# Density Matrix Renormalization Group

Vishal Kumar Sharma

*A dissertation submitted for the partial fulfillment of*
*BS-MS dual degree in Science*


Department of Physical Sciences
Indian Institute of Science Education and Research
Mohali

April 2019

# Certificate of Examination

This is to certify that the dissertation titled "**Density Matrix Renormalization Group**" submitted by Vishal Kumar Sharma (Reg. No. MS14041) for the partial fulfillment of BS-MS dual degree programme of the institute, has been examined by the thesis committee duly appointed by the institute. The committee finds the work done by the candidate satisfactory by the institute and recommends that the report be accepted.

Dr. Yogesh Singh | Dr. Goutam Sheet | Dr. Sanjeev Kumar (Supervisor)

Dated: April 26, 2019

# Declaration

The work presented in this dissertation has been carried out by me under guidance of Dr. Sanjeev Kumar at the Indian Institute of Science Education and Research Mohali.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bona-fide record of original work done by me and all sources listed within have detailed in the bibliography.

Vishal Kumar Sharma
(Candidate)

Dated: April 26, 2019

In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Sanjeev Kumar
(Supervisor)

# *Acknowledgements*

I am grateful to my thesis adviser Dr. Sanjeev Kumar for the useful discussions and motivation throughout the year. I found him always welcome for any discussion. His diligence and professionalism have always aspired me to become a better researcher and a better person. I thank Dr. Sandeep Goyal for teaching me Quantum mechanics; my understanding of Quantum mechanics is due to him. I thank Dr. Goutam Sheet for the first introduction to the exciting world of condensed matter physics. It will be no exaggeration to say that my interest in the condensed matter rests on whatever he and Dr. Sanjeev has taught me throughout the years. I would also like to thank Ayushi Singhania for useful discussion. I want to thank my friend Sanjay Kapoor for scintillating discussions and help in programming and latex. He has always been a good friend. I have found him as a motivator in darkest of the times at IISER Mohali.

I want to thank my friends Harsh Verma, Dharmendra Kumar, Shivam Mishra, Ramandeep Singh Arora, Rishabh, Raman Chaudhary, Shashank Mishra, Anjani Gupta, Pawan Suthar and Vasudev. It is not possible to express in words whatever I have learned from them; Probably their influence will be reflected in my actions.

I want to thank my relatives for constant support and help. Getting admission in IISERM and Completing Masters from would have been a formidable task without them.

Finally, I want to thank my Mother, Father, Sisters, and Brothers for everything, they have always been my motivation.

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# Abbreviations

| | |
|---|---|
| **RSRG** | **R**eal **S**pace **R**enormalization **G**roup |
| **DMRG** | **D**ensity **M**atrix **R**enormalization **G**roup |

# Contents

*I dedicate this thesis to my grandfather who was probably the first in my family to understand the importance of education, and then fostered it in my family.*

# *Abstract*

The dimension of the Hilbert space of many-body quantum system increases exponentially with the number of particles. When there is the possibility of having the variable number of particles at each position, then the dimension of Hilbert space increases exponentially with the number of possible position a particle can acquire, called as the site. Due to this reason, the exact diagonalization simulation of systems in condensed matter physics is impossible for a large size system. For most of the system in condensed matter physics, the analytical solution does not exist. Hence, one must find a way to simulate these many-body interacting system. Here we discuss a numerical algorithm which is designed to solve the many-body quantum system with excellent accuracy. In this article, we will discuss the algorithm as well as a result obtained by the algorithm for one-dimensional Tight-binding model and one dimensional Heisenberg chain.

# Chapter 1

# Real-Space Quantum Renormalization Group

Real Space Renormalization group is a method for the study of low lying states of one-dimensional single particle Hamiltonian, by an iterative increase of system size to reach a required system size. This method, like any renormalization method, relies on physically motivated throwing out some degree of freedom to reduce the degree of freedom, in a way that the remaining states contain essentially all the information needed for the calculation of relevant quantities. In this method, the problem of diagonalizing a bigger matrix reduced to diagonalization of much smaller matrices. The method constructs the ground state of a larger system with low lying states of smaller blocks with different boundary conditions.

The concept of renormalization method first introduced by Wilson Wilson [1975] despite being very successful for the solution of Kondo problem, performed very poorly for various Hamiltonian (Lee [1979], Bray und Chui [1979]). The reason for the failure was not very well understood until one of Wilson's student applied this renormalization method for the study of a particle on a box and one-dimensional tight binding problem. He also provided a new renormalization method which was mainly based on the old one but treated the boundary conditions carefully. The new renormalization method gives excellent result for the single particle Hamiltonian (White und Noack [1992]). In this chapter, we will discuss why Wilson's renormalization method did not work. We will also discuss the new modified algorithm.

## 1.1 The model system

The system we are studying is a single spin-less particle in a tight binding Hamiltonian. The element of the matrix for tight binding Hamiltonian can be managed to be same as that of the particle in a 1-dimensional box in a continuum limit.

### 1.1.1 Hamiltonian of the model system

Tight binding Hamiltonian H with nearest neighbour hopping is given by,

$$H = 2\left|0\right\rangle\left\langle 0\right| - \left|0\right\rangle\left\langle 1\right| + \left(\sum_{i=1}^{L-1} 2\left|i\right\rangle\left\langle i\right| - \left|i\right\rangle\left\langle i+1\right| - \left|i\right\rangle\left\langle i-1\right|\right) + 2\left|L\right\rangle\left\langle L\right| - \left|L\right\rangle\left\langle L-1\right| \tag{1.1}$$

Hamiltonian for particle in a 1-dimensional box is written in continuous position basis as,

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \tag{1.2}$$

for solving this Hamiltonian we first assume that the 1-dimensional box of collection of points very close to each other the distance between two points is h.

$$\frac{\partial^2\psi(x)}{\partial x^2} = \lim_{h\to 0}\frac{2\psi(i) - \psi(i-1) - \psi(i+1)}{h^2} \tag{1.3}$$

Equation 1.2 can be solved for system of given size and given boundary conditions using matrix methods for solving differential equation.
For example, if we want to impose free boundary on the first site $\psi'(1) = 0$ and fixed $\psi(N+1) = \psi(0) = 0$ then,

$$\psi'(1) = \frac{\psi(1) - \psi(0)}{h} = 0 \tag{1.4}$$

$$\psi(0) = \psi(1) \tag{1.5}$$

also at first site $x = 1$ (Equation 1.3) reduced to,

$$\frac{-\hbar^2}{2m}\frac{(-\psi(0) + 2\psi(1) - \psi(2))}{h^2} = E\psi(0) \tag{1.6}$$

Assuming a unit where,

$$\frac{-\hbar^2}{2mh^2} = 1 \tag{1.7}$$

Hence, Using Equation 1.5 , Equation 1.6 reduced to,

$$\psi(1) - \psi(2) = E\psi(1) \tag{1.8}$$

Hence Schrodinger equation for a particle in 1-dimensional box for free fixed boundary conditions in the site basis is written as,

$$\begin{pmatrix} 1 & -1 & 0 & 0 & \dots & \dots \\ -1 & 2 & -1 & 0 & \dots & \dots \\ 0 & -1 & 2 & -1 & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \\ 0 & 0 & 0 & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} \psi(1) \\ \psi(2) \\ \psi(3) \\ \vdots \\ \psi(N) \end{pmatrix} = E \begin{pmatrix} \psi(1) \\ \psi(2) \\ \psi(3) \\ \vdots \\ \psi(N) \end{pmatrix} \tag{1.9}$$

Similarly other boundary conditions can be implemented.

## 1.2 Wilson's renormalization method

The standard renormalization method for many body systems Wilson [1975] posits that we can make ground state out of low lying eigenstates of a smaller system. The algorithm devised by Wilson is following.

1. Start with a system of size L. The size L of the system must be small so that one can diagonalize it's Hamiltonian exactly to find it's eigenvalues and eigenvectors.

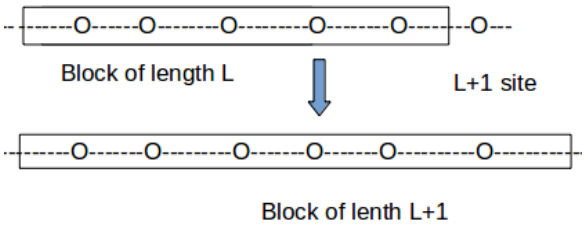


FIGURE 1.1: Pictorial Description of Wilson's Algorithm

2. Choose first few (say m) low lying energy eigenstates and form a matrix made of these low lying states as columns. Do "similarity like transformation" [1] to change the basis of all relevant operators of this block of L site system from the original basis to space of these chosen energy eigenstates. We call this transformation as rotation and truncation of operators.

$$\bar{H}_L = O_L^\dagger H_L O_L \tag{1.10}$$

$$\bar{A}_L = O_L^\dagger A_L O_L \tag{1.11}$$

where $O_L$ contains the m lowest eigenstates as columns

3. Add one more site to the block and write Hamiltonian and other operator for the Larger block of size L+1 considering the interaction between block and the site (see figure 1.1) . Total Hamiltonian of block and site can be devided into three parts.

$$H_{L+1} = H_L + H_{site} + H_{interaction} \tag{1.12}$$

4. Repeat the procedure form the first step considering L+1 block system as new block.

5. When you reach the system size of interest then calculate the properties of system using the energy eigenstate of approximate Hamiltonian and other approximate operators. Using these approximate operators and approximate energy eigenstate we can calculate the approximate expectation value of the relevant operators.

[1] Not exactly a similarity transformation, because similarity transformation, transforms the operator written in one complete basis to another complete basis. On the other hand, In this transformation, the states, in which operators are projected do not form a complete basis

### 1.2.1 Wilson's Renormalization method for the particle in 1-D box and Tight Binding Hamiltonian.

For a single particle in a 1-D box the size of Hilbert space increases linearly with the number of sites. Hence, The Algorithm for a particle in the 1-D box remains the same, but instead of adding one site we double the number of sites at each step (White und Noack [1992]). Hamiltonian for the larger system which is made of two smaller block of equal size can be written in matrix form as following,

$$H = \left[\begin{array}{c|c} H_L & T_{RL} \\ \hline T_{LR} & H_R \end{array}\right]$$

Where $H_L$ and $H_R$ are Hamiltonian for the left and right blocks. $T_{LR}$ and $T_{RL}$ are matrices which include the hopping between two blocks. They are called connection matrices. Since Hamiltonian is Hermitian $T_{LR} = T_{RL}^{\dagger}$

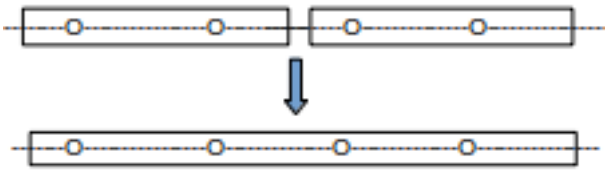

FIGURE 1.2: Pictorial Description of Wilson's Renormalization Method

For example, Consider a system of four sites. We can write it's Hamiltonian in position basis for fixed-fixed boundary condition on each end of the block as,

$$H_{foursite} = \left[\begin{array}{cc|cc} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ \hline 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{array}\right]$$

We can consider it to be made of two, two site blocks Whose Hamiltonian is written as,

$$H_{twosite} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

In position basis. The connection matrix is given by given by,

$$T_{LR} = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

The nonzero elements in connection Hamiltonian correspond to the hopping of particle from the last site of the left block to the first site of right block.

To insert the truncation, we much first choose the number of states we want to keep for the algorithm. Suppose we decided that we want to keep "m" states for the description of a block. Then we can project all operators based on the most probable states (least energetic states) of the block using the procedure describe in Equation 1.10 and Equation 1.11.

