormalization procedure; it consists in keeping the states of a system that contribute the more in the ground state of the whole system. To do this, he had recourse to statistical mechanics and especially to the concept of density matrix, which tells us how much a part of a system is "involved" in the ground state of a bigger system and which states contribute the more.

Technically, the basic idea of DMRG algorithm consists in increasing the size of the system by adding two sites at a time while the corresponding Hilbert space is kept constant. In the warm--up phase, the Hamiltonian operator and connection operators of each block in the system are renormalized and then stored to be used later. This is followed by a sweeping procedure which iterates the process on the full system until convergence is reached. The development of the DMRG method has opened a possibility to a variety of quantum systems (Spin systems, Hubbard model, Kondo insulator, etc.) to be solved numerically with extremely high accuracy, with system size much larger than those solved by exact diagonalization.

In the other hand, the interest in one-dimensional spin-S Heisenberg Hamiltonians is renewed in recent years by theoretical and experimental motivations. Thus, in the seventies, several families of magnetic compounds with linear chain structures were discovered and their properties were analyzed from models developped earlier [6]. In fact, wide number of molecular clusters containing relatively a small number of magnetic ions can be synthesized ([7], [8]), and the essential of their low energy magnetic

properties is captured by such a model. In other hand, there are several material systems (*e.g* Y_2BaNiO_5) which are well represented by the one-dimensional Heisenberg model [9]. Also, spin ladders systems containing $CuCl_3$ and $CuBr_3$ were found to be ideal models of a ferromagnetic and antiferromagnetic alternating Heisenberg chains with $S=\frac{1}{2}$ [10]. The advent of high temperature superconductors has also triggered the interest ([11], [12]).

In the present paper we will use the fact that the ground state eigenfunction belongs to the subspace corresponding to $S_T^z=0$, S_T^z being the total z-component spin of the system. This will reduce considerably the computational effort in diagonalizing matrices but demands, in other hand, more dexterity in dealing with a such case.

II. GROUND STATE EIGENFUNCTION

One can write the ground state of the the superblock (system+environment), as it is shown in Fig. 1, in a basis that is a tensor product of the basis vectors of the system (one of the enlarged blocks) and the environment (the other enlarged block)

$$|\Psi_0\rangle = \sum_{i=1}^{m_l\times D}\sum_{j=1}^{m_r\times D} a_{ij}\,|b_i^l\rangle_e \otimes |b_j^r\rangle_e . \tag{1}$$

Where $|b_i^l\rangle_e$ and $|b_j^r\rangle_e$ are the basis for left (system) and right (environment) enlarged blocks in Hilbert space of dimensions $m_l\times D$ and $m_r\times D$, respectively. Each enlarged block basis is a tensor product of the block $m_{l,r}-$ dimensional basis and the $D-$dimensional basis of the added site.

Thus

$$|b_i^l\rangle_e = |b_p^l\rangle\otimes|d_q\rangle$$
$$|b_k^r\rangle_e = |d_t\rangle\otimes|b_s^r\rangle .$$

Where $|b_i^l\rangle$ and $|b_k^r\rangle$ are the bases of the left and right blocks, respectively, while $|d_i\rangle$ represent the basis of a single site within a *D*--dimensional space. In the case of the Heisenberg model, there are two basis vectors on each site: $|d_1\rangle = |\uparrow\rangle$, and $|d_2\rangle = |\downarrow\rangle$, so that *D* is equal to 2. Note that in further steps, $m_{l,r}-$ will represent the number of states kept for each block. The left and right blocks are enlarged by a site at a time. We assume that the right block can be obtained from left block through reflection symmetry, which is not the case when we deal, for example, with a disordered system; where reflection symmetry is broken. It is necessary to number the enlarged block states as follows (this is not the only way): $k=(i-1)D+j$.

The density matrix ρ is given by

$$\rho_{ii'} = \sum_{j=1}^{D\times m_r} a_{ij}a_{i'j}^{*}. \tag{2}$$

After the density matrix ρ is built and diagonalized, m_l eigenvectors corresponding to the highest eigenvalues of the latter are chosen to build truncature operator *O*, needed to renormalize the operators of enlarged blocks (*i.e*. keep the dimension of the Hilbert space constant while the number of sites is increasing). This is the very basic idea of renormalization algorithm. The operator *O* is a $m_l\times(m_l\times D)$ matrix, whose rows are the m_l eigenvectors corresponding to the highest eigenvalues of ρ. Open boundary conditions are applied to the superblock.

