Numerical and Analytical Explorations in the Matrix Product Representations for Qudit States

Dissertation submitted to
Visvesvaraya National Institute of Technology, Nagpur
in partial fulfillment of requirement for the award of degree of

Master of Science
In
Physics

By
Bhute Utkarsha Prasad Sanjeevani
(MS20PHY009)

Under the supervision of

Dr. M. S. Ramkarthik
Assistant Professor
Department of Physics,
VNIT Nagpur

DEPARTMENT OF PHYSICS
VISVESVARAYA NATIONAL INSTITUTE OF TECHNOLOGY, NAGPUR
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Dedicated to my mother Sanjeevani Bhute and father Prasad Bhute

VISVESVARAYA NATIONAL INSTITUTE OF TECHNOLOGY, NAGPUR

DEPARTMENT OF PHYSICS

Dissertation approval sheet

Dissertation entitled "Numerical and Analytical Explorations in the Matrix Product Representations for Qudit States" by **Bhute Utkarsha Prasad Sanjeevani** is approved for the degree of Master of Science in Physics.

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(*Name*:)	(*Name*:)
Supervisor	**External Examiner**

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(*Name*:)
Chairman

Department of PHYSICS

Visvesvaraya National Institute of Technology, Nagpur

Declaration

I, **Bhute Utkarsha Prasad Sanjeevani,** hereby declare that this dissertation titled **"Numerical and Analytical Explorations in the Matrix Product Representations for Qudit States"** is carried out by me in the Department of Physics of Visvesvaraya National Institute of Technology, Nagpur. The work is original and has not been submitted earlier whole or in part for the award of any degree/diploma at this or any other Institution / University.

Name: Bhute Utkarsha Prasad Sanjeevani

Date:

Certificate

This to certify that the dissertation titled "**Numerical and Analytical Explorations in the Matrix Product Representations for Qudit States"** is submitted by **Bhute Utkarsha Prasad Sanjeevani** in partial fulfillment of the requirements for the award of the degree of Master of Science in, VNIT Nagpur. The work is comprehensive, complete and fit for finale valuation.

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Date:

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Certified that M.Sc. Dissertation titled "**Numerical and Analytical Explorations in the Matrix Product Representations for Qudit States**" submitted by **Bhute Utkarsha Prasad Sanjeevani** Enrollment No. MS20PHY009, ID No. 25112 is original in nature and not copied from any literature material. Due credit has been given to the original researcher wherever referred.

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ORIGINALITY REPORT

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Bhute Utkarsha Prasad Sanjeevani

ABSTRACT

Quantum many-body systems are challenging to deal with because the underlying Hilbert space grows exponentially. As a result, the *matrix product state* (MPS) representation is ideal for quantum many-body states where correlations are formed in a 'local' manner. The density matrix renormalization group (DMRG) technique, which is the foundation for a large number of recent breakthroughs in quantum information and condensed matter theory, is based on this MPS representation.

This thesis examines the left canonical MPS (LCMPS), right canonical MPS (RCMPS), and mixed canonical MPS (MCMPS) representations in depth, with a special emphasis on the reshaped matrices obtained in the representation for any qudit state. With analytical and numerical calculations, we have discussed the whole procedure of the MPS representation in depth. We have discovered interesting patterns and regions pertaining to the reshaped matrices. Using the novel methods we have developed, one can predict the dimensions of the reshaped matrices very easily for any qudit state. Generalized codes are written for LCMPS, RCMPS and MCMPS which can work for *any* value of d and L and thus for any pure quantum state of any qudits and for *any* partition p (in case of MCMPS). We have also worked on several operations on the MPS representation of a quantum state, such as overlap, matrix elements, and expectation value, and developed generalised codes for these operations. In addition, the procedure for obtaining reduced density operators from MPS representations of any qudit quantum state has been thoroughly explained and the generalized codes are written for it which can work for any pure quantum state and any bipartition.

List of Figures

Contents

Chapter 1

Introduction

1.1 The qubit system

A classical bit of information is represented by a system that can be in either of two states 0 or 1 like a two way electrical switch. Just as a classical bit, the two most common states for a qubit (quantum bit) are the states $|0\rangle$ and $|1\rangle$. A qubit is the fundamental quantum state representing the smallest unit of quantum information containing one bit of classical information accessible by measurement [1]. The actual difference between a classical and quantum state is that, a classical bit can have a state only of either 0 or 1 whereas a qubit can be in a linear combination of states, also known as superposition. In other words, we can write a quantum state in a more general form as,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{1.1}$$

where α and β are complex numbers satisfying the condition $|\alpha|^2 + |\beta|^2 = 1$.

We can also think of $|\psi\rangle$ as a vector in the Hilbert space $\mathcal{H}_2$ of dimension 2 spanned by the two linearly independent orthonormal basis states $|0\rangle$ and $|1\rangle$. A Hilbert space is an inner product space which is complete with respect to the norm induced by the inner product. The qubits can be realized physically by the two states of an electron orbiting an atom or by the two directions of the spin (intrinsic angular momentum) of a particle or by the two polarizations of a photon. Let's take a spin-half particle as an example. If we were to measure its spin along the Z-axis, we would observe that it is either up (in $+Z$ direction) or down (in $-Z$ direction). In

many physics papers, the two states are denoted as $|\uparrow\rangle$ and $|\downarrow\rangle$. For computational purposes, we can simply regard them as $|0\rangle$ and $|1\rangle$.

1.1.1 Matrix representation of a qubit state

A quantum state in the qubit space can be represented as a unit (column) vector in the $\mathcal{H}_2$ space, spanned by the following two basis states,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1.2}$$

which are the eigenstates of the Paulli Z matrix and are also called as the computational basis states. Hence, we can write a general single qubit state $|\psi\rangle$ as,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \tag{1.3}$$

1.1.2 Multi-qubit system

A general single qubit state can be written as,

$$|\psi_1\rangle = C_0|0\rangle + C_1|1\rangle = \sum_{i_1=0}^{1} C_{i_1}|i_1\rangle. \tag{1.4}$$

The dimension of the Hilbert space $\mathcal{H}_2$ for a single qubit is 2, as it as only two basis states $\{|0\rangle, |1\rangle \in \mathcal{H}_2\}$. Now for a two qubit system, we have four possible computational basis states, namely $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. Thus the dimension of the Hilbert space $\mathcal{H}_2^{\otimes 2}$ for a two qubit system is $2^2 = 4$ and we can write a general form of the two-qubit state as follows,

$$|\psi_2\rangle = C_{00}|00\rangle + C_{01}|01\rangle + C_{10}|10\rangle + C_{11}|11\rangle = \sum_{i_1=0}^{1}\sum_{i_2=0}^{1} C_{i_1 i_2}|i_1\rangle|i_2\rangle. \tag{1.5}$$

Similarly, the dimension of the Hilbert space $\mathcal{H}_2^{\otimes 3}$ for a three qubit system is $2^3 = 8$ and a general three qubit state can be written as,

$$|\psi_3\rangle = \sum_{i_1=0}^{1}\sum_{i_2=0}^{1}\sum_{i_3=0}^{1} C_{i_1 i_2 i_3}|i_1\rangle|i_2\rangle|i_3\rangle. \tag{1.6}$$

Now consider a system of n qubits where each qubit is described by a two-dimensional Hilbert space $\mathcal{H}_2$ which corresponds to a single qubit orthonormal basis $\{|0\rangle, |1\rangle \in \mathcal{H}_2\}$. Then the dimension of the Hilbert space $\mathcal{H}_2^{\otimes n}$ for a n qubit system is 2^n and a general pure state of n qubits $|\psi_n\rangle \in \mathcal{H}_2^{\otimes n}$ is given by,

$$|\psi_n\rangle = \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_n=0}^{1} C_{i_1 i_2 \cdots i_n} \, |i_1 \, i_2 \cdots i_n\rangle. \tag{1.7}$$

We can see that as the number of qubits (n) increases, the dimension of the Hilbert space grows exponentially as 2^n.

1.1.3 Matrix representation of a multi-qubit state

Consider a general two qubit state Eq.[1.5]. It can be represented as a unit (column) vector in the $\mathcal{H}_2^{\otimes 2}$ space, spanned by the following four basis states,

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{1.8}$$

So, we can write a general two qubit state $|\psi\rangle$ as,

$$|\psi\rangle = C_{00} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + C_{01} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + C_{10} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + C_{11} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} C_{00} \\ C_{01} \\ C_{10} \\ C_{11} \end{pmatrix}. \tag{1.9}$$

The matrix representing a single qubit state will be of dimension $[2 \times 1]$ and the matrix representing a two qubit state will be of dimension $[2^2 \times 1]$. Similarly, a quantum state in the n-qubit space can be represented as a unit (column) vector in the $\mathcal{H}_2^{\otimes n}$ space, spanned by 2^n basis states and the matrix representing this quantum state will be of dimension $[2^n \times 1]$.

1.2 The qudit system

We have seen that a state of single qubit in the $2-$dimensional Hilbert space is a superposition of 2 basis states $\{|0\rangle, |1\rangle \in \mathcal{H}_2\}$. Suppose we consider a particle whose state is in superposition of d basis states. We will call this particle a 'qudit'. Thus a state in the $d-$dimensional qudit space [2] is a superposition of d basis states and it can be written as,

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + \cdots + \alpha_{d-1}|d-1\rangle, \tag{1.10}$$

where $|\alpha_0|^2 + |\alpha_1|^2 + \cdots + |\alpha_{d-1}|^2 = 1$.

A Hilbert space $\mathcal{H}$ of dimension $d = 2$ is referred to as a qubit space, one with $d = 3$ is referred to as a qutrit space and the generic term for any $d > 2$ is the qudit space. A spin-half particle, like an electron, is a natural 'qubit' system, whereas a spin-1 particle, like a system of two electrons, is a 'qutrit' system [3]. Theoretically the particles are allowed to have spin quantum number of 0, $\frac{1}{2}$, 1, $\frac{3}{2}$, $2, \cdots$ etc. $d = 2s + 1$, where s is the spin of particle. For spin-half particle $s = \frac{1}{2}$, we get $d = 2$ 'qubit system' and for spin-one particle $s = 1$, we get $d = 3$ 'qutrit system'.

We can consider an example to better understand the concept of 'qudit'. A qubit is having only two states; so we can realize it as a two way switch. A 'qutrit' is a three way switch. Similarly a 'qudit' is a switch with d states. This is schematically shown in Fig.[1.1] below.

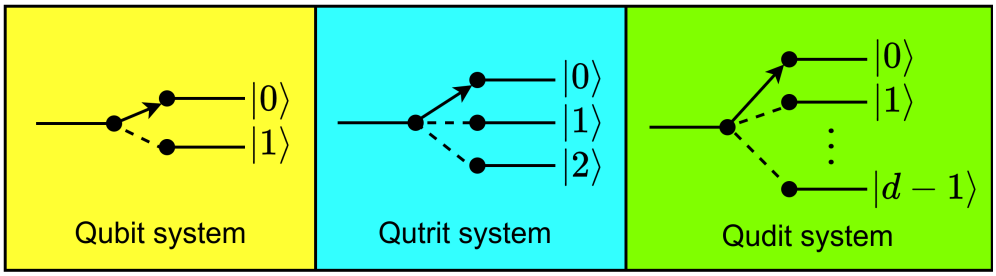


Figure 1.1: Difference between qubit and qudit system

1.2.1 Matrix representation of a qudit state

A quantum state in the qubit system can be represented as a unit (column) vector in the $\mathcal{H}_2$ space, spanned by the two basis states $\{|0\rangle, |1\rangle \in \mathcal{H}_2\}$. Similarly, a qudit state is a unit vector in $\mathcal{H}_d$ space, spanned by the d basis states, $\{|0\rangle, |1\rangle, \cdots, |d-1\rangle \in \mathcal{H}_d\}$, given as,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \; |1\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}, \; \cdots, \; |d-1\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}. \tag{1.11}$$

Then we can write a general state $|\psi\rangle$ as,

$$|\psi\rangle = \sum_{i=0}^{d-1} \alpha_i |i\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{d-1} \end{pmatrix}. \tag{1.12}$$

1.2.2 Multi-qudit system

A general single qudit state can be written as,

$$|\psi_1\rangle = \sum_{i_1=0}^{d-1} C_{i_1}|i_1\rangle. \tag{1.13}$$

The dimension of the Hilbert space $\mathcal{H}_d$ for a single qudit is d, as it as d basis states $\{|0\rangle, |1\rangle, \cdots, |d-1\rangle \in \mathcal{H}_d\}$.

Now for a two qudit system, we have d^2 possible computational basis states, namely $|00\rangle,\ |01\rangle, \cdots, |0d\rangle,\ |10\rangle,\ |11\rangle, \cdots, |1d\rangle,\ \cdots, |d0\rangle,\ |d1\rangle, \cdots, |dd\rangle$. Thus the dimension of the Hilbert space $\mathcal{H}_d^{\otimes 2}$ for a two qudit system is d^2, and we can write a general form of the two-qudit state as follows,

$$|\psi_2\rangle = \sum_{i_1=0}^{d-1}\sum_{i_2=0}^{d-1} C_{i_1 i_2}|i_1\rangle|i_2\rangle. \tag{1.14}$$

Similarly, the dimension of the Hilbert space $\mathcal{H}_d^{\otimes 3}$ for a three qudit system is d^3, and a general three qudit state can be written as,

$$|\psi_3\rangle = \sum_{i_1=0}^{d-1}\sum_{i_2=0}^{d-1}\sum_{i_3=0}^{d-1} C_{i_1 i_2 i_3}|i_1\rangle|i_2\rangle|i_3\rangle. \tag{1.15}$$

Now consider n qudits where each qudit is described by a $d-$dimensional Hilbert space $\mathcal{H}_d$ which corresponds to a single qudit orthonormal basis $\{|0\rangle, |1\rangle, \cdots |d-1\rangle \in \mathcal{H}_d\}$. So the dimension of the Hilbert space $\mathcal{H}_d^{\otimes n}$ for a n qubit system is d^n, and a general pure state of n qudits $|\psi_n\rangle \in \mathcal{H}_d^{\otimes n}$ is given by,

$$|\psi_n\rangle = \sum_{i_1=0}^{d-1}\sum_{i_2=0}^{d-1}\cdots\sum_{i_n=0}^{d-1} C_{i_1 i_2 \cdots i_n}\ |i_1\ i_2 \cdots i_n\rangle. \tag{1.16}$$

We can see that as the number of qudits (n) increases, the dimension of the Hilbert space grows exponentially as d^n.

1.2.3 Matrix representation of a multi-qudit state

Consider a general two qudit state Eq.[1.14]. It can be represented as a unit (column) vector in the $\mathcal{H}_d^{\otimes 2}$ space. Let us consider $d = 3$ which is a 'qutrit' state. So the dimension of the Hilbert space will be $d^2 = 3^2 = 9$, spanned by the following nine basis states: $|00\rangle$, $|01\rangle$, $|02\rangle$, $|10\rangle$, $|11\rangle$, $|12\rangle$, $|20\rangle$, $|21\rangle$ and $|22\rangle$ where,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{1.17}$$

So, we can write a general two qudit state $|\psi\rangle$ as:

$$|\psi\rangle = \begin{pmatrix} C_{00} \\ C_{01} \\ C_{02} \\ C_{10} \\ C_{11} \\ C_{12} \\ C_{20} \\ C_{21} \\ C_{22} \end{pmatrix}. \tag{1.18}$$

To summarize, the matrix representing single qudit state will be of dimension $[d \times 1]$ and the matrix representing two qudit state will be of dimension $[d^2 \times 1]$. On the similar lines, a quantum state in the n-qudit space can be represented as a unit (column) vector in the $\mathcal{H}_d^{\otimes n}$ space, spanned by d^n basis states and the matrix representing this quantum state will be of dimension $[d^n \times 1]$.

1.3 The density operator

A ket vector in the Hilbert space denoted as $|\psi\rangle$ is actually not the most general way of defining a quantum state. The most general representation of a quantum system is written in terms of an operator $\hat{\rho}$ called the density operator, or density matrix [4].

Suppose a quantum system is in one of a number of states $|\psi_i\rangle$, where i is an index, with respective probabilities p_i. $\{p_i, |\psi_i\rangle\}$ is an ensemble of pure states. The density operator for the system is defined as,

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{1.19}$$

where $\sum_i p_i = 1$ and $0 \leqslant p_i \leqslant 1$. The density matrix is a positive semi-definite, Hermitian operator and $tr(\hat{\rho}) = 1$, which is the normalization condition of the density matrix.

1.3.1 Pure and mixed states

If all the p_i's in Eq.[1.19] are zero except one, the state is pure. In this case the density operator is simply $\hat{\rho} = |\psi\rangle\langle\psi|$. However if more than one p_i's in Eq.[1.19] are non zero then we call the state described by $\hat{\rho}$ as a mixed state. It is said to be a mixture of the different pure states in the ensemble for $\hat{\rho}$. There is a simple criterion for determining whether a state is pure or mixed: a pure state satisfies $tr(\hat{\rho}^2) = 1$, while a mixed state satisfies $tr(\hat{\rho}^2) < 1$.

1.3.2 The reduced density operator

If we have a system AB made up of 2 subsystems A and B, then if we know the combined state of the system as ρ^{AB}, the reduced density operator ρ^A will be the state of subsystem A and the reduced density operator ρ^B will be the state of subsystem B. ρ^A is formed from the density operator of the entire system by taking the partial trace over the state of system B. This represents the maximum information which is available about the system A alone, irrespective of the state of system B.

Suppose we have physical systems A and B, whose state is described by a density operator ρ^{AB}. The reduced density operator for system A is defined by,

$$\rho^A = tr_B(\rho^{AB}), \tag{1.20}$$

where tr_B is a map of operators known as the partial trace over system B. The partial trace is defined by,

$$tr_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) = |a_1\rangle\langle a_2|tr(|b_1\rangle\langle b_2|) = |a_1\rangle\langle a_2|\langle b_1|b_2\rangle, \tag{1.21}$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space of A, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of B.

Similarly the reduced density operator for system B is defined by,

$$\rho^B = tr_A(\rho^{AB}), \tag{1.22}$$

where tr_A is a map of operators known as the partial trace over system A. The partial trace is defined by,

$$tr_A(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) = |b_1\rangle\langle b_2|tr(|a_1\rangle\langle a_2|) = |b_1\rangle\langle b_2|\langle a_1|a_2\rangle, \tag{1.23}$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space of A, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of B.

1.3.3 Entanglement

We can look at entanglement from the point of view of subsystem states. Let us take a joint state of two systems A and B in a pure state $|\psi\rangle_{AB}$ as,

$$|\psi\rangle_{AB} = \frac{|0\rangle_A|1\rangle_B - |1\rangle_A|0\rangle_B}{\sqrt{2}}. \tag{1.24}$$

The joint system AB is made of two subsystems A and B. We trace over the subsystem A or B using the joint state $|\psi\rangle_{AB}$ to get the state of the individual systems A and B. The resulting density matrix ρ^A and ρ^B will describe the state of the subsystem A and B respectively as,

$$\rho^A = tr_B(\rho^{AB}), \qquad\qquad \rho^B = tr_A(\rho^{AB}). \tag{1.25}$$

The reduced density operators are used to calculate the entanglement between two sub-systems making a composite system. Calculating ρ^A and ρ^B for the state given in Eq.[1.24], we see

$$\rho^A = tr_B(\rho^{AB}) =_B \langle 0|(|\psi\rangle_{AB\ AB}\langle\psi|)|0\rangle_B +_B \langle 1|(|\psi\rangle_{AB\ AB}\langle\psi|)|1\rangle_B = \frac{I_A}{2}. \tag{1.26}$$

here I_A is the $[2 \times 2]$ identity matrix. Similarly it can be shown that ρ^B is also $I_B/2$. The quantity $tr(\rho^A)^2 = tr(\rho^B)^2 = 1/2 < 1$. This shows that although the state of the joint system $|\psi\rangle_{AB}$ is pure, the subsystem states ρ^A and ρ^B are in a mixed state. This means that the subsystem states cannot determine the joint pure state $|\psi\rangle_{AB}$ and in the process of describing the subsystems we have lost some information.

It can also be written as $\rho^{AB} \neq \rho^A \otimes \rho^B$ if the state $|\psi\rangle_{AB}$ is *entangled*, however if $|\psi\rangle_{AB}$ is an *unentangled* state then $\rho^{AB} = \rho^A \otimes \rho^B$. In other words entangled pure states are those whose subsystem states are in a mixed state. However unentangled pure states have subsystem states which are in pure states. All states that are not separable are called entangled. Operationally, in an entangled state (for two systems A, B) if we measure state A we typically know also about state B with 100% certainty even without making any measurement on it [5].

So far we discussed the matrix representation of the qubit and qudit states and also the density matrix representation of a system. We also studied how the entanglement content is related to the reduced density matrices of the subsystems. Now we will look at some decompositions which we will be using in the next chapters.

1.4 The singular value decomposition (SVD)

Every complex $[M \times N]$ rectangular matrix A has the following decomposition,

$$A = USV^{\dagger}, \tag{1.27}$$

where the matrix U of dimension $[M \times min(M, N)]$ has orthonormal columns (the left singular vectors), *i.e.* $U^{\dagger}U = I$. If $M \leqslant N$ then $UU^{\dagger} = I$ which means U is unitary.[6]

The matrix S of dimension $[min(M, N) \times min(M, N)]$ is a diagonal matrix with non-negative entries S_a called singular values ($s_1 \geqslant s_2 ... \geqslant s_r > 0 \geqslant ... \geqslant 0$). The number of non-zero singular values is the (Schmidt) rank r of M.

The matrix $V^{\dagger}$ of dimension $[min(M, N) \times N]$ has orthonormal rows (the right singular vectors), *i.e.* $V^{\dagger}(V^{\dagger})^{\dagger} = V^{\dagger}V = I$. If $M \geqslant N$ then $VV^{\dagger} = I$ which means V is unitary.

Suppose the dimension of the matrix A is $[M \times N]$, then the dimensions of the matrices U, S and $V^{\dagger}$ after performing SVD will be $[M \times r]$, $[r \times r]$ and $[r \times N]$, where r is the rank of matrix A. This is shown in the Fig.[1.2] for the cases $M > N$ and $M < N$.

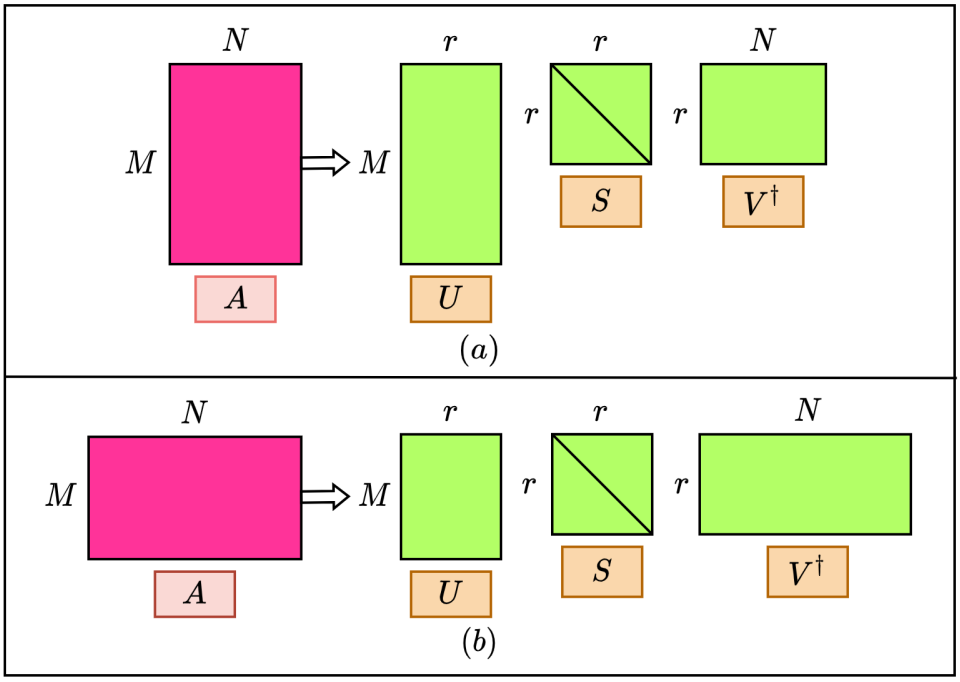


Figure 1.2: Dimensions of the matrices after performing the SVD on a matrix A of dimensions $[M \times N]$ (a) with $M > N$ and (b) with $M < N$

Example of SVD

$$\underbrace{\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{U} \times \underbrace{\begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \end{pmatrix}}_{S} \times \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{V^\dagger}$$

1.5 QR decomposition

The QR decomposition gives the decomposition $A = QR$ for any matrix A, where Q is a unitary matrix and R is an upper triangular matrix [7]. Suppose the dimension of the matrix A is $[M \times N]$, then the dimensions of the matrices Q and R after performing QR decomposition will be $[M \times M]$, $[M \times N]$. This is called *full* QR decomposition. It is shown in the Fig.[1.3] for the cases $M > N$ and $M < N$.

Example of QR decomposition

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{\sqrt{-2}}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} \end{pmatrix}}_{Q} \times \underbrace{\begin{pmatrix} \sqrt{3} & \frac{2}{\sqrt{3}} & \frac{2}{\sqrt{3}} \\ 0 & \frac{\sqrt{2}}{\sqrt{3}} & \frac{-1}{\sqrt{6}} \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}}_{R}$$

If the dimension of the matrix A is $[M \times N]$ such that $M > N$, then the bottom $(M - N)$ rows of R are zero, and we can write,

$$A = QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 R_1$$

Hence, now the dimensions of the matrices Q_1 and R_1 will be $[M \times N]$ and $[N \times N]$, and while $Q_1^\dagger Q_1 = I$, in general $Q_1 Q_1^\dagger \neq I$. This is called *thin* QR decomposition.

Example of thin QR decomposition

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 1 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & \frac{-1}{\sqrt{2}} \\ 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}}_{Q} \times \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{2} \end{pmatrix}}_{R}$$

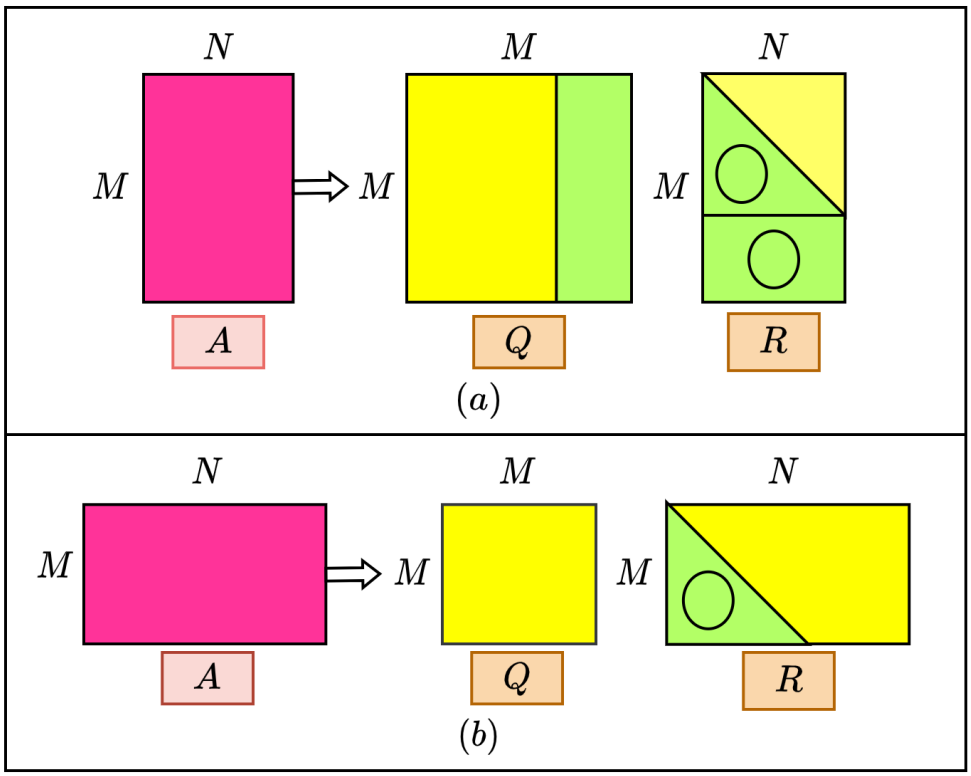


Figure 1.3: Dimensions of the matrices after performing the QR decomposition on a matrix A of dimensions $[M \times N]$ (a) with $M > N$ and (b) with $M < N$

1.6 The Schmidt decomposition

Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_A\rangle$ for system A, and orthonormal states $|i_B\rangle$ for system B such that,

$$|\psi\rangle = \sum_i \lambda_i \, |i_A\rangle |i_B\rangle, \tag{1.28}$$

where λ_i are non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$ known as Schmidt coefficients and the number of non-zero values λ_i is called the Schmidt number (χ) for the state $|\psi\rangle$. The Schmidt number quantifies the 'amount' of entanglement between systems A and B for a composite system. The bases $|i_A\rangle$ and $|i_B\rangle$ are called the Schmidt bases for A and B, respectively, and $\langle i_A|j_A\rangle = \delta_{ij}$, $\langle i_B|j_B\rangle = \delta_{ij}$ [8].

