# Density matrix renormalization group

Yu-An Chen, Hung-I Yang*†
*MIT Department of Physics*
(Dated: May 18, 2014)

We give an introduction to Numerical Renormalization Group (NRG) and point out the reason it fails. We then discuss the procedure of the more sophisticated Density Matrix Renormalization Group (DMRG) and the advantages it provides. As an example, we apply DMRG to spin-$\frac{1}{2}$ Heisenberg model, and show that even with very low computational power, DMRG can give reasonable results of the ground state energy.

## 1. INTRODUCTION

Exactly solving an interacting quantum system with many degree of freedom is extremely hard. For example, 1-D chain of spin-$\frac{1}{2}$ system with the nearest neighbor interaction:

$$H = \sum_{i=1}^{L-1} S_i \cdot S_{i+1} \tag{1}$$

Its Hilbert space has dimension $2^L$, where $N$ is typically of order $10^{23}$ for thermodynamics limit. Diagnalizing the whole Hamiltonian is impossible.

The density matrix renormalization group (DMRG) is invented by Steve White in 1992 [1]. It is a numerical variational technique for the simulation of 1-dimensional strongly correlated quantum lattice systems [2]. It is able to obtain the low energy physics of quantum many-body systems with high accuracy. The key idea of this method is that we only focus on a small number of states in the huge Hilbert space.

## 2. THEORY

### 2.1. Numerical Renormalization Group (NRG)

Renormalization group is a technique to deal with the problem by increasing the length of the system iteratively. In the algorithm, we keep track of only certain number of states to keep the size of the Hilbert space manageable. The most important part of this algorithm is *decimation procedure*, the way we choose the most relevant states for our problem. If we are interested in ground state, it may be intuitive to choose the $D$ states with the least energy (often $D$ is a few hundred). For example, once we have $D$ basis states for a system with size $l$, we double the size. The new system contains block A and block B, each of them has size $l$, as shown in Fig. 1. Then, for any state in combined system AB, we can express it as:

$$|\psi\rangle = \sum_{i,j}^{D} \Psi_{ij} |i\rangle_A |j\rangle_B \tag{2}$$

Now, the dimension of Hamiltonian $H_{AB}$ is $D^2 \times D^2$ in basis $\{|\psi\rangle\}$. We diagonalize the Hamiltonian $H_{AB}$ and choose the only $D$ states with the least energy as a basis of the system AB. We can continue this procedure to double the size iteratively.

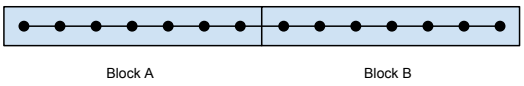


FIG. 1: Basis of states is $\{|i\rangle_A\}$ in block A and $\{|j\rangle_B\}$ in block B, where $1 \le i, j \le D$.

If we do this procedure $n$ times, the size of the system becomes $2^n$. With a small number of steps, we can get to $l \to \infty$ limit quite easily. This method seems efficient and easy to do, but it is actually a terribly uncontrolled technique. A simple example is solving the ground state energy of 1-dimensional tight-binding model:

$$H = -t \sum_i (|i\rangle\langle i+1| + |i+1\rangle\langle i|) \tag{3}$$

This model can be solved exactly by doing a Fourier transform ($H$ is diagonal in $k$-space). On the other hand, the NRG procedure does not give the correct results. The reason is that if we only focus on the lowest energy, we lost information about the boundary effects. For example, the ground state for particles in a quantum well with length $2L$ cannot be well approximated by linear combination of low energy eigenstates of two quantum wells with length $L$ each. NRG is not enough and we need a more clever way to choose $D$ relevant states.