In order to estimate the accuracy of the truncation procedure, it is useful to compute the following quantity

$$P = 1-\sum_{\alpha=1}^{m}\omega_\alpha , \tag{3}$$

where ω_α are the *m* eigenvalues of the density matrix ($m=m_l$ for left block) whose eigenvectors are to be kept to form the "truncation" operators.

FIGURE 1. The superblock configuration: two blocks and two sites to add at each step of the DMRG procedure.

III. PROCEDURE

In this section we present a detailed example of the application of the DMRG method to Heisenberg model. In fact, the Hamiltonian of a one-dimensional isotropic Heisenberg spin-- $\frac{1}{2}$ chain with *N* spin is

$$H = J\sum_i^N S_iS_{i+1} = J\sum_i^N[\frac{1}{2}(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+) + S_i^zS_{i+1}^z], \tag{4}$$

where $S_i=(S_i^x,S_i^y,S_i^z)$ is the quantum mechanical operator spin at site *i* with $S_i^\pm = S_i^x \pm iS_i^y$. *J* is taken to be unity and only interactions between nearest neighbors sites are to be considered. In matrix form, spin matrices at single sites are given by

$$S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

The left enlarged block of a heisenberg chain writes, in the basis $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, as

$$H_l^{(1)}(4,2) = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (6)$$

Note that digit 4 in Hamiltonian above stands for number of basis vectors, digit 2 is the number of effective sites the Hamiltonian matrix is representing, while the superscript 1 terms the first renormalization step. The right enlarged one has a similar matrix. We need also to construct rightmost/leftmost sites spin matrices, that are used to connect each block to the added site, $S_r^+, S_r^-, S_l^+, S_l^-, S_l^z$ and S_r^z, to be renormalized. For example, S_r^+, S_l^z are the right most spin S^+, and the left most spin S^z, respectively. They write as

$$S_r^+ = I_2 \otimes S^+ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$S_l^z = S^z \otimes I_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

where I_2 is a unit matrix of order 2. Thus, the superblock Hamiltonian writes

$$H_{sup} = H_l^{(1)} \otimes I_2 + I_2 \otimes H_r^{(1)} + \frac{1}{2}(S_r^+ \otimes S_l^- + S_r^- \otimes S_l^+) + S_r^z \otimes S_l^z. \quad (7)$$

There are 16 basis vectors for the superblock Hamiltonian, but there are, in fact, only 6 basis vectors that span the subspace $Sz = 0$. These basis vectors are

$$\begin{pmatrix} |\uparrow\uparrow\downarrow\downarrow\rangle \\ |\uparrow\downarrow\uparrow\downarrow\rangle \\ |\uparrow\downarrow\downarrow\uparrow\rangle \\ |\downarrow\uparrow\uparrow\downarrow\rangle \\ |\downarrow\uparrow\downarrow\uparrow\rangle \\ |\downarrow\downarrow\uparrow\uparrow\rangle \end{pmatrix}.$$

TABLE I. Eigenvalues, eigenvectors and corresponding total Sz of de density matrix for the left enlarged block,

N	eigenvector	eigenvalue	Sz	state
1	(1, 0, 0, 0)	$2.232909936926020 \times 10^{-2}$	1	$\|1\rangle = \|\uparrow\uparrow\rangle$
2	$(0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$	0.933012701892219	0	$\|2\rangle = \frac{1}{\sqrt{2}}(\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle)$
3	$(0, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$	$2.232909936926041 \times 10^{-2}$	0	$\|3\rangle = \frac{1}{\sqrt{2}}(\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle)$
4	(0, 0, 0, 1)	$2.232909936926016 \times 10^{-2}$	-1	$\|4\rangle = \|\downarrow\downarrow\rangle$

and the corresponding Hamiltonian block, in this bsis, is

$$H_{sup}^{Sz=0} = \frac{1}{4}\begin{pmatrix} 1 & 0 & 2 & 0 & 0 & 0 \\ 0 & -1 & 2 & 2 & 0 & 0 \\ 2 & 2 & -3 & 0 & 2 & 0 \\ 0 & 2 & 0 & -3 & 2 & 2 \\ 0 & 0 & 2 & 2 & -1 & 0 \\ 0 & 0 & 0 & 2 & 0 & 1 \end{pmatrix}. \quad (8)$$

The diagonalization of the above matrix gives, among others, the ground state eigenfunction; which enables us to build the density matrix ρ. Note that the Hamiltonian $H_l^{(1)}(4,2)$ and the density matrix ρ have the same block--diagonal structure, *i.e.* they have the same eigenvectors with different eigenvalues.