Proof

We will give the proof for the case where the state spaces of systems A and B are of the same dimension. Let $|j\rangle$ and $|k\rangle$ be any fixed orthonormal bases for systems A and B, respectively. Then $|\psi\rangle$ can be written as,

$$|\psi\rangle = \sum_{jk} a_{jk} \, |j\rangle|k\rangle, \tag{1.29}$$

for some matrix a of complex numbers a_{jk}. By the singular value decomposition, $a = udv$, where d is a diagonal matrix with non-negative elements, and u and v are unitary matrices. Thus,

$$|\psi\rangle = \sum_{ijk} u_{ji} d_{ii} v_{ik} \, |j\rangle|k\rangle. \tag{1.30}$$

Defining,

$$|i_A\rangle = \sum_{j} u_{ji}|j\rangle, \qquad\qquad |i_B\rangle = \sum_{k} v_{ik}|k\rangle, \tag{1.31}$$

and $\lambda_i = d_{ii}$, we see that this gives,

$$|\psi\rangle = \sum_{i} \lambda_i \, |i_A\rangle|i_B\rangle. \tag{1.32}$$

The unitarity of u and the orthonormality of $|j\rangle$ make it obvious that they constitute an orthonormal set $|i_A\rangle$. Similarly $|i_B\rangle$ also form an orthonormal set.

The entanglement properties of a pure state can be found from the Schmidt coefficients. If there is only one Schmidt coefficient λ_i for example in the Eq.[**??**] which is unity with all the others being zero, then the state $|\psi\rangle_{AB}$ is unentangled, however if more than one non zero Schmidt coefficient exists, it means that the state $|\psi\rangle_{AB}$ is an entangled state.

1.7 Motivation for matrix product states (MPS)

Now that we are familier with SVD and QR decomposition, we can proceed to MPS representation of state. We will first see the motivation behind it. We are familier with the concept of vectors from linear algebra. A tensor is just a generalization of the vector concept (in fact a vector is a rank 1 tensor, and even a scalar can be considered a rank 0 tensor). A tensor is just an $n-$dimensional array with n indices.

Vectors are familiar geometric objects with invariant magnitude and direction. In diagram form, a vector can be visualized as a object having only one arm showing one free index as shown in Fig.[1.4 (a)]. Mathematically, it can be written as,

$$|A\rangle = \sum_{i_1=1}^{m} A_{i_1}|i_1\rangle. \tag{1.33}$$

This is just a column vector of dimension $[m \times 1]$ whose elements are A_{i_1}. So there will be m matrix elements. Any vector is a rank 1 tensor.

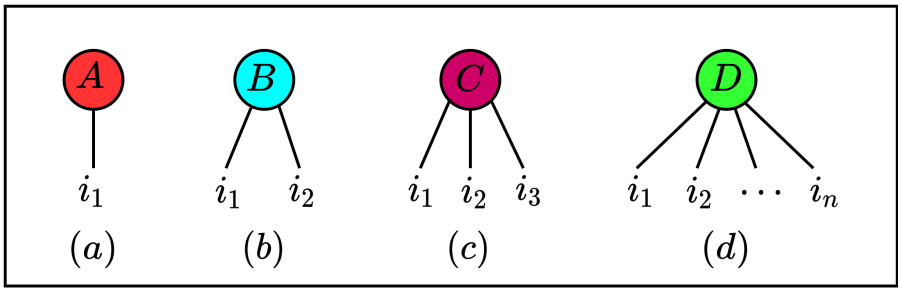


Figure 1.4: Diagramatical represenation of a vector, a matrix and a tensor

Next a matrix can be visualized as a object having two arms showing two free indices as shown in Fig.[1.4 (b)]. Mathematically, it can be written as,

$$|B\rangle = \sum_{i_1=1}^{m} \sum_{i_2=1}^{n} B_{i_1 i_2} |i_1\rangle |i_2\rangle. \tag{1.34}$$

This is a two dimensioal matrix of dimension $[m \times n]$ whose elements are $B_{i_1 i_2}$. So there will be mn matrix elements. Any matrix is a rank 2 tensor.

Next a tensor of rank 3 can be visualized as a object having three arms showing three free indices as shown in Fig.[1.4 (c)]. Mathematically, it can be written as,

$$|C\rangle = \sum_{i_1=1}^{m} \sum_{i_2=1}^{n} \sum_{i_3=1}^{l} C_{i_1 i_2 i_3} |i_1\rangle |i_2\rangle |i_3\rangle. \tag{1.35}$$

This is a three dimensioal matrix of dimension $[m \times n \times l]$ whose elements are $C_{i_1 i_2 i_3}$. So there will be mnl matrix elements.

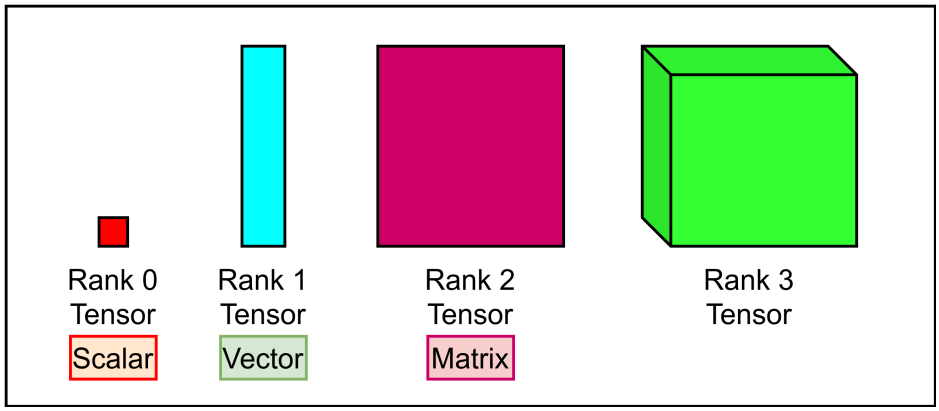


Figure 1.5: Scalar, vector, matrix and tensor

Tensors extend the description of vectors to geometric objects that have magnitude and any number of directions. The order of a tensor is equal to the number of

its free indices. An order n tensor will have n arms showing n free indices as shown in Fig.[1.4 (d)] and in index notation it will have n indices. Mathematically, it can be written as,

$$|C\rangle = \sum_{i_1=1}\sum_{i_2=1}\cdots\sum_{i_n=1} C_{i_1 i_2 \cdots i_n}|i_1\rangle|i_2\rangle\cdots|i_n\rangle. \tag{1.36}$$

As shown in Fig.[1.5], a scalar is a rank 0 tensor, a vector is a rank 1 tensor and a matrix is a rank 2 tensor. This figure clearly explains the concept of tensor.

A pure quantum qudit state of L particles is desctribed by a tensor of rank L. Now, a tensor is not a scalar, a vector or anything. It's just an abstract quantity that obeys the coordinate transformation law [9]. A tensor is a multilinear function, so it will be easier if we could represent this tensor in terms of matrices. The matrix product state representation does exactly the same thing.

In the next chapters we have given detailed theory for a decomposition of a pure state into matrix products called MPS representation. Consider a system that has L sites, each site corresponds to a d-dimensional local state space (basis) $\{\sigma_i\}$ where $i = 1, ..., L$ which are the qudits. A general pure quantum qudit state is,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d}\sum_{\sigma_2=1}^{d}...\sum_{\sigma_L=1}^{d} C_{\sigma_1\sigma_2...\sigma_L}|\sigma_1\rangle|\sigma_2\rangle...|\sigma_L\rangle. \tag{1.37}$$

Let us represent the coefficients $C_{\sigma_1...\sigma_L}$ as a green box (with rounded edges), where the physical indices σ_1 to σ_L stick out vertically as shown in Fig.[1.6]. $C_{\sigma_1\sigma_2...\sigma_L}$ represents an tensor of order L.

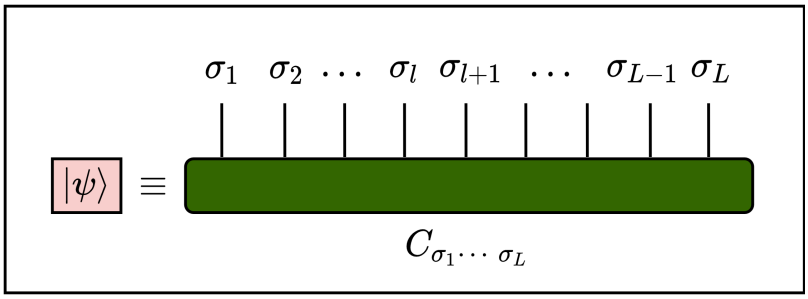


Figure 1.6: Graphical representation of an arbitrary qudit state $|\psi\rangle$ of L spins

The number of C coefficients is d^L and the vector $|\Psi\rangle$ in matrix form has dimension $[d^L \times 1]$. MPS gives a **change in representation of these state coefficients** which is very useful in performing a plethora of tasks with less computational time.

We assume that this quantum state is normalized. If not, normalization can be done easily. Our motive is to find more local notion of the state (that is its decomposition into product of local matrices). There are three ways of doing this, which we will discuss in detail in this thesis. To sum up, any state vector in matrix form will have dimension $[d^L \times 1]$ and we are interested in its decomposition into 'product' of local matrices which we call *Matrix Product States* (MPS).

1.7.1 Advantages and applications of matrix product states

With a increasing number of particles (qudits), the Hilbert space's dimension expands exponentially. As a result, dealing with the many-body problem is difficult [10], because we have to work with tensors of greater ranks. MPS converts this tensor into a product of **local** matrices at each site having lower dimensions compared to the d^L dimensional matrix totally for the state, thus we have to deal with matrices rather than tensors. The fundamental benefit of MPS is that it requires far fewer parameters than the d^L parameters required to describe a general quantum state.

MPS is extensively used in effective computation using Many-body sytems like Ising Model [11], AKLT model [12] and Heisenberg model [13]. The Density Matrix Renormalization Group (DMRG) [16] is a numerical variational technique used to obtain the low-energy physics of quantum many-body systems with high accuracy. It is one of the most efficient algorithm to solve quantum many body system.

1.8 Summary and conclusions

In this chapter, we discussed about the qubit and qudit states and their matrix representations. Also we looked at the density matrix approach, which is mathematically equivalent to the state vector approach and we also glanced through its application. We also discussed about Singular Value Decomposition, QR Decomposition and Schmidt Decomposition which will be constantly used throughout this thesis. Lastly we focused on the motivation and importance of Matrix Product States.

Chapter 2

The Vidal decomposition

The first effort to write a pure state in terms of local matrices was the Vidal decomposition [14], which we will see in detail in this chapter with various examples.

Consider n interacting spin qubits or in general a multi-qubit state of n particles, each one described by a two-dimensional Hilbert space $\mathcal{H}_2$ which corresponds to a single qubit linearly independent orthonormal basis $\{|0\rangle, |1\rangle \in \mathcal{H}_2\}$.

A general *pure* state of n qubits $|\psi\rangle \in \mathcal{H}_2^{\otimes n}$ is,

$$|\psi\rangle = \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_n=0}^{1} C_{i_1 i_2 \cdots i_n} \, |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle. \tag{2.1}$$

Expressing $|\psi\rangle$ like this requires 2^n complex numbers $C_{i_1 i_2 \cdots i_n}$. Simulating such a large system and computing its evolution in time is not simple. The point is that, generally for the description of the state of n interacting qubits we need $\mathcal{O}(exp(n))$ parameters and the Vidal decomposition of pure state scales down the number of required parameters as it requires $\mathcal{O}(poly(n))$ parameters. This clearly is an indication of the reduction in the computational time.

We intend to find out the following decomposition of these 2^n coefficients as given by Eq.(2.1) in terms of n tensors Γ and $n-1$ vectors λ such that,

$$C_{i_1 i_2 \cdots i_n} = \sum_{\alpha_1} \cdots \sum_{\alpha_{n-1}} \Gamma^{[1] i_1}_{\alpha_1} \, \lambda^{[1]}_{\alpha_1} \, \Gamma^{[2] i_2}_{\alpha_1 \alpha_2} \, \lambda^{[2]}_{\alpha_2} \, \cdots \, \Gamma^{[n] i_n}_{\alpha_{n-1}}. \tag{2.2}$$

In compact form, we can write the coefficients as,

$$C_{i_1 i_2 \cdots i_n} = \Gamma^{[1]i_1}\ \lambda^{[1]}\ \Gamma^{[2]i_2}\ \lambda^{[2]}\ \cdots\ \Gamma^{[n]i_n}, \tag{2.3}$$

where we have replaced the repeated sums over $\alpha_1, \alpha_2\ \cdots\ \alpha_{n-1}$ by the matrix multiplications. Plugging Eq.(2.3) in Eq.(2.1) gives the total state in a new form as under,

$$|\psi\rangle = \sum_{i_1=0}^{1} \cdots \sum_{i_n=0}^{1}\ \Gamma^{[1]i_1}\ \lambda^{[1]}\ \Gamma^{[2]i_2}\ \lambda^{[2]}\ \cdots\ \Gamma^{[n]i_n}\ |i_1\rangle \otimes \cdots \otimes |i_n\rangle. \tag{2.4}$$

This is the Vidal decomposition of a *pure* state $|\psi\rangle$.

2.1 Defining χ (measure of entanglement)

Consider a pure state $|\psi\rangle \in \mathcal{H}_2^{\otimes n}$ of a n-qubit system. Now we bipartition this state into A and B. The Schimdt Decomposition (SD) of $|\psi\rangle$ with respect to the partition $A : B$ is,

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_A} \lambda_\alpha |\Phi_\alpha^{[A]}\rangle |\Phi_\alpha^{[B]}\rangle, \tag{2.5}$$

where $|\phi_\alpha^{[A]}\rangle$ is an eigenvector of the reduced density matrix $\rho^{[A]}$ with eigenvalues $(\lambda_\alpha^2 > 0)$ and $|\phi_\alpha^{[B]}\rangle$ is an eigenvector of the reduced density matrix $\rho^{[B]}$ with same non zero eigenvalues $(\lambda_\alpha^2 > 0)$. λ_α is the Schmidt coefficient satisfying $\sum_\alpha \lambda_\alpha^2 = 1$.

The Schmidt rank χ_A is a natural measure of the entanglement between the qubits in A and B. The state $|\psi\rangle$ is unentangled if and only if there is only one non-zero Schmidt coefficient λ_α which has to be unity. If more than one Schmidt coefficient is non-zero, then the state is entangled. If all the Schmidt coefficients are non-zero and they are all equal, then the state is said to be maximally entangled. Accordingly, we quantify the entanglement of state $|\psi\rangle$ by χ which is defined as,

$$\chi = max_A(\chi_A), \tag{2.6}$$

that is, the maximal Schmidt rank over all possible bipartite splittings $A : B$ of n qubits.

2.2 The structure of Vidal decomposition

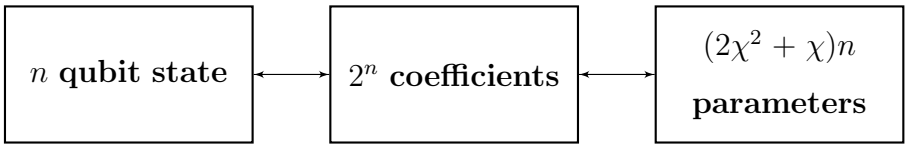
Vidal Decomposition is a local decomposition of the state $|\psi\rangle \in \mathcal{H}_2^{\otimes n}$ in terms of n tensors $\{\Gamma^{[l]}\}_{l=1}^{n}$ and $n-1$ vectors $\{\lambda^{[l]}\}_{l=1}^{n-1}$. It is local in a sense that, when a

two-qubit gate is applied to qubits l and $l+1$, only $\Gamma^{[l]}$, $\lambda^{[l]}$ and $\Gamma^{[l+1]}$ needs to be updated during computation or in effect, it means only the labels l and $l+1$ are operated upon. Now consider,

$$C_{i_1 i_2 \cdots i_n} \longleftrightarrow \Gamma^{[1]}\, \lambda^{[1]}\, \Gamma^{[2]}\, \lambda^{[2]} \cdots\, \Gamma^{[l]} \cdots\, \lambda^{[n-1]}\, \Gamma^{[n]}. \tag{2.7}$$

where we have replaced the repeated sums over $\alpha_1, \alpha_2\ \cdots\ \alpha_{n-1}$ by the matrix multiplication. Here, tensor $\Gamma^{[l]i}_{\alpha\,\alpha'}$ is assigned to qubit l and has (at most) three indices α, $\alpha^{'}$ and i, where $\alpha = 1\ \cdots\ \chi$, $\alpha' = 1\ \cdots\ \chi$ and $i = 0, 1$. Here χ is the Schmidt rank (Schmidt number) for that particular Schmidt decomposition and $\lambda^{[l]}$ is a vector whose components $\lambda^{[l]}_{\alpha'}$ store the Schmidt coefficients of the splitting $[1\ \cdots\ l] : [(l+1)\ \cdots\ n]$ for a $n-$qubit state.

The 2^n coefficients $C_{i_1 i_2 \cdots i_n}$ of the state $|\psi\rangle$ are expressed in terms of about $(2\chi^2 + \chi)n$ parameters, a number that grows only linearly in n for a fixed value of χ and not exponentially like the naive Hilbert space.



This decomposition (but not χ) depends on the particular way qubits have been ordered from 1 to n, and consists of a concatenation of $n-1$ Schmidt decompositions.

2.3 Mathematical details about the Vidal decomposition of a pure state

We first compute the Schmidt decomposition of a n qubit pure quantum state $|\psi\rangle$ according to the bipartite splitting of the system into qubit 1 and the $(n-1)$ remaining qubits,

$$|\psi\rangle = \sum_{\alpha_1=1}^{\chi} \lambda^{[1]}_{\alpha_1}\, |\Phi^{[1]}_{\alpha_1}\rangle\, |\Phi^{[2\,\cdots\,n]}_{\alpha_1}\rangle. \tag{2.8}$$

Then expand each Schmidt vector $|\Phi^{[1]}_{\alpha_1}\rangle$ in terms of the local basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 1 as,

$$|\Phi^{[1]}_{\alpha_1}\rangle = \sum_{i_1=0}^{1} \Gamma^{[1]i_1}_{\alpha_1}\, |i_1\rangle. \tag{2.9}$$

Note that here the summation over i_1 runs from 0 to 1 because we are considering qubit states. That gives,

$$|\psi\rangle = \sum_{\alpha_1=1}^{\chi} \sum_{i_1=0}^{1} \Gamma_{\alpha_1}^{[1]i_1} \lambda_{\alpha_1}^{[1]} |i_1\rangle |\Phi_{\alpha_1}^{[2\cdots n]}\rangle. \tag{2.10}$$

Then we have to follow the next three steps:

Step 1 : Expand each Schmidt vector $|\Phi_{\alpha_1}^{[2\cdots n]}\rangle$ in terms of the local basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 2,

$$|\Phi_{\alpha_1}^{[2\cdots n]}\rangle = \sum_{i_2=0}^{1} |\tau_{\alpha_1 i_2}^{[3\cdots n]}\rangle |i_2\rangle. \tag{2.11}$$

Step 2 : Write each (possibly unnormalized) vector $|\tau_{\alpha_1 i_2}^{[3\cdots n]}\rangle$ in terms of at most χ Schmidt vectors $\left\{|\Phi_{\alpha_2}^{[3\cdots n]}\rangle\right\}_{\alpha_2=1}^{\chi}$ (*i.e.* the eigenvectors of $\rho^{[3\cdots n]}$) and the corresponding Schmidt coefficients $\lambda_{\alpha_2}^{[2]}$ such that,

$$|\tau_{\alpha_1 i_2}^{[3\cdots n]}\rangle = \sum_{\alpha_2=1}^{\chi} \Gamma_{\alpha_1\alpha_2}^{[2]i_2} \lambda_{\alpha_2}^{[2]} |\Phi_{\alpha_2}^{[3\cdots n]}\rangle. \tag{2.12}$$

Step 3 : Substituting Eq.(2.12) in Eq.(2.11) and then in Eq.(2.10), we get,

$$|\psi\rangle = \sum_{\alpha_1=1}^{\chi} \sum_{\alpha_2=1}^{\chi} \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \Gamma_{\alpha_1}^{[1]i_1} \lambda_{\alpha_1}^{[1]} \Gamma_{\alpha_1\alpha_2}^{[2]i_2} \lambda_{\alpha_2}^{[2]} |i_1 i_2\rangle |\Phi_{\alpha_2}^{[3\cdots n]}\rangle. \tag{2.13}$$

Iterating steps 1 to 3 for the Schmidt vectors $|\Phi_{\alpha_2}^{[3\cdots n]}\rangle$,$|\Phi_{\alpha_3}^{[4\cdots n]}\rangle, \cdots, |\Phi_{\alpha_{n-1}}^{[n]}\rangle$, one can express the state $|\psi\rangle$ in terms of tensors $\Gamma^{[l]}$ and vectors $\lambda^{[l]}$ to get,

$$|\psi\rangle = \sum_{i_1=0}^{1} \cdots \sum_{i_n=0}^{1} C_{i_1\cdots i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle, \tag{2.14}$$

where,

$$C_{i_1\ldots i_n} = \sum_{\alpha_1=1}^{\chi} \cdots \sum_{\alpha_{n-1}=1}^{\chi} \Gamma_{\alpha_1}^{[1]i_1} \lambda_{\alpha_1}^{[1]} \Gamma_{\alpha_1\alpha_2}^{[2]i_2} \lambda_{\alpha_2}^{[2]} \Gamma_{\alpha_2\alpha_3}^{[3]i_3} \cdots \Gamma_{\alpha_{n-1}}^{[n]i_n}. \tag{2.15}$$

2.4 The connection between Schmidt decomposition and Vidal decomposition

The Vidal Decomposition as given by Eq.(2.15) readily gives the Schmidt Decomposition of $|\psi\rangle$ according to the bipartite splitting $[1\cdots l] : [(l+1)\cdots n]$ *i.e.* the bipartite splitting $A : B$ such that A contains the first l qubits and B contains the rest of them which can be written as,

$$|\psi\rangle = \sum_{\alpha_l} \lambda^{[l]}_{\alpha_l} \, |\Phi^{[1 \cdots l]}_{\alpha_l}\rangle \, |\Phi^{[(l+1 \cdots n]}_{\alpha_l}\rangle. \tag{2.16}$$

It can be checked by induction over l that,

$$|\Phi^{[1 \cdots l]}_{\alpha_l}\rangle \longleftrightarrow \Gamma^{[1]}_{\alpha_1} \, \lambda^{[1]}_{\alpha_1} \, \cdots \, \lambda^{[l-1]}_{\alpha_{l-1}} \, \Gamma^{[l]}_{\alpha_{l-1}\alpha_l}, \tag{2.17}$$

meaning that,

$$|\Phi^{[1 \cdots l]}_{\alpha_l}\rangle = \sum_{\alpha_1 \cdots \alpha_{l-1}} \Gamma^{[1]i_1}_{\alpha_1} \, \lambda^{[1]}_{\alpha_1} \, \cdots \, \lambda^{[l-1]}_{\alpha_{l-1}} \, \Gamma^{[l]i_l}_{\alpha_{l-1}\alpha_l} |i_1 \, \cdots \, i_l\rangle. \tag{2.18}$$

and by construction we already have,

$$|\Phi^{[l+1 \cdots n]}_{\alpha_l}\rangle \longleftrightarrow \Gamma^{[l+1]}_{\alpha_l\alpha_{l+1}} \, \lambda^{[l+1]}_{\alpha_{l+1}} \, \cdots \, \lambda^{[n-1]}_{\alpha_{n-1}} \, \Gamma^{[n]}_{\alpha_{n-1}}, \tag{2.19}$$

meaning that,

$$|\Phi^{[l+1 \cdots n]}_{\alpha_l}\rangle = \sum_{\alpha_{l+1}} \cdots \sum_{\alpha_{n-1}} \Gamma^{[l+1]i_{l+1}}_{\alpha_l\alpha_{l+1}} \, \lambda^{[l+1]}_{\alpha_{l+1}} \, \cdots \, \lambda^{[n-1]}_{\alpha_{n-1}} \, \Gamma^{[n]i_n}_{\alpha_{n-1}}, |i_1 \, \cdots \, i_l\rangle. \tag{2.20}$$

So we have obtained the Schmidt decomposition of the state in terms of Γ tensors and λ vectors.

2.5 Analytical calculation of the Vidal decomposition and illustrative examples

2.5.1 Vidal decomposition of a two-qubit Bell state

Now consider a two-qubit bell state as under,

$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}. \tag{2.21}$$

In matrix form $|\psi\rangle$ can be written as a $[4 \times 1]$ column vector as,

$$|\psi\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} C_{00} \\ C_{01} \\ C_{10} \\ C_{11} \end{pmatrix}.$$

We first compute the SD of $|\psi\rangle$ for a bipartite splitting $[1] : [2]$,

$$|\psi\rangle = \sum_{\alpha_1=0}^{1} \lambda^{[1]}_{\alpha_1} \, |\Phi^{[1]}_{\alpha_1}\rangle \, |\Phi^{[2]}_{\alpha_1}\rangle.$$

The reduced density matrix for qubit 1 is,

$$\rho^{[1]} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

and the reduced density matrix for qubit 2 is,

$$\rho^{[2]} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

Now, $|\Phi_{\alpha_1}^{[1]}\rangle$ are the eigenvectors of the reduced density matrix $\rho^{[1]}$ given by,

$$|\Phi_0^{[1]}\rangle = |0\rangle, \qquad |\Phi_1^{[1]}\rangle = |1\rangle.$$

We will write $|\Phi_{\alpha_1}^{[1]}\rangle$ in terms of the basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 1 as below,

$$|\Phi_0^{[1]}\rangle = |0\rangle = \Gamma_0^{[1]0}\,|0\rangle + \Gamma_0^{[1]1}\,|1\rangle,$$

$$|\Phi_1^{[1]}\rangle = |1\rangle = \Gamma_1^{[1]0}\,|0\rangle + \Gamma_1^{[1]1}\,|1\rangle.$$

That gives, $\Gamma_0^{[1]0} = 1$, $\Gamma_1^{[1]0} = 0$, $\Gamma_0^{[1]1} = 0$, $\Gamma_1^{[1]1} = 1$, so the corresponding matrices which describe the tensor can be written as,

$$\boxed{\Gamma^{[1]0} = \begin{pmatrix} 1 & 0 \end{pmatrix},} \qquad \boxed{\Gamma^{[1]1} = \begin{pmatrix} 0 & 1 \end{pmatrix}.} \tag{2.22}$$

However, $\lambda_{\alpha_1}^{[1]}$ are the square roots of the eigenvalues of $\rho^{[1]}$ which are,

$$\lambda_0^{[1]} = \frac{1}{\sqrt{2}}, \quad \lambda_1^{[1]} = \frac{1}{\sqrt{2}},$$

this implies,

$$\boxed{\lambda^{[1]} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}.} \tag{2.23}$$

Now, $|\Phi_{\alpha_1}^{[2]}\rangle$ are the eigenvectors of reduced density matrix $\rho^{[2]}$ which are,

$$|\Phi_0^{[2]}\rangle = |0\rangle, \qquad |\Phi_1^{[2]}\rangle = |1\rangle.$$

We will write $|\Phi_{\alpha_1}^{[2]}\rangle$ in terms of the basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 2 as,

$$|\Phi_0^{[2]}\rangle = |0\rangle = \Gamma_0^{[2]0}\,|0\rangle + \Gamma_0^{[2]1}\,|1\rangle,$$

$$|\Phi_1^{[2]}\rangle = |1\rangle = \Gamma_1^{[2]0}\,|0\rangle + \Gamma_1^{[2]1}\,|1\rangle.$$

That gives, $\Gamma_0^{[2]0} = 1,\ \ \Gamma_1^{[2]0} = 0,\ \ \Gamma_0^{[2]1} = 0,\ \ \Gamma_1^{[2]1} = 1$. Then we have as before,

$$\boxed{\Gamma^{[2]0} = \begin{pmatrix} 1 \\ 0 \end{pmatrix},} \qquad \boxed{\Gamma^{[2]1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.} \tag{2.24}$$

The coefficients $C_{i_1 i_2}$ in terms of the Γ and λ matrices are given by,

$$C_{i_1 i_2} = \Gamma^{[1]i_1}\ \lambda^{[1]}\ \Gamma^{[2]i_2}.$$

Explicitly we can write,

$$|\psi\rangle = \begin{pmatrix} C_{00} = \Gamma^{[1]0}\ \lambda^{[1]}\ \Gamma^{[2]0} = \dfrac{1}{\sqrt{2}} \\ C_{00} = \Gamma^{[1]0}\ \lambda^{[1]}\ \Gamma^{[2]1} = 0 \\ C_{00} = \Gamma^{[1]1}\ \lambda^{[1]}\ \Gamma^{[2]0} = 0 \\ C_{00} = \Gamma^{[1]1}\ \lambda^{[1]}\ \Gamma^{[2]1} = \dfrac{1}{\sqrt{2}} \end{pmatrix},$$

which exactly matches with the coefficients of the state considered.