*Yu-An Chen wrote the introduction, theory, and procedure of DMRG. Hung-I Yang wrote the code and produce the results for the Heisenberg model.
†Electronic address: chenyuan@mit.edu, hung_i@mit.edu

### 2.2. Density Matrix Renormalization Group (DMRG)

We will give the sketch of infinite-system DMRG first, and then justify the reason behind the procedure (there is also finite-system DMRG version, but we will not discuss it in this paper). In infinite-system DMRG (Fig. 2), we introduce left and right block A and B, which contains one spin (or site) in the initial step (so the total length is 2). This can be solved exactly by diagonalizing the Hamiltonian. Longer chains are built iteratively by inserting pairs of spins between the blocks such that the chain grows to length 4,6, and so on. At each step, spins are distributed into left and right blocks, so the size of one block grows as 2,3, and so on. This causes the exponential growth of the full block space by $d^l$, where $d$ describe the dimension of spin at one site (e.g. $d = 2$ for spin-$\frac{1}{2}$), and $l$ is the length of the block. Our chain always has a structure of block-site-site-block, $A \bullet \bullet B$.

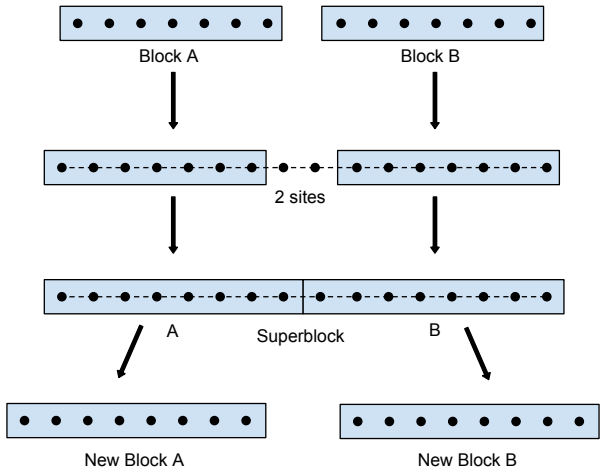


FIG. 2: Basis of states is $\{|i\rangle_A\}$ in block A and $\{|j\rangle_B\}$ in block B, where $1 \leq i, j \leq D$.

Now we give a truncation $D$ as the reduced block space dimension. In practice, $D$ will be order of hundred or thousand. For block A, we have effective $D$-dimension reduce Hilbert space with orthonormal basis $\{|a_l\rangle_A\}$. Similarly, we have $\{|a_l\rangle_B\}$ as an effective $D$-dimension basis for block B. For very small blocks, the basis dimension may be less than $D$. For larger block, the truncation will occur.

In this framework, the question becomes what the ground state of the $A \bullet \bullet B$ system is and how we find the $D$-dimension reduced Hilbert space for new blocks $A\bullet$ and $\bullet B$.

Analogous to Eq. 2, any state of the superblock $A\bullet\bullet B$ can be expressed as:

$$|\psi\rangle = \sum_{a_A\sigma_A\sigma_B a_B} \psi_{a_A\sigma_A\sigma_B a_B}|a\rangle_A|\sigma\rangle_A|\sigma\rangle_B|a\rangle_B \quad (4)$$

$$\equiv \sum_{i_A, j_B} \psi_{i_A j_B}|i\rangle_A|j\rangle_B \quad (5)$$

where $\{|\sigma\rangle_A\}$ and $\{|\sigma\rangle_B\}$ are the the basis states with dimension $d$ of the site next to A and B, respectively. $\{|i\rangle_A\}$ and $\{|i\rangle_B\}$ are combined states for the new blocks A and B (each with dimension $Dd$). By numerically diagonalization of $\hat{H}_{A\bullet\bullet B}$ in basis $|\psi\rangle$, we can find the ground state $|\psi_0\rangle$ which minimizes the energy

$$E = \langle\psi_0|\hat{H}_{A\bullet\bullet B}|\psi_0\rangle \quad (6)$$

This answers the first question: finding the ground state.