Then write the Hamiltonian for the larger block as a matrix of size $2m \times 2m$,

$$H = \left[\begin{array}{c|c} \bar{H}_L & \bar{T}_{LR} \\ \hline \bar{T}^{\dagger}_{LR} & \bar{H}_R \end{array}\right]$$

and connection matrix for the larger block as,

$$T_{LR} = \left[\begin{array}{c|c} 0 & 0 \\ \hline \bar{T}_{LR} & 0 \end{array}\right]$$

We can repeat the same procedure by finding the eigenstates of new Hamiltonian and using m most probable states, low lying energy eigenstates, to rotated and truncate the Hamiltonian in the space of "m" most probable states and then to form Hamiltonian and connection matrix for the new even bigger Block.

### 1.2.2 Failure of Wilson's renormalization method for particle in 1-D box and tight binding Hamiltonian

The Reason behind the failure of the renormalization method can be assigned to the treatment of boundary and heuristic argument can be given for the poor performance of the algorithm. The justification of this heuristic argument rests on the almost exact result obtained by a closely related algorithm given by White und Noack [1992] which handle boundary condition(s) in a slightly different way.

| Energy level | Exact diagonalization | Wilson's Renormalization |
|---|---|---|
| Ground state | $2.3508003329019117 \times 10^{-06}$ | $1.920736 \times 10^{-2}$ |
| First excited state | $9.40319580475781 \times 10^{-06}$ | $1.920909 \times 10^{-2}$ |
| Second excited state | $2.1157169836989935 \times 10^{-05}$ | $1.921412 \times 10^{-2}$ |

TABLE 1.1: Result of Wilson's renormalization method for energy calculation

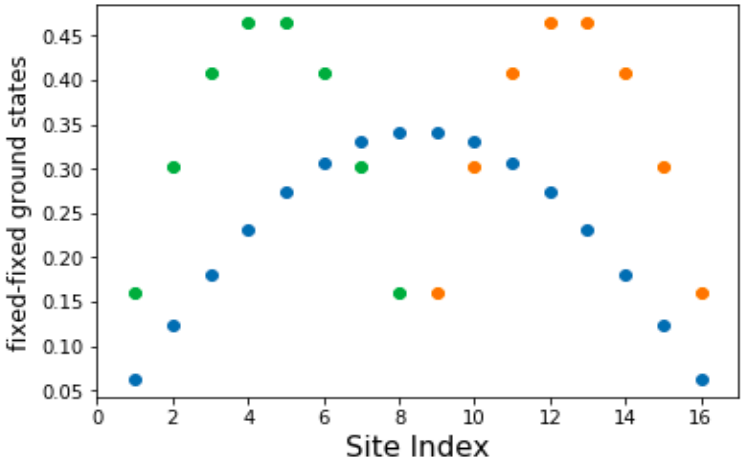


FIGURE 1.3: Pictorial description of mistake in Wilson's renormalization method.

For example, If we try to form a ground state for the 16 site system out of states of smaller 8 site system Figure 1.3, lowest of which is shown in Figure 1.3, has nodes on the ends. The states form out of these few (but not all) low lying state will necessarily will have dip in the middle, whereas the ground state of bigger block has maxima in middle. If one tries to implement other boundary condition then also due to the only nearest neighbour hopping only fixed boundary can be used to whenever two blocks are joined together. Hence, the assumption that the ground state of larger system can be made out of low lying states with a given boundary condition of smaller system is faulty.

One must note that The procedure is nothing but a change of basis if one takes into consideration all state of the smaller block, in other word do not perform any truncation of states. This procedure, of not throwing out any state, also gives the same result as the exact diagonalization method.

## 1.3 White and Noack's renormalization method

White and Noack posited that the to obtain low lying states of larger block one should use the low lying states of smaller blocks, but with different boundary conditions. These states of the smaller blocks must be used to construct energy eigenstates of larger blocks with various boundary conditions. To be more specific the algorithm which uses eigenstates with a combination of fixed and free boundary condition is discussed next.

### 1.3.1 Real space renormalization method

The Renormalization method algorithm provided by Steven R. White and R. M. Noack (White und Noack [1992]) is following.

1. Start with a block of smaller size L (a block of a single site is also fine) the dimension of Hilbert space of this block should be is easily handlable.

2. If started with the single site then form the Hamiltonian for the two site block with different boundary conditions on each end of the block. If you have started with more then one site block, then write it's Hamiltonian for different boundary conditions on each edge. There are four possibilities fixed-fixed, fixed-free, free-fixed and free-free boundary condition.

3. Diagonalize the Hamiltonian for all four boundary conditions to find energy eigenstates with particular boundary condition. Suppose you want to take into consideration only "m" number of states for the further calculations then choose "$m/4$" lowest energy eigenstates from each boundary condition.

4. Perform Gram Schmidt procedure to form an orthonormal set made out of these states. Form a matrix O whose columns are these orthonormal states. Project all four Hamiltonian with different boundary conditions and other relevant operators of the block in the space of these states.

$$\bar{H}_L = O_L^\dagger H_L O_L \tag{1.13}$$

$$\bar{A}_L = O_L^\dagger A_L O_L \tag{1.14}$$

$$\bar{T}_{LR} = O_L^{\dagger} T_{LR} O_L \tag{1.15}$$

5. Form Hamiltonian for larger 2L site block with different boundary condition at each edge.

$$H_{2L}^{b,b'} = \left[\begin{array}{c|c} \bar{H}_L^{b,fixed} & \bar{T}_L \\ \hline \bar{T}_L^{\dagger} & \bar{H}_L^{fixed,b'} \end{array}\right]$$

   Here b and b' specify boundary condition on edge. They can take two possible arguments fixed and free. $H_L$ is L site Hamiltonian with specified boundary condition. Here also there are four different possibilities of boundary conditions. Note that fixed boundary condition is being used whenever two blocks are joined.

$$T_{2L} = \left[\begin{array}{c|c} 0 & 0 \\ \hline \bar{T}_L & 0 \end{array}\right]$$

   Where $T_{2L}$ is connection matrix for the larger block.

6. Now repeat the whole procedure till you reach a desired system size.

7. Then calculate the Energy eigenvalue for the fixed-fixed boundary condition at the end of step 2.

This algorithm calculated energy for the particle in a box is almost exact. Below we provide the table for comparison with exact diagonalization.

| Energy level | Exact diagonalization | Real Space renormalization |
|---|---|---|
| Ground state | $2.3508003329019 \times 10^{-06}$ | $2.3508003336985 \times 10^{-6}$ |
| First excited state | $9.40319580475 \times 10^{-06}$ | $9.403195807395 \times 10^{-6}$ |
| Second excited state | $2.1157169836989 \times 10^{-05}$ | $2.1157169843449 \times 10^{-5}$ |

TABLE 1.2: Result of Real space renormalization method

The fact that the combination of fixed free performed so well is not just an accident. We can choose other combinations of boundary conditions which rest on the same physical argument of constructing energy eigenvectors of the larger block from the eigenvectors of the smaller block with different boundary condition. One possibility is using the eigenvectors with periodic and anti-periodic boundary condition for the algorithm. This method also gives the almost exact result (White und Noack [1992]).

### 1.3.2 Superblock method

A most general approach is constructed given where we do not need to take care of boundary condition deliberately, where the algorithm itself takes care of finding appropriate boundary conditions of energy eigenstates of smaller blocks (cf. White und Noack [1992]).

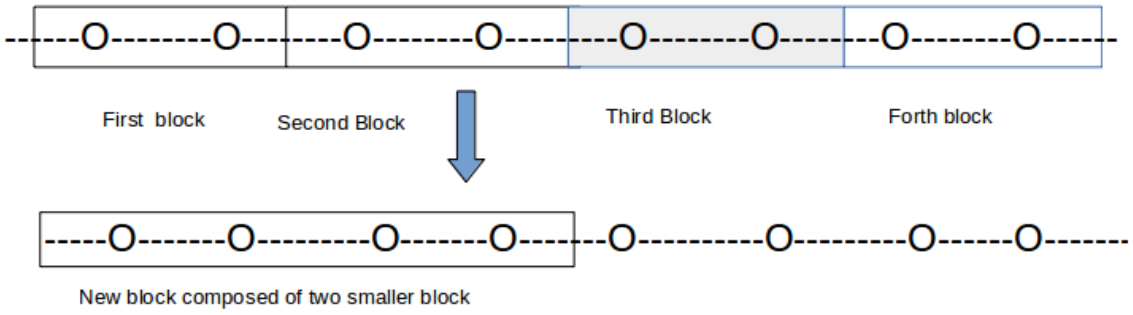


FIGURE 1.4: Pictorial Description of superblock method

The Algorithm can be given as follows,

1. Start with a block of small size, then choose a superblock composed of many identical blocks with a boundary condition (say p, where $p > 2$).
2. Solve the Hamiltonian of the superblock to extract first m eigenvectors of the superblock.
3. Take the projection of these states for the first two blocks.
4. Now consider the new larger block composed of two block as the new block. Again start with step 1 to construct Hamiltonian of superblock compose of p ($p \geq 2$) number of identical block.
5. Repeat the same procedure till you reach the superblock of appropriate size. Then calculate the energy and eigenstate of the superblock.

This algorithm has the advantage that we do not need to impose boundary conditions deliberately. We will see later that the generalization of this algorithm will be useful for the renormalization methods for the many-body quantum system.

## 1.4 Summary and concluding remarks

Real space Renormalization group can be used to calculate the energies and other properties of 1-dimensional, single particle quantum system with a given Hamiltonian. We have seen that the first few eigenstates of the smaller block can be used to form "approximate" operator for the block which can be used to "approximately" construct the operators of a larger block. The quantities (in our case, energy) calculated with these operators are almost exact.

However, we are interested in the calculation of quantities that describe the physical properties of the many-particle interacting system. Although the method provided here is for the single particle systems, one can develop renormalization algorithm for the many-particle interacting system on the same spirit of constructing operators and eigenstate of larger system using operators and eigenstates of the smaller systems (White [1993]). The many-body algorithm has a close resemblance to the superblock method discussed in this chapter. In the next chapter we will discuss the underlying theoretical background for a Renormalization Method called as, Density Matrix renormalization group, for the many-body interacting systems.

# Chapter 2

# Density Matrix Renormalization Group: Theory

The motivation behind the Renormalization methods is to circumvent large matrix diagonalization, to represent operators and calculate the properties of the system in a given state without diagonalizing an extremely large matrix. We will see in this chapter that the problem of diagonalizing a large matrix can be reduced to diagonalization and operations on small matrix much time for calculation of a predestined quantity of interest. This chapter is dedicated to the underlying theory of such an algorithm. The purpose of the discussion is to provide a theoretical base for the algorithm to be discussed in later chapters.

## 2.1 Concept of reduced density matrix

The problem that reduced density matrix deals with is the following: Given a state of the universe which, contain a system S and an environment E, How to determine the state of the system?

**Case I: When universe is in a pure state**
Suppose I have a Universe divided in a system S and environment E. State of the

Universe is in state $|\psi\rangle_{SE}$ of S and E can be written using Schmidt decomposition as

$$|\psi\rangle_{SE} = \sum_k |\phi_k\rangle_S |k\rangle_E \tag{2.1}$$

Without loss of generality, the set $\{ |k\rangle \}$ can be chosen to be an orthonormal basis of environment E.

If we can calculate the expectation value of all local operator of S, then I can know everything that can be known about system S.