2.5.2 Vidal decomposition of a 3-qubit GHZ state

Now consider a 3-qubit GHZ state as under,

$$|\psi\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}. \tag{2.25}$$

In matrix form $|\psi\rangle$ is written as a $[2^3 \times 1]$ column vector,

$$|\psi\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} C_{000} \\ C_{001} \\ C_{010} \\ C_{011} \\ C_{100} \\ C_{101} \\ C_{110} \\ C_{111} \end{pmatrix}.$$

We first compute the SD of $|\psi\rangle$ for a bipartite splitting $[1] : [23]$,

$$|\psi\rangle = \sum_{\alpha_1=0}^{1} \lambda_{\alpha_1}^{[1]}\ |\Phi_{\alpha_1}^{[1]}\rangle\ |\Phi_{\alpha_1}^{[23]}\rangle.$$

The reduced density matrix for qubit 1 is,

$$\rho^{[1]} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

and the reduced density matrix for qubit 2 and 3 is,

$$\rho^{[23]} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}.$$

Now, $|\Phi_{\alpha_1}^{[1]}\rangle$ are the eigenvectors of reduced density matrix $\rho^{[1]}$ given by,

$$|\Phi_0^{[1]}\rangle = |0\rangle, \qquad |\Phi_1^{[1]}\rangle = |1\rangle.$$

Now, we will write $|\Phi_{\alpha_1}^{[1]}\rangle$ in terms of the basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 1 as,

$$|\Phi_0^{[1]}\rangle = |0\rangle = \Gamma_0^{[1]0}\,|0\rangle + \Gamma_0^{[1]1}\,|1\rangle,$$

$$|\Phi_1^{[1]}\rangle = |1\rangle = \Gamma_1^{[1]0}\,|0\rangle + \Gamma_1^{[1]1}\,|1\rangle.$$

That gives, $\Gamma_0^{[1]0} = 1$, $\Gamma_1^{[1]0} = 0$, $\Gamma_0^{[1]1} = 0$, $\Gamma_1^{[1]1} = 1$ and finally we get,

$$\Gamma^{[1]0} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad \Gamma^{[1]1} = \begin{pmatrix} 0 & 1 \end{pmatrix}. \tag{2.26}$$

Now, $\lambda_{\alpha_1}^{[1]}$ are the square roots of eigenvalues of $\rho^{[1]}$ which are, $\lambda_0^{[1]} = \frac{1}{\sqrt{2}}$, $\lambda_1^{[1]} = \frac{1}{\sqrt{2}}$,

$$\lambda^{[1]} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \tag{2.27}$$

However, $|\Phi_{\alpha_1}^{[23]}\rangle$ are the eigenvectors of $\rho^{[23]}$ which are,

$$|\Phi_0^{[23]}\rangle = |00\rangle, \qquad |\Phi_1^{[23]}\rangle = |11\rangle.$$

Now we will write $|\Phi_{\alpha_1}^{[23]}\rangle$ in terms of the basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 2 as,

$$|\Phi_0^{[23]}\rangle = |00\rangle = |\tau_{00}^{[3]}\rangle\,|0\rangle + |\tau_{01}^{[3]}\rangle\,|1\rangle,$$

$$|\Phi_1^{[23]}\rangle = |11\rangle = |\tau_{10}^{[3]}\rangle\,|0\rangle + |\tau_{11}^{[3]}\rangle\,|1\rangle.$$

That gives, $|\tau_{00}^{[3]}\rangle = |0\rangle,\ \ |\tau_{01}^{[3]}\rangle = 0,\ \ |\tau_{10}^{[3]}\rangle = 0,\ \ |\tau_{11}^{[3]}\rangle = |1\rangle.$

Now we write $|\tau_{\alpha_1 i_2}^{[3]}\rangle$ in terms of the Schmidt vectors $|\phi_{\alpha_2}^{[3]}\rangle$ (*i.e.* eigenvectors of $\rho^{[3]}$) and the Schmidt coefficient $\lambda_{\alpha_2}^{[2]}$ as,

$$|\tau_{\alpha_1 i_2}^{[3]}\rangle = \sum_{\alpha_2} \Gamma_{\alpha_1\alpha_2}^{[2]i_2}\ \lambda_{\alpha_2}^{[2]}\ |\phi_{\alpha_2}^{[3]}. \tag{2.28}$$

The reduced density matrix for qubit 3 is given by,

$$\rho^{[3]} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

$|\Phi_{\alpha_2}^{[3]}\rangle$ are the eigenvectors of $\rho^{[3]}$ which are,

$$|\Phi_0^{[3]}\rangle = |0\rangle, \qquad\qquad |\Phi_1^{[3]}\rangle = |1\rangle.$$

and $\lambda_0^{[2]} = \dfrac{1}{\sqrt{2}},\ \ \lambda_1^{[2]} = \dfrac{1}{\sqrt{2}}$, and hence we get,

$$\boxed{\lambda^{[2]} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}.} \tag{2.29}$$

Now we will consider the following cases to get $\Gamma_{\alpha_1\alpha_2}^{[2]i_2}$ values using Eq.[2.28] and

$$|\Phi_0^{[3]}\rangle = |0\rangle, \qquad |\Phi_1^{[3]}\rangle = |1\rangle, \qquad \lambda_0^{[1]} = \frac{1}{\sqrt{2}}, \qquad \lambda_1^{[1]} = \frac{1}{\sqrt{2}}.$$

1. $\boxed{\alpha_1 = 0,\ \ i_2 = 0}$

$$|\tau_{00}^{[3]}\rangle = \Gamma_{00}^{[2]0}\ \lambda_0^{[2]}\ |\phi_0^{[3]}\rangle + \Gamma_{01}^{[2]0}\ \lambda_1^{[2]}\ |\phi_1^{[3]}\rangle,$$

$$|0\rangle = \Gamma_{00}^{[2]0}\ \frac{1}{\sqrt{2}}\ |0\rangle + \Gamma_{01}^{[2]0}\ \frac{1}{\sqrt{2}}\ |1\rangle.$$

That gives, $\Gamma_{00}^{[2]0} = \sqrt{2},\ \ \Gamma_{01}^{[2]0} = 0.$

2. $\boxed{\alpha_1 = 0,\ \ i_2 = 1}$

$$|\tau_{01}^{[3]}\rangle = \Gamma_{00}^{[2]1}\ \lambda_0^{[2]}\ |\phi_0^{[3]}\rangle + \Gamma_{01}^{[2]1}\ \lambda_1^{[2]}\ |\phi_1^{[3]}\rangle,$$

$$0 = \Gamma_{00}^{[2]1}\ \frac{1}{\sqrt{2}}\ |0\rangle + \Gamma_{01}^{[2]1}\ \frac{1}{\sqrt{2}}\ |1\rangle.$$

That gives, $\Gamma_{00}^{[2]1} = 0,\ \ \Gamma_{01}^{[2]1} = 0.$

3. $\alpha_1 = 1, \;\; i_2 = 0$

$$|\tau_{10}^{[3]}\rangle = \Gamma_{10}^{[2]0}\, \lambda_0^{[2]}\, |\phi_0^{[3]}\rangle + \Gamma_{11}^{[2]0}\, \lambda_1^{[2]}\, |\phi_1^{[3]}\rangle,$$

$$0 = \Gamma_{10}^{[2]0}\, \frac{1}{\sqrt{2}}\, |0\rangle + \Gamma_{11}^{[2]0}\, \frac{1}{\sqrt{2}}\, |1\rangle.$$

That gives, $\Gamma_{10}^{[2]0} = \sqrt{2}, \;\; \Gamma_{11}^{[2]0} = 0.$

4. $\alpha_1 = 1, \;\; i_2 = 1$

$$|\tau_{11}^{[3]}\rangle = \Gamma_{10}^{[2]1}\, \lambda_0^{[2]}\, |\phi_0^{[3]}\rangle + \Gamma_{11}^{[2]1}\, \lambda_1^{[2]}\, |\phi_1^{[3]}\rangle,$$

$$|1\rangle = \Gamma_{10}^{[2]1}\, \frac{1}{\sqrt{2}}\, |0\rangle + \Gamma_{11}^{[2]1}\, \frac{1}{\sqrt{2}}\, |1\rangle.$$

That gives, $\Gamma_{10}^{[2]1} = \sqrt{2}, \;\; \Gamma_{11}^{[2]1} = 0.$ Finally in matrix form,

$$\Gamma^{[2]0} = \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 0 \end{pmatrix}, \qquad \Gamma^{[2]1} = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2} \end{pmatrix}. \tag{2.30}$$

Now we will write $|\Phi_{\alpha_2}^{[3]}\rangle$ in terms of the basis vectors $\{|0\rangle, |1\rangle\}$ for qubit 3 as,

$$|\Phi_0^{[3]}\rangle = |0\rangle = \Gamma_0^{[3]0}\, |0\rangle + \Gamma_0^{[3]1}\, |1\rangle,$$

$$|\Phi_1^{[3]}\rangle = |1\rangle = \Gamma_1^{[3]0}\, |0\rangle + \Gamma_1^{[3]1}\, |1\rangle.$$

That gives, $\Gamma_0^{[3]0} = 1, \;\; \Gamma_1^{[3]0} = 0, \;\; \Gamma_0^{[3]1} = 0, \;\; \Gamma_1^{[2]1} = 1,$ so we get,

$$\Gamma^{[3]0} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \Gamma^{[3]1} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.31}$$

The coefficients $C_{i_1 i_2 i_3}$ in terms of the Γ and λ matrices are,

$$C_{i_1 i_2} = \Gamma^{[1]i_1}\, \lambda^{[1]}\, \Gamma^{[2]i_2}\, \lambda^{[2]}\, \Gamma^{[3]i_3}$$

and hence,

$$|\psi\rangle = \begin{pmatrix} C_{000} = \Gamma^{[1]0}\,\lambda^{[1]}\,\Gamma^{[2]0}\,\lambda^{[2]}\,\Gamma^{[3]0} = \dfrac{1}{\sqrt{2}} \\ C_{001} = \Gamma^{[1]0}\,\lambda^{[1]}\,\Gamma^{[2]0}\,\lambda^{[2]}\,\Gamma^{[3]1} = 0 \\ C_{010} = \Gamma^{[1]0}\,\lambda^{[1]}\,\Gamma^{[2]1}\,\lambda^{[2]}\,\Gamma^{[3]0} = 0 \\ C_{011} = \Gamma^{[1]0}\,\lambda^{[1]}\,\Gamma^{[2]1}\,\lambda^{[2]}\,\Gamma^{[3]1} = 0 \\ C_{100} = \Gamma^{[1]1}\,\lambda^{[1]}\,\Gamma^{[2]0}\,\lambda^{[2]}\,\Gamma^{[3]0} = 0 \\ C_{101} = \Gamma^{[1]1}\,\lambda^{[1]}\,\Gamma^{[2]0}\,\lambda^{[2]}\,\Gamma^{[3]1} = 0 \\ C_{110} = \Gamma^{[1]1}\,\lambda^{[1]}\,\Gamma^{[2]1}\,\lambda^{[2]}\,\Gamma^{[3]0} = 0 \\ C_{111} = \Gamma^{[1]1}\,\lambda^{[1]}\,\Gamma^{[2]1}\,\lambda^{[2]}\,\Gamma^{[3]1} = \dfrac{1}{\sqrt{2}} \end{pmatrix},$$

which exactly matches with the coefficients of the state considered.

2.6 Summary and conclusion

The Vidal decomposition was one of the earlier attempts to express a quantum state in terms of matrices at local sites in an effort to bring down the computational time when we perform operations with these states. In this chapter the procedure to obtain Vidal Decomposition for any pure quantum state of n qubits was discussed in detail. The whole procedure is explained in detail with the help of an analytical calculation of two examples. As was expected, the Vidal decomposition helps in accessing the state locally, meaning at each site rather that writing it as a single column vector. It is however to be noted that the coefficients are products of tensors and vectors and the split up is also a little "messy". In the forthcoming chapters we will study a clean localization of a pure quantun state called the Matrix Product State Representation.

Chapter 3

The left canonical matrix product state (LCMPS)

We have discussed the motivation for matrix product states in detail in section (1.7). Now in this chapter we will start with a general pure quantum qudit state and proceed to study a decomposition of a pure state into matrix products which we call as a Left Canonical Matrix Product State (LCMPS) representation [7]. Analytical and numerical studies have been done for any qudit state of arbitrary number of spins. As we travel along the chapter, we give illustrative examples for a deep understanding.

A general pure quantum qudit state is,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} \sum_{\sigma_2=1}^{d} ... \sum_{\sigma_L=1}^{d} C_{\sigma_1\sigma_2...\sigma_L} |\sigma_1\rangle|\sigma_2\rangle...|\sigma_L\rangle. \tag{3.1}$$

3.1 Procedure to obtain the left canonical matrix product state (LCMPS) for any qudit state

The first step is to reshape the state vector Eq.(3.1) with d^L elements into a matrix ψ of dimension $[d \times d^{L-1}]$, that is,

$$C_{(\sigma_1...\sigma_L),(1)} = \psi_{(\sigma_1),(\sigma_2...\sigma_L)}. \tag{3.2}$$

SVD of matrix $\psi_{(\sigma_1),(\sigma_2\ldots\sigma_L)}$ on RHS of Eq.(3.2) gives,

$$\psi_{(\sigma_1),(\sigma_2\ldots\sigma_L)} = \sum_{a_1=1}^{r_1} U_{(\sigma_1),(a_1)} S_{(a_1),(a_1)} (V^\dagger)_{(a_1),(\sigma_2\ldots\sigma_L)}. \tag{3.3}$$

The dimensions of the matrices U, S and $V^\dagger$ will be $[d \times d]$, $[d \times d]$ and $[d \times d^{L-1}]$ respectively. But here instead of considering the full matrices, we can focus on only the non-zero singular values along the diagonal of matrix S which is called as the rank. The rank $r_1 \leqslant d$. So we restrict the sum to run only over the first r_1 positive non-zero singular values, so the number of operations to be performed is now decreased. Now the dimensions of the matrices U, S and $V^\dagger$ will be $[d \times r_1]$, $[r_1 \times r_1]$ and $[r_1 \times d^{L-1}]$ respectively. Throughout this thesis we will be using this optimal approximation.

$$U_{d,d} S_{d,d} (V^\dagger)_{d,d^{L-1}} \rightarrow U_{d,r_1} S_{r_1,r_1} (V^\dagger)_{r_1,d^{L-1}}.$$

S and $V^\dagger$ are multiplied and the resulting matrix has been reshaped back into a vector given by,

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1} U_{(\sigma_1),(a_1)} C_{(a_1),(\sigma_2\ldots\sigma_L)}. \tag{3.4}$$

Now we decompose the matrix U into a collection of d row vectors A^{σ_1} of dimension $[1 \times r_1]$ with entries $A^{\sigma_1}_{(1),(a_1)} = U_{(\sigma_1),(a_1)}$ where $U_{(\sigma_1),(a_i)}$ is the $i-$th row of U matrix which can be visualized as,

$$\begin{pmatrix} U_{(\sigma_1),(a_1=1)} \\ U_{(\sigma_1),(a_1=2)} \\ \vdots \\ U_{(\sigma_1),(a_1=r_1)} \end{pmatrix} = \begin{pmatrix} A^{\sigma_1}_{(1),(a_1=1)} \\ A^{\sigma_1}_{(1),(a_1=2)} \\ \vdots \\ A^{\sigma_1}_{(1),(a_1=r_1)} \end{pmatrix}.$$

Also we reshape $C_{(a_1),(\sigma_2\ldots\sigma_L)}$ into a matrix $\psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}$ of dimension $r_1 d \times d^{L-2}$, to give,

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1} A^{\sigma_1}_{a_1} \psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}. \tag{3.5}$$

Graphically, the result after the first decomposition is represented as shown below in Fig.(3.1), where we have on the left hand side a red circle representing $A^{\sigma_1}_{a_1}$ and on the right $C_{(a_1),(\sigma_2\ldots\sigma_L)}$.

The auxiliary degrees of freedon (a_1) are represented by horizontal lines, and the rule is that **connected lines are summed over**. $A^{\sigma_1}_{a_1}$ has only two two connected lines meaning it is representing a matrix whereas $C_{(a_1),(\sigma_2 \ldots \sigma_L)}$ is a tensor.

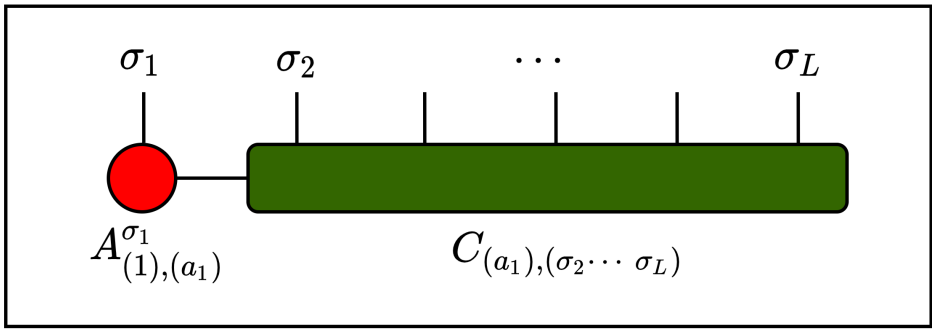


Figure 3.1: Graphical representation of A^{σ_1} after the first SVD

Again doing an SVD of matrix $\psi_{(a_1\sigma_2),(\sigma_3 \ldots \sigma_L)}$ on RHS of Eq.(3.5) gives,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{a_1} \left[U_{(a_1\sigma_2),(a_2)} S_{(a_2),(a_2)} (V^\dagger)_{(a_2),(\sigma_3 \ldots \sigma_L)} \right]. \tag{3.6}$$

The rank is $r_2 \leqslant r_1 d \leqslant d^2$. Multiply S and $V^\dagger$ and reshape into a matrix ψ of dimension $[r_2 d \times d^{L-3}]$ to get,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),(a_2)} \underbrace{S_{(a_2),(a_2)} (V^\dagger)_{(a_2),(\sigma_3 \ldots \sigma_L)}}_{\psi_{(a_2\sigma_3),(\sigma_4 \ldots \sigma_L)}}. \tag{3.7}$$

Replace U by a set of d matrices A^{σ_2} of dimension $[r_1 \times r_2]$ with entries

$$A^{\sigma_2}_{(a_1),(a_2)} = U_{(a_1\sigma_2),(a_2)},$$

Now,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{(a_1),(a_2)} \psi_{(a_2\sigma_3),(\sigma_4 \ldots \sigma_L)}. \tag{3.8}$$

After the second decomposition, we have $A^{\sigma_1}_{(1),(a_1)}$, then $A^{\sigma_1}_{(a_1),(a_2)}$ and on the right $C_{(a_2),(\sigma_3 \ldots \sigma_L)}$, with all the connected lines summed over as shown in Fig.(3.2).

Upon further SVDs in the same way as done earlier, we obtain

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} \cdots \sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} \cdots A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} A^{\sigma_L}_{(a_{L-1}),(1)}. \tag{3.9}$$

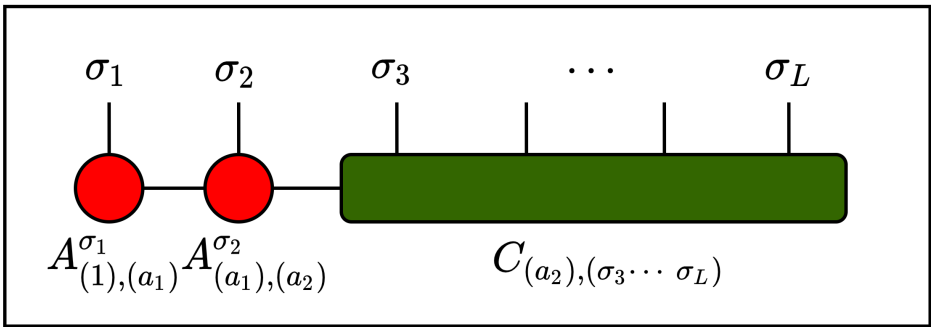


Figure 3.2: Graphical representation of A^{σ_1} and A^{σ_2} after the second SVD

So, we have arrived at L number of $A-$matrices multiplied together and labelled by physical indices. $\sigma_1, \sigma_2, ...$ are the physical indices as they refer to the index of lattice sites and $a_1, a_2, ...$ are the matrix indices which come from the SVD decomposition. A site l is represented by a solid red circle and the physical index σ_l by a vertical line. The first and last site are row and column vectors respectively, connected by only one horizontal line indicating one matrix index. All other sites are matrices connected by two horizontal lines indicating two matrix indices as shown in Fig.(3.3).

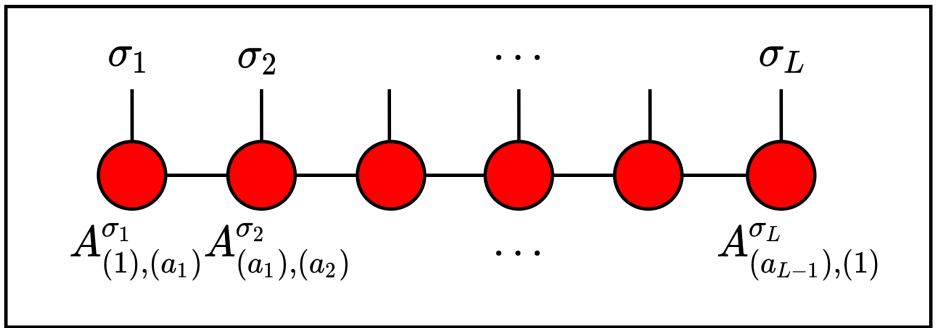


Figure 3.3: Graphical representation of the product of A matrices making up the complete matrix product state

In compact form, we have,

$$C_{\sigma_1 ... \sigma_L} = A^{\sigma_1} A^{\sigma_2} ... A^{\sigma_{L-1}} A^{\sigma_L}, \tag{3.10}$$

where we have replaced the sums over $a_1, a_2, ...$ by matrix multiplications to get a neat form as below,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} ... \sum_{\sigma_L=1}^{d} A^{\sigma_1} A^{\sigma_2} ... A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1\rangle ... |\sigma_L\rangle. \tag{3.11}$$

The (arbitrary) quantum state of qudits is now represented exactly in the form of a matrix product state as we wanted.

3.1.1 Dimensions of the A matrices

Now let us see what will be the dimensions of these A matrices. Suppose SVD is performed on a matrix of dimension $[m \times n]$ then the maximal dimensions of the matrices are reached when the number of non-zero singular values is equal to the upper bound (the lesser of the dimensions of the matrix to be decomposed), which is infact major advantage in any SVD.

- If $m > n$ then we get $U_{m,n} S_{n,n} (V^\dagger)_{n,n}$.
- If $m < n$ then we get $U_{m,m} S_{m,m} (V^\dagger)_{m,n}$.

For even L, the dimensions of the matrices will be $[1 \times d], [d \times d^2], ..., [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2-1}], ..., [d^2 \times d], [d \times 1]$. For odd L, the dimensions of the matrices will be $[1 \times d], [d \times d^2], ..., [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2}], [d^{L/2} \times d^{L/2-1}], ..., [d^2 \times d], [d \times 1]$.

LCMPS gives dL number of $A-$matrices of which first d matrices are the row matrices and last d matrices are the column matrices.

3.1.2 Properties of the A matrices

For each SVD, $U^\dagger U = I$ holds.

$$\delta_{a_l, a_l'} = \sum_{a_{l-1}=1}^{r_{l-1}} \sum_{\sigma_l=1}^{d} (U^\dagger)_{(a_l),(a_{l-1}\sigma_l)} U_{(a_{l-1}\sigma_l),(a_l')} = I. \tag{3.12}$$

Now, we will replace U by a set of A matrices.

$$\sum_{a_{l-1}=1}^{r_{l-1}} \sum_{\sigma_l=1}^{d} (A^{\sigma_l})^\dagger_{(a_l),(a_{l-1})} A^{\sigma_l}_{(a_{l-1}),(a_l')} = \sum_{\sigma_l=1}^{d} ((A^{\sigma_l})^\dagger A^{\sigma_l})_{(a_l),(a_l')} = I. \tag{3.13}$$

This implies,

$$\sum_{\sigma_l}(A^{\sigma_l})^\dagger A^{\sigma_l} = I. \tag{3.14}$$

Matrices that obey this condition are referred to as left-normalized. Matrix product states that consist only of left-normalized matrices are called left-canonical MPS or in short LCMPS.

3.2 Clear steps involved in LCMPS using SVD

We have studied the procedure to obtain the left canonical matrix product state (LCMPS) for any qudit state. Here we will give all the steps involved in it for clarity and deep understanding. We will start with Eq.(3.2),

$$\begin{aligned}
& C_{(\sigma_1\ldots\sigma_L),(1)} \\
= \;& \psi_{(\sigma_1),(\sigma_2\ldots\sigma_L)}, \\
= \;& \sum_{a_1=1}^{r_1} \underbrace{U_{(\sigma_1),(a_1)}}_{A^{\sigma_1}_{(1),(a_1)}} \underbrace{S_{(a_1),(a_1)}(V^\dagger)_{(a_1),(\sigma_2\ldots\sigma_L)}}_{\psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}}, \\
= \;& \sum_{a_1=1}^{r_1} A^{\sigma_1}_{(1),(a_1)}\psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}, \\
= \;& \sum_{a_1=1}^{r_1}\sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)} \underbrace{U_{(a_1\sigma_2),(a_2)}}_{A^{\sigma_2}_{(a_1),(a_2)}} \underbrace{S_{(a_2),(a_2)}(V^\dagger)_{(a_2),(\sigma_3\ldots\sigma_L)}}_{\psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}}, \\
= \;& \sum_{a_1=1}^{r_1}\sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)}A^{\sigma_2}_{(a_1),(a_2)}\psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}, \\
& \qquad\qquad \vdots \\
= \;& \sum_{a_1=1}^{r_1}\ldots\sum_{a_{L-2}=1}^{r_{L-2}} A^{\sigma_1}_{(1),(a_1)}A^{\sigma_2}_{(a_1),(a_2)}\ldots A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})}\psi_{(a_{L-2}\sigma_{L-1}),(\sigma_L)}, \\
= \;& \sum_{a_1=1}^{r_1}\ldots\sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)}\ldots A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})} \underbrace{U_{(a_{L-2}\sigma_{L-1}),(a_{L-1})}}_{A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}} \underbrace{S_{(a_{L-1}),(a_{L-1})}(V^\dagger)_{(a_{L-1}),(\sigma_L)}}_{A^{\sigma_L}_{(a_{L-1}),(1)}}, \\
= \;& \sum_{a_1=1}^{r_1}\ldots\sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)}\ldots A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})}A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}A^{\sigma_L}_{(a_{L-1}),(1)}.
\end{aligned}$$

3.3 Left canonical MPS using QR decomposition

Left canonical MPS can also be generated by using the QR decomposition as follows. First step is to reshape the state vector Eq.(3.1) into the matrix $\psi_{(\sigma_1),(\sigma_2\ldots\sigma_L)}$ and then perform the QR decomposition,

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \psi_{(\sigma_1),(\sigma_2\ldots\sigma_L)} = \sum_{a_1=1}^{r_1} Q_{(\sigma_1),(a_1)} R_{(a_1),(\sigma_2\ldots\sigma_L)}. \tag{3.15}$$

Now we decompose the matrix Q into a collection of d row vectors A^{σ_1} of dimension $[1 \times r_1]$ with entries $A^{\sigma_1}_{(1),(a_1)} = Q_{(\sigma_1),(a_1)}$. It is quite similar to the SVD procedure.

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1} A^{\sigma_1}_{(1),(a_1)} \psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}. \tag{3.16}$$

The next QR decomposition gives,

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1}\sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)} Q_{(a_1\sigma_2),(a_2)} R_{(a_2),(\sigma_3\ldots\sigma_L)}. \tag{3.17}$$

Replace Q by a set of d matrices A^{σ_2} of dimension $[r_1 \times r_2]$ with entries

$$A^{\sigma_2}_{(a_1),(a_2)} = Q_{(a_1\sigma_2),(a_2)}.$$

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1}\sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} \psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}. \tag{3.18}$$

and so on to finally obtain,

$$C_{(\sigma_1\ldots\sigma_L),(1)} = \sum_{a_1=1}^{r_1}\sum_{a_2=1}^{r_2}\ldots\sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} \ldots A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} A^{\sigma_L}_{(a_{L-1}),(1)}. \tag{3.19}$$

3.3.1 Dimensions of the A matrices

Suppose QR decomposition is performed on a matrix of dimension $[m \times n]$ then the maximal dimesions of the matrices Q and R are $[m \times m]$ and $[m \times n]$ respectively. With this, the matrix dimensions of A matrices for even L will be $[1 \times d], [d \times d^2], \ldots, [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2+1}], [d^{L/2+1} \times d^{L/2+2}]$ and so on.