If we take $\{|i\rangle_A\}$ as a basis for block $A\bullet$, the dimension is $Dd$. Since we do not want exponential growth, we choose the $D$ most relevant states for block $A\bullet$ and similarly for $\bullet B$. The procedure is following: we first consider the reduced density operator for $A\bullet$

$$\hat{\rho}_{A\bullet} \equiv \mathrm{Tr}_{\bullet B}|\psi_0\rangle\langle\psi_0| \quad (7)$$

With Eq. 15, we can write it explicitly as

$$(\rho_{A\bullet})_{ii'} = \sum_j \psi_{ij}\psi^*_{i'j} \quad (8)$$

where we omit the subscript 0 for simplicity. The eigenvalues and eigenstates of $\hat{\rho}_{A\bullet}$ can be solved by exact diagonalization. The choice is to choose the $D$ eigenstates with the largest weight (eigenvalues). It makes sense to choose in this way since we are interested in ground state and this procedure gives $D$ states which "contribute" to the ground state the most. There is a more rigorous reason, which is related to minimizing the difference between $|\psi_0\rangle$ and approximated state $|\tilde{\psi}_0\rangle$ with rank $D$, and it will be discussed later.

Now we have found the $D$-dimension reduced Hilbert space for new block A, and we can continue doing the same procedure to get the ground state and reduced Hilbert space for larger size $l$. In this case the length increases by 1 at each step and the procedure is normally done for hundreds of times.

### 2.3. Reason Behind the Decimation Procedure of DMRG

#### *2.3.1. The Minimization Problem*

We have a state $|\psi\rangle$ and we want to approximate it by some $|\tilde{\psi}\rangle$ spanned over state spaces of superblock that have dimension $D$ only. In the words, we want to minimize the 2-norm:

$$|||\psi\rangle - |\tilde{\psi}\rangle||_2^2 \equiv |||\psi'\rangle||_2^2 = \sum_{ij}|\Psi'_{ij}|^2 = ||\Psi'||_F^2 \quad (9)$$

where $|\psi'\rangle = \sum_{ij} \Psi'_{ij}|i\rangle_A|j\rangle_B$ and the 2-norm of the vector equals to Frobenius norm of the matrix $\Psi$ since set $\{|i\rangle\}$ and $\{|j\rangle\}$ are orthonormal.

#### 2.3.2. Singular Value Decomposition (SVD) and Schmidt Decomposition

*Singular value decomposition* is a very useful technique in linear algebra, from which we are able to get a very compact representation of quantum states living in the bipartite parts AB, the *Schmidt decomposition*.

SVD theorem states that for arbitrary (rectangular) matrix $M$ of dimension $N_A \times N_B$, there exists a decomposition

$$M = USV^\dagger \tag{10}$$

where $U$ is of dimension $N_A \times min(N_A, N_B)$ with orthonormal columns, $S$ is of dimension $min(N_A, N_B) \times min(N_A, N_B)$ with non-negative entries $S_{aa} \equiv s_a$ on the diagonal, and $V^\dagger$ is of $min(N_A, N_B) \times N_B$ with orthonormal rows. Without loss of generality, we assume $s_1 \geq s_2 \geq ... \geq s_r > 0$. $\{s_i\}$ are called singular values. Rank of a matrix, $r$, is defined as number of non-zero singular values.

Singular values and vectors have some interesting properties. One of them is in the optimal approximation of $M$ (rank $r$) by a matrix $M'$ (rank $r' < r$) in the Frobenius norm $||M||_F^2$. It is given by

$$M' = US'V^\dagger \quad \text{where} \quad S' = diag(s_1, s_2, ..., s_{r'}, 0, ...) \tag{11}$$

This gives the answer to the minimization problem.