Suppose M is an local operator of system S. We want to calculate the expectation value of M. which is given by $\langle\psi| M \otimes I |\psi\rangle$

$$\langle\psi| M \otimes I |\psi\rangle = \left( \sum_l \langle l| \langle\phi_l| \right) M \otimes I \left( \sum_k |k\rangle |\phi_k\rangle \right) \tag{2.2}$$

$$= \sum_{k,l} \langle l|k\rangle \langle\psi_l| M |\phi_k\rangle \tag{2.3}$$

$$= \sum_l \langle\psi_l| M |\phi_l\rangle \tag{2.4}$$

let $\{ |\alpha\rangle \}$ and $\{ |\beta\rangle \}$ be complete orthonormal basis of systems Hilbert space of system. Then above equation can be written as

$$= \sum_{\alpha,\beta,l} \langle\phi_l|\alpha\rangle \langle\alpha| M |\beta\rangle \langle\beta|\phi_l\rangle = \sum_{\alpha,\beta,l} \langle\beta|\phi_l\rangle \langle\phi_l|\alpha\rangle \langle\alpha| M |\beta\rangle$$

Since $\{ |\alpha\rangle \}$ is complete.

$$\sum_{\beta,l} \langle\beta|\phi_l\rangle \langle\phi_l| M |\beta\rangle = tr \left( \left( \sum_l |\phi_l\rangle \langle\phi_l| \right) M \right) \tag{2.5}$$

The expression $\sum_l |\phi_l\rangle \langle\phi_l|$ is reduced density matrix for system and is obtained by taking partial trace of $|\psi\rangle \langle\psi|$ with respect to environment basis. Hence Density matrix $\rho_A$ for system is obtained by

$$\rho_s = tr_E \left( |\psi\rangle \langle\psi| \right) \tag{2.6}$$

**Case II : When universe is in a mixed state**

In this situation, the state of the combined system of S and E can be only written as a density matrix $\rho_{SE}$.

Suppose as before; we want to calculate properties of system S by calculating the expectation value of local operators of system S. In another word the problem is following: Given the density matrix of the Universe composed of S and E. How to determine the expectation value of operator $M_S$. Operating $M_S$ on system S is same as operating $M_S \otimes I_E$ on the combined system AB. Hence, the problem is of finding a matrix $\rho_S$ such that,

$$tr(M_S \rho_S) = tr((M_S \otimes I_E)\rho_{SE}) \tag{2.7}$$

Suppose $\{ |i\rangle \}$ are orthonormal complete basis of system S and $\{ |j\rangle \}$ are complete basis of Environment E. Then $\{ |i\rangle \otimes |j\rangle \}$ for all possible combination of i and j is a basis for the combined system SE. Hence,

$$tr((M_S \otimes I_E)\rho_{SE}) \tag{2.8}$$

$$= \sum_{i,j} \langle i| \langle j| ((M_S \otimes I_E) \rho_{SE}) |i\rangle |j\rangle \tag{2.9}$$

$$= \sum_{k,l} \sum_{i,j} \langle ij| (M_S \otimes I_E) |kl\rangle \langle kl| \rho_{SE} |ij\rangle \tag{2.10}$$

$$= \sum_{ijkl} (\langle i| M_S |k\rangle \langle j|l\rangle)(\langle kl| \rho_{SE} |ij\rangle) \tag{2.11}$$

$$= \sum_{ijkl} (\langle i| M_S |k\rangle \delta(j,l))(\langle kl| \rho_{SE} |ij\rangle) \text{ since, } \langle j|l\rangle = \delta(j,l) \tag{2.12}$$

$$= \sum_{ikj} \langle i| M_S |k\rangle \langle kj| \rho_{SE} |ij\rangle \tag{2.13}$$

since $\{ |k\rangle \}$ is complete or $\sum_K |k\rangle \langle k| = 1$. Hence, the above equation can be written as,

$$= \sum_{i,j} \langle i| M_A \left( \sum_k (|k\rangle \langle k| \right) \langle j| \rho_{AB} |ij\rangle \tag{2.14}$$

$$= \sum_i \langle i| M_A \left( \sum_j \langle j| \rho_{AB} |j\rangle \right) |i\rangle \tag{2.15}$$

The expression $\sum_j \langle j| \rho_{AB} |j\rangle$ is called reduced density matrix $\rho_A$ for system A.

$$\langle M_A \rangle = \sum_i \langle i| M_A \rho_A |i\rangle \tag{2.16}$$

For all operator $M_A$.

The reduced density matrix of system S is obtained by taking a partial trace of, density matrix of the universe, with environment E for both pure and mixed state of the universe (Preskill [1998] and Nielsen und Chuang [2002]).

## 2.2 Heuristic theory for the DMRG algorithm

The basic idea of renormalization method is to describe the state of the system in a small number of states (say, m) which are very small compared to the size of the Hilbert space of the system. This chapter, we will show how to choose these m states which contain almost all the information and discuss the possible consequences of choosing only a few states.

**Notation** : In condensed matter convention we call universe composed of system S and Environment E as a superblock (not universe).

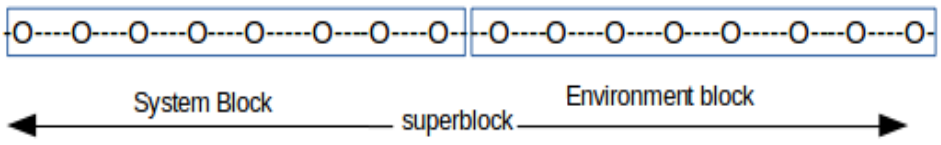


FIGURE 2.1: Pictorial description of a superblock compose of system and environment block

Renormalization group method aims to "approximate" all the relevant operators and states of system, environment, and Superblock in a matrix of the size which is much smaller than the dimension of original Hilbert space of system, environment, and superblock respectively. In a way that this smaller degree of freedom contains almost all the relevant information. What we want is to describe the System with a few numbers of states compared with the size of Hilbert space. In the next section, we will discuss how we can achieve this goal, assuming we want to study the physical properties of a pure state of Hamiltonian.

### 2.2.1 Expectation Value Optimization

Suppose we are assuming that the superblock is in some state $|\psi\rangle$ then we want to specify the state of system block with only a few numbers of states. If the Schmidt decomposition of the state is written as,

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle |j\rangle \tag{2.17}$$

where $\{ |i\rangle \}$ and $\{ |j\rangle \}$ are orthonormal basis of system and environment respectively. Then reduced density matrix of system is written as,

$$\rho_S = tr_E |\psi\rangle \langle\psi| \tag{2.18}$$

Where the states of environment is traced out.

$$\langle i| \rho_S |i'\rangle = \sum_j \psi_{ij} \psi^*_{i'j}$$

Suppose the dimension of Hilbert space is $N^S$ and we want to keep only $M^S$ state. Since reduced density matrix is Hermitian we can do perform spectral decomposition of the reduced density matrix of System. After Schmidt decomposition we can write,

$$\rho_A = \sum_\alpha w_\alpha |w_\alpha\rangle \langle w_\alpha| \tag{2.19}$$

Since trace of reduced density matrix is 1. Hence,$\sum_\alpha w_\alpha = 1$

Now the exact expectation value of any operator is written as,

$$\langle A \rangle = \sum_{\alpha=1}^{N^S} w_\alpha \langle w_\alpha | A | w_\alpha \rangle \tag{2.20}$$

Suppose that the $w_\alpha$ are shorted in a way that $w_1 \geq w2 \geq w_3 \ldots$ then we can approximate the expectation value as follows,

$$\langle A \rangle = \sum_{\alpha=1}^{M^S} w_\alpha \langle w_\alpha | A | w_\alpha \rangle \tag{2.21}$$

Hence the error in expectation value is given by,

$$\langle A \rangle_{error} = \sum_{\alpha>M^S}^{N^S} w_\alpha \langle w_\alpha | A | w_\alpha \rangle \tag{2.22}$$

If the operator $\hat{A}$ is bounded by $c_A$ then, the the error in $\langle A \rangle$ is also bounded,

$$| \langle A \rangle_{approx} - \langle A \rangle | \leq \left( \sum_{\alpha>M^s}^{N^S} w_\alpha \right) c_A = \epsilon_\rho c_A \tag{2.23}$$

Where $\hat{A}$ is bounded by $c_A$ means,

$$\langle \phi | \hat{A} | \phi \rangle \leq c_A \tag{2.24}$$

for all normal vector $|\phi\rangle$. We observed from Equation 2.23 that the quantity in bracket $\epsilon_\rho$ is a measure of error in calculated value. If the quantity $\epsilon_\rho$ is sufficiently small then the error is marginal.

For example, suppose we want to calculate two-point correlation function $\left\langle S_i^Z S_j^Z \right\rangle$ for spin chain and $\epsilon_\rho$ turns out to be say, $10^{-5}$ (cf.Table 4.1). We know that the two-point spin correlation operator for spin half is bounded by 0.25 then we know that the error in any two-point correlation is also bounded by $0.25 \times 10^{-5}$, quite insignificant!

Hence, **if we want to represent system in a few number of states then it's extremely important that the density matrix eigenvalue $w_\alpha$ decay fast** (Schollwöck [2005] and White [1998]).

### 2.2.2 Approximate Operator representation in Density Matrix Renormalization Group

Given that the system is in a given density matrix which in terms predict one of the possible probabilistic decomposition of the system as a mixed state of some states. Assuming that the eigenvalue of density matrix decreases very fast we can write an approximate operator $\hat{A}_{Approximate}$ for every operator $\hat{A}$.

This operator are also obtained using the same "similarity like equation" discussed in chapter 1 Equation 1.13 and Equation 1.14. Suppose a Hermitian operator $\hat{A}$ we can do spectral decomposition of this operator.

$$\hat{A} = \sum_i a_i \left|a_i\right\rangle \left\langle a_i\right| \tag{2.25}$$

Since $\left\{ \left|w_\alpha\right\rangle \right\}, \alpha = [1, N_S]$ are complete basis of system's Hilbert space we can write the Equation 2.25 as,

$$\sum_{\alpha,\beta,i} a_i \left|w_\alpha\right\rangle \left\langle w_\alpha|a_i\right\rangle \left\langle a_i|w_\beta\right\rangle \left\langle w_\beta\right| \tag{2.26}$$

which can be rearrange as,

$$\sum_{\alpha,\beta} \left(a_i \left\langle w_\alpha|a_i\right\rangle \left\langle a_i|w_\alpha\right\rangle\right) \left|w_\alpha\right\rangle \left\langle w_\beta\right| \tag{2.27}$$

This is the Exact operator in $\left\{ \left|w_\alpha\right\rangle \right\}, \alpha = [1, N_S]$ basis. However the approximate operator is written as follows,

$$\sum_{\alpha=1}^{M^S} \sum_{\beta=1}^{M_S} \left(a_i \left\langle w_\alpha|a_i\right\rangle \left\langle a_i|w_\alpha\right\rangle\right) \left|w_\alpha\right\rangle \left\langle w_\beta\right| \tag{2.28}$$

It follows from the orthonormalization property and sufficient small $\epsilon_\rho$ that the calculate expectation values are almost exact for this approximate local and bounded operator.

### 2.2.3 Optimization of wave function

Another completely different line of argument justifies the method of choosing the states with the highest eigenvalue of reduced density operator.

Distance between two states in a vector space is defined as follows, Given two arbitrary vectors in a vector space V the distance D(x,y) between them is a map $V \times V \to R$ such that,

$$D(x,y) \geq 0 \quad \forall x, y, \text{ 0 only for x=y} \tag{2.29}$$

$$D(x,y) = D(y,x) \tag{2.30}$$

$$D(x,y) \leq D(x,z) + D(y,z) \tag{2.31}$$

It turns out that $||\,|x\rangle - |y\rangle\,||^2$ is a valid map for distance.