But with thin QR Decomposition or the reduced QR decomposition, if $m > n$ then the maximal dimesions of the matrices Q and R are $[m \times n]$ and $[n \times n]$

respectively and then for even L, the matrix dimensions of the A matrices will be $[1 \times d], [d \times d^2], ..., [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2-1}], ..., [d^2 \times d], [d \times 1]$. Hence thin QR is required here, as an analysis of the dimension shows.

Now we have $Q^\dagger Q = I$, which means $A-$matrices are left normalized.

However by using QR decomposition, we do not see the spectrum of the singular values. We are also not able to determine the ranks $r_1, r_2, ...$ which means that, this decomposition fully exploits the maximal $A-$matrix dimensions.

3.4 Clear steps involved in the LCMPS using QR

Now we will give all the steps involved in obtaining LCMPS using QR decomposition for clarity and deep understanding. We will start with Eq.(3.2),

$$
\begin{aligned}
&C_{(\sigma_1 ... \sigma_L),(1)} \\
&\quad = \psi_{(\sigma_1),(\sigma_2 ... \sigma_L)}, \\
&\quad = \sum_{a_1=1}^{r_1} \underbrace{Q_{(\sigma_1),(a_1)}}_{A^{\sigma_1}_{(1),(a_1)}} \underbrace{R_{(a_1),(\sigma_2 ... \sigma_L)}}_{\psi_{(a_1\sigma_2),(\sigma_3 ... \sigma_L)}}, \\
&\quad = \sum_{a_1=1}^{r_1} A^{\sigma_1}_{(1),(a_1)} \psi_{(a_1\sigma_2),(\sigma_3 ... \sigma_L)}, \\
&\quad = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)} \underbrace{Q_{(a_1\sigma_2),(a_2)}}_{A^{\sigma_2}_{(a_1),(a_2)}} \underbrace{R_{(a_2),(\sigma_3 ... \sigma_L)}}_{\psi_{(a_2\sigma_3),(\sigma_4 ... \sigma_L)}}, \\
&\quad = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} \psi_{(a_2\sigma_3),(\sigma_4 ... \sigma_L)}, \\
&\qquad\qquad \vdots \\
&\quad = \sum_{a_1=1}^{r_1} ... \sum_{a_{L-2}=1}^{r_{L-2}} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} ... A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})} \psi_{(a_{L-2}\sigma_{L-1}),(\sigma_L)}, \\
&\quad = \sum_{a_1=1}^{r_1} ... \sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)} ... A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})} \underbrace{Q_{(a_{L-2}\sigma_{L-1}),(a_{L-1})}}_{A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}} \underbrace{R_{(a_{L-1}),(\sigma_L)}}_{A^{\sigma_L}_{(a_{L-1}),(1)}}, \\
&\quad = \sum_{a_1=1}^{r_1} ... \sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{(1),(a_1)} ... A^{\sigma_{L-2}}_{(a_{L-3}),(a_{L-2})} A^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} A^{\sigma_L}_{(a_{L-1}),(1)}.
\end{aligned}
$$

3.5 Analytical calculation and discussion of LCMPS with one example

Now let us consider one example for clarity and completeness. We will find the LCMPS representation for a 4-qubit $W-$state as given below,

$$|\psi\rangle = \frac{1}{2}\left[|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle\right].$$

Here $d = 2$ and $L = 4$ meaning a 2-qubit space containing 4 particles, hence this state in the matrix form will have $d^L = 16$ elements and the total dimension will be $[d^L \times 1]$ which is $[16 \times 1]$ column vector.

- Step 1 - Reshape $|\psi\rangle$ into matrix of dimension $[d \times d^{L-1}]$,

$$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Step 2 - Do a QR Decomposition of the above matrix,

$$\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}}_{R}.$$

- Step 3 - Form A^{σ_1} matrices from the Q matrix,

$$A^{\sigma_1 0} = \begin{pmatrix} 0 & 1 \end{pmatrix},$$

$$A^{\sigma_1 1} = \begin{pmatrix} 1 & 0 \end{pmatrix}.$$

- Step 4 - Reshape R into a matrix of dimension $[d^2 \times d^{L-2}]$,

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & 0 \end{pmatrix}.$$

- Step 5 - QR Decomposition of the above matrix to get,

$$\underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{-1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{R}.$$

- Step 6 - Form A^{σ_2} matrices from the Q matrix as follows,

$$A^{\sigma_2 0} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{-1}{\sqrt{2}} \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$A^{\sigma_2 1} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

- Step 7 - Reshape R into a matrix of dimension $[d^3 \times d^{L-3}]$,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \\ 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

- Step 8 - QR Decomposition of the above matrix,

$$\underbrace{\begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & 0 \\ 0 & 1 \\ \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}}_{R}.$$

- Step 9 - Form A^{σ_3} matrices from the Q matrix found above,

$$A^{\sigma_3 0} = \begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad A^{\sigma_3 1} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

- Step 10 - Form A^{σ_4} matrices from the R matrix obtained in step 8 as,

$$A^{\sigma_4 0} = \begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} \\ 0 \end{pmatrix}, \quad \text{and} \quad A^{\sigma_4 1} = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}.$$

3.6 Flowchart diagram indicating the steps for LCMPS using QR decomposition with explanation

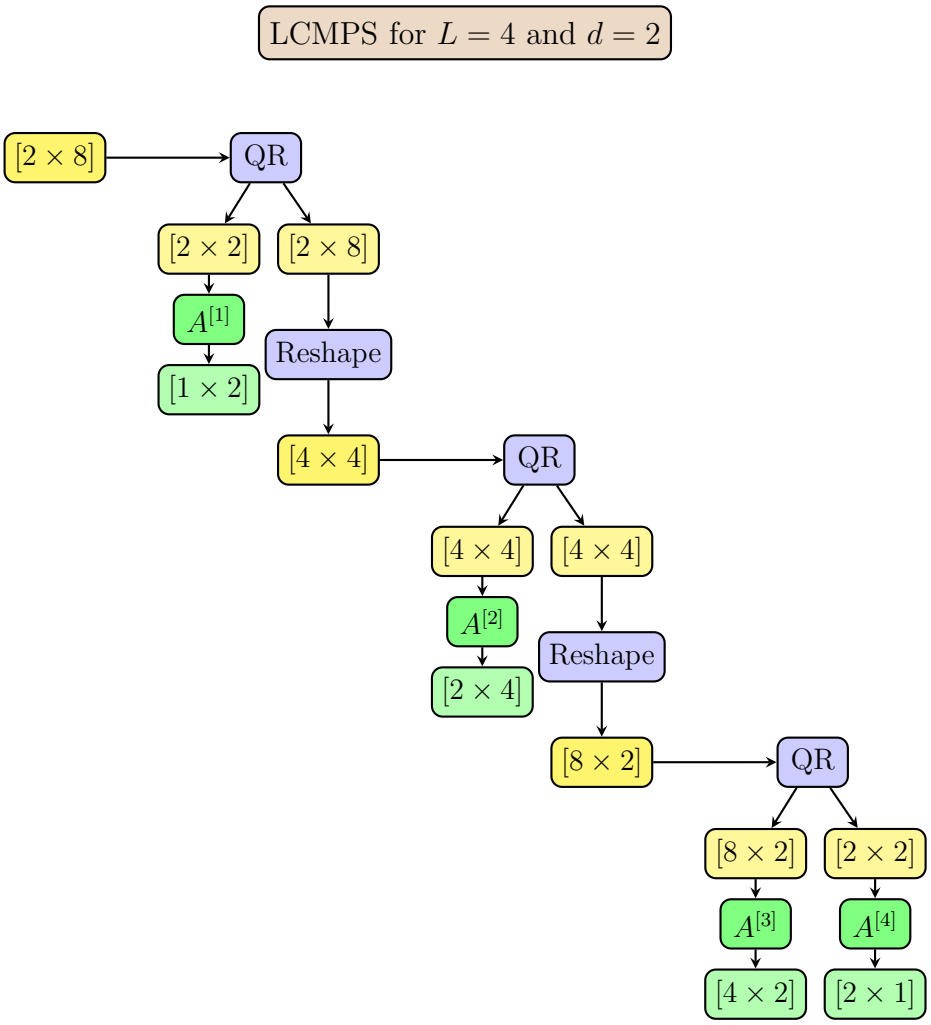


Figure 3.4: Flowchart Diagram indicating the steps for LCMPS using QR decomposition

Now for $L = 4$ and $d = 2$ the number of state coefficients will be $d^L = 2^4 = 16$ which we will represent as a matrix of dimension $[16 \times 1]$. Now the first step is to reshape it into a matrix of dimension $[2 \times 8]$. The first QR decomposition will give two matrices Q and R of dimensios $[2 \times 2]$ and $[2 \times 8]$ respectively. We will form the $A-$matrices for the first physical index from this Q matrix. Later the R matrix will be reshaped into a matrix of dimension $[4 \times 4]$. The last QR decomposition will give two matrices Q and R of dimensions $[8 \times 2]$ and $[2 \times 2]$ respectively from which we

will form the $A-$matrices for the third and fourth physical index as it is shown in the Fig.(3.4).

3.7 Figure for the dimensions of A matrices for $L = 2$ to $L = 10$

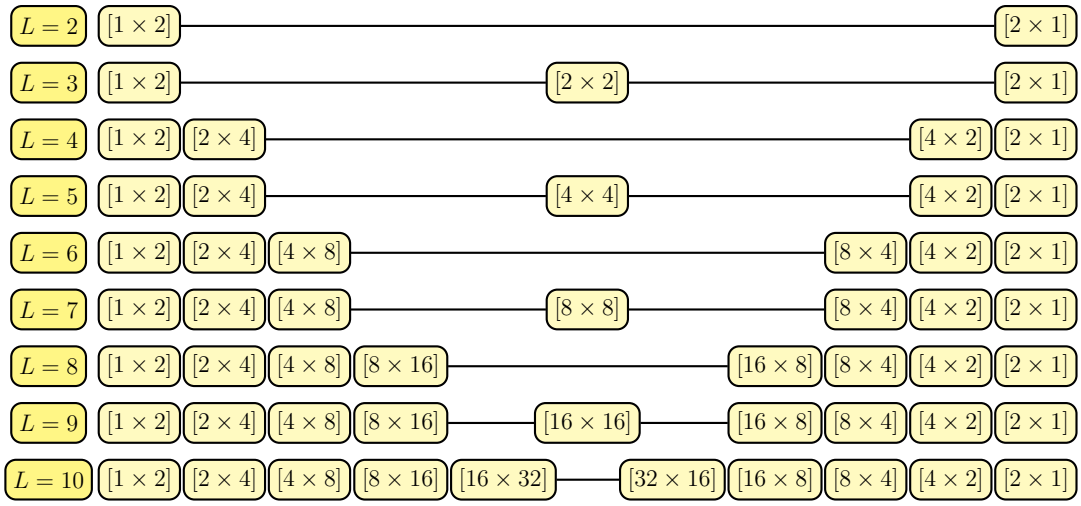


Figure 3.5: Figure for the dimensions of A matrices for $L = 2$ to $L = 10$

For any L we will get dL number of $A-$matrices in LCMPS representation. The dimension of these $A-$matrices for each L is shown in Fig.(3.5). Here for $L = 2$ we get only $2d$ number of $A-$matrices of dimensions $[1 \times 2]$ and $[2 \times 1]$ respectively. Similarly for $L = 7$ we get $7d$ number of $A-$matrices of dimensions $[1 \times 2]$, $[2 \times 4]$, $[4 \times 8]$, $[8 \times 8]$, $[8 \times 4]$, $[4 \times 2]$ and $[2 \times 1]$. Along the horizontal direction for each L, the dimensions of the $A-$matrices increases at first, reaches to a maximum and then decreases again. Along the vertical direction as L increases, the number of $A-$matrices increases with L.

3.8 General structure of the reshaped matrices giving rise to LCMPS for any d and L

We have seen that for any L we get L number of $A-$matrices of dimensions specificed in Fig.(3.5). Now we are in a position to predict the dimensions of the $A-$matrices

for any L. For that, we assign index variable 's' to these $A-$matrices. The following conditions and matrix structure corresponds to a particular row of Fig.(3.5). If $L = 3$ then there will be 3 number of $A-$matrices and s which is the index of $A-$matrices will take three values $s = 1, 2, 3$. The dimensions of the $A-$matrices depend on s, d and L. The conditions for the dimensions of the $A-$matrices for odd and even L are given below.

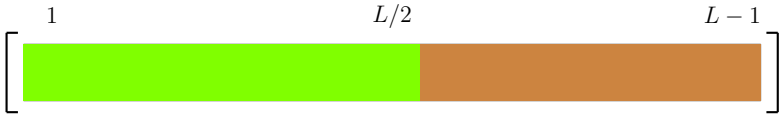
For Even L

Conditions $f(d, s, L)$

For even L, we will get dL number of $A-$matrices. In this case if $s \leqslant L/2$, we see that the dimension of the $A-$matrix will be $[d^{s-1} \times d^s]$ where s is the 'index variable' which basically refers to the particular lattice site. Also if $s > L/2$, we see that the dimension of the $A-$matrix will be $[d^{L+1-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $A-$ matrices show two separate regions. This is indicated in the following figure.

if $(s \leqslant L/2)$:	**if** $(s > L/2)$:
$[d^{s-1} \times d^s]$	$[d^{L+1-s} \times d^{L-s}]$

Matrix Structure



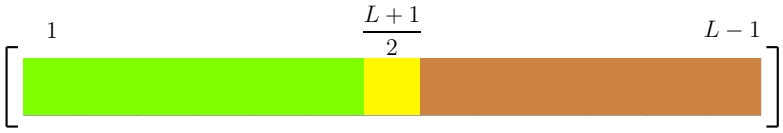
For Odd L

Conditions $f(d, s, L)$

For odd L also, we will get dL number of $A-$matrices. In this case if $s < (L+1)/2)$, we see that the dimension of the $A-$matrix will be $[d^{s-1} \times d^s]$. If $s == (L+1)/2$, we see that the dimension of the $A-$matrix will be $[d^{s-1} \times d^{s-1}]$ and if $s > (L+1)/2)$, we see that the dimension of the $A-$matrix will be $[d^{L+1-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $A-$ matrices show three separate regions. This is indicated in the following figure.

if $(s < (L+1)/2)$: $[d^{s-1} \times d^{s}]$	**if** $(s == (L+1)/2)$: $[d^{s-1} \times d^{s-1}]$	**if** $(s > (L+1)/2)$: $[d^{L+1-s} \times d^{L-s}]$

Matrix Structure



So if we know only the value of d and L, then we can easily predict the dimensions of the A matrices for any arbitrary qudit state, which is the highlight of our work.

3.9 Flowchart for the numerical implementation of LCMPS

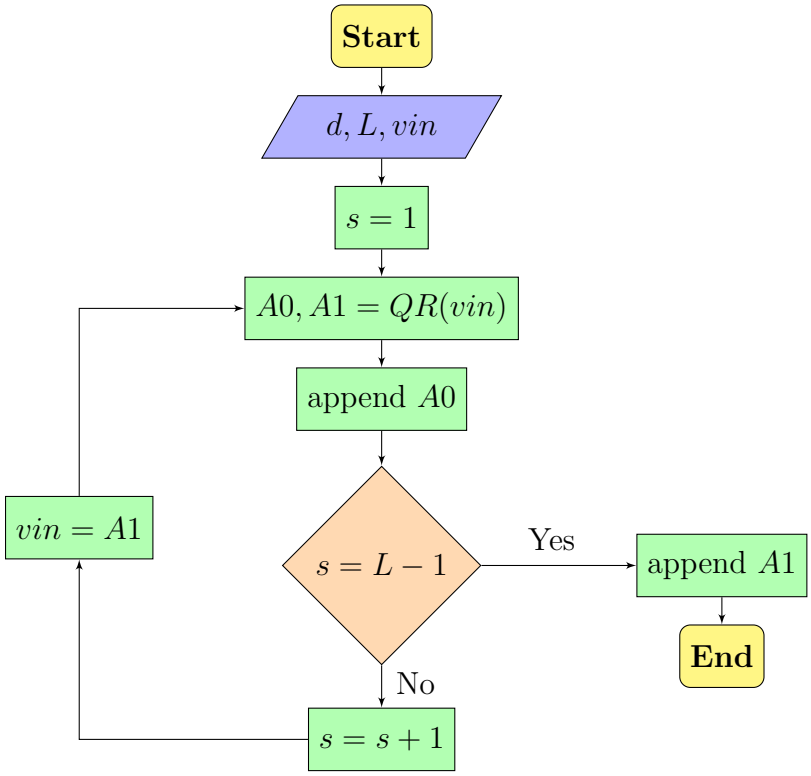


Figure 3.6: Flowchart for the python code of LCMPS

3.10 Python code for LCMPS for any d and L

```
def leftCanonicalMPS(d, L, vin, count):
    global i1, i2, dc
    if (count <= L-1):
        A0, A1 = np.linalg.qr(vin.reshape((int(len(vin[0])/(d**(L-
    count))), d**(L-count))), mode='reduced')
        for i1 in range (0, d):
            dc = i1
            A = []
            x = d**(count-1)
            if (count > (L+1)//2):
                x = d**(L+1-count)
            for i2 in range (0, int(len(A0)/d)):
                A.append(A0[dc])
                dc = dc + d
            matricesA.append(np.array(A).reshape(x, int(len(np.array
    (A).reshape((1,-1))[0])/x)))
        if (count == L-1):
            A1 = A1.T
            for i1 in range (0, d):
                matricesA.append(A1[i1].reshape((-1,1)))
        count = count + 1
        leftCanonicalMPS(d, L, A1.reshape((1,-1)), count)
    return matricesA
```

3.11 Output from the code of LCMPS for any d and any L giving A matrices and state coefficients

Let us see the output of this code that we have written for obtaining LCMPS.

4-qubit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0000\rangle + |1111\rangle\right)$$

Input to the program: $d = 2$, $L = 4$ and $|\psi\rangle$. The program returns 8 number of A matrices and also checks if the obtained matrices are giving back the original state. $A-$Matrices:

```
A0 =
[[1. 0.]]
A1 =
[[-0.  1.]]
A2 =
[[ 1.  0.  0.  0.]
 [-0. -0.  1.  0.]]
A3 =
[[-0.  1.  0.  0.]
 [-0. -0. -0.  1.]]
A4 =
[[ 1.  0.]
 [-0. -0.]
 [-0. -0.]
 [-0. -0.]]
A5 =
[[-0.  0.]
 [-0. -0.]
 [-0. -0.]
 [-0. -1.]]
A6 =
[[0.70710678]
 [0.        ]]
A7 =
[[ 0.        ]
 [-0.70710678]]
```

$$A^{\sigma_1 0} = A0 = \begin{pmatrix} 1. & 0. \end{pmatrix},$$
$$A^{\sigma_1 1} = A1 = \begin{pmatrix} 0. & 1. \end{pmatrix},$$

$$A^{\sigma_1 0} = A2 = \begin{pmatrix} 1. & 0. & 0. & 0. \\ 0. & 0. & 1. & 0. \end{pmatrix},$$

$$A^{\sigma_2 1} = A3 = \begin{pmatrix} 0. & 1. & 0. & 0. \\ 0. & 0. & 0. & 1. \end{pmatrix},$$

$$A^{\sigma_3 0} = A4 = \begin{pmatrix} 1. & 0. \\ 0. & 0. \\ 0. & 0. \\ 0. & 0. \end{pmatrix},$$

$$A^{\sigma_3 1} = A5 = \begin{pmatrix} 0. & 0. \\ 0. & 0. \\ 0. & 0. \\ 0. & -1. \end{pmatrix},$$

$$A^{\sigma_4 0} = A6 = \begin{pmatrix} 0.70710678 \\ 0. \end{pmatrix},$$

$$A^{\sigma_4 1} = A7 = \begin{pmatrix} 0. \\ -0.70710678 \end{pmatrix}.$$

The values of the coefficients making up the state are,

$$|\psi\rangle = \begin{pmatrix} A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 0}A^{\sigma_4 0} = 0.70710678 \\ A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 0}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 1}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 1}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 0}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 0}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 1}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 1}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 0}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 0}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 1}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 1}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 0}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 0}A^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 1}A^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 1}A^{\sigma_4 1} = 0.70710678 \end{pmatrix},$$

which are the correct values of the coefficients for the state considered.

3-qutrit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left(|000\rangle + |111\rangle + |222\rangle\right)$$

Input to the program: $d = 3$, $L = 3$ and $|\psi\rangle$. The program returns 9 number of A matrices and also checks if the obtained matrices are giving back the original state. $A-$Matrices:

```
A0 =
[[1. 0. 0.]]
A1 =
[[-0.  1.  0.]]
A2 =
[[-0. -0.  1.]]
```

```
A3 =
[[ 1.   0.   0.]
 [-0. -0. -0.]
 [-0. -0. -0.]]
A4 =
[[-0.   0.   0.]
 [-0. -1. -0.]
 [-0. -0. -0.]]
A5 =
[[-0. -0.   0.]
 [-0. -0. -0.]
 [-0. -0. -1.]]
A6 =
[[0.57735027]
 [0.         ]
 [0.         ]]
A7 =
[[ 0.         ]
 [-0.57735027]
 [ 0.         ]]
A8 =
[[ 0.         ]
 [ 0.         ]
 [-0.57735027]]
```

$A-$Matrices:

$$A^{\sigma_1 0} = A0 = \begin{pmatrix} 1. & 0. & 0. \end{pmatrix},$$
$$A^{\sigma_1 1} = A1 = \begin{pmatrix} 0. & 1. & 0. \end{pmatrix},$$
$$A^{\sigma_1 2} = A2 = \begin{pmatrix} 0. & 0. & 1. \end{pmatrix},$$
$$A^{\sigma_2 0} = A3 = \begin{pmatrix} 1. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$
$$A^{\sigma_2 1} = A4 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & -1. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$

$$A^{\sigma_2 2} = A5 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & -1. \end{pmatrix},$$

$$A^{\sigma_3 0} = A6 = \begin{pmatrix} 0.57735027 \\ 0. \\ 0. \end{pmatrix},$$

$$A^{\sigma_3 1} = A7 = \begin{pmatrix} 0. \\ -0.57735027 \\ 0. \end{pmatrix},$$

$$A^{\sigma_3 2} = A8 = \begin{pmatrix} 0. \\ 0. \\ -0.57735027 \end{pmatrix}.$$

The values of the state coefficients are,

$$|\psi\rangle = \begin{pmatrix} A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 0} = 0.57735027 \\ A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 1} = 0.57735027 \\ A^{\sigma_1 1}A^{\sigma_2 1}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}A^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}A^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}A^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}A^{\sigma_3 2} = 0.57735027 \end{pmatrix},$$

which are in perfect match with the coefficients for the state considered.

3.12 Summary and conclusion

In this chapter the procedure to obtain Left Canonical Matrix Product State (LCMPS) for any qudit quantum state using both SVD and QR was discussed in detail. The dimensions and properties of the left normalized A matrices were analysed. The whole procedure was explained in detail with the help of an analytical calculation and numerical results for the case of qubit and qutrit state. A flowchart diagram was also provided for illustrating all the steps involved. A generalized code was written in Python which can work for any value of d and L and thus for any pure quantum qudit state. The regions for odd and even qudit cases were separately studied and the structure of the reshaped matrices and novel results were obtained for the A matrices.

Chapter 4

The right canonical matrix product state (RCMPS)

4.1 Procedure to obtain the right canonical matrix product state (RCMPS) for any qudit state

A general pure quantum state is,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} \sum_{\sigma_2=1}^{d} ... \sum_{\sigma_L=1}^{d} C_{\sigma_1\sigma_2...\sigma_L} |\sigma_1\rangle|\sigma_2\rangle...|\sigma_L\rangle. \tag{4.1}$$

In similar manner as LCMPS, we can start from the right and go towards left that is from L to 1 [7]. First step is to reshape this state vector with d^L elements into a matrix ψ of dimension $[d^{L-1} \times d]$

$$C_{(\sigma_1...\sigma_L),(1)} = \psi_{(\sigma_1...\sigma_{L-1}),(\sigma_L)}. \tag{4.2}$$

SVD of ψ gives,

$$C_{(\sigma_1...\sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} U_{(\sigma_1...\sigma_{L-1}),(a_{L-1})} S_{(a_{L-1}),(a_{L-1})} (V^\dagger)_{(a_{L-1}),(\sigma_L)}. \tag{4.3}$$

The rank $r_{L-1} \leqslant d$. So we restrict the sum to run only over the first r_{L-1} positive non-zero singular values, so the number of operations to be performed has decreased. This is an optimal approximation.

$$U_{d^{L-1},d} S_{d,d} (V^\dagger)_{d,d} \rightarrow U_{d^{L-1},r_{L-1}} S_{r_{L-1},r_{L-1}} (V^\dagger)_{r_{L-1},d}.$$

U and S are multiplied and the resulting matrix has been reshaped back into a vector.

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} C_{(\sigma_1 \ldots \sigma_{L-1}),(a_{L-1})} (V^\dagger)_{(a_{L-1}),(\sigma_L)}. \tag{4.4}$$

Now we decompose the matrix $V^\dagger$ into a collection of d column vectors B^{σ_L} of dimension $[r_{L-1} \times 1]$ with entries $B^{\sigma_L}_{a_{L-1},(1)} = (V^\dagger)_{(a_{L-1}),(\sigma_L)}$ where $(V^\dagger)_{(a_i),(\sigma_L)}$ is the $i-$th column of the $V^\dagger$ matrix. Also we reshape $C_{(\sigma_1 \ldots \sigma_{L-1}),(a_{L-1})}$ into a matrix $\psi_{(\sigma_1 \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})}$ of dimension $[d^{L-2} \times r_{L-1} d]$, to give

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1 \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.5}$$

Graphically, the result after the first decomposition is represented as shown below in Fig.(4.1), where we have on the right hand side a blue circle representing $B^{\sigma_L}_{(a_{L-1}),(1)}$ and on the left $C_{(\sigma_1 \ldots \sigma_{L-1}),(a_{L-1})}$. The auxiliary degrees of freedon (a_{L-1}) are represented by horizontal lines, and the rule is that **connected lines are summed over**.

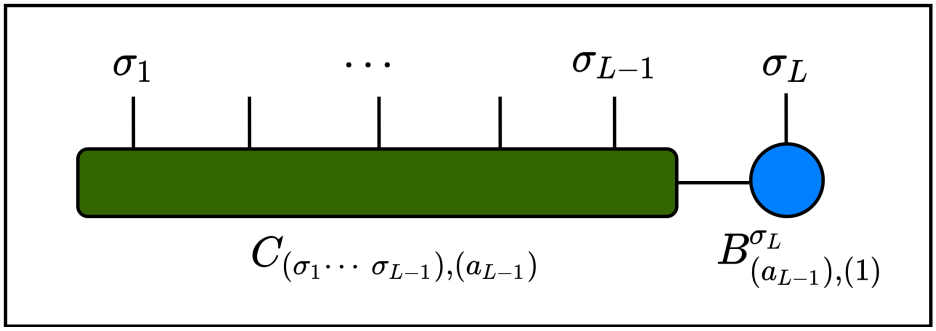


Figure 4.1: Graphical representation of $B^{\sigma_{L-1}}$ after the first SVD

SVD of ψ gives,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} \sum_{a_{L-2}=1}^{r_{L-2}} U_{(\sigma_1 \ldots \sigma_{L-2}),(a_{L-2})} S_{(a_{L-2}),(a_{L-2})} (V^\dagger)_{(a_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.6}$$

The rank is $r_{L-2} \leqslant r_{L-1} d \leqslant d^2$. Multiply U and S and reshape into a matrix ψ of dimension $[d^{L-3} \times r_{L-2} d]$ to get,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} \sum_{a_{L-2}=1}^{r_{L-2}} \underbrace{U_{(\sigma_1 \ldots \sigma_{L-2}),(a_{L-2})} S_{(a_{L-2}),(a_{L-2})}}_{\psi_{(\sigma_1 \ldots \sigma_{L-3}),(\sigma_{L-2} a_{L-2})}} (V^\dagger)_{(a_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.7}$$

Replace $V^\dagger$ by a set of d matrices $B^{\sigma_{L-1}}$ of dimension $[r_{L-2} \times r_{L-1}]$ with entries

$$B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} = (V^\dagger)_{(a_{L-2}),(\sigma_{L-1}a_{L-1})}.$$

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} \sum_{a_{L-2}=1}^{r_{L-2}} \psi_{(\sigma_1 \ldots \sigma_{L-3}),(\sigma_{L-2}a_{L-2})} B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.8}$$

After the second decomposition, we have $B^{\sigma_L}_{(a_{L-1}),(1)}$, then $B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}$ and on the left $C_{(\sigma_1 \ldots \sigma_{L-2}),(a_{L-2})}$, with all the connected lines summed over as shown in Fig.(4.2).