With SVD, we can derive the *Schmidt decomposition* for arbitrary quantum states. For any state,

$$|\psi\rangle = \sum_{i,j} \Psi_{ij}|i\rangle_A|j\rangle_B \tag{12}$$

where $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ are orthonormal bases of A and B with dimension $N_A$ and $N_B$ respectively. We perform SVD for matrix $\Psi_{ij}$ in Eq. 12 and obtain

$$|\psi\rangle = \sum_{ij} \sum_{a=1}^{min(N_A,N_B)} U_{ia} S_{aa} V^*_{ja} |i\rangle_A|j\rangle_B \tag{13}$$

$$= \sum_{a=1}^{min(N_A,N_B)} \left(\sum_i U_{ia}|i\rangle\right) s_a \left(\sum_j V^*_{ja}|j\rangle\right) \tag{14}$$

$$= \sum_{a=1}^{min(N_A,N_B)} s_a|a\rangle_A|a\rangle_B \tag{15}$$

By the orthonormality properties of $U$ and $V^\dagger$, the set $\{|a\rangle_A\}$ and $\{|a\rangle_B\}$ are orthonormal and can be extended to be orthonormal bases for new block A and B. We can restrict the sum only over $r \leq min(N_A, N_B)$ positive singular values and obtain so called *Schmidt decomposition*

$$|\psi\rangle = \sum_{a=1}^{r} s_a|a\rangle_A|a\rangle_B \tag{16}$$

With Schmidt decomposition, we can write down reduced density matrix $\hat{\rho}_A$ for block $A\bullet$ very conveniently:

$$\hat{\rho}_A = \sum_{a=1}^{r} s_a^2 |a\rangle_{A\,A}\langle a| \tag{17}$$

The eigenvalues are the squares of the singular values, $w_a = s_a^2$. The answer of the minimization problem is to pick out the largest $r'$(we called it $D$ in previous section) singular values, and this is the same as approximating $\hat{\rho}_A$ by

$$\hat{\rho}_A = \sum_{a=1}^{r'} s_a^2 |a\rangle_{A\,A}\langle a| \tag{18}$$

In other words, we choose the eigenstates with largest $r'$ eigenvalues as a basis for reduced Hilbert space, and this is exactly what we described in the previous section. The decimation procedure will give the least deviation from the true ground state.

## 3. APPLICATION OF DMRG

### 3.1. Spin-$\frac{1}{2}$ chain: Heisenberg Model

We choose spin-$\frac{1}{2}$ chain as our trial model:

$$H = \sum_{i=1}^{L-1} S_i \cdot S_{i+1} \tag{19}$$

With the magnetic field m, the Hamiltonian can be written as:

$$\hat{H} = -\sum_{j=1}^{l} \sigma_j \sigma_{j+1} - m \sum_{j=1}^{l} \sigma_j \tag{20}$$

We start with $l = 1$ and basis $\{|\uparrow\rangle, |\downarrow\rangle\}$, and run the DMRG algorithm written in mathematica code. With the limited computational power and time, we set D to be 5 and run a few hundred iterations until $l \approx 300-500$.

The spin-$\frac{1}{2}$ Heisenberg model can be solved exactly using the Bethe ansatz, which gives a ground state energy per site $-(\ln(2) - \frac{1}{4}) \approx -0.44$ without any magnetic field [3][4] . In Fig.3 The ground state energy without magnetic field converge to $-0.40 \pm 0.01$ as $l$ increase to a few hundred. With $D$ as small as 5, we are already able to calculate the ground state energy with reasonable accuracy.

We repeat the same procedure with magnetic field $m$ ranging from 0 to 3.0. The result of $m = 1.0$ is shown in

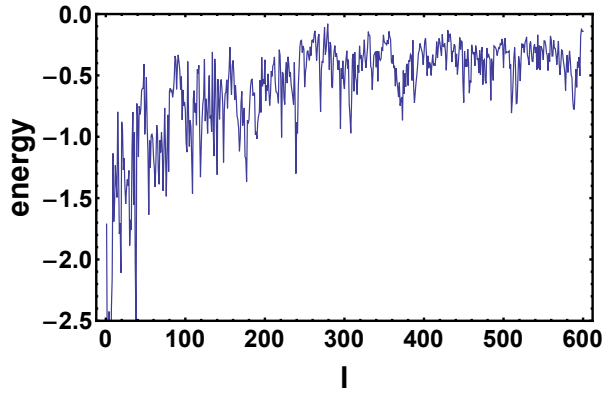


FIG. 3: The ground state energy per site of the spin 1/2 chain at different iteration $l$. With enough iteration, the ground state energy converge to around $-0.40 \pm 0.01$.