Suppose the state of is given as,

$$|\psi\rangle = \sum_{i=1}^{N^S} \sum_{j=1}^{N^E} \psi_{ij} \,|i\rangle\,|j\rangle \tag{2.32}$$

where $\{\,|i\rangle\,\}$ and $\{\,|j\rangle\,\}$ is complete basis for the system and environment respectively and $N^s$ and $N^E$ is dimension of hilbert space of system and environment respectively. If one tries to approximate the total wavefunction of superblock by an approximate representation of system such that the approximate state of the superblock is written as,

$$\left|\tilde{\psi}\right\rangle = \sum_{\alpha=1}^{M^S} \sum j = 1^{N^E} a_{\alpha,j} \,|\alpha\rangle\,|j\rangle \tag{2.33}$$

The problem is this: Given $M^S$ how to choose $a_{\alpha,j}$ such that distance is minimum. The problem can be solved using singular value decomposition. I have provided a more pedestrian solution to the problem. Distance between $|\psi\rangle$ and $\left|\tilde{\psi}\right\rangle$ can be written as,

$$\left(\sum_{i',j} \psi^*_{i',j} \,\langle i'|\,\langle j| - \sum_{\alpha',j} a^*_{\alpha',j} \,\langle \alpha'|\,\langle j|\right) \left(\sum_{ii,j} \psi_{i,j} \,|i\rangle\,|j\rangle - \sum_{\alpha,j} a_{\alpha,j} \,|\alpha\rangle\,|j\rangle\right) \tag{2.34}$$

$$\sum_{ij} |\psi_{ij}|^2 - \sum_{i',j,\alpha} \psi^*_{i'j} a_{\alpha,j} \,\langle i'|\alpha\rangle - \sum_{i,j,\alpha'} a^*_{\alpha',j} \psi_{i,j} \,\langle \alpha'|i\rangle - \sum_{\alpha,j} |a_{\alpha,j}|^2 \tag{2.35}$$

Since $|\psi\rangle$ is normal. Hence, $\sum_{ij} |\psi_{ij}|^2 = 1$ Hence, the problem reduces to minimization of

$$1 - \sum_{i',j,\alpha} \psi^*_{i'j} a_{\alpha,j} \langle i'|\alpha\rangle - \sum_{i,j,\alpha'} a^*_{\alpha',j} \psi_{i,j} \langle \alpha'|i\rangle - \sum_{\alpha,j} |a_{\alpha,j}|^2 \tag{2.36}$$

with respect to $a_{\alpha,j}$ and $\langle\alpha|i\rangle$ Taking partial derivative with $a_{\alpha j}$ for minimization condition gives,

$$-\sum_i \psi^*_{i,j} + a^*_{\alpha j} = 0 \text{ for all } \alpha, j \tag{2.37}$$

Inserting the minimization condition in Equation 2.36 gives,

$$1 - \sum_{j,\alpha} |a_{\alpha j}|^2 - \sum_{j,\alpha} |a_{\alpha j}|^2 + \sum_{\alpha,j} |a_{\alpha,j}|^2 \tag{2.38}$$

$$1 - \sum_{\alpha,j} |a_{\alpha j}|^2 \tag{2.39}$$

From Equation 2.37 and Equation 2.39 we can write the Equation 2.39 as follows,

$$1 - \sum_{\alpha,j} \left( \sum_i \psi_{ij} \langle \alpha|i\rangle \right) \left( \sum_{i'} \psi^*_{i',j} \langle i'|\alpha\rangle \right) \tag{2.40}$$

$$1 - \sum_{i,i',\alpha,j} \psi_{i,j} \psi^*_{i',j} \langle \alpha|i\rangle \langle i'|\alpha\rangle \tag{2.41}$$

Since,

$$\langle i'| \rho_S |i\rangle = \sum_j \psi i, j \psi^*_{i',j} \tag{2.42}$$

Hence, from Equation 2.41 and Equation 2.42 the Equation 2.41 can be written as,

$$1 - \sum_{i,i',\alpha} \langle i| \rho_S |i'\rangle \langle \alpha|i\rangle \langle i'|\alpha\rangle \tag{2.43}$$

If the specral decompositon if $\rho_s$ is written as $\sum_{w_\beta} w_\beta |w_\beta\rangle \langle w_\beta|$ then the above equation can be written as,

$$1 - \sum_{i,i',\alpha,\beta} w_\beta \langle i|w_\beta\rangle \langle w_\beta|i\rangle \langle \alpha|i\rangle \langle i|\alpha\rangle \tag{2.44}$$

Due to completeness of $\{ |i\rangle \}$ above equation reduces to,

$$1 - \sum_{\beta,\alpha} w_\beta \langle \alpha | w_\beta \rangle \langle w_\beta | \alpha \rangle \tag{2.45}$$

Now since $\langle \alpha | w_\beta \rangle \leq 1$. Hence, it seems obvious that if we choose the $|\alpha\rangle$ eigenvectors with the highest $M^S$ eigenvalue of the reduced density matrix, then the distance is minimum. In this case, the distance is given by,

$$1 - \sum_{\beta > M^S}^{N^s} w_\beta \tag{2.46}$$

Which is the same as the quantity $\epsilon_\rho$; defined in Equation 2.23. Hence, we see that the $\epsilon_\rho$ is a measure of the error in eigenstate approximation.

We observed that choosing the states with the highest eigenvalue of the reduced density matrix of system is the best way to approximate the state of system and superblock. Also, we have proved that the quantity $\epsilon_\rho$ defined in Equation 2.23 is a measure of the error in algorithm.

### 2.2.4 Optimization of entropy

For a bipartite Universe composed of a system s and environment E, a pure state of system is called entangled if the state can not written as a product state of system S and environment E. In other words the Schmidt number of the state is more than one.

$$|\psi\rangle_{SE} \text{ cannot not be written as } \quad |\phi\rangle_S \otimes |\xi\rangle_E \tag{2.47}$$

For more general discussion (Nielsen und Chuang [2002] and Preskill [1998]). There is an important measure of the entanglement between system and environment, called as Von Neumann Entropy Which is given by following expressionHorodecki u. a. [2009].

$$S = \sum_\alpha w_\alpha \log_2 w_\alpha \tag{2.48}$$

Where the $w_\alpha$ are the eigenstate of reduced density matrix both system and environment.Hence, we see that by choosing the states with highest eigenvalue we are

retaining the entanglement entropy system and system. Many author has proved that the success of DMRG algorithm rests on this entropy preservation technique.(Osborne und Nielsen [2002])

## 2.3 Summary and concluding remarks

We have observed in the previous sections that the optimal approximation for the system states is eigenvectors with the highest eigenvalues. Also, we have seen that the quantity $\epsilon_\rho$, called as **truncation error**, in Equation 2.23 is a valid measure for the error in calculated values using the renormalization method. Hence, the decay of eigenvalue of the reduced density matrix of the system is essential for the method to work. This result remains a fact to be proved by empirical observations in later chapters (cf. Figure 4.1).

We will see in the next chapter that the Density matrix renormalization method is a iterative method. The process of estimating keeping track of this error as we move along the algorithm becomes a convoluted task. In general, the error observed is an order of magnitude larger than the calculated truncation error because truncation error culminates after each iteration. In the next chapter, we will discuss the renormalization algorithm which we were set out for.

# Chapter 3

# Density Matrix Renormalization Group: Algorithms

In this chapter we will discuss the Density Matrix Renormalization Group (DMRG) algorithm for the many body interacting system. We will discuss the empirical observation associated with the DMRG algorithm. The empirical observation will be drawn from a particular model but the trend remain similar for any many body system where DMRG works fine.

Density matrix renormalization group algorithms can be divided into two categories depending upon the how system and environment behave to form the superblock.

The first is called as, Infinite System Method where system and environment increase in size after every step and we are often interested in local properties far from the boundary, where boundary effect is insignificant. Hence, In this method, the calculated quantities turn out to be very close to the value we obtain for the infinitely long system.

The second is called a finite system method, where system and environment are in such a way that the superblock is of finite size. Hence, we deliberately impose the boundary effect. The quantity calculated in this method can be local as well as global, for the full superblock. This method is used to calculate the finite system properties.

The Density matrix renormalization method we discuss here is for the one-dimensional many-body system. The states of superblock used to form the reduced density matrix

of the system are called target states. For calculation of ground state properties of a non-degenerate ground state, it is sufficient to choose target state as the ground state of the superblock. For degenerate ground state case, we need to have to uniquely pick the state with energy and an additional quantum number for some other conserved operator. We will discuss the algorithm for the non-degenerate ground state.

## 3.1 Infinite System Algorithm

We will first explain the algorithm concisely here. For convenience, we have divided the whole algorithm into various parts. While writing computer programs for the method, one can make divide the computer program into modules where each module perform one part of the algorithm Garrison und Mishmash [2013] [1].

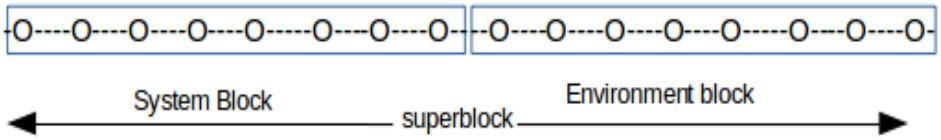


FIGURE 3.1: Superblock composed of system and environemt

### Initiation

- Start with a system and environment of small size such that the dimension of Hilbert space is for the superblock operator is small and Hamiltonian of the superblock is easily diagonalizable. Write the relevant operators for the system, environment, and Superblock. Using these operators write the Hamiltonian of the superblock. (Cf. figure 3.1)

### Diagonalization and expectation value calculation

- Diagonalize the Hamiltonian of the superblock to find the target states (for the study of ground state properties only ground state of Hamiltonian of the superblock is sufficient) for the superblock.

[1] This method of programming is considered good habit by programming community(cf. Guttag [2016])

- *After diagonalization, we will have Target states and operators for the superblock. Hence, We calculate the expectation value of relevant superblock operators for the target states here.*

### Rotation and truncation

- Find the reduced density matrix of the system and environment for the chosen target state. Diagonalize the reduced density matrix to find a few (Always a chooses number, much smaller than the size of Hilbert space of system) most probable (states with the highest eigenvalues) of the reduced density matrix.
- Project all operator of system and environment on the subspace of these most probable states for system and environment. For system block, This is done by constructing a matrix (T) whose column is the "m" (the number of states we choose to keep) most probable states of the system. Then performing "similarity like transformation[2]" for all operator as below,

$$\bar{A} = T^{\dagger} A T \tag{3.1}$$

For all system operator $\hat{A}$, We call $\bar{A}$ as the rotated truncated operator. Do Similarly for the environment.

### System and environment enlargement

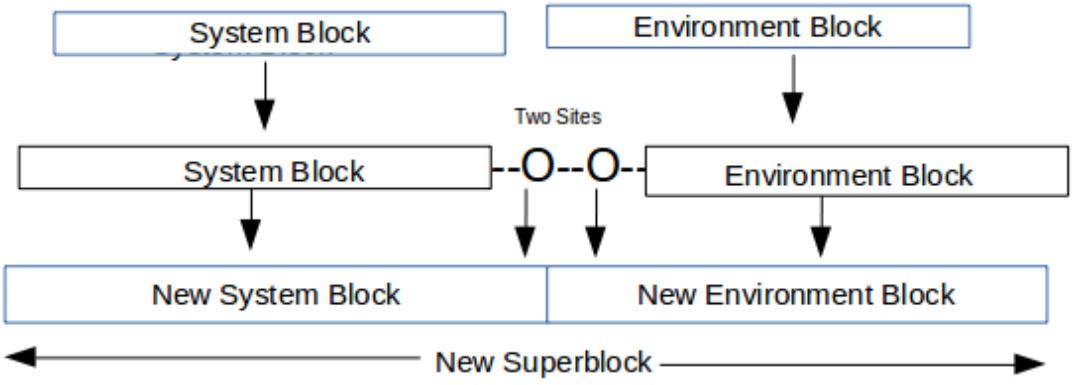


FIGURE 3.2: System and environment enlargement

[2]not precisely similarity transformation

- Add one site to *both* system and environment block. This system and site block combine to form a new enlarged system. Similarly, the environment and a site combine to form a new enlarged environment (cf. figure 3.2).
- Write the relevant operator for the new enlarged block and enlarged environment using the rotated and truncated system and environment block operators. Form the relevant operator including the Hamiltonian of new superblock composed of new enlarged system and environment.

**Iretation**

- Repeat the whole procedure beginning form the diagonalization and expectation value calculation part.

One must iterate the whole procedure many time to reach a Larger system and environment size. Then calculate the properties like per site energy, and correlation $\langle S_i^Z S_j^Z \rangle$ between two sites i and j from the middle of chain where the boundary effect is minimum and negligible (cf figure3.3).