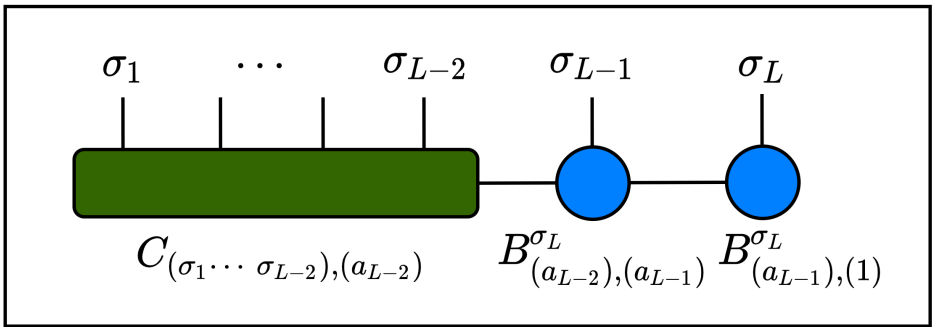


Figure 4.2: Graphical representation of $B^{\sigma_{L-2}}$ and $B^{\sigma_{L-1}}$ after the second SVD

Upon further SVDs, we obtain

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_1=1}^{r_1} \sum_{a_2=1}^{r_2} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} B^{\sigma_1}_{(1),(a_1)} B^{\sigma_2}_{(a_1),(a_2)} \ldots B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.9}$$

So, we have arrived at L number of $B-$matrices multiplied together and labelled by physical indices as shown in Fig.(4.3). $\sigma_1, \sigma_2, \ldots$ are the physical indices and $a_1, a_2, \ldots$ are the matrix indices. A site l is represented by a solid blue circle and the physical index σ_l by a vertical line. The first and last site are row and column vectors respectively, connected by only one horizontal line indicating one matrix index. All other sites are matrices connected by two horizontal lines indicating two matrix indices. The graphical representation of $B-$matrices is same as that of $A-$matrices.

In compact form,

$$C_{\sigma_1 \ldots \sigma_L} = B^{\sigma_1} B^{\sigma_2} \ldots B^{\sigma_{L-1}} B^{\sigma_L}. \tag{4.10}$$

where we have replaced the sums over $a_1, a_2, \ldots$ by matrix multiplications.

We obtain an MPS of the form

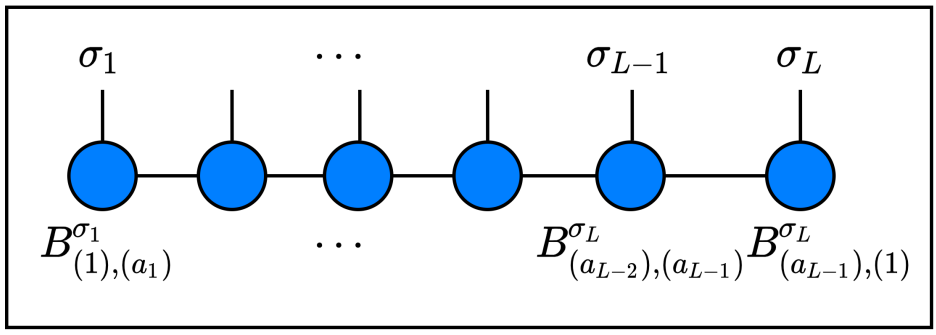


Figure 4.3: Graphical representation of the product of B matrices making up the complete matrix product state

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} ... \sum_{\sigma_L=1}^{d} B^{\sigma_1} B^{\sigma_2} ... B^{\sigma_{L-1}} B^{\sigma_L} |\sigma_1\rangle ... |\sigma_L\rangle. \tag{4.11}$$

The (arbitrary) quantum qudit state is now represented exactly in the form of a matrix product state.

4.1.1 Dimensions of the B matrices

The dimensions of the $B-$matrices are same as the $A-$matrices. For even L, the dimensions of the $B-$matrices will be $[1 \times d], [d \times d^2], ..., [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2-1}], ..., [d^2 \times d], [d \times 1]$. For odd L, the dimensions of the $B-$matrices will be $[1 \times d], [d \times d^2], ..., [d^{L/2-1} \times d^{L/2}], [d^{L/2} \times d^{L/2}], [d^{L/2} \times d^{L/2-1}], ..., [d^2 \times d], [d \times 1]$. RCMPS gives dL number of $B-$matrices of which the first d matrices are row matrices and last d matrices are column matrices.

4.1.2 Properties of the B matrices

For each SVD, the $V^\dagger$ matrix is right normalized meaning that $V^\dagger \left(V^\dagger\right)^\dagger = I$. Hence $V^\dagger V = I$ holds for each SVD.

$$\delta_{a_l, a_l'} = \sum_{a_{l-1}=1}^{r_{l-1}} \sum_{\sigma_l=1}^{d} (V^\dagger)_{(a_l),(a_{l-1}\sigma_l)} V_{(a_{l-1}\sigma_l),(a_l')} = I. \tag{4.12}$$

Now, we will replace V by a set of B matrices as given by,

$$\sum_{a_{l-1}=1}^{r_{l-1}} \sum_{\sigma_l=1}^{d} B^{\sigma_l}_{(a_l),(a_{l-1})} (B^{\sigma_l})^{\dagger}_{(a_{l-1}),(a_l')} = \sum_{\sigma_l=1}^{d} (B^{\sigma_l}(B^{\sigma_l})^{\dagger})_{(a_l),(a_l')} = I. \tag{4.13}$$

This implies,

$$\sum_{\sigma_l} B^{\sigma_l}(B^{\sigma_l})^{\dagger} = I. \tag{4.14}$$

Matrices that obey this condition are referred to as right-normalized. Matrix product states that consist only of right-normalized matrices are called right-canonical MPS.

4.2 Clear steps involved in RCMPS using SVD

We have studied the procedure to obtain the right canonical matrix product state (RCMPS) for any qudit state. Here we will give all the steps involved in it for clarity and deep understanding. We will start with Eq.(4.2),

$$\begin{aligned}
& C_{(\sigma_1 \ldots \sigma_L),(1)} \\
= \;& \psi_{(\sigma_1 \ldots \sigma_{L-1}),(\sigma_L)}, \\
= \;& \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{U_{(\sigma_1 \ldots \sigma_{L-1}),(a_{L-1})} S_{(a_{L-1}),(a_{L-1})}}_{\psi_{(\sigma_1 \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})}} \underbrace{(V^{\dagger})_{(a_{L-1}),(\sigma_L)}}_{B^{(\sigma_L),(1)}_{a_{L-1}}}, \\
= \;& \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1 \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
= \;& \sum_{a_{L-2}=1}^{r_{L-2}} \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{U_{(\sigma_1 \ldots \sigma_{L-2}),(a_{L-2})} S_{(a_{L-2}),(a_{L-2})}}_{\psi_{(\sigma_1 \ldots \sigma_{L-3}),(\sigma_{L-2} a_{L-2})}} \underbrace{(V^{\dagger})_{(a_{L-2}),(\sigma_{L-1} a_{L-1})}}_{B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
= \;& \sum_{a_{L-2}=1}^{r_{L-2}} \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1 \ldots \sigma_{L-3}),(\sigma_{L-2} a_{L-2})} B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
& \qquad \vdots \\
= \;& \sum_{a_2=1}^{r_2} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1),(\sigma_2 a_2)} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}, \\
= \;& \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{U_{(\sigma_1),(a_1)} S_{(a_1),(a_1)}}_{B^{\sigma_1}_{(1),(a_1)}} \underbrace{(V^{\dagger})_{(a_1),(\sigma_2 a_2)}}_{B^{\sigma_2}_{(a_1),(a_2)}} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}, \\
= \;& \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} B^{\sigma_1}_{(1),(a_1)} B^{\sigma_2}_{(a_1),(a_2)} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}.
\end{aligned}$$

4.3 Right canonical MPS using QR decomposition

Right canonical MPS can also be generated by using the QR decomposition. But here we do not QR-decompose the matrix $\psi = QR$, but instead $\psi^\dagger = QR$, such that $\psi = R^\dagger Q^\dagger$. We form the $B-$matrices from $Q^\dagger$ as under,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \psi_{(\sigma_1 \ldots \sigma_{L-1}),\sigma_L} = \sum_{a_{L-1}=1}^{r_{L-1}} R^\dagger_{(\sigma_1 \ldots \sigma_{L-1}),a_{L-1}} Q^\dagger_{a_{L-1},\sigma_L}. \tag{4.15}$$

Now we decompose the matrix $Q^\dagger$ into a collection of d column vectors $B^{\sigma_{L-1}}$ of dimension $[r_{L-1} \times 1]$ with entries $B^{\sigma_{L-1}}_{(a_{L-1}),(1)} = Q^\dagger_{a_{L-1},\sigma_L}$. It is similar to the SVD procedure. Reshape $R^\dagger \to \psi$

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1) \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{4.16}$$

Then we continue by QR decomposition of $\psi^\dagger$, thin QR is required here, as an analysis of the dimension shows (as given in sec.[3.3.1]).

This implies that the MPS representation of a state is not unique, as we have obtained various different exact representations of $|\psi\rangle$ in the MPS form.

4.4 Clear steps involved in the RCMPS using QR

Now we will give all the steps involved in obtaining RCMPS using QR decomposition for clarity and deep understanding. We will start with Eq.(4.2),

$$
\begin{aligned}
&C_{(\sigma_1\ldots\sigma_L),(1)} \\
&= \psi_{(\sigma_1\ldots\sigma_{L-1}),(\sigma_L)}, \\
&= \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{Q_{(\sigma_1\ldots\sigma_{L-1}),(a_{L-1})}}_{\psi_{(\sigma_1\ldots\sigma_{L-2}),(\sigma_{L-1}a_{L-1})}} \underbrace{R_{(a_{L-1}),(\sigma_L)}}_{B^{\sigma_L}_{(a_{L-1}),(1)}}, \\
&= \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1\ldots\sigma_{L-2}),(\sigma_{L-1}a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_{L-2}=1}^{r_{L-2}} \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{Q_{(\sigma_1\ldots\sigma_{L-2}),(a_{L-2})}}_{\psi_{(\sigma_1\ldots\sigma_{L-3}),(\sigma_{L-2}a_{L-2})}} \underbrace{R_{(a_{L-2}),(\sigma_{L-1}a_{L-1})}}_{B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})}} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_{L-2}=1}^{r_{L-2}} \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1\ldots\sigma_{L-3}),(\sigma_{L-2}a_{L-2})} B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&\qquad\qquad\qquad\qquad \vdots \\
&= \sum_{a_2=1}^{r_2} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(\sigma_1),(\sigma_2 a_2)} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{Q_{(\sigma_1),(a_1)}}_{B^{\sigma_1}_{(1),(a_1)}} \underbrace{R_{(a_1),(\sigma_2 a_2)}}_{B^{\sigma_2}_{(a_1),(a_2)}} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} B^{\sigma_1}_{(1),(a_1)} B^{\sigma_2}_{(a_1),(a_2)} B^{\sigma_3}_{(a_2),(a_3)} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}.
\end{aligned}
$$

4.5 Analytical calculation and discussion of RCMPS with one example

Now let us consider one example to clear the mist in performing the RCMPS. We will find the RCMPS representation for the 4-qubit $W-$state given by,

$$
|\psi\rangle = \frac{1}{2}\left[|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle\right]. \tag{4.17}
$$

Here $d = 2$ and $L = 4$, hence this state in the matrix form will have $d^L = 16$ elements.

- Step 1 - Reshape the state in Eq.(4.17) into matrix of dimension $[d^{L-1} \times d]$,

$$\begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

- Step 2 - Perform a QR Decomposition,

$$\underbrace{\begin{pmatrix} 0 & 1 \\ \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 \\ \frac{1}{2} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{\sqrt{3}}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}}_{R}.$$

- Step 3 - Form B^{σ_4} matrices from the R matrix,

$$B^{\sigma_4 0} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ 0 \end{pmatrix}, \qquad \text{and} \qquad B^{\sigma_4 1} = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}.$$

- Step 4 - Reshape Q into matrix of dimension $[d^{L-2} \times d^2]$,

$$\begin{pmatrix} 0 & 1 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Step 5 - Perform QR Decomposition of the above matrix,

$$\underbrace{\begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 1 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{R}.$$

- Step 6 - Reshape R into matrix of dimension $[d^{L-1} \times d]$,

$$\begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & 0 \\ 0 & 1 \\ \frac{1}{3} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

- Step 7 - Form B^{σ_3} matrices from the R matrix,

$$B^{\sigma_3 0} = \begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix},$$

$$B^{\sigma_3 1} = \begin{pmatrix} 0 & 0 \\ \frac{1}{3} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

- Step 8 - Reshape Q into matrix of dimension $[d^{L-3} \times d^3]$,

$$\begin{pmatrix} 0 & 1 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

- Step 9 - Perform QR Decomposition of the above matrix,

$$\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix}}_{R}.$$

- Step 10 - Reshape R into a matrix of dimension $[d^{L-2} \times d^2]$,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix}.$$

- Step 11 - Form B^{σ_2} matrices from the R matrix as below,

$$B^{\sigma_2 0} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$B^{\sigma_2 1} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} & 0 \end{pmatrix}.$$

- Step 12 - Form B^{σ_1} matrices from the Q matrix,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$B^{\sigma_1 0} = \begin{pmatrix} 0 & 1 \end{pmatrix},$$

$$B^{\sigma_1 1} = \begin{pmatrix} 1 & 0 \end{pmatrix}.$$

4.6 Flowchart diagram indicating the steps for RCMPS using QR decomposition with explanation

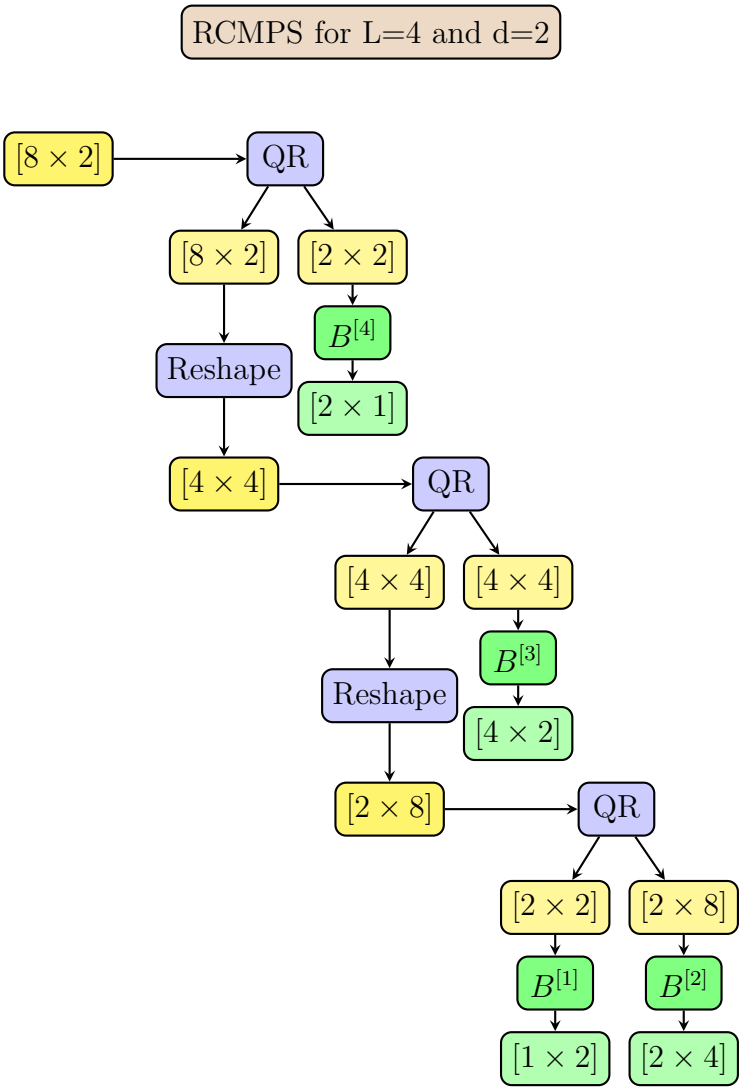


Figure 4.4: Flowchart Diagram indicating the steps for RCMPS using QR decomposition

Now for $L = 4$ and $d = 2$ the number of state coefficients will be $d^L = 2^4 = 16$ which we will represent as a matrix of dimension $[16 \times 1]$. Now the first step is to reshape it into a matrix of dimension $[8 \times 2]$. The first QR decomposition will give two matrices Q and R of dimensions $[8 \times 2]$ and $[2 \times 2]$ respectively. We will form the $B-$matrices for the first physical index from this R matrix. Later the Q matrix will be reshaped into a matrix of dimension $[4 \times 4]$. The same procedure will be followed for $L - 1$ times as it is shown in the Fig.(4.4).

4.7 Figure for the dimensions of B matrices for $L = 2$ to $L = 10$

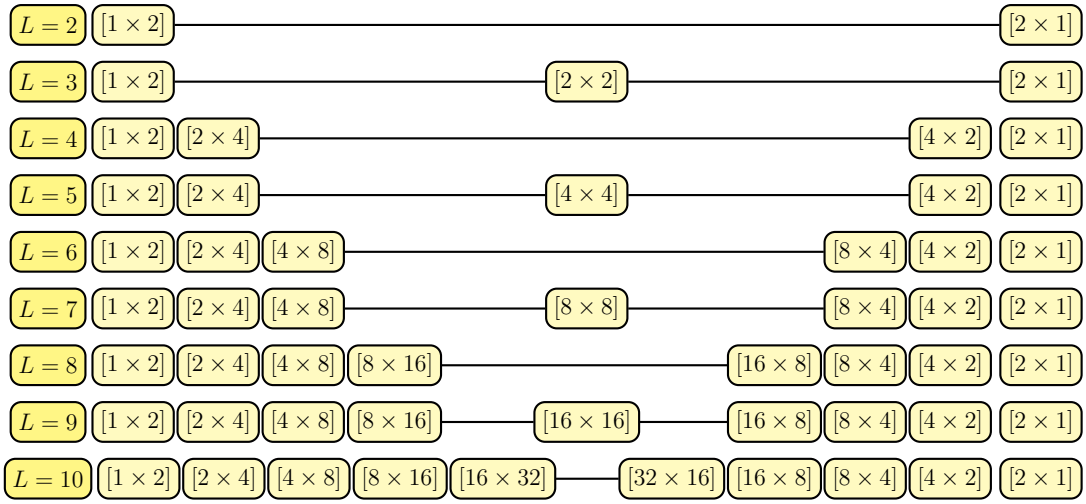


Figure 4.5: Figure for the dimensions of B matrices for $L = 2$ to $L = 10$

For any L we will get dL number of $B-$matrices in the RCMPS representation. The dimension of these $B-$matrices for each L is shown in the Fig.(4.5). Here for $L = 2$ we get only $2d$ number of $B-$matrices of dimensions $[1 \times 2]$ and $[2 \times 1]$ respectively. Similarly for $L = 7$ we get $7d$ number of $B-$matrices of dimensions $[1 \times 2]$, $[2 \times 4]$, $[4 \times 8]$, $[8 \times 8]$, $[8 \times 4]$, $[4 \times 2]$ and $[2 \times 1]$. Along the horizontal direction for each L, the dimensions of the $B-$matrices increases at first, reaches to a maximum and then decreases again. Along the vertical direction as L increases, the number of $B-$matrices increases with L.

4.8 General structure of the reshaped matrices giving rise to RCMPS for any d and L

We have seen that for any L we get dL number of $B-$matrices of dimensions specificed in the Fig.(4.5). Now we are in a position to predict the dimensions of the $B-$matrices for any L. For that, we assign index variable 's' to these $B-$matrices. The following conditions and matrix structure corresponds to particular row of Fig.(4.5). If $L = 3$ then there will be 3 number of $B-$matrices and s which is the index of $B-$matrices

will take three values $s = 1, 2, 3$. The dimensions of the $B-$matrices depend on s, d and L. The conditions for the dimensions of the $B-$matrices for odd and even L are given below.

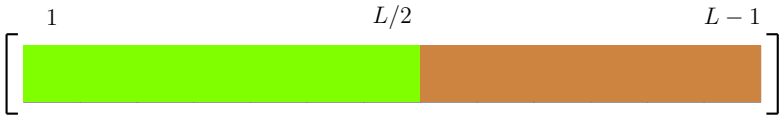
For Even L

Conditions $f(d, s, L)$

For even L, we will get dL number of $B-$matrices. In this case if $s \leqslant L/2$, we see that the dimension of the $B-$matrix will be $[d^{s-1} \times d^s]$ where s is the 'index variable' which basically refers to the particular lattice site. Also if $s > L/2$, we see that the dimension of the $B-$matrix will be $[d^{L+1-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $B-$ matrices show two separate regions. This is indicated in the following figure.

if $(s \leqslant L/2)$:	**if** $(s > L/2)$:
$[d^{s-1} \times d^s]$	$[d^{L+1-s} \times d^{L-s}]$

Matrix Structure



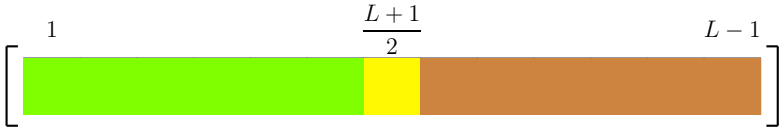
For Odd L

Conditions $f(d, s, L)$

For odd L also, we will get dL number of $B-$matrices. In this case if $s < (L+1)/2)$, we see that the dimension of the $B-$matrix will be $[d^{s-1} \times d^s]$. If $s == (L+1)/2$, we see that the dimension of the $B-$matrix will be $[d^{s-1} \times d^{s-1}]$ and if $s > (L+1)/2)$, we see that the dimension of the $B-$matrix will be $[d^{L+1-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $B-$ matrices show three separate regions. This is indicated in the following figure.

if $(s < (L+1)/2)$: $[d^{s-1} \times d^{s}]$	**if** $(s == (L+1)/2)$: $[d^{s-1} \times d^{s-1}]$	**if** $(s > (L+1)/2)$: $[d^{L+1-s} \times d^{L-s}]$

Matrix Structure



So if we know only the value of d and L, then we can easily predict the dimensions of the $B-$ matrices for any arbitrary qudit state, which is the highlight of our work.

4.9 Flowchart for the numerical implementation of RCMPS

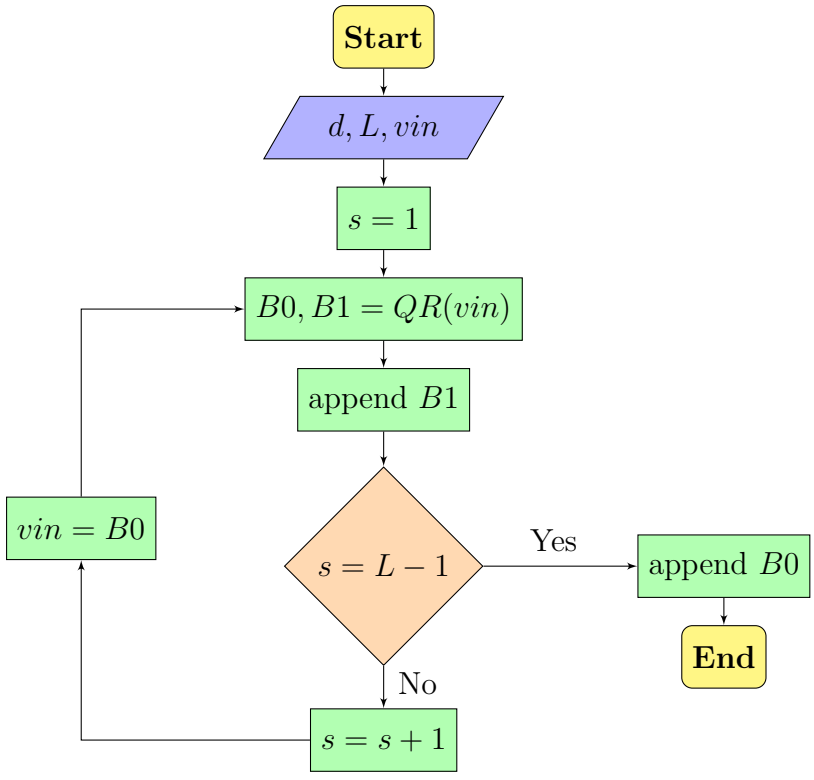


Figure 4.6: Flowchart for the python code of RCMPS

4.10 Python code for RCMPS for any d and L

```
def rightCanonicalMPS(d, L, vin, count):
    global i1, i2, dc
    if (count <= L-1):
        B0, B1 = np.linalg.qr(vin.reshape(( d**(L-count), int(len(
    vin[0])/(d**(L-count))))), mode='reduced')
        for i1 in range (0, d):
            dc = i1
            B = []
            x = d**(count-1)
            if (count > (L+1)//2):
                x = d**(L+1-count)
            B1 = B1.reshape(int(len(B1.reshape((1,-1))[0])/x), x)
            for i2 in range (0, int(len(B1)/d)):
                B.append(B1[dc])
                dc = dc + d
            matricesB.append(np.array(B).reshape(int(len(np.array(B)
    .reshape((1,-1))[0])/x), x))
        if (count == L-1):
            for i1 in range (0, d):
                matricesB.append(B0[i1].reshape((1,-1)))
        count = count + 1
        rightCanonicalMPS(d, L, B0.reshape((1,-1)), count)
    return matricesB
```

4.11 Output from the code of RCMPS for any d and any L giving B matrices and state coefficients

Let us see the output of this code that we have written for obtaining RCMPS.

4-qubit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0000\rangle + |1111\rangle\right)$$

Input to the program: $d = 2$, $L = 4$ and $|\psi\rangle$. The program returns 8 $B-$ matrices and also checks if the obtained matrices are giving back the original state.

$B-$Matrices:

```
B0 =
[[0.70710678]
 [0.        ]]
B1 =
[[ 0.        ]
 [-0.70710678]]
B2 =
[[1. 0.]
 [0. 0.]
 [0. 0.]
 [0. 0.]]
B3 =
[[-0.  0.]
 [ 0.  0.]
 [ 0.  0.]
 [ 0. -1.]]
B4 =
[[ 1.  0.  0.  0.]
 [ 0. -0.  1.  0.]]
B5 =
[[ 0.  1.  0.  0.]
 [ 0. -0. -0.  1.]]
B6 =
[[1. 0.]]
B7 =
[[-0.  1.]]
```

$B-$Matrices:

$$B^{\sigma_1 0} = B6 = \begin{pmatrix} 1. & 0. \end{pmatrix},$$

$$B^{\sigma_1 1} = B7 = \begin{pmatrix} 0. & 1. \end{pmatrix},$$

$$B^{\sigma_1 0} = B4 = \begin{pmatrix} 1. & 0. & 0. & 0. \\ 0. & 0. & 1. & 0. \end{pmatrix},$$

$$B^{\sigma_2 1} = B5 = \begin{pmatrix} 0. & 1. & 0. & 0. \\ 0. & 0. & 0. & 1. \end{pmatrix},$$

$$B^{\sigma_3 0} = B2 = \begin{pmatrix} 1. & 0. \\ 0. & 0. \\ 0. & 0. \\ 0. & 0. \end{pmatrix},$$

$$B^{\sigma_3 1} = B3 = \begin{pmatrix} 0. & 0. \\ 0. & 0. \\ 0. & 0. \\ 0. & -1. \end{pmatrix},$$

$$B^{\sigma_4 0} = B0 = \begin{pmatrix} 0.70710678 \\ 0. \end{pmatrix},$$

$$B^{\sigma_4 1} = B1 = \begin{pmatrix} 0. \\ -0.70710678 \end{pmatrix}.$$

The values of the coefficients making up the state are,

$$|\psi\rangle = \begin{pmatrix} B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 0}B^{\sigma_4 0} = 0.70710678 \\ B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 1}B^{\sigma_4 1} = 0.70710678 \end{pmatrix},$$

which are the correct values of the coefficients for the state considered.

3-qutrit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left(|000\rangle + |111\rangle + |222\rangle\right)$$

Input to the program: $d = 3$, $L = 3$ and $|\psi\rangle$. The program returns 9 $B-$matrices and also checks if the obtained matrices are giving back the original state.