One picks up two eigenvectors, corresponding to the highest eigenvalues of the density matrix, to build the truncature operators, such that

$$O = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}. \quad (9)$$

Thus, the renormalized Hamiltonian of the left block is given by

$$H_l^{'(1)}(2,2) = OH_l^{(1)}(4,2)O^{\dagger} = \frac{1}{4}\begin{pmatrix} -3 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (10)$$

This 2x2 matrix represents the Hamiltonian of a block of 2 sites with just two basis vectors (it depends on the number of the states kept; in our case 2 states): $|2\rangle$ and $|3\rangle$, both representing a basis vector of total Sz equal to zero; as cited in Table I. All other operators are also renormalized. For example:

$$S_r^{'} + (2,2) = OS_r^{+}O^{\dagger} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}; S_r^{'z}(2,2) = OS_r^{z}O^{\dagger} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. (11)$$

The superblock Hamiltonian is then constructed in the new basis. The Fig. 2 displays the effective superblock.

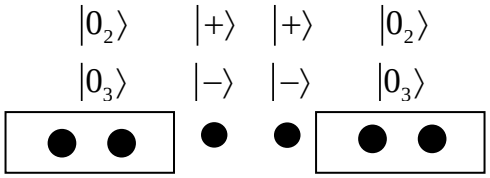

FIGURE 2. Basis vectors for both right and left blocks and the two added sites.

Number 0 stands for total Sz of each state with a subscript referring to the number of state in Table I, whereas + and - stand for spin up and spin down, respectively. There are effectively 16 basis vectors

$$\begin{pmatrix} |0_2 \uparrow\uparrow 0_2\rangle \\ |0_2 \uparrow\uparrow 0_3\rangle \\ |0_2 \uparrow\downarrow 0_2\rangle \\ \vdots \\ |0_3 \downarrow\uparrow 0_3\rangle \\ |0_3 \downarrow\downarrow 0_2\rangle \\ |0_3 \downarrow\downarrow 0_3\rangle \end{pmatrix}.$$

Among these 16 vectors there are only 8 basis vectors which span the subspace $Sz = 0$. These 8 vectors are

$$\begin{pmatrix} |0_2 \uparrow\downarrow 0_2\rangle \\ |0_2 \downarrow\uparrow 0_2\rangle \\ |0_2 \uparrow\downarrow 0_3\rangle \\ |0_2 \downarrow\uparrow 0_3\rangle \\ |0_3 \uparrow\downarrow 0_2\rangle \\ |0_3 \downarrow\uparrow 0_2\rangle \\ |0_3 \uparrow\downarrow 0_3\rangle \\ |0_3 \downarrow\uparrow 0_3\rangle \end{pmatrix}.$$

The superblock Hamiltonian is then rewritten in the reduced subspace (8 basis vectors) to get the ground state. The density matrix is then built again and the truncature operators constructed. Now we need to construct the operators of the left block and see what are the new basis vectors. Thus

$$H_l^{(2)}(4,3) = H_l^{'(1)}(2,2) \otimes I_2 + \frac{1}{2}(S_l^{'+}(2,2) \otimes S_d^{-} + S_l^{'-}(2,2) \otimes S_d^{+}) + S_r^{'z}(2,2) \otimes S_d^{z}. \qquad (12)$$

This matrix is written in the basis $(|0_2 \uparrow\rangle, |0_2 \downarrow\rangle, |0_3 \uparrow\rangle, |0_3 \downarrow\rangle)$

$$H_l^{(2)}(4,3) = \frac{1}{4}\begin{pmatrix} -3 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\left[\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] + \frac{1}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (13)$$

where the spin operators matrices are the same as in the first iteration. This is not true in general, but in our case it is for we have decided to keep only two states, which makes the spin operator of the rightmost site of the left block writes as

$$S_r^{+} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \qquad (14)$$

If, for example, we decide to keep three states then,

$$S_r^{+} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \qquad (15)$$

Let's remind that the density matrix for the left block and the left block Hamiltonian share the same structure, so that

the eigenvectors of the density matrix are a linear combination of the 4 basis vectors stated for the left block.

Again we have to pick up the first two highest eigenvalues of the density matrix in order to use their corresponding eigenvectors in building the truncature operators.