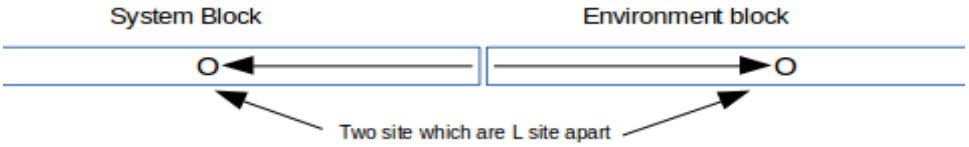


FIGURE 3.3: Choosing site for correlation calculation Using Infinite algorithm

If Hamiltonian has reflection symmetry than it can be proved that the basis vectors of the environment can be chosen in a way that all operators of environment can we taken to be identical to the system block (White und Noack [1992],Schollwöck [2005]). This property holds for both exact and truncated rotated operators. Using this property reduces the time taken by the algorithm by almost half (Schollwöck [2005]).

The Infinite System Algorithm does not always give a satisfactory result, and there is a system where this algorithm failed is failed to be implemented (cf. section II.D Schollwöck [2005]). In such a case, there-there is another method which is slightly more computational resource demanding but significantly more useful.

## 3.2 Finite System Algorithm

As we have already mentioned earlier in this chapter that the finite system method is used for the calculation of finite system properties. We will see in this section that this algorithm inevitably imposes the finite system constraints. We will again divide the whole algorithm into parts for convenience. Suppose we want to calculate the properties of L site long system. Here also we divide the algorithm into many parts; each part can be implemented as a module in a computer program.

**Part I: Warm-up**

This part of the algorithm is nothing but the Infinite system algorithm, but here we have to store the operator after every step for all the system and environment size.

- Start with a system of system and environment of equal and small size. Perform the infinite system algorithm until you reach a superblock of size L. At every stem store in the hard-disk of the computer the all relevant rotated truncated operator[3] for system and environment of all possible size.

**Part II: Sweep System size enlargement on the cast of environment size shrink**

- Now increase the system size by one site by decreasing the size of the environment block by one site.
- Write operators for the new enlarged system block and shrunk environment block. For obtaining an operator for the shrunken environment block of a particular size use the stored, rotated truncated operator of the same sized environment from the warm-up part. In order to calculate an operator in the enlarged system block, use the stored operator of system block from the warmup part and tensor product structure of the operators.

**Rotation and Truncation**

[3]Defined earlier in Infinite System Algorithm section

- Write the Hamiltonian for the superblock using the rotated truncated operator of system and environment block. Diagonalise the Hamiltonian of superblock to obtain the target states. Then find the reduced density matrix of system and environment.

- Diagonalize the Reduced density matrix to obtain the most probable state of the system. Form the transformation matrix as we did in Infinite system method. Perform the "similarity like transformation." Equation 3.1 to obtain the rotated truncated operator for the system. Similarly for the environment. Store the new rotated truncated operator for the enlarged system and shrunken environment.

Each block is labeled by two things first whether it is system block or environment block. Second by its size. For each system and environment block of various length, we have some operator which are being replaced by the new operators calculated in the step above.

- Perform the step above until the environment shrinks to the single site.

- Then enlarge the environment on the cast of shrinkage of the system till the system is reduced to a single size, as depicted in Figure 3.4.

- Again Increase the system size till you reach to the superblock where system and environment have the same size.

The whole procedure explained in the "sweep" part is illustrated in figure 3.4.

The whole procedure described in part II is called as "a single sweep" *At this step one Have the superblock operator for various relevant quantities including Hamiltonian and target states. One can calculate various properties.* it is not expected that the calculated properties will be correct just after one sweep. One must perform additional (typically 3-4) sweep. Sometime even when the results are converging it is considered good practice to do few more sweeps. It is also advised to check the result for various m, number of states considered. (cf. section II.D Schollwöck [2005]).

For calculation of properties of infinite systems where infinite system method does not work or impossible to implement (cf. Schollwöck [2005]) then we can calculate properties of finite system and then do extrapolate the result for infinite length. In

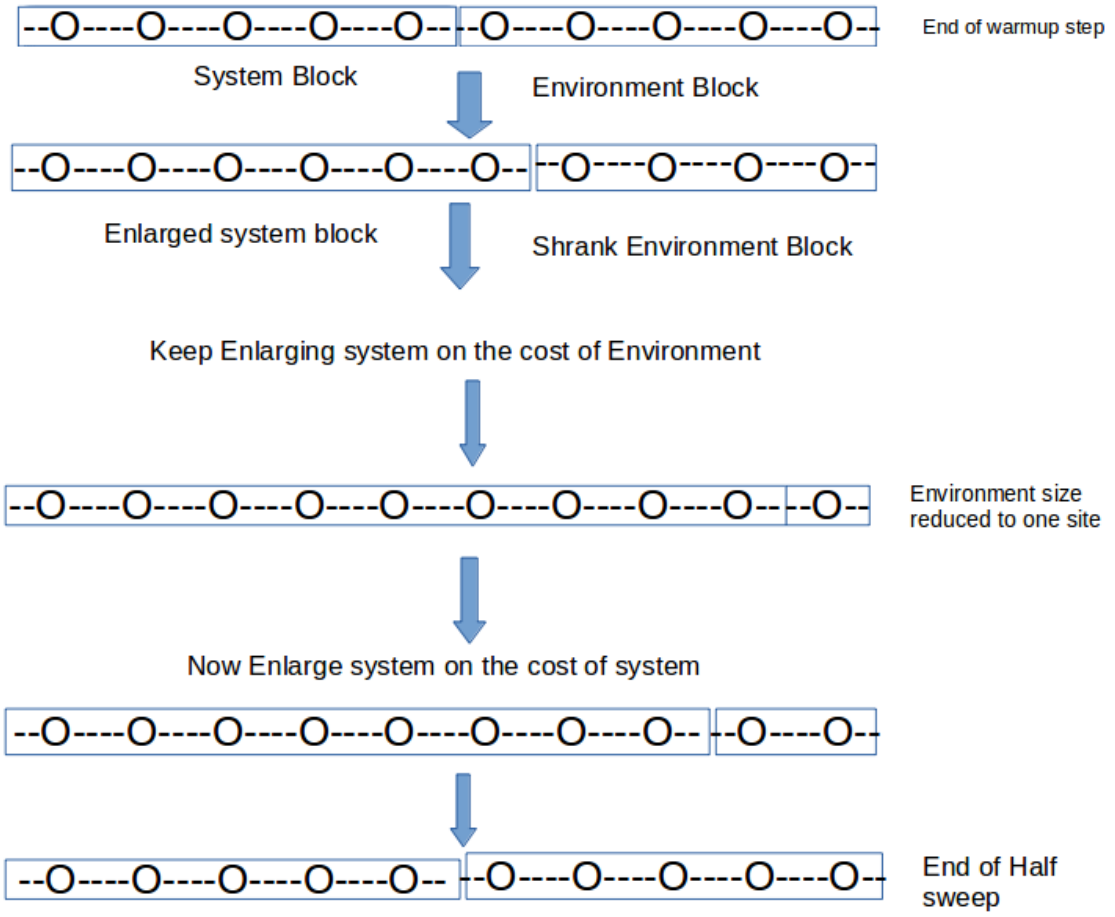


FIGURE 3.4: Pictorial Disciption of Half sweep

such situation it become important to calculate the properties of finite system with excellent accuracy. To obtain better accuracy it is advised that we should calculate the result for different possible m (number of state kept for calculation) then calculate the truncation error for all m. Finally interpolate the result for zero truncation error. It is found that the error in obtain result varies linearly with truncation error ( cf. White und Huse [1993] , Liang [1990] and Section II.F Schollwöck [2005])

## 3.3 Good Quantum Numbers in Density Matrix Renormalization Group

For some system, it's impossible to uniquely pick a single state for the study. Then we must look for another quantum label other than energy to uniquely pick the state.

For Ferromagnetic Heisenberg chain the Ground state is a degenerate state. But for the Heisenberg chain the total spin operator $\sum_i S_i^z$ is a conserved quantity. It turns out that we can uniquely pick the state using energy and total spin operator value.

In Density matrix renormalization group it's possible to pick the states labeled by a given set of quantum numbers. Using this we can further decrease the considerable degree of freedom which makes the algorithm much more faster. We will discuss the consequence of using this property in Section 4.6.

## 3.4 Targeting more then one states

When calculating properties like excitation spectra or energy gap between states. If we are unable to use the good quantum number properties of states. Then we must target more than one state. In such a situation one must use the density matrix of superblock as an equally weighted sum of all the states we need to consider. In other words, we need to construct the density matrix of superblock a density matrix with equal probability density of targeted pure states,

$$\rho_{superblock} = \frac{1}{N} \sum_i |\psi_i\rangle \langle\psi_i| \tag{3.2}$$

Where N is the total number of pure states targeted. In such cases, the algorithm converses much slowly. The reason is that in such situation the probability (eigenvalue) of the states is distributed and do not decay very fast.

## 3.5 Summary and concluding remarks

We have discussed, in detail, the Density Matrix Renormalization Group Algorithm for the study of Infinite and finite size systems. A more detailed discussion can be found Feiguin [2011],Peschel u. a. [1999]. Next chapter we will move on to the implementation of these algorithms for the study of a model system called as 1-dimensional Heisenberg chain. We will learn about some empirical observation characterizing the DMRG methods as well as we will try to calculate physical quantities related to the Heisenberg chain.

# Chapter 4

# Result and Conclusion

In this chapter, we will discuss various results; some of them are about the empirical observation for the characterization of the DMRG algorithm other results are related to the physical properties of the model system. All of this result is acquired for a particular model system called 1-dimensional Heisenberg Chain. We will discuss the result obtained from the DMRG algorithm for the model system. I would like to intimate that all the results we mention here is just a reproduction of results from various research papers (White [1992], White [1993],White und Huse [1993]) with the purpose of learning the algorithms.

## 4.1 Heisenberg Hamiltonian

Hamiltonian for Heisenberg chain is given by

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{4.1}$$

Where i is the site index. We would like to determine the properties of this system using the DMRG algorithm. For $J \geq 0$ the system is called anti-ferromagnetic and for $J \leq 0$ the system is ferromagnetic. We have studied the system with J=1 with open boundary condition.

## 4.2 Result obtained for the system

***Fast decay of Probability of states of reduced density matrix of system***

We have seen in earlier chapter 2 ( Equation 2.23) that the very fast decay of probability of states is essential for the DMRG algorithm to work properly. Here we will plot the result for 32 site spin half with m=50. Note the logarithmic scale.

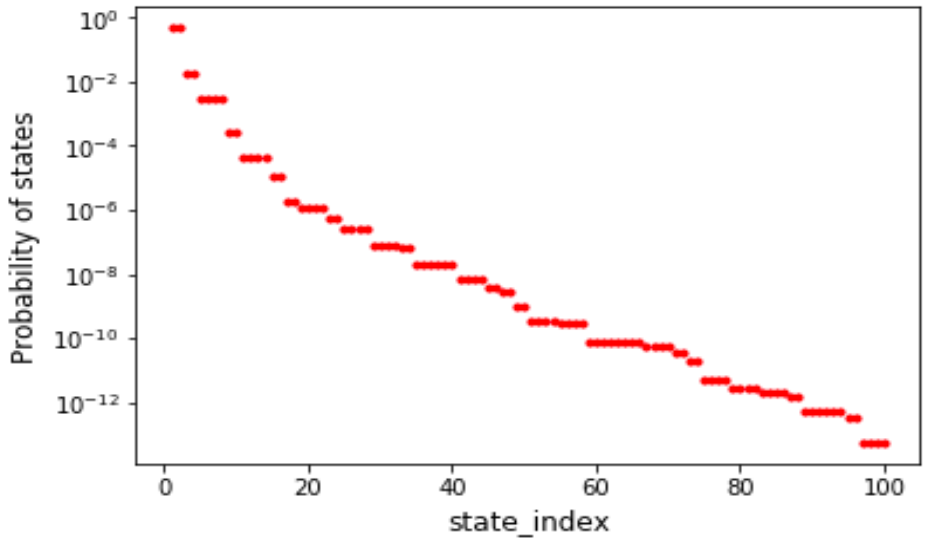


FIGURE 4.1: Probabilities of different states for spin half chain are plotted. Fast Decay of probability is conspicuous

In figure 4.2 we have plotted the sum of probability in the states vs the number of most probable states in the x-axis. It is visible in figure 4.2 that the first few states contain almost all the probability. A similar result is obtained for 32 sites spin-one chain with m=50.