$B-$Matrices:

```
B0 =
[[0.57735027]
 [0.        ]
 [0.        ]]
B1 =
[[ 0.        ]
 [-0.57735027]
```

```
 [ 0.         ]]
B2 =
[[ 0.         ]
 [ 0.         ]
 [-0.57735027]]
B3 =
[[1. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]
B4 =
[[-0.  0.  0.]
 [ 0. -1.  0.]
 [ 0.  0.  0.]]
B5 =
[[-0. -0.  0.]
 [ 0.  0.  0.]
 [ 0.  0. -1.]]
B6 =
[[1. 0. 0.]]
B7 =
[[0. 1. 0.]]
B8 =
[[ 0. -0.  1.]]
```

$B-$Matrices:

$$B^{\sigma_1 0} = B6 = \begin{pmatrix} 1. & 0. & 0. \end{pmatrix},$$

$$B^{\sigma_1 1} = B7 = \begin{pmatrix} 0. & 1. & 0. \end{pmatrix},$$

$$B^{\sigma_1 2} = B8 = \begin{pmatrix} 0. & 0. & 1. \end{pmatrix},$$

$$B^{\sigma_2 0} = B3 = \begin{pmatrix} 1. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$

$$B^{\sigma_2 1} = B4 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & -1. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$

$$B^{\sigma_2 2} = B5 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & -1. \end{pmatrix},$$

$$B^{\sigma_3 0} = B0 = \begin{pmatrix} 0.57735027 \\ 0. \\ 0. \end{pmatrix},$$

$$B^{\sigma_3 1} = B1 = \begin{pmatrix} 0. \\ -0.57735027 \\ 0. \end{pmatrix},$$

$$B^{\sigma_3 2} = B2 = \begin{pmatrix} 0. \\ 0. \\ -0.57735027 \end{pmatrix}.$$

The values of the state coefficients are,

$$|\psi\rangle = \begin{pmatrix} B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 0} = 0.57735027 \\ B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 0}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 1}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 2}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 2}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 0}B^{\sigma_2 2}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 0}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 1} = 0.57735027 \\ B^{\sigma_1 1}B^{\sigma_2 1}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 2}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 2}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 1}B^{\sigma_2 2}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 0}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 0}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 0}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 1}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 1}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 1}B^{\sigma_3 2} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 2}B^{\sigma_3 0} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 2}B^{\sigma_3 1} = 0. \\ B^{\sigma_1 2}B^{\sigma_2 2}B^{\sigma_3 2} = 0.57735027 \end{pmatrix},$$

which are in perfect match with the coefficients for the state considered.

4.12 Summary and conclusion

In this chapter the procedure to obtain Right Canonical Matrix Product State (RCMPS) for any quantum qudit state using both SVD and QR was discussed in detail. The dimensions and properties of the right normalized $B-$matrices was analysed. The whole procedure was explained in detail with the help of an analytical calculation using one example for qubit and qutrit. A flowchart diagram was also provided for clearly indicating all the steps involved. A generalized code was introduced which can work for any value of d and L and thus for any pure quantum qudit state. This code was presented along with the flowchart and some illustrative examples.

Chapter 5

The mixed canonical matrix product state (MCMPS)

In the previous chapters we have seen the details about LCMPS and RCMPS and we obtained,

LCMPS:

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{5.1}$$

RCMPS:

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} B^{\sigma_1} B^{\sigma_2} \cdots B^{\sigma_{L-1}} B^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{5.2}$$

For LCMPS we performed SVD from left and for RCMPS we performed SVD from right, we can also mix the decomposition of the state from the left and from the right [7].

5.1 Procedure to obtain the mixed canonical matrix product state (MCMPS) for any qudit state

We will start with general pure quantum state,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} \sum_{\sigma_2=1}^{d} ... \sum_{\sigma_L=1}^{d} C_{\sigma_1 \sigma_2 ... \sigma_L} |\sigma_1\rangle |\sigma_2\rangle ... |\sigma_L\rangle. \tag{5.3}$$

Now consider a decomposition of $|\Psi\rangle$ from left up to site l,

$$C_{(\sigma_1 \ldots \sigma_L),(1)} = \sum_{a_l} (A^{\sigma_1} \ldots A^{\sigma_l})_{(1),(a_l)} S_{(a_l),(a_l)} (V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)}. \tag{5.4}$$

Graphically, the result after the first l decomposition is represented as shown below in Fig.(5.1), where we have on the left hand side l number of red circles representing $A^{\sigma_1} \cdots A^{\sigma_l}$ and on the left $C_{a_l,(\sigma_{l+1} \cdots \sigma_L)}$.

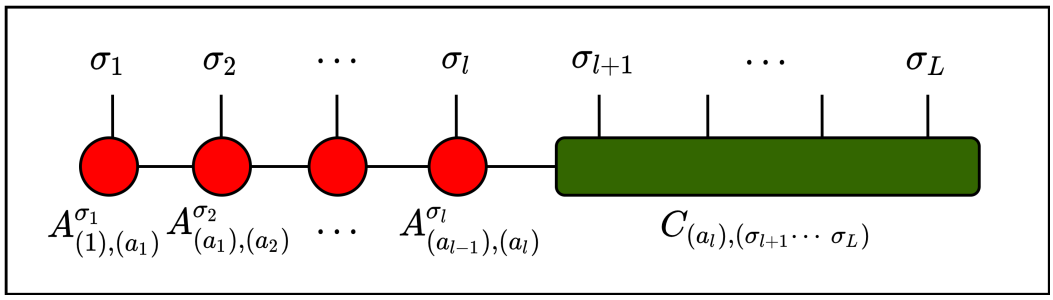


Figure 5.1: Graphical representation of $A^{\sigma_1} \cdots A^{\sigma_l}$ after the first l number of SVDs from left

We reshape $V^\dagger$ as matrix $\psi_{(a_l \sigma_{l+1} \ldots \sigma_{L-1}),(\sigma_L)}$ and carry out successive SVDs as in the original right canonical decomposition from the right, up to and including the site σ_{l+2} to get,

$$(V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)} \rightarrow \psi_{(a_l \sigma_{l+1} \ldots \sigma_{L-1}),(\sigma_L)}.$$

Graphically, the result after the first decomposition from right is represented as shown below in Fig.(5.2), where we have on the right hand side blue circle representing $B^{\sigma_{L-1}}$ and on the left $C_{a_l,(\sigma_{l+1} \cdots \sigma_{L-1}),(a_{L-1})}$.

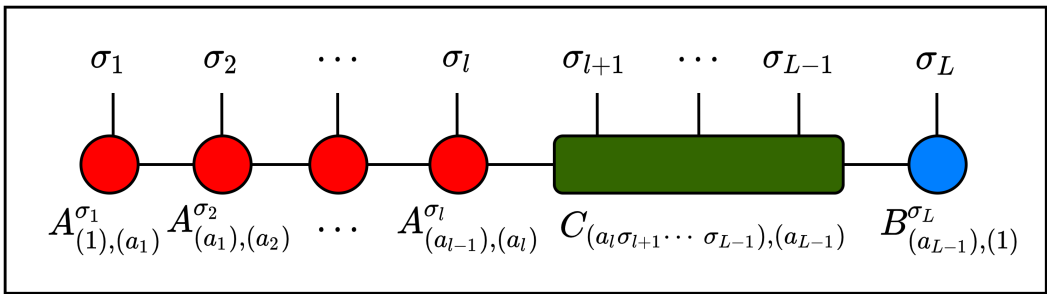


Figure 5.2: Graphical representation of $B^{\sigma_{L-1}}$ after the first SVD from right

In the last SVD $U_{(a_l \sigma_{l+1}),(a_{l+1})} S_{(a_{l+1}),(a_{l+1})}$ remains, which we reshape to $B^{\sigma_{l+1}}_{(a_l),(a_{l+1})}$. Thus we get,

$$(V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)} = \sum_{a_{l+1}=1}^{r_{l+1}} \cdots \sum_{a_{L-1}=1}^{r_{L-1}} B^{\sigma_{l+1}}_{(a_l),(a_{l+1})} B^{\sigma_{l+2}}_{(a_{l+1}),(a_{l+2})} B^{\sigma_{l+3}}_{(a_{l+2}),(a_{l+3})} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}. \tag{5.5}$$

All the steps are given in section [5.2] for clear understanding. So finally from Eq.(5.4) and Eq. (5.5) we get,

$$C_{\sigma_1 \ldots \sigma_L} = \sum_{a_1=1}^{r_1} \ldots \sum_{a_l=1}^{r_l} A^{\sigma_1}_{1,a_1} \ldots A^{\sigma_l}_{a_{l-1},a_l} S_{a_l,a_l} \sum_{a_{l+1} \ldots a_{L-1}} B^{\sigma_{l+1}}_{a_l a_{l+1}} B^{\sigma_{l+2}}_{a_{l+1} a_{l+2}} \ldots B^{\sigma_L}_{a_{L-1},1}, \tag{5.6}$$

$$C_{\sigma_1 \ldots \sigma_L} = \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{1,a_1} \ldots A^{\sigma_l}_{a_{l-1},a_l} S_{a_l,a_l} B^{\sigma_{l+1}}_{a_l a_{l+1}} \ldots B^{\sigma_L}_{a_{L-1},1}. \tag{5.7}$$

All $A-$matrices are left normalized and all $B-$matrices are right normalized. We have arrived at $dL+1$ number of matrices multiplied together and labelled by physical indices. $\sigma_1, \sigma_2, \ldots$ are the physical indices as they refer to the index of lattice sites and $a_1, a_2, \ldots$ are the matrix indices which come from the SVD decomposition. A site represented by a solid red circle represents $A-$matrices and the site represented by a solid blue circle represents $B-$matrices. The S matrix is represented by a diamond shape. The physical index σ_l is indicated by a vertical line. The first and last site are row and column vectors respectively, connected by only one horizontal line indicating one matrix index. All other sites are matrices connected by two horizontal lines indicating two matrix indices as shown in Fig.[5.3].

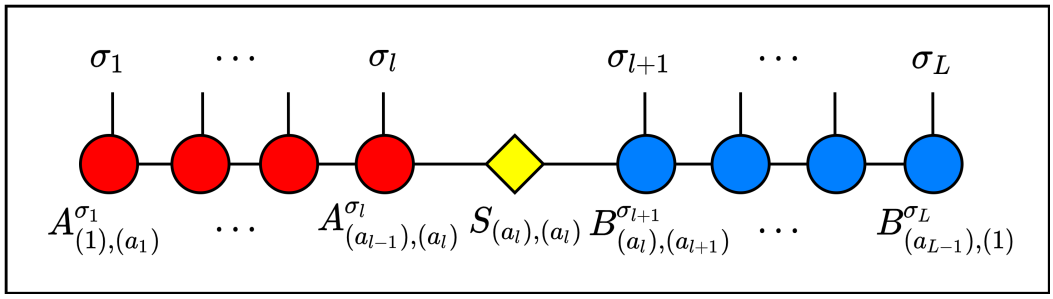


Figure 5.3: Graphical representation of the product of A matrices, S matrix and B matrices making up the complete matrix product state

In compact form,

$$C_{\sigma_1 \ldots \sigma_L} = A^{\sigma_1} \cdots A^{\sigma_l} S B^{\sigma_{l+1}} \cdots B^{\sigma_L}. \tag{5.8}$$

We obtain an MPS of the form,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} A^{\sigma_1} \cdots A^{\sigma_l} S B^{\sigma_{l+1}} \cdots B^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{5.9}$$

S contains singular values on the bond $(l, l+1)$.

For the partition, $[1, \cdots, l] : [l+1, \cdots, L]$ we have,

$$|a_l\rangle_A = \sum_{a_1 \ldots a_l} (A^{\sigma_1} \ldots A^{\sigma_l})_{1,a_l} |\sigma_1, \ldots, \sigma_l\rangle,$$

$$|a_l\rangle_B = \sum_{a_{l+1} \ldots a_{L-1}} (B^{\sigma_{l+1}} \ldots B^{\sigma_L})_{a_l,1} |\sigma_{l+1}, \ldots, \sigma_L\rangle,$$

and $S_{a_l a_l} = S_{a_l}$.

$$|\Psi\rangle = \sum_{a_l} S_{a_l} |a_l\rangle_A |a_l\rangle_B. \tag{5.10}$$

This is the Schmidt Decomposition provided the states on A and B are orthonormal respectively, which indeed is the case by construction.

5.2 Clear steps involved in MCMPS using SVD

We have seen the procedure to obtain the mixed canonical matrix product state (MCMPS) in brief. Now we will give all the detailed steps involved in it for clarity and deep understanding. We will start with Eq.[5.4],

$$\begin{aligned}
C_{(\sigma_1 \ldots \sigma_L),(1)} &= \sum_{a_1=1}^{r_1} \ldots \sum_{a_{l-1}=1}^{r_{l-1}} A^{\sigma_1}_{(1),(a_1)} A^{\sigma_2}_{(a_1),(a_2)} \ldots A^{\sigma_{l-1}}_{(a_{l-2}),(a_{l-1})} \psi_{(a_{l-1}\sigma_l),(\sigma_{l+1} \ldots \sigma_L)}, \\
&= \sum_{a_1=1}^{r_1} \ldots \sum_{a_l=1}^{r_l} A^{\sigma_1}_{(1),(a_1)} \ldots A^{\sigma_{l-1}}_{(a_{l-2}),(a_{l-1})} \underbrace{U_{(a_{l-1}\sigma_l),(a_l)}}_{A^{\sigma_l}_{(a_{l-1}),(a_l)}} S_{(a_l),(a_l)} (V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)}, \\
&= \sum_{a_1=1}^{r_1} \ldots \sum_{a_{l-1}=1}^{r_{l-1}} A^{\sigma_1}_{(1),(a_1)} \ldots A^{\sigma_{l-1}}_{(a_{l-2}),(a_{l-1})} A^{\sigma_l}_{(a_{l-1}),(a_l)} S_{(a_l),(a_l)} (V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)}, \\
&= \sum_{a_l} (A^{\sigma_1} \ldots A^{\sigma_l})_{(1),(a_l)} S_{(a_l),(a_l)} (V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)}.
\end{aligned}$$

Now consider,

$$\begin{aligned}
(V^\dagger)_{(a_l),(\sigma_{l+1} \ldots \sigma_L)} &= \psi_{(a_l \sigma_{l+1} \ldots \sigma_{L-1}),(\sigma_L)}, \\
&= \sum_{a_{L-1}=1}^{r_{L-1}} U_{(a_l \sigma_{l+1} \ldots \sigma_{L-1}),(a_{L-1})} S_{(a_{L-1}),(a_{L-1})} (V^\dagger)_{(a_{L-1}),(\sigma_L)}, \\
&= \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(a_l \sigma_{l+1} \ldots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_{L-2}=1}^{r_{L-2}} \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(a_l \sigma_{l+1} \ldots \sigma_{L-3}),(\sigma_{L-2} a_{L-2})} B^{\sigma_{L-1}}_{(a_{L-2}),(a_{L-1})} B^{\sigma_L}_{(a_{L-1}),(1)},
\end{aligned}$$

continuing with SVD from right hand side we get,

$$
\begin{aligned}
&(V^{\dagger})_{(a_l),(\sigma_{l+1}\ldots\sigma_L)} \\
&= \sum_{a_{l+2}=1}^{r_{l+2}} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \psi_{(a_l\sigma_{l+1}),(\sigma_{l+2}a_{l+2})} B^{\sigma_{l+3}}_{(a_{l+2}),(a_{l+3})} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_{l+1}=1}^{r_{l+1}} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} \underbrace{U_{(a_l\sigma_{l+1}),(a_{l+1})} S_{(a_{l+1}),(a_{l+1})}}_{B^{\sigma_{l+1}}_{(a_l),(a_{l+1})}} \underbrace{(V^{\dagger})_{(a_{l+1}),(\sigma_{l+2}a_{l+2})}}_{B^{\sigma_{l+2}}_{(a_{l+1}),(a_{l+2})}} B^{\sigma_{l+3}}_{(a_{l+2}),(a_{l+3})} \ \ldots \ B^{\sigma_L}_{(a_{L-1}),(1)}, \\
&= \sum_{a_{l+1}=1}^{r_{l+1}} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} B^{\sigma_{l+1}}_{(a_l),(a_{l+1})} B^{\sigma_{l+2}}_{(a_{l+1}),(a_{l+2})} B^{\sigma_{l+3}}_{(a_{l+2}),(a_{l+3})} \ldots B^{\sigma_L}_{(a_{L-1}),(1)}.
\end{aligned}
$$

That gives,

$$
C_{\sigma_1\ldots\sigma_L} = \sum_{a_1=1}^{r_1} \ldots \sum_{a_l=1}^{r_l} A^{\sigma_1}_{1,a_1} \ldots A^{\sigma_l}_{a_{l-1},a_l} S_{a_l,a_l} \sum_{a_{l+1}\ldots a_{L-1}} B^{\sigma_{l+1}}_{a_l a_{l+1}} B^{\sigma_{l+2}}_{a_{l+1}a_{l+2}} \ldots B^{\sigma_L}_{a_{L-1},1},
$$

$$
C_{\sigma_1\ldots\sigma_L} = \sum_{a_1=1}^{r_1} \ldots \sum_{a_{L-1}=1}^{r_{L-1}} A^{\sigma_1}_{1,a_1} \ldots A^{\sigma_l}_{a_{l-1},a_l} S_{a_l,a_l} B^{\sigma_{l+1}}_{a_l a_{l+1}} \ldots B^{\sigma_L}_{a_{L-1},1}.
$$

5.3 Analytical calculation and discussion of MCMPS with one example

Now let us consider one example. We will find the MCMPS representation for the 5-qubit $GHZ-$state for partition $[123] : [45]$ i.e. $p = 3$

$$
|\psi\rangle = \frac{1}{\sqrt{2}} \left[|00000\rangle + |11111\rangle\right]
$$

Here $d = 2$ and $L = 5$, hence this state in the matrix form will have $d^L = 32$ elements.

- Step 1 - Reshape $|\psi\rangle$ into a matrix of dimension $[d \times d^{L-1}]$,

$$
\begin{pmatrix}
\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}}
\end{pmatrix}.
$$

- Step 2 - Perform SVD of the above matrix,

$$
\underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{U} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}}_{S} \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}}_{V^{\dagger}}.
$$

- Step 3 - Form the A^{σ_1} matrices from the U matrix as below,

$$A^{\sigma_1 0} = \begin{pmatrix} 0 & 1 \end{pmatrix}, \qquad A^{\sigma_1 1} = \begin{pmatrix} 1 & 0 \end{pmatrix}.$$

- Step 4 - Multiply matrices S and $V^\dagger$ and reshape it into a matrix of dimension $[d^2 \times d^{L-2}]$,

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Step 5 - Perform SVD of the above matrix to get,

$$\underbrace{\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}}_{U} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{S} \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}}_{V^\dagger}.$$

- Step 6 - Form A^{σ_2} matrices from the U matrix to get,

$$A^{\sigma_2 0} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad A^{\sigma_2 1} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

- Step 7 - Multiply matrices S and $V^\dagger$ and reshape it into a matrix of dimension $[d^3 \times d^{L-3}]$,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Step 8 - Perfrom SVD of the above matrix to obtain,

$$\underbrace{\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}}_{U} \underbrace{\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{S} \underbrace{\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}}_{V^\dagger}.$$

- Step 9 - Form the A^{σ_3} matrices from the U matrix as given below,

$$A^{\sigma_3 0} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad A^{\sigma_3 1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

- Step 10 - Form the S matrix as under,

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

- Step 11 - Reshape matrix $V^\dagger$ into a matrix of dimension $[d^{L-p+1} \times d]$,

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

- Step 12 - Perfrom QR Decomposition of the above matrix to get,

$$\underbrace{\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \\ 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix}}_{R}.$$

- Step 13 - Form B^{σ_5} matrices from the R matrix above to get,

$$B^{\sigma_5 0} = \begin{pmatrix} \sqrt{2} \\ 0 \end{pmatrix} \quad \text{and} \quad B^{\sigma_5 1} = \begin{pmatrix} 0 \\ \sqrt{2} \end{pmatrix}.$$

- Step 14 - Form B^{σ_4} matrices from the Q matrix above to get,

$$B^{\sigma_4 0} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \quad \text{and} \quad B^{\sigma_4 1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \end{pmatrix}.$$

5.4 Flowchart diagram indicating the steps for MCMPS using both SVD and QR decomposition with explanation

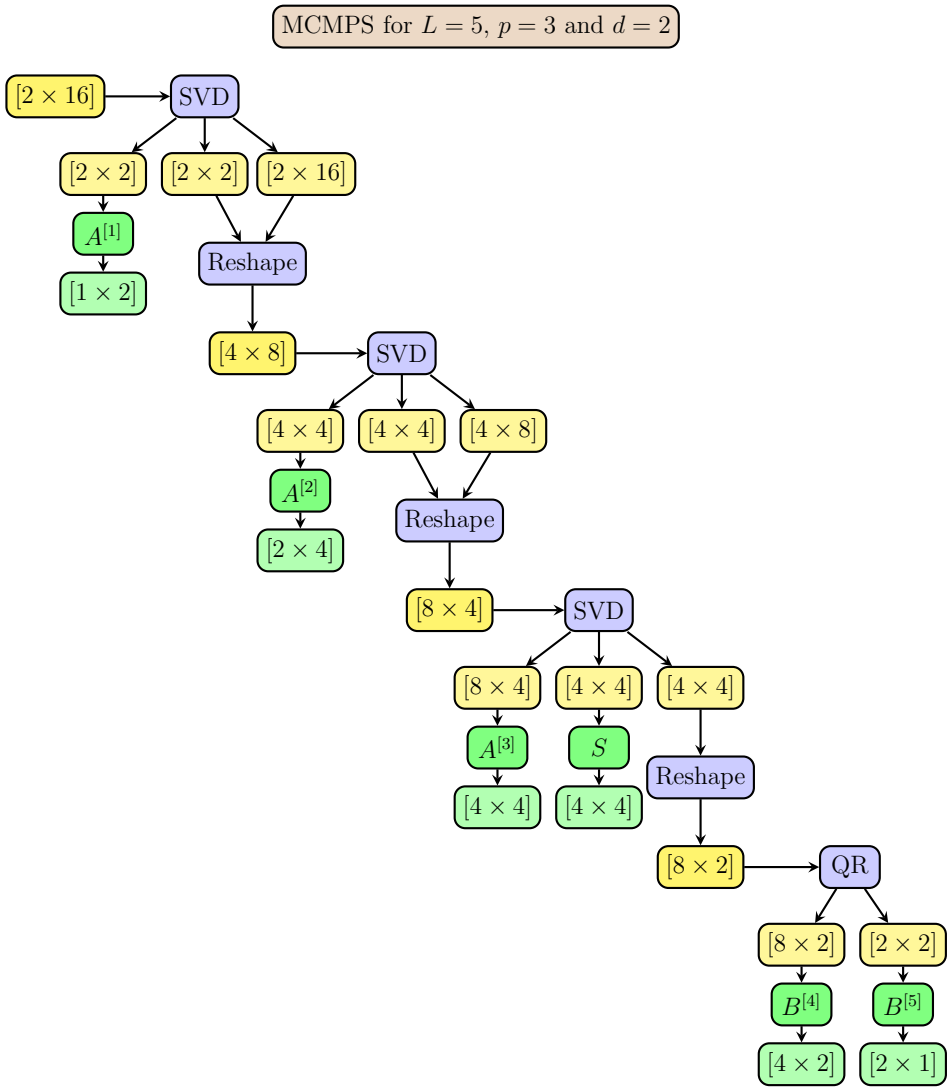
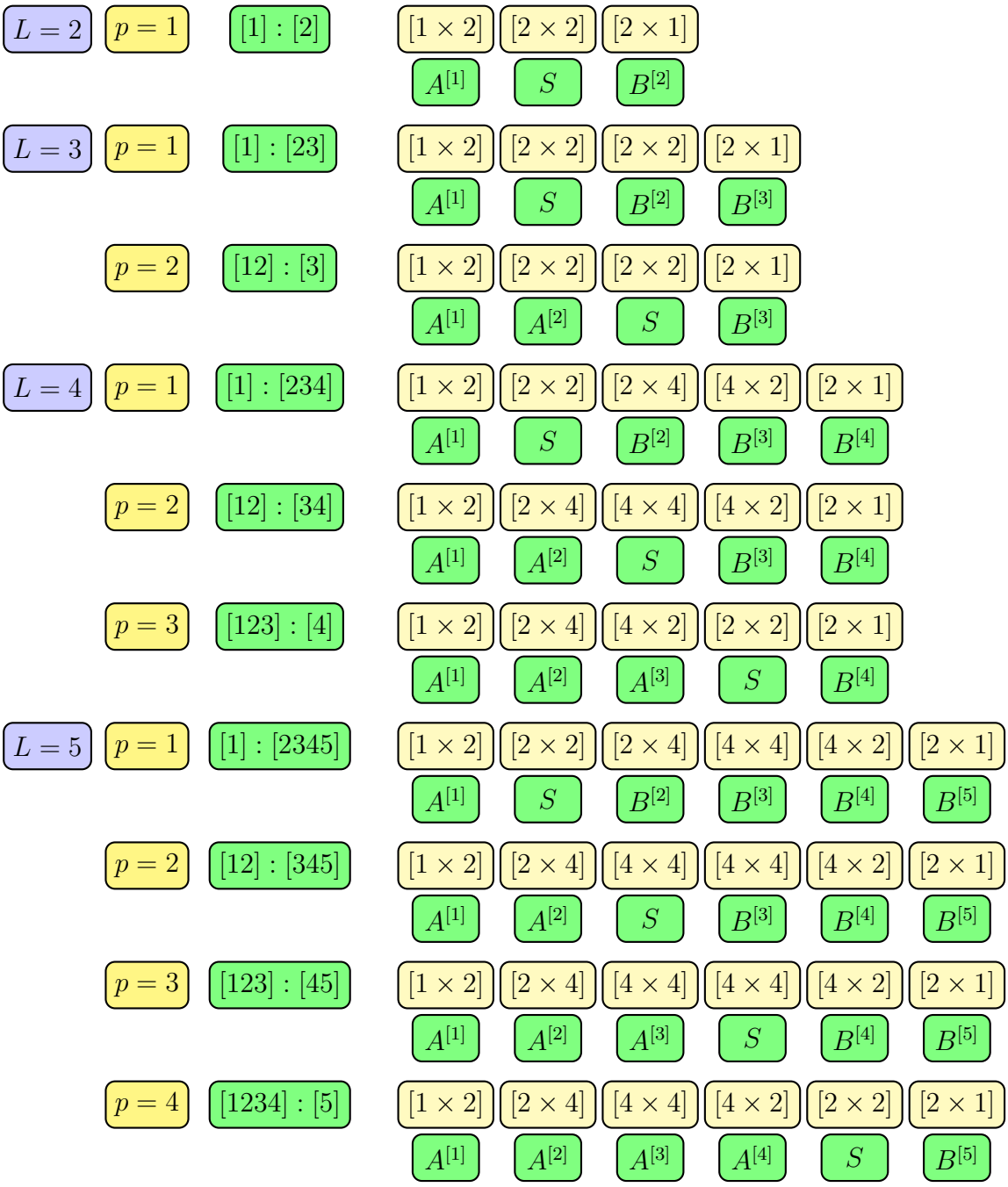


Figure 5.4: Flowchart Diagram indicating the steps for MCMPS using both SVD and QR decomposition

Now for $L = 5$ and $d = 2$ the number of state coefficients will be $d^L = 2^4 = 32$ which we will represent as a matrix of dimension $[32 \times 1]$. Now, the first step is to reshape it into a matrix of dimension $[2 \times 16]$. The first SVD will give three matrices U, S and $V^\dagger$ of dimensions $[2 \times 2]$, $[2 \times 2]$ and $[2 \times 16]$ respectively. We will form the $A-$matrices for the first physical index from this U matrix. Later the S and $V^\dagger$

matrices will be multiplied and reshaped into a matrix of dimension $[4 \times 8]$. The same procedure will be followed for p times as it is shown in this Fig.(5.4). After the third SVD, we will form the $A-$matrices for the third physical index from this U matrix and also take the S matrix. Later, reshape matrix $V^{\dagger}$ into a matrix of dimension $d^{L+1-p} \times d$ and perform QR decomposition. This QR decomposition will give two matrices Q and R of dimensions $[8 \times 2]$ and $[2 \times 2]$ respectively. We will form the $B-$matrices for the fifth physical index from the R matrix and $B-$matrices for the fourth physical index from the Q matrix as shown.

5.5 Possible partitions for certain values of L (for $L = 2$ to $L = 5$) and the dimensions of the matrix product states



5.6 The dimensions of the reshaped matrices giving rise to MCMPS for $L = 2$ to $L = 10$

For any L, we will get $(dL + 1)$ number of matrices in the MCMPS representation. The dimensions of these matrices for partition $p = 1$ and $p = L - 1$ for each L is shown in following figures.

5.6.1 For partition $p = 1$

For partition $p = 1$ we get for any L, $1d$ number of $A-$matrices, S matrix of dimension $[2 \times 2]$ and $(L - 1)d$ number of $B-$matrices. Here for $L = 4$ we get $1d$ number of $A-$matrices of dimension $[1 \times 2]$, S matrix of dimension $[2 \times 2]$ and $3d$ number of $B-$matrices of dimension $[2 \times 4]$, $[4 \times 2]$ and $[2 \times 1]$ respectively.