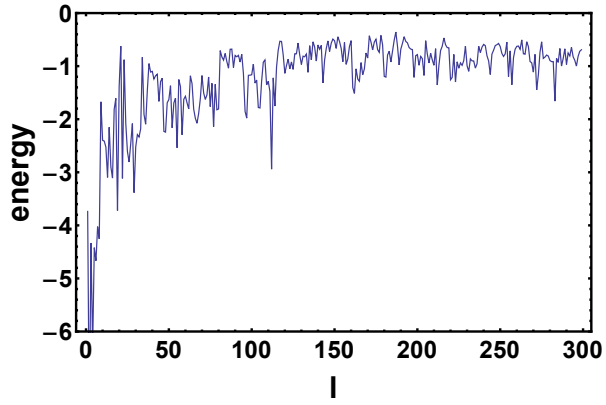


FIG. 4: The ground state energy converge to around -0.84 with a magnetic field $m = 1.0$.

Fig.4 as an example. As the magnetic field increases, we expect the spins to align with the magnetic field, which will lower the ground state energy. This is in fact what we see in our result shown in Fig.5.

### 3.2. DISCUSSION

In our results, the ground state energy per site does not converge very well, which may be due to the small $D = 5$. In practice, $D \sim O(100)$ is usually used to get more accurate results. To use larger $D$, we must improve some details in the algorithm. For example, to obtain ground state from $\hat{H}_{A\bullet\bullet B}$, we need $H_{A\bullet\bullet B}$ in sparse form and use Lanczos or Jacobi-Davidson methods to solve the eigensystem.

Another technical issue we face is that the eigensystem of the reduced density matrix $\hat{\rho}_{A\bullet}$ has only two non-zero eigenvalues. The remaining eigenvalues are zeros with floating point errors, and this continues to be the case for large $l$. When we choose the $D$ basis of largest weights, this gives rise to some ambiguity and may result in choosing the irrelevant eigenstates. Since the algorithm is run iteratively, choosing the wrong basis at one step will affect the result in all the following steps.

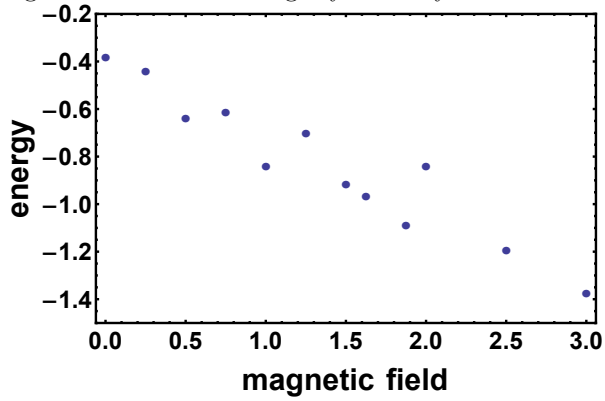


FIG. 5: Ground state energies per site under different magnetic field. As the magnetic field increases, the ground state energy decreases.

## 4. CONCLUSIONS

The renormalization group is a powerful technique to determine low energy properties of one-dimension many body system. From our trial model, we produced the ground state energy without magnetic field, and verified that the ground state energy decreases as the magnetic field is increased. With low computational cost, we have shown that the DMRG method is one of the most efficient algorithm to solve quantum many body system.


[1] S. White. *Density-matrix algorithms for quantum renormalization groups*. Phys. Rev. B 48, 10345 (1993).

[2] U. Schollwoeck. *The density-matrix renormalization group in the age of matrix product states*. Annals of Physics 326, 96 (2011).

[3] M. Karbach and G. Mller. *Introduction to the Bethe ansatz I*. Computers in Physics 11 (1997), 36-43.

[4] M. Karbach, K. Hu, and G. Mller.*Introduction to the Bethe ansatz II*. Computers in Physics 12 (1998), 565-573.