For this second iteration, we have two same highest eigenvalues: E_g=0.499898832190182 with eigenvectors (0.9921, 0, -0.1257, 0) and (0, -0.9921, 0, -0.1257), so that the truncature operator writes

$$O = \begin{pmatrix} 0.9921 & 0.000 & -0.1257 & 0.000 \\ 0.000 & -0.9921 & 0.000 & -0.1257 \end{pmatrix}. \qquad (16)$$

All this means that we have made a basis change to a new two--vectors basis

$$|1\rangle = 0.9921\,|0_2\uparrow\rangle - 0.1257\,|0_3\uparrow\rangle, \qquad (17)$$

and

$$|2\rangle = -0.9921\,|0_2\downarrow\rangle - 0.1257\,|0_3\downarrow\rangle. \qquad (18)$$

For the first state $|1\rangle$ the total Sz is equal to $\frac{1}{2}$, while it is equal to $-\frac{1}{2}$ for the second state $|2\rangle$.

At this stage, the two values of Sz are passing through this basis change, and the figure of the effective superblock looks like this

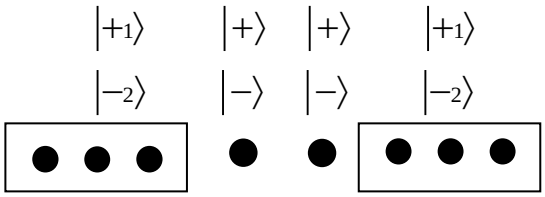

FIGURE 3. Basis vectors for both right and left blocks and the two added sites.

The subscripts 1 and 2 refer to the states kept for the renormalization, so that $|+_1\rangle = |1\rangle$ and $|+_2\rangle = |2\rangle$, whereas + and - refer to the total Sz for each state.

As the truncature operator is built, all block operators are obtained and then the superblock is built in a basis with 16 vectors

$$\begin{pmatrix} |+_1\uparrow\uparrow+_1\rangle \\ |+_1\uparrow\uparrow-_2\rangle \\ |+_1\uparrow\downarrow+_1\rangle \\ \vdots \\ |-_2\downarrow\uparrow-_2\rangle \\ |-_2\downarrow\downarrow+_1\rangle \\ |-_2\downarrow\downarrow-_2\rangle \end{pmatrix}.$$

Among these 16 vectors there are only 6 basis vectors which span the subspace $Sz = 0$. These 6 vectors are

$$\begin{pmatrix} |+_1\uparrow\downarrow-_2\rangle \\ |+_1\downarrow\uparrow-_2\rangle \\ |+_1\downarrow\downarrow+_1\rangle \\ |-_2\uparrow\uparrow-_2\rangle \\ |-_2\uparrow\downarrow+_1\rangle \\ |-_2\downarrow\uparrow+_1\rangle \end{pmatrix}.$$

All the above steps, called the warm--up phase, are repeated until a desired size is reached. All truncature operators are stored to be used later.

Note that the results out of the warm--up phase, also named the *infinite size* method, are not so accurate, and, consequently, S. White [1] had suggested a number of sweeping cycles to be achieved in order to improve the accuracy of results. In fact, once the warm--up phase is achieved a sweep cycle begins, when the left and right blocks are representing the same number of effective sites. Therefore, the left block is enlarged while the right block retrieves, until it will contain only one site. Then the configuration is reversed: the right block becomes the left block while the left block becomes the right one. Thus, the renormalization steps restart following the procedure explained above. For more accuracy, the eigenvalues and eigenvectors are taken when the configuration of the superblock is symmetric. Technical aspects of the sweeping phase, named also *finite size* method, are abundantly explained in DMRG literature; see for example [1, 2, 3].

IV. CONCLUSIONS

In this paper, we have presented a detailed example of DMRG procedure applied to antiferromagnetic Heisenberg model. It permits to compute low states energies of a spin-$\frac{1}{2}$ chain. This example could be an introductory application of the DMRG method to simple systems. It helps to understand more or less the spirit of the method, and then to

move to a higher level where the number of states kept is very large.

In other hand, we have shown that if we consider system symmetries, this will reduce considerably the computational effort, especially if we are interested to just ground state and low-lying states properties. Thus, we have used the fact that the ground state belongs to the subspace of $S_T^z = 0$ to limit the diagonalization to only matrices whose total spin-z of the basis vectors is equal to zero. Therefore, if we are concerned by the excited states, we have to enquire about the subspace those excited states are belonging to.

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