We have seen from the Results in this subsection that the probability distribution is decaying fast, which was necessary for the DMRG algorithm to work properly. So we can now move on to study other results related to the study of our model system.

On the other hand, the probability decays much slower for more than one target state. In Figure 4.5 we plot the probability distribution for 32 site spin 1 chain. The much slower decay concerning a single target state is evident in Figure 4.5.

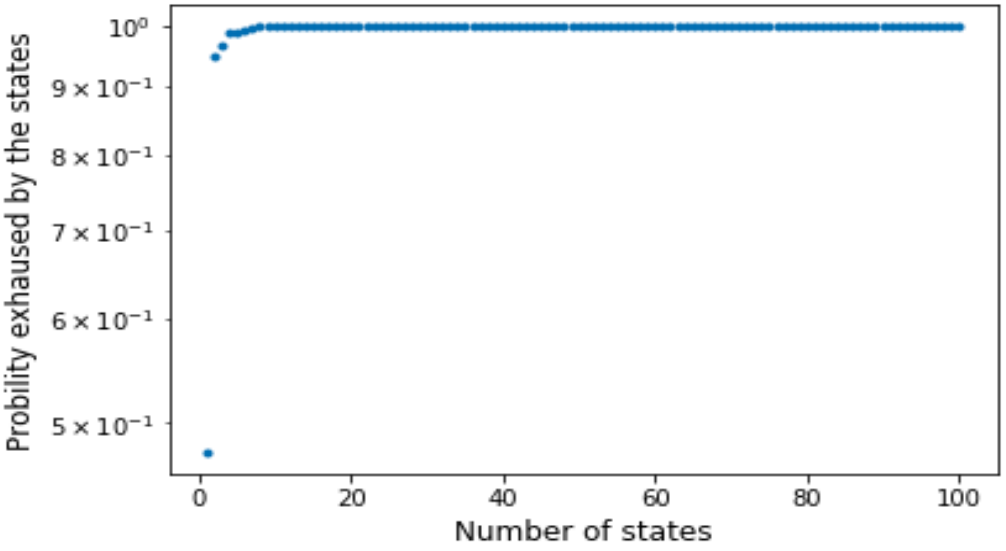


FIGURE 4.2: Probability contain in states is plotted

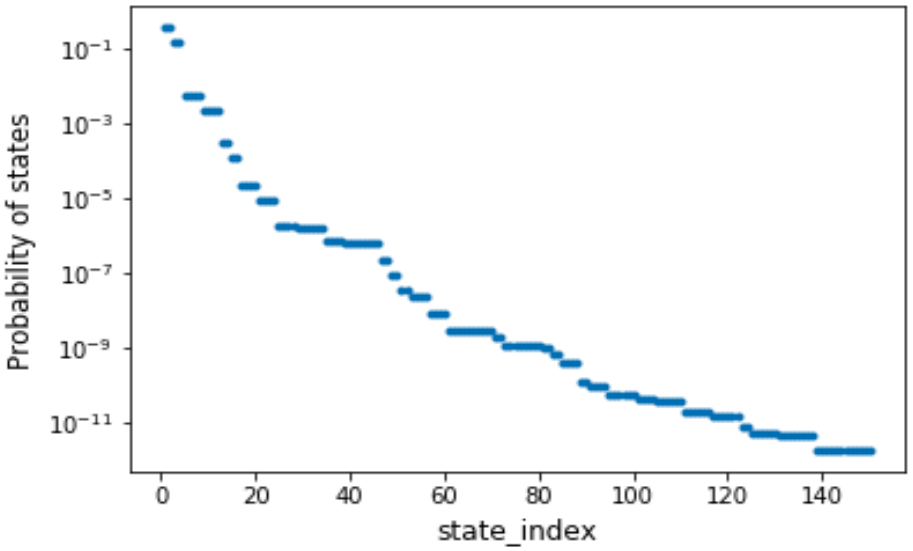


FIGURE 4.3: Probability of states is plotted
Fast decay of probability is again conspicuous

## 4.3 Energy calculation for Infinite and finite Systems

In this section, we discuss the energy calculated using the finite and infinite system DMRG.

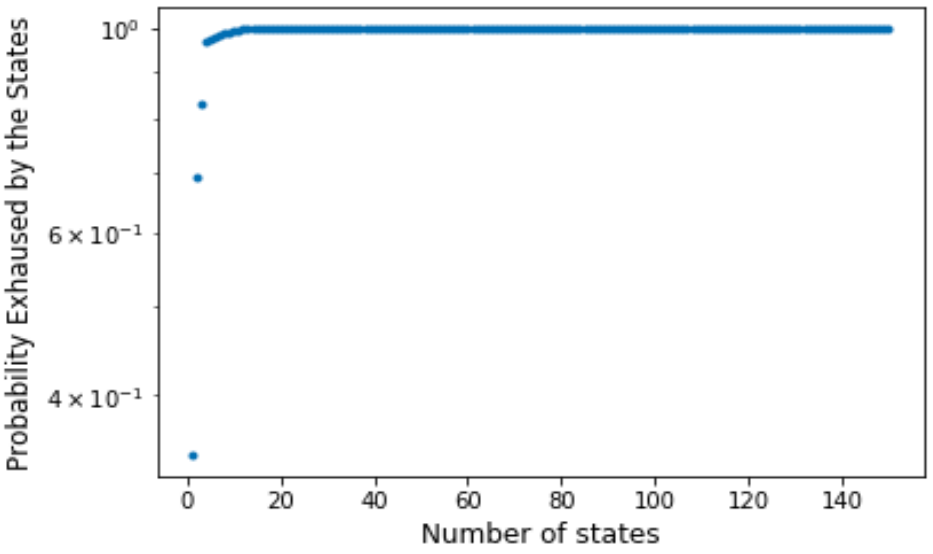


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FIGURE 4.4: Probability contained in the states is plotted

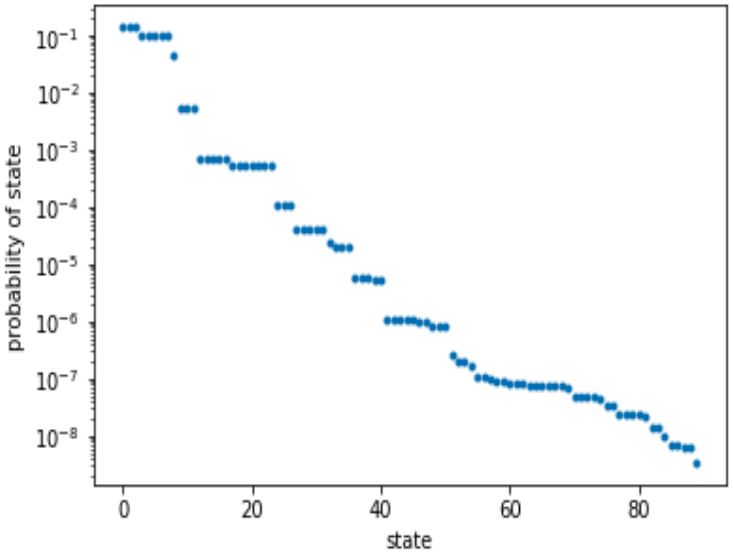


FIGURE 4.5: Probability Distribution when targeting first four state of the spin one chain

### 4.3.1 Ground energy for the infinite Spin half and Spin 1 Heisenberg chain

The energy calculated here is for j=1 in Equation 4.1. We have calculated per site energy for Spin half and Spin one Heisenberg chain. The energy calculated was obtained by the change in energy from one iteration to next till the energy obtained was

converged to eight decimal point. The target state used for the calculation was only the ground state of the superblock.

For infinite long spin half chain the calculated per site energy is given in Table 4.1 for various values of number of states kept (m).

| m | Energy | Truncation error |
|---|---|---|
| 16 | $-0.44307726$ | $4.4812 \times 10^{-6}$ |
| 24 | $-0.4431308$ | $2.6820 \times 10^{-6}$ |
| 32 | $-0.44313896$ | $1.8903 \times 10^{-6}$ |
| 48 | $-0.4431442$ | $3.7802 \times 10^{-7}$ |

TABLE 4.1: Per site Energy for infinitely long spin Half chain

For spin one chain the persite energy calculated is given below.

| m | Energy | Truncation error |
|---|---|---|
| 16 | $-1.40141925$ | $1.0665 \times 10^{-5}$ |
| 24 | $-1.40148143$ | $3.9377 \times 10^{-7}$ |

TABLE 4.2: Per site Energy for infinitely long spin 1 chain

For Spin half chain the exact energy is calculated using the Bathe-ansatz the exact per site energy for the spin half chain is $-\ln 2 + \frac{1}{4} = -0.443147....$ The Result calculated using DMRG is correct to the fifth decimal point. Energy calculated using Infinite DMRG for Spin 1 chain is also matching with the energy calculate with monte-carlo method (Nightingale und Blöte [1986], Liang [1990],White [1992]).

### 4.3.2 Low lying energy calculated for the finite system

We can calculate ground state and first excited energy for the finite Spin half and spin chain using finite DMRG algorithm. We have compared the outcome with the exact diagonalization. In Table 4.4 we show the calculated relative error $|\frac{E_{DMRG}-E_{exact}}{E_{exact}}|$ in energy. From Table 4.4 it is obvious that the energy calculated using DMRG is almost exact.

We have already seen that the energy calculated using the DMRG algorithm is exceptionally accurate. Also we have observed that the accuracy of result increases with increasing m. We would like to see the effect of keeping more number of state (m) for the calculation of energy. The Figure 4.6 provides the relative error in ground state

| L | $\Delta E_{gs}$ | $\Delta E_{1^{st}ES}$ |
|---|---|---|
| 12 | $3.49 \times 10^{-15}$ | $2.19 \times 10^{-15}$ |
| 14 | $6.28 \times 10^{-14}$ | $3.19 \times 10^{-12}$ |
| 16 | $1.89 \times 10^{-12}$ | $3.51 \times 10^{-11}$ |
| 18 | $1.11 \times 10^{-11}$ | $6.52 \times 10^{-11}$ |
| 20 | $3.61 \times 10^{-11}$ | $3.06 \times 10^{-10}$ |

TABLE 4.3: Relative error in energy of spin half chain of length L

energy of a 32 site Spin half and Spin one chain. Exact energy is calculated using the DMRG itself. The exact result is obtained for very large m.

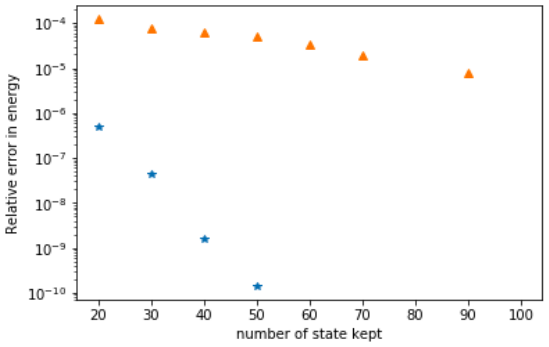


FIGURE 4.6: Relative Error in energy
calculated by keeping different degree of freedom

In Figure 4.6 the red triangles are for spin 1, and blue stars are for spin half. We see that the decrease in relative error in energy is approximately exponential with an increase in m (note the "almost" linear curve and logarithmic y-axis).

## 4.4 Gap calculation

In the study of the quantum spin chain the gap calculation if considered as an important phenomenon. We have calculated the gap for the spin half and spin one chain. According to Haldane prediction, we found a finite gap for the infinitely long spin chain. We also found that the gap for the spin half chain is zero, predicted by Bathe-ansatz.