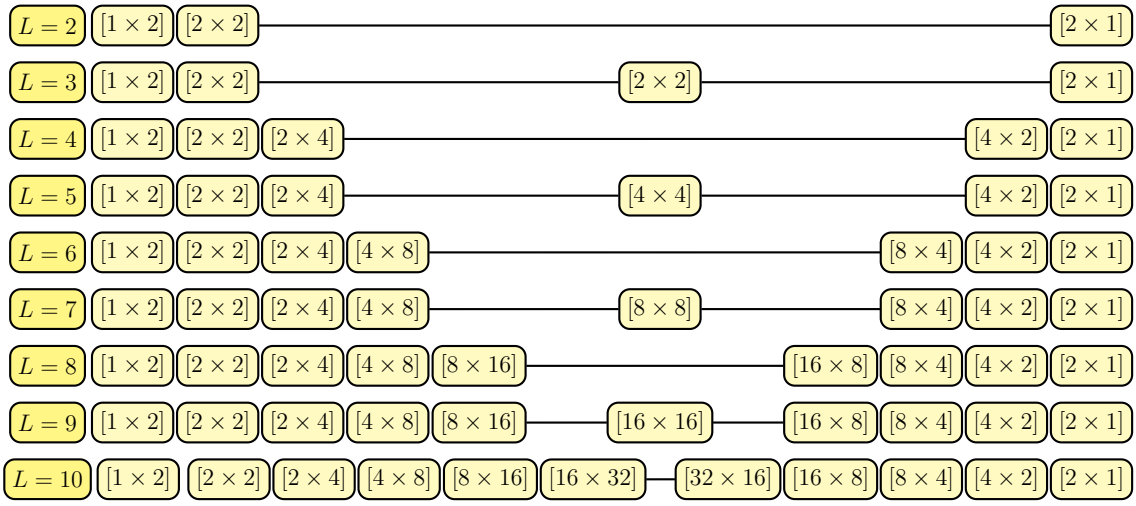


Figure 5.5: Figure for the dimensions of matrices for $L = 2$ to $L = 10$ for $p = 1$

5.6.2 For partition $p = L - 1$

For partition $p = L - 1$ we get for any L, $(L-1)d$ number of $A-$matrices, S matrix of dimension $[2 \times 2]$ and $1d$ number of $B-$matrices. Here for $L = 4$ we get $3d$ number of $A-$matrices of dimension $[1 \times 2]$, $[2 \times 4]$ and $[4 \times 2]$ respectively, S matrix of dimension $[2 \times 2]$ and $1d$ number of $B-$matrices of dimension $[2 \times 1]$.

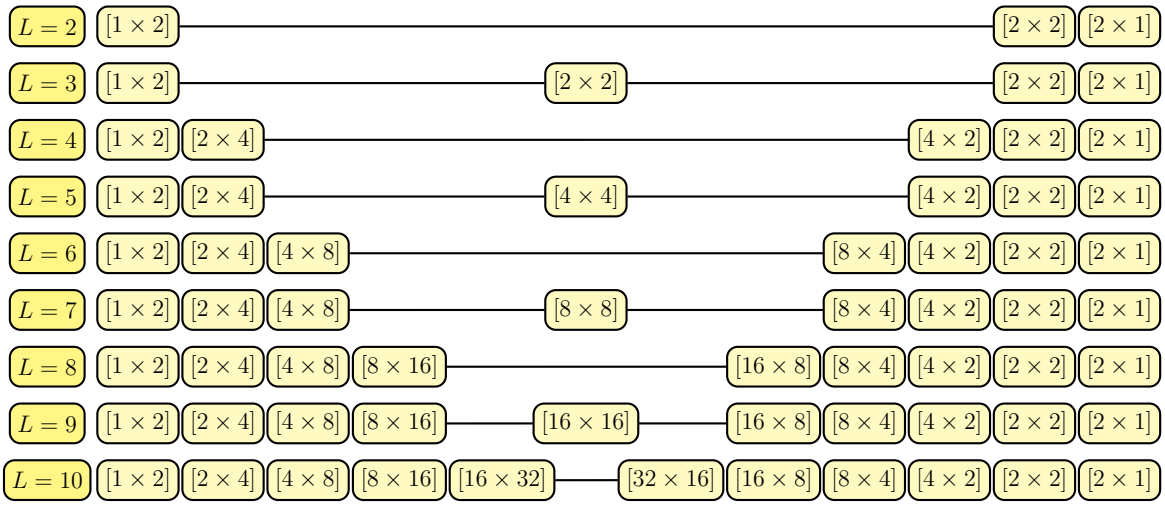


Figure 5.6: Figure for the dimensions of matrices for $L = 2$ to $L = 10$ for $p = L - 1$

5.7 General structure of reshaped matrices giving rise to MCMPS for arbitrary partition p and any d and L

We have seen that for any L, we get $(dL + 1)$ matrices of dimensions specified in the diagrams in section (5.6). Now we are in a position to predict the dimensions of the matrices for any L and any p. For that we assign index variable 's' to these matrices. The dimensions of the matrices depend on s, d, p and L. For even L, we will get $(dL + 1)$ number of matrices. If $s < p$ we get the $A-$matrices, if $s = p$ we get the S matrix and if $s > p$ we get the $B-$matrices. The conditions for the dimensions of the matrices for odd and even L are given below.

For Even L

Conditions $f(L, d, p, s)$

The condition $s < p$ gives the $A-$matrices for any d, L and p. We see that if $s < L/2$ then the dimension of the $A-$matrix will be $[d^s \times d^{s+1}]$ and if $s \geqslant L/2$ then the dimension of the $A-$matrix will be $[d^{L-s} \times d^{L-s-1}]$. These conditions are mentioned below and also the structure the dimensions of $A-$ matrices show two separate regions. This is indicated in the following figure by the lower triangular part.

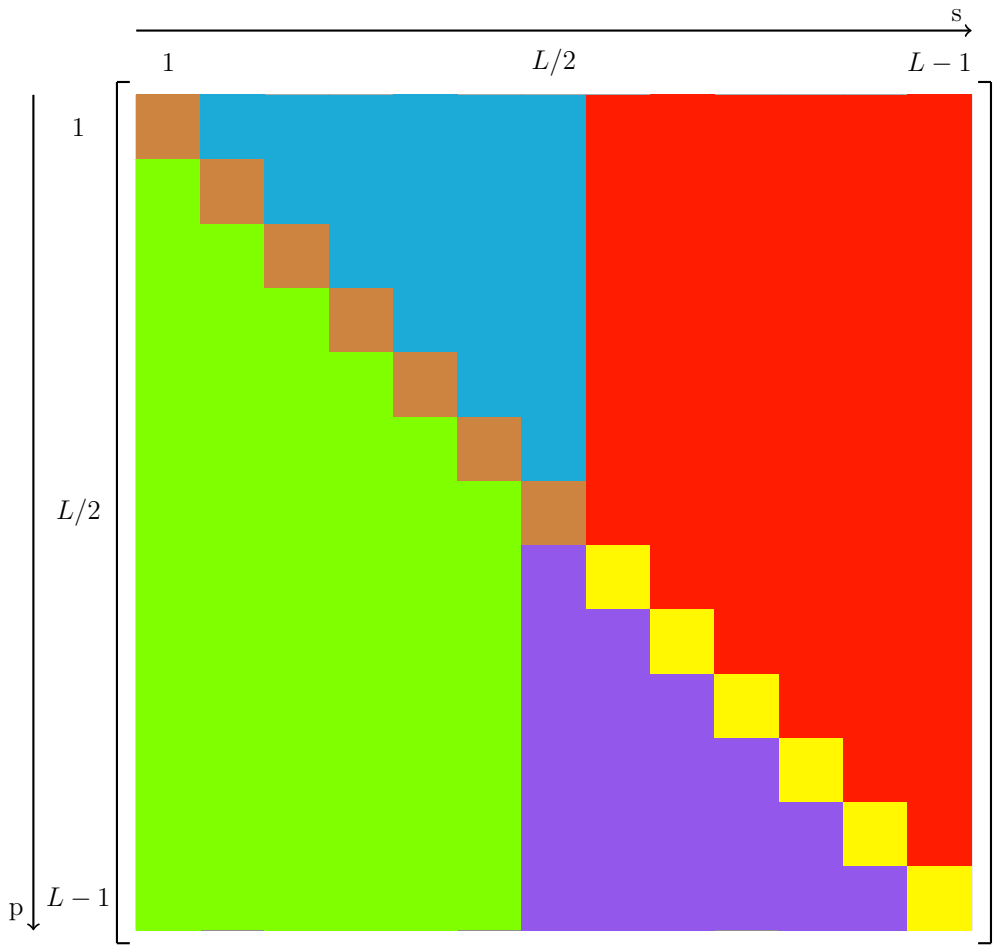
Similarly the condition $s > p$ gives the $B-$matrices for any d, L and p. If $s \leqslant L/2$ then the dimension of the $B-$matrix will be $[d^{s-1} \times d^s]$ and if $s > L/2$ then the dimension of the $B-$matrix will be $[d^{L-s+1} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $B-$ matrices show two separate regions. This is indicated in the following figure by the upper triangular part.

Also the condition $s = p$ gives the S matrix for any d, L and p. If $s \leqslant L/2$ then the dimension of the S matrix will be $[d^s \times d^s]$ and if $s > L/2$ then the dimension of the S matrix will be $[d^{L-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of S matrices show two separate regions. This is indicated in the following figure by the diagonal part.

So, for even L we get a total of 6 different regions as showed in following figure. Same colors are used for indicating the regions and the corresponding conditions for clear understanding.

if $(s < p)$:	if $(s == p)$:	if $(s > p)$:
if $(s < L//2)$: $[d^s \times d^{s+1}]$	**if** $(s \leqslant L//2)$: $[d^s \times d^s]$	**if** $(s \leqslant L//2)$: $[d^{s-1} \times d^s]$
if $(s \geqslant L//2)$: $[d^{L-s} \times d^{L-s-1}]$	**if** $(s > L//2)$: $[d^{L-s} \times d^{L-s}]$	**if** $(s > L//2)$: $[d^{L-s+1} \times d^{L-s}]$

Matrix Structure



For Odd L

Conditions $f(L,d,p,s)$

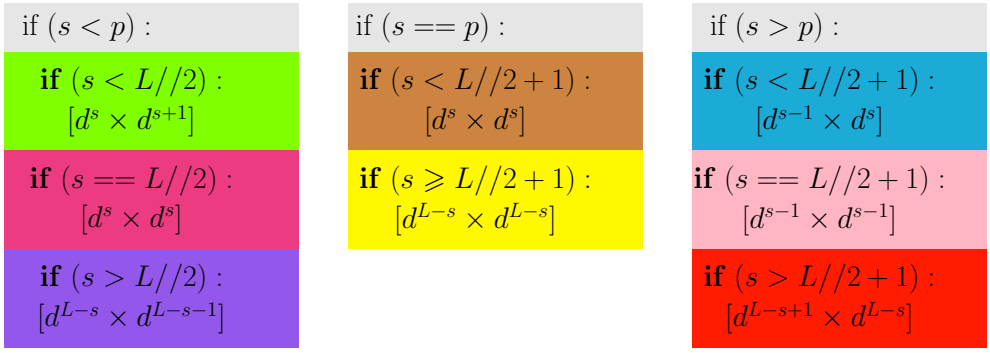
The condition $s < p$ gives the $A-$matrices for any d, L and p. We see that if $s < (L-1)/2$ then the dimension of the $A-$matrix will be $[d^s \times d^{s+1}]$, if $s = (L-1)/2$ then the dimension of the $A-$matrix will be $[d^s \times d^s]$ and if $s \geqslant (L-1)/2$ then the dimension of the $A-$matrix will be $[d^{L-s} \times d^{L-s-1}]$. These conditions are mentioned below and also the structure the dimensions of $A-$ matrices show three separate regions. This is indicated in the following figure by the lower triangular part.

Similarly the condition $s > p$ gives the $B-$matrices for any d, L and p. If $s < (L+1)/2$ then the dimension of the $B-$matrix will be $[d^{s-1} \times d^s]$, if $s = (L+1)/2$ then the dimension of the $B-$matrix will be $[d^{L-s} \times d^{L-s}]$ and if $s > (L+1)/2$ then the

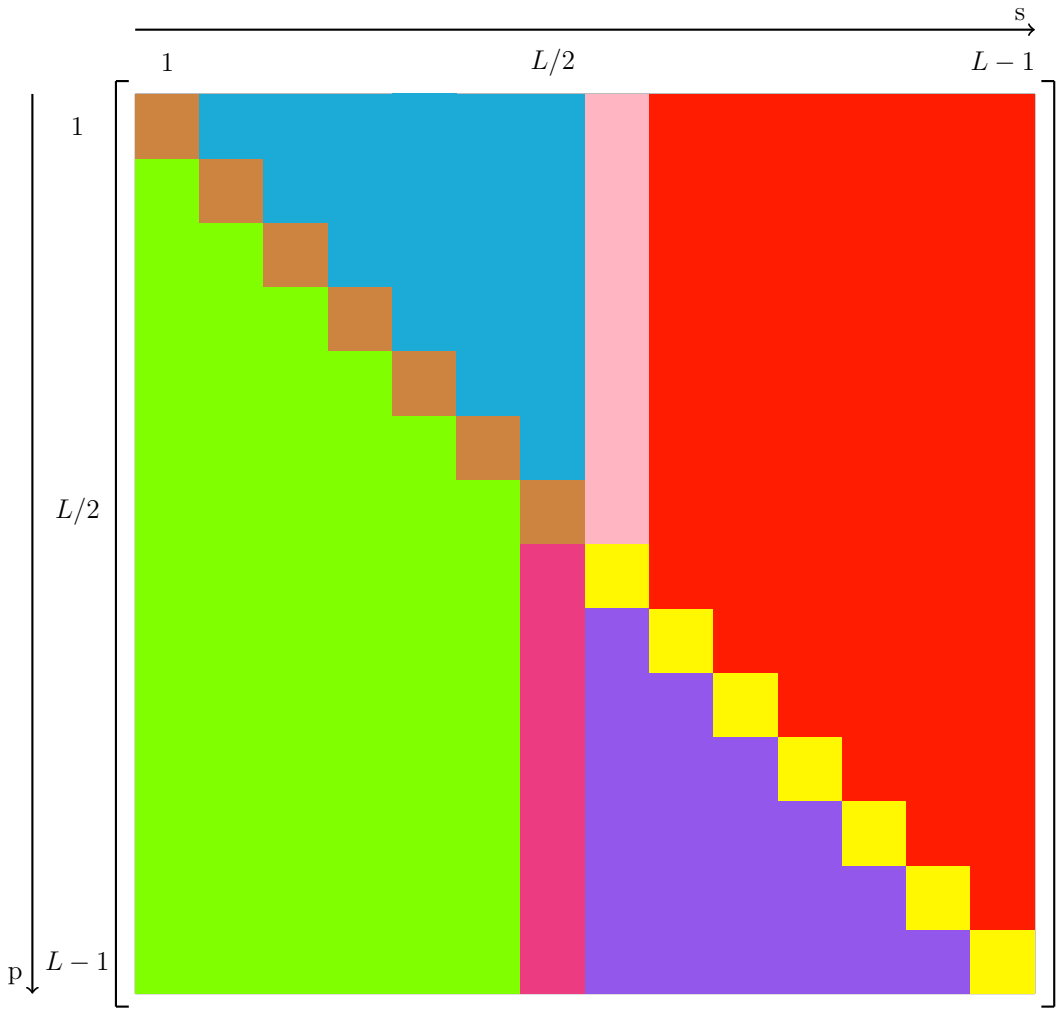
dimension of the $B-$matrix will be $[d^{L-s+1} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of $B-$ matrices show three separate regions. This is indicated in the following figure by the upper triangular part.

Also the condition $s = p$ gives the S matrix for any d, L and p. If $s < (L+1)/2$ then the dimension of the S matrix will be $[d^s \times d^s]$ and if $s \geqslant (L+1)/2$ then the dimension of the S matrix will be $[d^{L-s} \times d^{L-s}]$. These conditions are mentioned below and also the structure the dimensions of S matrices show two separate regions. This is indicated in the following figure by the diagonal part.

So, for odd L we get a total of 8 different regions as showed in following figure. Same colors are used for indicating the regions and the corresponding conditions for clear understanding. It is obvious from the figures that the matrix structure for odd and even L are similar except for the part where $s = (L+1)/2 > p$ and $s = (L-1)/2 < p$ for odd L.



Matrix Structure



So if we know only the value of d, p and L, then we can easily predict the dimensions of the $A-$ matrices, S matrix and $B-$matrices for any arbitrary qudit state.

For $L = 14$ (Even)

$p = 1$	$[1 \times 2]$	$[2 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 2$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 3$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 4$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 5$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 6$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 7$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 8$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 9$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 10$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 11$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 12$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 13$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 2]$	$[2 \times 1]$

For $L = 15$ (Odd)

$p = 1$	$[1 \times 2]$	$[2 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 2$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 3$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 4$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 5$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 6$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 7$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 8$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 9$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 10$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 11$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 12$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 13$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 4]$	$[4 \times 2]$	$[2 \times 1]$
$p = 14$	$[1 \times 2]$	$[2 \times 4]$	$[4 \times 8]$	$[8 \times 16]$	$[16 \times 32]$	$[32 \times 64]$	$[64 \times 128]$	$[128 \times 128]$	$[128 \times 64]$	$[64 \times 32]$	$[32 \times 16]$	$[16 \times 8]$	$[8 \times 4]$	$[4 \times 2]$	$[2 \times 2]$	$[2 \times 1]$

5.8 Flowchart for the numerical implementation process of MCMPS

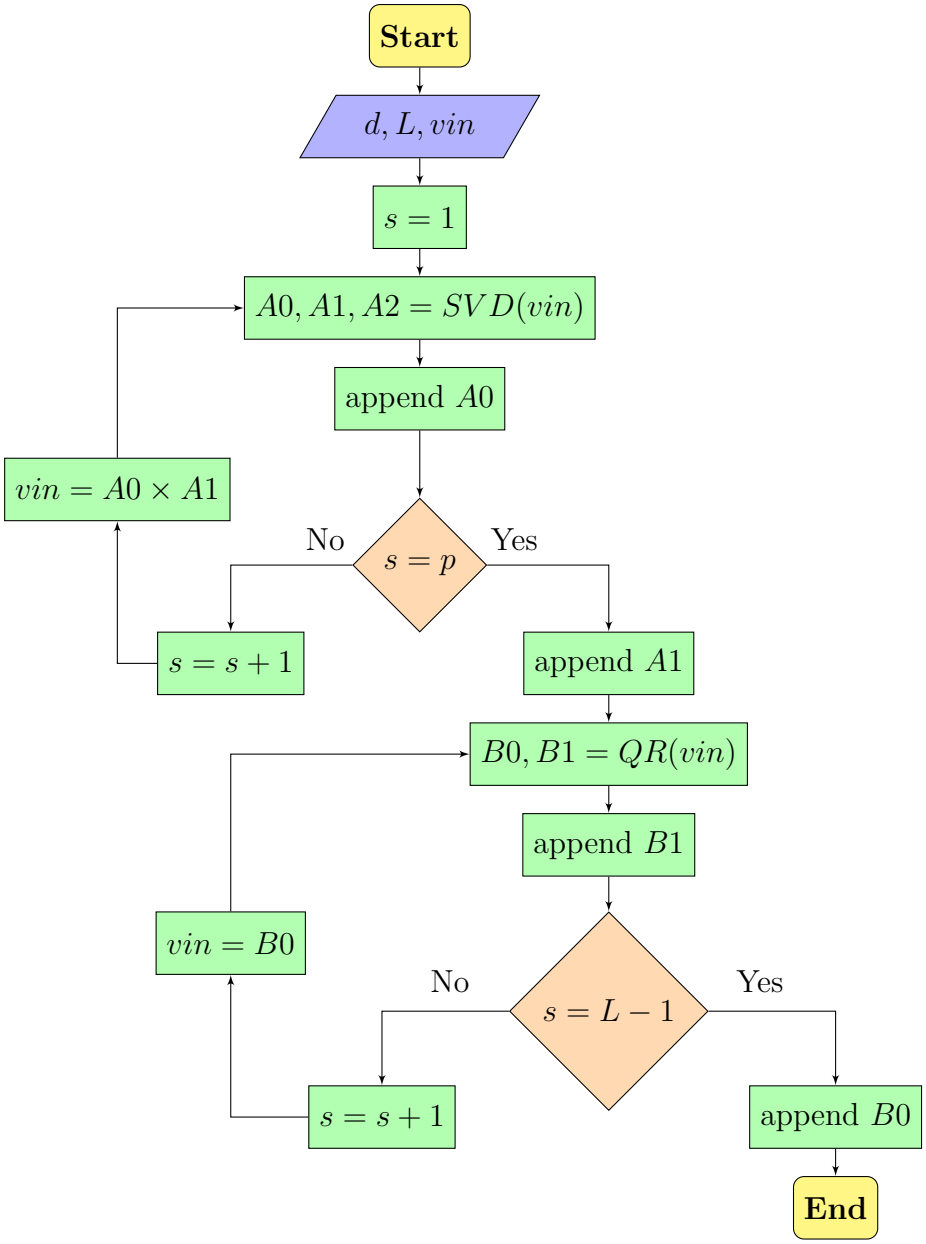


Figure 5.7: Flowchart for the python code of MCMPS

5.9 Python code for MCMPS for any d,L and p

```
def mixedCanonicalMPS(d, L, vin, count, p):
    if (count <= L-1):
        if (count <= p):
            A0, A1, A2 = np.linalg.svd(vin.reshape((int(len(vin[0])
   /(d**(L-count))), d**(L-count))), full_matrices=False)
            A1 = np.diag(A1)
            x = d**(count-1)
            appendA(A0, x, count, p)
            if (count < p):
                A0 = np.dot(A1, A2)
            if (count == p):
                matrices.append(A1)
                A0 = A2
        if (count > p):
            x = int(len(vin[0])/d**(L-count+p))
            A0, A1, A2 = np.linalg.svd(vin.reshape(( d**(L-count+p),
    x)), full_matrices=False)
            A1 = np.diag(A1)
            A0 = np.dot(A0, A1)
            appendA(A2, x//d, count, p)
            if (count == L-1):
                appendA(A0, x, count, p)
        count = count + 1
        mixedCanonicalMPS(d, L, A0.reshape((1,-1)), count, p)
    return matrices
```

5.10 Output from the code of MCMPS for any d, L and any p giving A matrices, S matrix and B matrices and state coefficients

Let us see the output of this code that we have written for obtaining MCMPS.

4-qubit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0000\rangle + |1111\rangle\right)$$

Input to the program: $d = 2$, $L = 4, p = 2$ and $|\psi\rangle$. The program returns 4 $A-$matrices, S matrix and 4 $B-$matrices and also checks if the obtained matrices are giving back the original state.

$A-$Matrices:

```
A0 =
[[1. 0.]]
A1 =
[[0. 1.]]
A2 =
[[1. 0. 0. 0.]
 [0. 0. 0. 1.]]
A3 =
[[0. 0. 1. 0.]
 [0. 1. 0. 0.]]
S =
[[0.70710678 0.         0.         0.        ]
 [0.         0.70710678 0.         0.        ]
 [0.         0.         0.         0.        ]
 [0.         0.         0.         0.        ]]
B5 =
[[-1.]
 [-0.]]
B6 =
[[-0.]
 [-1.]]
B7 =
[[-1.  0.]
 [ 0.  0.]
 [ 0. -1.]
 [ 0.  0.]]
B8 =
[[ 0.  0.]
 [ 0. -1.]
 [ 0.  0.]
 [-1.  0.]]
```

$$A^{\sigma_1 0} = A0 = \begin{pmatrix} 1. & 0. \end{pmatrix},$$

$$A^{\sigma_1 1} = A1 = \begin{pmatrix} 0. & 1. \end{pmatrix},$$

$$A^{\sigma_1 0} = A2 = \begin{pmatrix} 1. & 0. & 0. & 0. \\ 0. & 0. & 0. & 1. \end{pmatrix},$$

$$A^{\sigma_2 1} = A3 = \begin{pmatrix} 0. & 0. & 1. & 0. \\ 0. & 1. & 0. & 0. \end{pmatrix},$$

$$S = \begin{pmatrix} 0.70710678 & 0. & 0. & 0. \\ 0. & 0.70710678 & 0. & 0. \\ 0. & 0. & 0. & 0. \\ 0. & 0. & 0. & 0. \end{pmatrix},$$

$$B^{\sigma_3 0} = B7 = \begin{pmatrix} -1. & 0. \\ 0. & 0. \\ 0. & -1. \\ 0. & 0. \end{pmatrix},$$

$$B^{\sigma_3 1} = B8 = \begin{pmatrix} 0. & 0. \\ 0. & -1. \\ 0. & 0. \\ -1. & 0. \end{pmatrix},$$

$$B^{\sigma_4 0} = B5 = \begin{pmatrix} -1. \\ 0. \end{pmatrix},$$

$$B^{\sigma_4 1} = B6 = \begin{pmatrix} 0. \\ -1. \end{pmatrix}.$$

The values of the coefficients making up the state are,

$$|\psi\rangle = \begin{pmatrix} A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 0}B^{\sigma_4 0} = 0.70710678 \\ A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 1}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 0}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 0}B^{\sigma_4 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 1}B^{\sigma_4 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 1}B^{\sigma_4 1} = 0.70710678 \end{pmatrix}.$$

These are the correct values of coefficients for the state considered.

3-qutrit GHZ state

$$|\psi\rangle = \frac{1}{\sqrt{3}}\left(|000\rangle + |111\rangle + |222\rangle\right)$$

Input to the program: $d = 3$, $L = 3$ and $p = 2$ and $|\psi\rangle$. The prgram returns 6 $A-$ matrices, S matrix and 3 $B-$ matrices and also checks if the obtained matrices are giving back the original state.

$A-$Matrices:

```
A0 =
[[1. 0. 0.]]
A1 =
[[0. 1. 0.]]
A2 =
[[0. 0. 1.]]
```

```
A3 =
[[1. 0. 0.]
 [0. 0. 0.]
 [0. 0. 0.]]
A4 =
[[ 0.  0.  0.]
 [ 0. -1.  0.]
 [ 0.  0.  0.]]
A5 =
[[ 0.  0.  0.]
 [ 0.  0.  0.]
 [ 0.  0. -1.]]
S =
[[0.57735027 0.         0.        ]
 [0.         0.57735027 0.        ]
 [0.         0.         0.57735027]]
B7 =
[[1.]
 [0.]
 [0.]]
B8 =
[[-0.]
 [-1.]
 [-0.]]
B9 =
[[-0.]
 [-0.]
 [-1.]]
```

$A-$Matrices:

$$A^{\sigma_1 0} = A0 = \begin{pmatrix} 1. & 0. & 0. \end{pmatrix},$$
$$A^{\sigma_1 1} = A1 = \begin{pmatrix} 0. & 1. & 0. \end{pmatrix},$$
$$A^{\sigma_1 2} = A2 = \begin{pmatrix} 0. & 0. & 1. \end{pmatrix},$$
$$A^{\sigma_2 0} = A3 = \begin{pmatrix} 1. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$

$$A^{\sigma_2 1} = A4 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & -1. & 0. \\ 0. & 0. & 0. \end{pmatrix},$$

$$A^{\sigma_2 2} = A5 = \begin{pmatrix} 0. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & -1. \end{pmatrix},$$

$$S = \begin{pmatrix} 0.57735027 & 0. & 0. \\ 0. & 0.57735027 & 0. \\ 0. & 0. & 0.57735027 \end{pmatrix},$$

$$B^{\sigma_3 0} = B7 = \begin{pmatrix} 1. \\ 0. \\ 0. \end{pmatrix},$$

$$B^{\sigma_3 1} = B8 = \begin{pmatrix} 0. \\ -1. \\ 0. \end{pmatrix},$$

$$B^{\sigma_3 2} = B9 = \begin{pmatrix} 0. \\ 0. \\ -1. \end{pmatrix}.$$

The values of the coefficients making up the state are,

$$|\psi\rangle = \begin{pmatrix} A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 0} = 0.57735027 \\ A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 0}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 1}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 0}A^{\sigma_2 2}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 0}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 1} = 0.57735027 \\ A^{\sigma_1 1}A^{\sigma_2 1}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 1}A^{\sigma_2 2}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 0}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 1}SB^{\sigma_3 2} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}SB^{\sigma_3 0} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}SB^{\sigma_3 1} = 0. \\ A^{\sigma_1 2}A^{\sigma_2 2}SB^{\sigma_3 2} = 0.57735027 \end{pmatrix},$$

which are infact precisely the values of the state coefficients.

5.11 Summary and conclusion

In this chapter the procedure to obtain Mixed Canonical Matrix Product State (MCMPS) for any quantum qudit state was discussed in detail. The whole procedure was explained in detail with the help of an analytical calculation using one example. A flowchart diagram was also provided for clearly indicating all the steps involved. A generalized code was introduced which can work for any value of d, p and L and thus for any pure quantum qudit state. This code was presented along with the flowchart and some examples for completeness and clarity.