We have seen that the gap for the infinitely long spin chain is going to zero for the spin half chain, on the other hand, the gap for the spin one chain is approximately 0.41 for spin one chain.

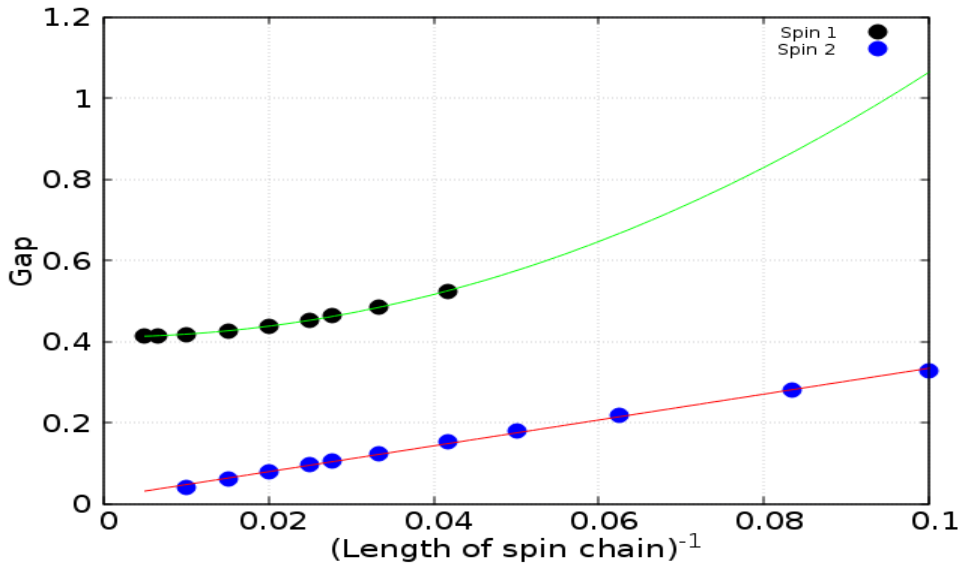


FIGURE 4.7: Finite gap of spin one Heisenberg chain

## 4.5 correlation

We have reproduced the $\langle S_i^z S_j^z \rangle$ correlation for spin one chain mentioned in White und Huse [1993]. The correlation was calculated using the method described in Figure 3.3. The correlation is expected to behave as,

$$c(l) \propto (-1)^l \left(\frac{\pi\xi}{2l}\right) \exp\left(-\frac{l}{\xi}\right) \tag{4.2}$$

In Figure 4.8, we can see the exponential decrease of the correlation with length (note the logarithmic y-axis).

## 4.6 Gap calculation using conserved Quantum number

We have discussed earlier 3.3 that we can use the conservation properties of Hamiltonian to pick states with a given sector. Since we are aware that the ground state of spin one anti-ferromagnetic Heisenberg chain has total Spin $S_i^z = 0$ and Next state has total spin $S_i^z = 1$. These four states are degenerate for the infinitely long chain.

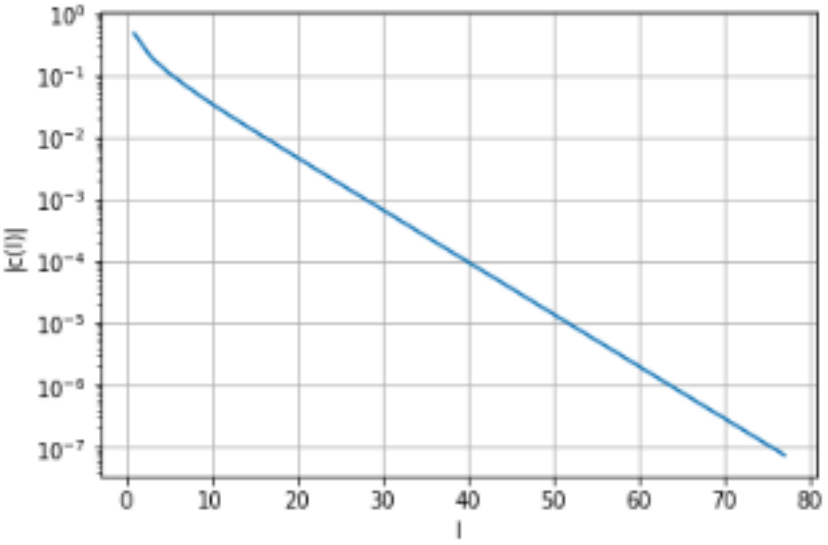


FIGURE 4.8: $\left\langle S_i^z S_j^z \right\rangle$ correlation using infinite system method, l is distance between the sites i and j.

But the energy of next states lies in spin sector $S_i^z = 2$ . We can use this property to pick ground energy with $S_i^z = 1$ and excited state with $S_i^z = 2$ and do the gap calculation once more with this method. The result obtained with this method converses very quickly compared to another method of calculating excitation energy. Here we provide the result obtained using the conserved quantum number method.

| L | *GroundState* | *ExcitedState* |
|---|---|---|
| 10 | −1.275622917649155 | −1.1990726099217743 |
| 12 | −1.2980723851656533 | −1.2404285104896537 |
| 16 | −1.3250375315880778 | −1.2875725273575762 |
| 20 | −1.3407105424292758 | −1.3134250848153275 |
| 26 | −1.3549130157090992 | −1.3357166808762275 |
| 40 | −1.3712699301414524 | −1.3599679321793097 |
| 50 | −1.3773166398625138 | −1.3685573347150555 |
| 150 | −1.3934285790225758 | −1.3906704451115068 |
| 200 | −1.3954424420369702 | −1.39338057146293 |

TABLE 4.4: Excitation energy calculation for the Spin one Heisenberg chain.

The time taken by the program for calculation of excitation energy using conserved quantum number is significantly less than the time taken by the program to calculate the excitation energy by targeting many states. The time taken by many state algorithm is about a few hours, whereas the time taken by the conserved quantum number algorithm is just a few minutes.

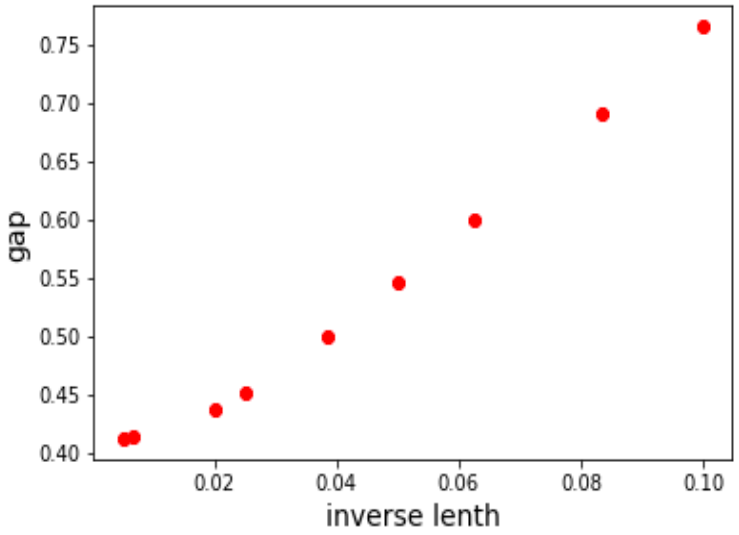


FIGURE 4.9: Gap Plot for spin one Using Conserved Quantum Number

## 4.7 Summary

In this chapter we verified the fact that the almost all of the probability of the states of system and environment is exhausted by very few states. This property make sure that the error in calculated value is negligible.

we calculated the ground state energy of finite and infinite, spin half and spin one Heisenberg chain. The result turns out be almost exact.

we calculated the gap for the spin half and spin one chain using two different methods. We found the well known result of finite gap for the infinite spin one chain and zero gap for the infinite spin half chain.

We also calculated the $\langle S_i^z S_j^Z \rangle$ correlation for spin one chain for particle and confirm the fact that the $\langle S_i^z S_j^Z \rangle$ correlation decay exponentially with distance between sites for site far from each other.

# Appendix A

# Program for the Wilson's Renormalization

```
import numpy as np
from numpy import linalg as LA

m=1
A=np.array([[2,-1],[-1,2]])
c=np.array([[0,0],[-1,0]])
#defining trucation
def trunc_diagonalize(x,y):
    e, v = LA.eigh(x)          #finding eigenvalue an eigenvetor of a hermitian matrix {in
     incerasing order of eigenvalues}
    print('e'+str(k)+'=',e)    #printing to know how many sites we are considering in each step
    V=v.copy()
    np.transpose(V)
    V=V.tolist()

    if 2*m > 8:
        w=np.zeros((2*m,8))
        w=v[0:2*m,0:8]              #filling first 8 column(fisr 8 eigenvectors) in blank matrix w
        v=w
    b=np.matmul(x,v)                #H{bar}=A{dagger}*H*A
    B=np.matmul(v.conj().T,b)       #above
    x=np.matmul(y,v)                #T{BAR}=A{DAGGER}*T*A
    C=np.matmul(v.conj().T,x)       #above
    d=C.copy()                      #T{dagger}
    D=d.conj().T                    #above
    return B,C,D                    # return H{BAR},T{BAR},T{BAR}{DAGGER}
k=1
B,C,D=trunc_diagonalize(A,c)
print('B=',B,'\n','C=',C,'\n','D=',D)
m=2
k=2
while k<12:

    print('eigenvalue'+str(k))
    if m >8:
        m=8
    A = np.zeros((2*m,2*m))
    A[0:m,0:m]=B
    A[m:2*m,m:2*m]=B
    A[0:m,m:2*m]=C
    A[m:2*m,0:m]=D

    c=np.zeros((2*m,2*m))
```

```
43          c[m:2*m, 0:m]=C
44          C=c
45
46          B,C,D=trunc_diagonalize(A, c)
47
48          m=2*m
49          k=k+1
```

# Appendix B

# Program for the White's Real Space Renormalization Method

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
"""
Created on Wed Apr  4 01:53:53 2018
@author: Vishal
"""

import numpy as np

from numpy import linalg as la

H1=np.zeros((8,8))   #fixed fixed
for i in range(8):
      for j in range(8):
          if i==j:
              H1[i][i]=2
          if i==j+1 or i==j-1:
              H1[i][j]=-1
H1[0][0]=2
H1[7][7]=2
H2=np.zeros((8,8))   #fixed freee
for i in range(8):
      for j in range(8):
          if i==j:
              H2[i][i]=2
          if i==j+1 or i==j-1:
              H2[i][j]=-1
H2[0][0]=2
H2[7][7]=1
H3=np.zeros((8,8))   #free fixed
for i in range(8):
      for j in range(8):
          if i==j:
              H3[i][i]=2
          if i==j+1 or i==j-1:
              H3[i][j]=-1
H3[0][0]=1
H3[7][7]=2
H4=np.zeros((8,8))    #free free
for i in range(8):
      for j in range(8):
          if i==j:
```

```
                H4[i][i]=2
            if i==j+1 or i==j-1:
                H4[i][j]=-1
H4[0][0]=1
H4[7][7]=1




U=np.zeros((8,8))
U[7][0]=-1


#defining scmidt decmposition will be used later
def Gram_schmidt(x):
    l=len(x[:,0])
    for i in range(8):
        y=np.zeros((l,1))
        y=x[:,i].copy()
        if i==0:
            x[:,0]=np.multiply(1/(np.linalg.norm(y)),y)
        if i>0:
            for j in range(i):
                y=np.subtract(y,np.multiply(np.matmul(x[:,j].conj().T,x[:,i]),x[:,j]))
            x[:,i]=np.multiply(1/(np.linalg.norm(y)),y)

    return(x)

k=8
i=3
m=8
while k<=2048:

    w=np.zeros((m,8))
    e,v1=la.eigh(H1)          #for 2048 block printing energy calculated by free fixed truncation
    if k==2048:
        print("energy=",e)
    w[0:m,0:2]=v1[0:m,0:2]  #defing blank matrix w and then filing its column by eigenvector
     obtained from various hamiltonian obtained by varions boundary condition
    e,v2=la.eigh(H2)
    w[0:m,2:4]=v2[0:m,0:2]
    e,v3=la.eigh(H3)
    w[0:m,4:6]=v3[0:m,0:2]
    e,v4=la.eigh(H4)
    w[0:m,6:8]=v4[0:m,0:2]

    y=w.copy()
    q=Gram_schmidt(y)   #gram scmidt process for orthogonalization of columns of matrice

    s=q.copy()
    t=q.copy()
    u=q.copy()
    v=q.copy()


    #changing the basis to colums of q
    a1=np.matmul(H1,s)
    A1=np.matmul(s.conj().T,a1)
    a2=np.matmul(H2,t)
    A2=np.matmul(t.conj().T,a2)
    a3=np.matmul(H3,u)
    A3=np.matmul(u.conj().T,a3)
    a4=np.matmul(H4,v)
    A4=np.matmul(v.conj().T,a4)


    t=np.matmul(U,q)
    T=np.matmul(q.conj().T,t)
    Copy=T.copy()
    Y=Copy.conj().T

```

```
113     #defining hamiltonian for bigger block consisting of two similer block
114
115     B1=np.zeros((16,16))
116     B1[0:8,0:8]=A1[0:8,0:8]
117     B1[8:16,8:16]=A1[0:8,0:8]
118     B1[0:8,8:16]=T[0:8,0:8]
119     B1[8:16,0:8]=Y[0:8,0:8]
120
121     B2=np.zeros((16,16))
122     B2[0:8,0:8]=A1[0:8,0:8]
123     B2[8:16,8:16]=A2[0:8,0:8]
124     B2[0:8,8:16]=T[0:8,0:8]
125     B2[8:16,0:8]=Y[0:8,0:8]
126
127     B3=np.zeros((16,16))
128     B3[0:8,0:8]=A3[0:8,0:8]
129     B3[8:16,8:16]=A1[0:8,0:8]
130     B3[0:8,8:16]=T[0:8,0:8]
131     B3[8:16,0:8]=Y[0:8,0:8]
132
133     B4=np.zeros((16,16))
134     B4[0:8,0:8]=A3[0:8,0:8]
135     B4[8:16,8:16]=A2[0:8,0:8]
136     B4[0:8,8:16]=T[0:8,0:8]
137     B4[8:16,0:8]=Y[0:8,0:8]
138
139     H1=B1
140     H2=B2
141     H3=B3
142     H4=B4
143
144     #defining connecting term of hamiltoian for bigger block
145     t=np.zeros((16,16))
146     t[8:16,0:8]=T[0:8,0:8]
147     U=t
148
149     m=16
150     k=2*k
151      i=i+1
```

# Appendix C

# Program for the Infinite system Algorithm for spin Half Heisenberg Chain

```
1
2  import numpy as np
3  from numpy import linalg as la
4  from scipy.sparse import kron, identity
5  from scipy.sparse.linalg import eigsh
6  #from scipy.sparse import csr_matrix
7
8  sp1=np.zeros((2,2))
9  sp1[0,1]=1.0
10 sm1=sp1.transpose().conjugate()
11
12 sz1=np.zeros((2,2))
13 sz1[0,0]=0.5
14 sz1[1,1]=-0.5
15 H1=np.zeros((2,2))
16 I=identity(2)
17 m=50
18
19
20 twositeH=np.kron(sz1,sz1)+(np.kron(sp1,sm1)+np.kron(sm1,sp1))*(1/2)
21 foursiteH=kron(kron(twositeH,I),I)+kron(I,kron(I,twositeH))+kron(I,kron(twositeH,I))
22
23 e,v=eigsh(foursiteH,k=1)
24
25 psi_gs=v[:,0]
26
27 def reduceddensitymatrix(psi,dimns):
28     reduceddensitymatrix=np.zeros((dimns,dimns))
29     for i in range(dimns):
30         for j in range(dimns):
31             a=0
32             for k in range(dimns):
33                 b=np.conjugate(psi[dimns*j+k])*psi[dimns*i+k]
34                 a=a+b
35             reduceddensitymatrix[i,j]=a
36     return reduceddensitymatrix
37
38
```

```
dim=4
rho=reduceddensitymatrix(psi_gs,dim)
k,v=la.eigh(rho)
#print('e=','\n',k)
#print('v=','\n',v)
transformation_matrix=v
#print(kron(I,sm1).shape)
#print(e,'\n',v)

H_rot_trun=transformation_matrix.conjugate().transpose().dot(twositeH.dot(transformation_matrix))
sz_rot_trun=transformation_matrix.conjugate().transpose().dot(kron(I,sz1).dot(
    transformation_matrix))
sp_rot_trun=transformation_matrix.conjugate().transpose().dot(kron(I,sp1).dot(
    transformation_matrix))
sm_rot_trun=transformation_matrix.conjugate().transpose().dot(kron(I,sm1).dot(
    transformation_matrix))

basis_size=4

def H2(sz_rot_trun,sp_rot_trun,sm_rot_trun,sz1,sp1,sm1):
    return kron(sz_rot_trun,sz1)+(1/2)*(kron(sp_rot_trun,sm1)+kron(sm_rot_trun,sp1))

def enlarge_block(basis_size,H_rot_trun,sz_rot_trun,sp_rot_trun,sm_rot_trun,sz1,sp1,sm1):
    sz=kron(identity(min(m,basis_size)),sz1)
    sp=kron(identity(min(m,basis_size)),sp1)
    sm=kron(identity(min(m,basis_size)),sm1)
    H_left_enlarge=kron(H_rot_trun,I)+H2(sz_rot_trun,sp_rot_trun,sm_rot_trun,sz1,sp1,sm1)
    return sz,sp,sm,H_left_enlarge
enlarge_block(basis_size,H_rot_trun,sz_rot_trun,sp_rot_trun,sm_rot_trun,sz1,sp1,sm1)

#def    superblock_Hamiltonian(sz,sp,sm,H_left_enlarge,basis_size):
#    superblock_Hamiltonian=kron(H_left_enlarge,identity(2*basis_size))+kron(identity(2*basis_size)
    ,H_left_enlarge)+H2(sz,sp,sm,sz,sp,sm)
#    return superblock_Hamiltonian

def rotate_and_truncate(sz,sp,sm,H_left_enlarge, transformation_matrix):
    sz_rot_trun=transformation_matrix.conjugate().transpose().dot(sz.dot(transformation_matrix))
    sp_rot_trun=transformation_matrix.conjugate().transpose().dot(sp.dot(transformation_matrix))
    sm_rot_trun=transformation_matrix.conjugate().transpose().dot(sm.dot(transformation_matrix))
    H_rot_trun=transformation_matrix.conjugate().transpose().dot(H_left_enlarge.dot(
    transformation_matrix))
    return sz_rot_trun,sp_rot_trun,sm_rot_trun,H_rot_trun
L=2

while L<=32:
    energy=[0,0]
    energy[0]=e
    sz,sp,sm,H_left_enlarge=enlarge_block(basis_size,H_rot_trun,sz_rot_trun,sp_rot_trun,
    sm_rot_trun,sz1,sp1,sm1)
    superblock_Hamiltonian=kron(H_left_enlarge,identity(min(2*m,2*basis_size)))+\
    kron(identity(min(2*m,2*basis_size)),H_left_enlarge)+H2(sz,sp,sm,sz,sp,sm)



    e,v=eigsh(superblock_Hamiltonian,k=1)
    q=2*L+2
    energy[1]=e

    psi_gs=v
    rho=reduceddensitymatrix(psi_gs,min(2*m,basis_size*2))


    g,v=la.eigh(rho)
    print(g)
    if 2*basis_size<=m:
        w=v
    else:

        w=v[:,2*min(m,basis_size)-m:2*min(m,basis_size)]
        print((energy[1]-energy[0])/2, 1-sum(g[2*min(m,basis_size)-m:2*min(m,basis_size)]),m)
    transformation_matrix=w
```

```
104
105     sz_rot_trun , sp_rot_trun , sm_rot_trun , H_rot_trun=rotate_and_truncate(sz , sp , sm, H_left_enlarge ,
         transformation_matrix)
106     basis_size=2*basis_size
107     L=L+1
```

# Bibliography


[Bray und Chui 1979] Bray, JW ; Chui, ST: Computer renormalization-group calculations of 2 k F and 4 k F correlation functions of the one-dimensional Hubbard model. In: *Physical Review B* 19 (1979), Nr. 10, S. 4876

[Feiguin 2011] Feiguin, Adrian E.: The Density Matrix Renormalization Group and its time-dependent variants. In: *AIP Conference Proceedings* Bd. 1419 AIP (Veranst.), 2011, S. 5–92

[Garrison und Mishmash 2013] Garrison, James R. ; Mishmash, Ryan V.: *Simple DMRG*. https://github.com/simple-dmrg/simple-dmrg/. 2013

[Guttag 2016] Guttag, John: *Introduction to Computation and Programming Using Python: With Application to Understanding Data*. MIT Press, 2016

[Horodecki u. a. 2009] Horodecki, Ryszard ; Horodecki, Paweł ; Horodecki, Michał ; Horodecki, Karol: Quantum entanglement. In: *Reviews of modern physics* 81 (2009), Nr. 2, S. 865

[Lee 1979] Lee, Patrick A.: Real-Space Scaling Studies of Localization. In: *Physical Review Letters* 42 (1979), Nr. 22, S. 1492

[Liang 1990] Liang, Shoudan: Monte Carlo calculations of the correlation functions for Heisenberg spin chains at T= 0. In: *Physical review letters* 64 (1990), Nr. 13, S. 1597

[Nielsen und Chuang 2002] Nielsen, Michael A. ; Chuang, Isaac: *Quantum computation and quantum information*. 2002

[Nightingale und Blöte 1986] Nightingale, MP ; Blöte, HWJ: Gap of the linear spin-1 Heisenberg antiferromagnet: A Monte Carlo calculation. In: *Physical Review B* 33 (1986), Nr. 1, S. 659

[Osborne und Nielsen 2002] Osborne, Tobias J. ; Nielsen, Michael A.: Entanglement, quantum phase transitions, and density matrix renormalization. In: *Quantum Information Processing* 1 (2002), Nr. 1-2, S. 45–53

[Peschel u. a. 1999] Peschel, I ; Wang, X ; Kaulke, M ; Hallberg, K: *Density-Matrix Renormalization, vol. 528 of Lecture Notes in Physics*. 1999

[Preskill 1998] Preskill, John: Lecture notes for physics 229: Quantum information and computation. In: *California Institute of Technology* 16 (1998)

[Schollwöck 2005] Schollwöck, Ulrich: The density-matrix renormalization group. In: *Reviews of modern physics* 77 (2005), Nr. 1, S. 259

[White 1992] White, Steven R.: Density matrix formulation for quantum renormalization groups. In: *Physical review letters* 69 (1992), Nr. 19, S. 2863

[White 1993] White, Steven R.: Density-matrix algorithms for quantum renormalization groups. In: *Physical Review B* 48 (1993), Nr. 14, S. 10345

[White 1998] White, Steven R.: Strongly correlated electron systems and the density matrix renormalization group. In: *Physics Reports* 301 (1998), Nr. 1-3, S. 187–204

[White und Huse 1993] White, Steven R. ; Huse, David A.: Numerical renormalization-group study of low-lying eigenstates of the antiferromagnetic S= 1 Heisenberg chain. In: *Physical Review B* 48 (1993), Nr. 6, S. 3844

[White und Noack 1992] White, Steven R. ; Noack, Reinhard M.: Real-space quantum renormalization groups. In: *Physical review letters* 68 (1992), Nr. 24, S. 3487

[Wilson 1975] Wilson, Kenneth G.: The renormalization group: Critical phenomena and the Kondo problem. In: *Reviews of modern physics* 47 (1975), Nr. 4, S. 773