Chapter 6

Operations with MPS

In this chapter we will give some interesting details on how to do some quantum mechanical operations using the MPS formulation. These are very effective when we computationally attempt to solve such problems and helps us to reduce computational time and gain more insight into the physics of the problem.

So far we have obtained three different exact representations of any general pure qudit state $|\psi\rangle$ in the MPS form, which are,

LCMPS:

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{6.1}$$

RCMPS:

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} B^{\sigma_1} B^{\sigma_2} \cdots B^{\sigma_{L-1}} B^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{6.2}$$

MCMPS:

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} A^{\sigma_1} \cdots A^{\sigma_l} S B^{\sigma_{l+1}} \cdots B^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle. \tag{6.3}$$

Here all the $A-$matrices are left normalized and all the $B-$matrices are right normalized. If we allow general matrices and do not worry about left, right or no normalization, we can simply multiply the S matrix in Eq.(6.3) into one of the adjacent A or B matrices, such that the general MPS appears as,

$$|\psi\rangle = \sum_{\sigma_1=1}^{d} \cdots \sum_{\sigma_L=1}^{d} M^{\sigma_1} \cdots M^{\sigma_L} |\sigma_1 \ \cdots \ \sigma_L\rangle, \tag{6.4}$$

More compactly, writing $|\sigma_1 \cdots \sigma_L\rangle = |\sigma\rangle$ we get,

$$|\psi\rangle = \sum_{\sigma} M^{\sigma_1} \cdots M^{\sigma_L} |\sigma\rangle, \tag{6.5}$$

here no assumption about the normalization is implied.

6.1 Overlap or inner product using the MPS representation

Let us consider an overlap between the states $|\psi\rangle$ and $|\phi\rangle$, described by matrices M and $\tilde{M}$ respectively [7].

$$|\psi\rangle = \sum_{\sigma'} M^{\sigma_1'} \cdots M^{\sigma_L'} |\sigma'\rangle, \tag{6.6}$$

$$|\phi\rangle = \sum_{\sigma} \tilde{M}^{\sigma_1} \cdots \tilde{M}^{\sigma_L} |\sigma\rangle. \tag{6.7}$$

Taking adjoint of $|\phi\rangle$, and calculating $\langle\phi|\psi\rangle$ gives the overlap,

$$\begin{aligned}
\langle\phi|\psi\rangle &= \sum_{\sigma} \tilde{M}^{\sigma_1^*} \cdots \tilde{M}^{\sigma_L^*} \langle\sigma| \sum_{\sigma'} M^{\sigma_1'} \cdots M^{\sigma_L'} |\sigma'\rangle, && (6.8)\\
&= \sum_{\sigma\ \sigma'} \tilde{M}^{\sigma_1^*} \cdots \tilde{M}^{\sigma_L^*} M^{\sigma_1'} \cdots M^{\sigma_L'} \underbrace{\langle\sigma|\sigma'\rangle}_{\delta_{\sigma\sigma'}}, && (6.9)\\
&= \sum_{\sigma} \underbrace{\tilde{M}^{\sigma_1^*} \cdots \tilde{M}^{\sigma_L^*}}_{scalar} \underbrace{M^{\sigma_1} \cdots M^{\sigma_L}}_{scalar}. && (6.10)
\end{aligned}$$

Transposing the scalar formed from $\left(\tilde{M}^{\sigma_1^*} \cdots \tilde{M}^{\sigma_L^*}\right)$ which is the identity operation.

$$\langle\phi|\psi\rangle = \sum_{\sigma} (\tilde{M}^{\sigma_1^*} \cdots \tilde{M}^{\sigma_L^*})^T M^{\sigma_1} \cdots M^{\sigma_L} = \sum_{\sigma} \tilde{M}^{\sigma_L^\dagger} \cdots \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} \cdots M^{\sigma_L}. \tag{6.11}$$

Here we have contractions (summations) over the matrix indices implicit in the matrix multiplications and over the physical indices. Each physical index $\sigma_1 \cdots \sigma_L$ runs from 1 to d. So if we contract first the matrix index and then the physical index, we have to sum over d^L strings of matrix multiplications, which is exponentially expensive. But we can regroup the sums cleverly as follows to get,

$$\boxed{\langle\phi|\psi\rangle = \sum_{\sigma_L=1}^{d} \tilde{M}^{\sigma_L^\dagger} \left(\cdots \left(\sum_{\sigma_2=1}^{d} \tilde{M}^{\sigma_2^\dagger} \left(\sum_{\sigma_1=1}^{d} \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} \right) M^{\sigma_2} \right) \cdots \right) M^{\sigma_L}.} \tag{6.12}$$

The first step is to multiply the column and row vectors $\tilde{M}^{\sigma_1^\dagger}$ and M^{σ_1} to form a matrix and sum over the first physical index. For the next step, we contract a three matrix multiplication over the second physical index and so on till last physical index. For the first step, we have multiplication of two matrices and for the second step, we have multiplication of three matrices. But from this step onwards, we will always have multiplication of three matrices. Thus totally we are carrying out $(2L-1)d$ multiplications. For simplicity we assume that the dimensions of all these matrices is $[D \times D]$. Thus the time complexity associated with multiplication of 2 matrices is $\mathcal{O}(D^3)$. Then the total operational count is $\mathcal{O}(LdD^3)$. Thus we go from exponential to weak polynomial complexity.

6.1.1 Analytical calculation of the overlap with one example

Let us consider an overlap between the 3-qubit GHZ state and the 3-qubit W state as follows,

$$|\psi\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}, \tag{6.13}$$

$$|\phi\rangle = \frac{|001\rangle + |010\rangle + |001\rangle}{\sqrt{3}}. \tag{6.14}$$

The matrix product state representation of the states $|\psi\rangle$ and $|\phi\rangle$ gives the matrices M and $\tilde{M}$ respectively. For the state $|\psi\rangle$, we get

$$M^{[1]0} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad M^{[1]1} = \begin{pmatrix} 0 & 1 \end{pmatrix},$$

$$M^{[2]0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad M^{[2]1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

$$M^{[3]0} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}, \qquad M^{[3]1} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

For the state $|\phi\rangle$, we get

$$\tilde{M}^{[1]0} = \begin{pmatrix} 0 & 1 \end{pmatrix}, \qquad \tilde{M}^{[1]1} = \begin{pmatrix} 1 & 0 \end{pmatrix},$$

$$\tilde{M}^{[2]0} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{pmatrix}, \qquad \tilde{M}^{[2]1} = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

$$\tilde{M}^{[3]0} = \begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} \\ 0 \end{pmatrix}, \qquad \tilde{M}^{[3]1} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{3}} \end{pmatrix}.$$

Next we perform the contractions,

$$\langle\phi|\psi\rangle = \sum_{\sigma_3=0}^{1} \tilde{M}^{\sigma_3^\dagger} \left(\sum_{\sigma_2=0}^{1} \tilde{M}^{\sigma_2^\dagger} \left(\sum_{\sigma_1=0}^{1} \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} \right) M^{\sigma_2} \right) M^{\sigma_3}, \tag{6.15}$$

We will consider each of these terms. Let,

$$\sum_{\sigma_1=0}^{1} \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} = X = \tilde{M}^{\dagger[1]0} M^{[1]0} + \tilde{M}^{\dagger[1]1} M^{[1]1}, \tag{6.16}$$

$$\begin{aligned} X &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix}, \\ &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

That gives,

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{6.17}$$

Now, consider

$$\sum_{\sigma_2=0}^{1} \tilde{M}^{\sigma_2^\dagger} \left(\sum_{\sigma_1=0}^{1} \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} \right) M^{\sigma_2} = \sum_{\sigma_2=0}^{1} \tilde{M}^{\sigma_2^\dagger} X M^{\sigma_2} = Y, \tag{6.18}$$

$$\begin{aligned} Y &= \tilde{M}^{\dagger[2]0} X M^{[2]0} + \tilde{M}^{\dagger[2]1} X M^{[2]1}, \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ &= \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

That gives,

$$Y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{6.19}$$

Now, consider

$$\sum_{\sigma_3=0}^{1} \tilde{M}^{\sigma_3^\dagger} \left(\sum_{\sigma_2=0}^{1} \tilde{M}^{\sigma_2^\dagger} \left(\sum_{\sigma_1=0}^{1} \tilde{M}^{\sigma_1^\dagger} M^{\sigma_1} \right) M^{\sigma_2} \right) M^{\sigma_3} = \sum_{\sigma_3=0}^{1} \tilde{M}^{\sigma_3^\dagger} Y M^{\sigma_3} = Z \tag{6.20}$$

$$
\begin{aligned}
Z &= \tilde{M}^{\dagger[3]0} Y M^{[3]0} + \tilde{M}^{\dagger[3]1} Y M^{[3]1}, \\
&= \begin{pmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \\
&= \begin{pmatrix} 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \\
&= 0.
\end{aligned}
$$

Everything finally boils down to,

$$\langle \phi | \psi \rangle = 0 \tag{6.21}$$

6.1.2 Python code for the overlap for any d and any L (multi-qudit state)

```
def overlap(d, L, z1, z2):
    d1 = np.zeros((d,d))
    for i in range (0,d):
        d1 = d1 + np.dot(np.transpose(np.conjugate(z2[i])),z1[i])
    for i0 in range (1, L-1):
        x = d**(L-(i0+1))
        if (i0 < L//2):
            x = d**(i0+1)
        elif (L % 2 == 1 and i0 == L//2):
            x = d**(i0)
        d2 = np.zeros((x,x))
        for i in range (0,d):
            d2 = d2 + np.dot(np.dot(np.transpose(np.conjugate(z2[i+
    i0*d])), d1), z1[i+i0*d])
        d1 = d2
    dn = np.zeros((1,1))
    for i in range (0,d):
        dn = dn + np.dot(np.dot(np.transpose(np.conjugate(z2[i+(L-1)
    *d])), d2),z1[i+(L-1)*d])
    return dn[0][0]
```

6.1.3 Output from the code for the overlap between 2 multi-qudit states (any d and any L)

Consider an overlap between the 3-qubit GHZ state and the 3-qubit W state as follows,

$$|\psi\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}, \tag{6.22}$$

$$|\phi\rangle = \frac{|001\rangle + |010\rangle + |001\rangle}{\sqrt{3}}. \tag{6.23}$$

```
Overlap:
0.0
```

6.2 Matrix elements using the MPS representation

The operator (matrix) O can be written as [7],

$$O = IOI = \sum_i |i\rangle\langle i|O\sum_j |j\rangle\langle j|. \tag{6.24}$$

where $\{|i\rangle\}$ and $\{|j\rangle\}$ form the complete orthonormal basis.

$$O = \sum_{i,j} \underbrace{\langle i|O|j\rangle}_{O^{i,j}} |i\rangle\langle j|. \tag{6.25}$$

So the operator O is written as,

$$O = \sum_{i,j} O^{i,j}|i\rangle\langle j|. \tag{6.26}$$

On the similar lines, the matrix element operator for site l is $(i \to \sigma_l)$ and $(j \to \sigma_l^{'})$,

$$\hat{O}^{[l]} = \sum_{\sigma_l,\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}|\sigma_l\rangle\langle\sigma_l^{'}|. \tag{6.27}$$

We can extend this operator on every site to get,

$$\begin{aligned}
\hat{O} &= \hat{O}^{[1]}\hat{O}^{[2]}...\hat{O}^{[L-1]}\hat{O}^{[L]}, \\
&= \left(\sum_{\sigma_1,\sigma_1^{'}} O^{\sigma_1,\sigma_1^{'}}|\sigma_1\rangle\langle\sigma_1^{'}|\right)\left(\sum_{\sigma_2,\sigma_2^{'}} O^{\sigma_2,\sigma_2^{'}}|\sigma_2\rangle\langle\sigma_2^{'}|\right)\cdots\left(\sum_{\sigma_L,\sigma_L^{'}} O^{\sigma_L,\sigma_L^{'}}|\sigma_L\rangle\langle\sigma_L^{'}|\right), \\
&= \sum_{\sigma,\sigma^{'}} O^{\sigma_1,\sigma_1^{'}}O^{\sigma_2,\sigma_2^{'}}...O^{\sigma_L,\sigma_L^{'}}|\sigma\rangle\langle\sigma^{'}|.
\end{aligned}$$

So the operator matrix element is,

$$O^{\sigma_1,\sigma_1^{'}} O^{\sigma_2,\sigma_2^{'}} \dots O^{\sigma_L,\sigma_L^{'}}.$$

Now consider two states,

$$|\psi\rangle = \sum_{\sigma^{''}} M^{\sigma_1^{''}} ... M^{\sigma_L^{''}} |\sigma^{''}\rangle.$$

$$|\phi\rangle = \sum_{\sigma^{'''}} \tilde{M}^{\sigma_1^{'''}} ... \tilde{M}^{\sigma_L^{'''}} |\sigma^{'''}\rangle.$$

We can write,

$$\langle\phi|\hat{O}|\psi\rangle = \left[\sum_{\sigma^{'''}} \tilde{M}^{\sigma_L^{'''\dagger}} ... \tilde{M}^{\sigma_1^{'''\dagger}} \langle\sigma^{'''}|\right] \left[\sum_{\sigma,\sigma^{'}} O^{\sigma_1,\sigma_1^{'}} ... O^{\sigma_L,\sigma_L^{'}} |\sigma\rangle\langle\sigma^{'}|\right] \left[\sum_{\sigma^{''}} M^{\sigma_1^{''}} ... M^{\sigma_L^{''}} |\sigma^{''}\rangle\right],$$

$$\begin{aligned}\langle\phi|\hat{O}|\psi\rangle &= \sum_{\sigma,\sigma^{'},\sigma^{''},\sigma^{'''}} \tilde{M}^{\sigma_L^{'''\dagger}} ... \tilde{M}^{\sigma_1^{'''\dagger}} O^{\sigma_1,\sigma_1^{'}} ... O^{\sigma_L,\sigma_L^{'}} M^{\sigma_1^{''}} ... M^{\sigma_L^{''}} \langle\sigma^{'''}|\sigma\rangle\langle\sigma^{'}|\sigma^{''}\rangle, \\ &= \sum_{\sigma\sigma^{'}} \tilde{M}^{\sigma_L^{\dagger}} ... \tilde{M}^{\sigma_1^{\dagger}} O^{\sigma_1,\sigma_1^{'}} ... O^{\sigma_L,\sigma_L^{'}} M^{\sigma_1^{'}} ... M^{\sigma_L^{'}}.\end{aligned}$$

We can regroup the sums to reduce the operational count in the similar way as it was done for the overlap.

$$\langle\phi|\hat{O}|\psi\rangle = \sum_{\sigma_L,\sigma_L^{'}} O^{\sigma_L,\sigma_L^{'}} \tilde{M}^{\sigma_L^{\dagger}} \left(... \left(\sum_{\sigma_2,\sigma_2^{'}} O^{\sigma_2,\sigma_2^{'}} \tilde{M}^{\sigma_2^{\dagger}} \left(\sum_{\sigma_1,\sigma_1^{'}} O^{\sigma_1,\sigma_1^{'}} \tilde{M}^{\sigma_1^{\dagger}} M^{\sigma_1} \right) M^{\sigma_2} \right) ... \right) M^{\sigma_L}. \tag{6.28}$$

6.2.1 Python code for the matrix elements for any d and any L

```
def matrixEle(d, L, z1, z2, O):
    d1 = np.zeros((d,d))
    for i in range (0,d):
        for j in range (0,d):
            d1 = d1 + O[0][i][j] * np.dot(np.transpose(np.conjugate(
   z2[i])),z1[i])
    if (L == 2):
        d2 = d1
    else:
        for i0 in range (1, L-1):
            x = d**(L-(i0+1))
```

```
            if (i0 < L//2):
                x = d**(i0+1)
            elif (L % 2 == 1 and i0 == L//2):
                x = d**(i0)
            d2 = np.zeros((x,x))
            for i in range (0,d):
                for j in range (0,d):
                    d2 = d2 + O[i0][i][j] * np.dot(np.dot(np.
transpose(np.conjugate(z2[i+i0*d])),d1),z1[i+i0*d])
            d1 = d2
    dn = np.zeros((1,1))
    for i in range (0,d):
        for j in range (0,d):
            dn = dn + O[L-1][i][j] * np.dot(np.dot(np.transpose(np.
conjugate(z2[i+(L-1)*d])), d2), z1[j+(L-1)*d])
    return dn[0][0]
```

6.3 Expectation value using the MPS representation

Now we will proceed to give details about obtaining expectation value of the operator using MPS formulation. The expectation value refers to the value of an operator one would 'expect' to find if one could repeat the measurement an infinite number of times and take the average of the values obtained. More formally, the expected value is a weighted average of all possible results.

Consider the state,

$$|\psi\rangle = \sum_{\sigma} M^{\sigma_1}...M^{\sigma_{l-1}}M^{\sigma_l}M^{\sigma_{l+1}}...M^{\sigma_L}|\sigma_1...\sigma_{l-1}\sigma_l\sigma_{l+1}...\sigma_L\rangle$$

We assume that the matrices to the left of site l are all left normalized and the matrices to the right of site l are all right normalized, the status of site l is arbitrary.

Then the expectation value is given by,

$$\langle\psi|\hat{O}|\psi\rangle = \left[\sum_{\sigma''} \tilde{M}^{\sigma_L''\dagger}...\tilde{M}^{\sigma_1''\dagger}\langle\sigma''|\right]\left[\sum_{\sigma_l,\sigma_l'} O^{\sigma_l,\sigma_l'}|\sigma_l\rangle\langle\sigma_l'|\right]\left[\sum_{\sigma'''} M^{\sigma_1'''}...M^{\sigma_L'''}|\sigma'''\rangle\right],$$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{\sigma^{''},\sigma^{'''}}\sum_{\sigma_l,\sigma_l^{'}} \tilde{M}^{\sigma_L^{''\dagger}}\cdots\tilde{M}^{\sigma_1^{''\dagger}} O^{\sigma_l,\sigma_l^{'}} M^{\sigma_1^{'''}}\cdots M^{\sigma_L^{'''}} \langle\sigma^{''}|\sigma_l\rangle\langle\sigma_l^{'}|\sigma^{'''}\rangle,$$

$$= \sum_{\sigma_1^{''}\cdots\sigma_l^{''}\cdots\sigma_L^{''}}\sum_{\sigma_1^{'''}\cdots\sigma_l^{'''}\ldots\sigma_L^{'''}}\sum_{\sigma_l,\sigma_l^{'}} \tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_1^{''\dagger}} O^{\sigma_l,\sigma_l^{'}} M^{\sigma_1^{'''}}\ldots M^{\sigma_L^{'''}} \langle\sigma_1^{''}\ldots\sigma_l^{''}\ldots\sigma_L^{''}|\sigma_l\rangle \times$$
$$\langle\sigma_l^{'}|\sigma_1^{'''}\ldots\sigma_l^{'''}\ldots\sigma_L^{'''}\rangle,$$

$$= \sum_{\sigma_1^{''}\ldots\sigma_{l-1}^{''}}\sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}}\sum_{\sigma_1^{'''}\ldots\sigma_{l-1}^{'''}}\sum_{\sigma_{l+1}^{'''}\ldots\sigma_L^{'''}}\sum_{\sigma_l\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}}\tilde{M}^{\sigma_{l-1}^{''\dagger}}\cdots\tilde{M}^{\sigma_1^{''\dagger}} \times$$
$$M^{\sigma_1^{'''}}\ldots M^{\sigma_{l-1}^{'''}} M^{\sigma_l^{'}} M^{\sigma_{l+1}^{'''}}\ldots M^{\sigma_L^{'''}} \langle\sigma_1^{''}\ldots\sigma_{l-1}^{''}\sigma_{l+1}^{''}\ldots\sigma_L^{''}|\sigma_1^{'''}\ldots\sigma_{l-1}^{'''}\sigma_{l+1}^{'''}\ldots\sigma_L^{'''}\rangle,$$

$$= \sum_{\sigma_1^{''}\ldots\sigma_{l-1}^{''}}\sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}}\sum_{\sigma_l\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}}\tilde{M}^{\sigma_{l-1}^{''\dagger}}\ldots\tilde{M}^{\sigma_1^{''\dagger}} \times$$
$$M^{\sigma_1^{''}}\ldots M^{\sigma_{l-1}^{''}} M^{\sigma_l^{'}} M^{\sigma_{l+1}^{''}}\ldots M^{\sigma_L^{''}}$$

Now we will use the fact that $M^{\dagger}M = I$ upto the left of site l.

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}}\sum_{\sigma_l\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}}\left(\sum_{\sigma_1^{''}\ldots\sigma_{l-1}^{''}}\tilde{M}^{\sigma_{l-1}^{''\dagger}}\ldots\tilde{M}^{\sigma_1^{''\dagger}} M^{\sigma_1^{''}}\ldots M^{\sigma_{l-1}^{''}}\right)\times$$
$$M^{\sigma_l^{'}} M^{\sigma_{l+1}^{''}}\ldots M^{\sigma_L^{''}},$$

$$= \sum_{\sigma_l}\sum_{\sigma_l^{'}}\sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}} O^{\sigma_l,\sigma_l^{'}}\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}} M^{\sigma_l^{'}} M^{\sigma_{l+1}^{''}}\ldots M^{\sigma_L^{''}},$$

$$= \sum_{\sigma_l}\sum_{\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}\sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}}\langle\sigma_{l+1}^{''}\ldots\sigma_L^{''}|\sigma_{l+1}^{''}\ldots\sigma_L^{''}\rangle\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}} M^{\sigma_l^{'}} M^{\sigma_{l+1}^{''}}\ldots M^{\sigma_L^{''}}\times$$
$$\langle\sigma_{l+1}^{''}\ldots\sigma_L^{''}|\sigma_{l+1}^{''}\ldots\sigma_L^{''}\rangle,$$

$$= \sum_{\sigma_l}\sum_{\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}}\sum_{\sigma_{l+1}^{''}\ldots\sigma_L^{''}}\langle\sigma_{l+1}^{''}\ldots\sigma_L^{''}|\times$$
$$\left[\tilde{M}^{\sigma_L^{''\dagger}}\ldots\tilde{M}^{\sigma_{l+1}^{''\dagger}}\tilde{M}^{\sigma_l^{\dagger}} M^{\sigma_l^{'}} M^{\sigma_{l+1}^{''}}\ldots M^{\sigma_L^{''}}|\sigma_{l+1}^{''}\ldots\sigma_L^{''}\rangle\langle\sigma_{l+1}^{''}\ldots\sigma_L^{''}|\right]|\sigma_{l+1}^{''}\ldots\sigma_L^{''}\rangle,$$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{\sigma_l}\sum_{\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}} Tr\left[\tilde{M}^{\sigma_L^{''}\dagger}...\tilde{M}^{\sigma_{l+1}^{''}\dagger}\tilde{M}^{\sigma_l^{\dagger}}M^{\sigma_l^{'}}M^{\sigma_{l+1}^{''}}...M^{\sigma_L^{''}}|\sigma_{l+1}^{''}...\sigma_L^{''}\rangle\langle\sigma_{l+1}^{''}...\sigma_L^{''}|\right]$$

We have, $Tr(ABC) = Tr(BCA) = Tr(CAB)$, that gives,

$$\begin{aligned}\langle\psi|\hat{O}|\psi\rangle &= \sum_{\sigma_l}\sum_{\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}} Tr\left[M^{\sigma_{l+1}^{''}}...M^{\sigma_L^{''}}\tilde{M}^{\sigma_L^{''}\dagger}...\tilde{M}^{\sigma_{l+1}^{''}\dagger}\tilde{M}^{\sigma_l^{\dagger}}M^{\sigma_l^{'}}\langle\sigma_{l+1}^{''}...\sigma_L^{''}|\sigma_{l+1}^{''}...\sigma_L^{''}\rangle\right], \\ &= \sum_{\sigma_l}\sum_{\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}} Tr\left[M^{\sigma_{l+1}^{''}}...M^{\sigma_L^{''}}\tilde{M}^{\sigma_L^{''}\dagger}...\tilde{M}^{\sigma_{l+1}^{''}\dagger}\tilde{M}^{\sigma_l^{\dagger}}M^{\sigma_l^{'}}\right],\end{aligned}$$

Now the matrices to the right of site l are right normalized $MM^{\dagger} = I$

$$\langle\psi|\hat{O}|\psi\rangle = \sum_{\sigma_l,\sigma_l^{'}} O^{\sigma_l,\sigma_l^{'}} Tr(\tilde{M}^{\sigma_l^{\dagger}}M^{\sigma_l}). \tag{6.29}$$

6.3.1 Python code for the expectation value for any d and any L

```
def expValue(d, L, z1, O, i0):
    dn = 0
    for i in range (0,d):
        for j in range (0,d):
            dn = dn + O[i][j] * np.trace(np.dot(np.transpose(np.
    conjugate(z1[i+i0*d])), z1[j+i0*d]))
    return dn
```

6.4 Summary and conclusion

In this chapter the procedure to perform various operations like overlap, matrix element and expectation value using the MPS representation of any qudit quantum state was discussed in detail. Generalized codes were written for any value of d and L and thus for any pure quantum state. These codes were presented along with some examples.

Chapter 7

MPS and reduced density operators

In previous chapter we have seen how to do some quantum mechanical operations using the MPS formulation. Now we will proceed to give details about obtaining reduced density operator using MPS formulation [7].

Now a general pure quantum qudit state of a system that has L sites is,

$$|\Psi\rangle = \sum_{\sigma_1=1}^{d} \sum_{\sigma_2=1}^{d} ... \sum_{\sigma_L=1}^{d} C_{\sigma_1\sigma_2...\sigma_L} |\sigma_1\rangle|\sigma_2\rangle...|\sigma_L\rangle. \tag{7.1}$$

We now bipartition the space into P and Q where P contains sites 1 to l and Q contains $l+1$ to L as shown in Fig.(7.1) below,

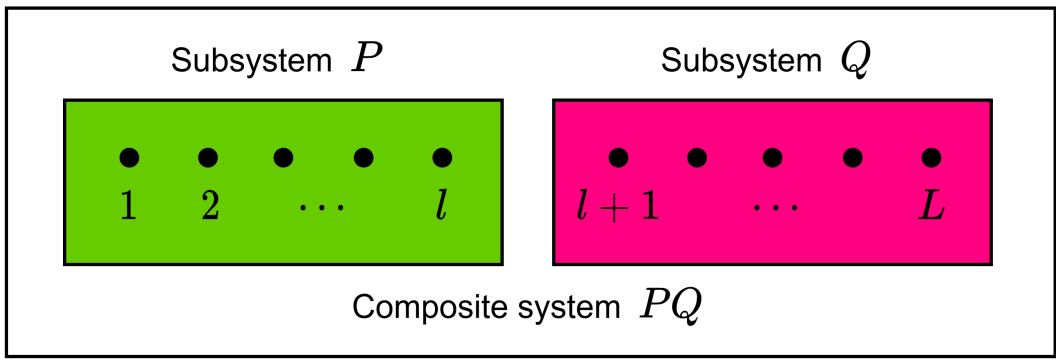


Figure 7.1: Schematic diagram showing the composite system PQ consisting of the two subsystems P and Q

We have a system PQ made up of 2 subsystems P and Q, then if we know the combined state of the systen as ρ^{PQ}, the reduced density operator ρ^P will be the state of subsystem P and the reduced density operator ρ^Q will be the state of subsystem Q. The reduced density matrices are used extensively in quantum

mechanics and quantum information theory, specially for the calculations pertaining to entanglement measures.

7.1 Reduced density operator for subsystem P

To get reduced density operator $\hat{\rho}_P^{[l]}$, we express the state in terms of $A-$matrices as,

$$|\psi\rangle = \sum_{\sigma} A^{\sigma_1}...A^{\sigma_L}|\sigma\rangle.$$

Now,

$$\begin{aligned}
|\psi\rangle\langle\psi| &= \sum_{\sigma,\sigma'} A^{\sigma_1}...A^{\sigma_L}A^{\sigma_L'^{\dagger}}...A^{\sigma_1'^{\dagger}}|\sigma\rangle\langle\sigma'|, \\
&= \sum_{\sigma_1...\sigma_L}\sum_{\sigma_1'...\sigma_L'} A^{\sigma_1}...A^{\sigma_l}A^{\sigma_{l+1}}...A^{\sigma_L}A^{\sigma_L'^{\dagger}}...A^{\sigma_{l+1}'^{\dagger}}A^{\sigma_l'^{\dagger}}...A^{\sigma_1'^{\dagger}} \times \\
&\quad |\sigma_1...\sigma_l\sigma_{l+1}...\sigma_L\rangle\langle\sigma_1'...\sigma_l'\sigma_{l+1}'...\sigma_L'|. \\
|\psi\rangle\langle\psi| &= \sum_{\sigma_1...\sigma_l\in P}\sum_{\sigma_1'...\sigma_l'\in P}\sum_{\sigma_{l+1}...\sigma_L\in Q}\sum_{\sigma_{l+1}'...\sigma_L'\in Q}(A^{\sigma_1}...A^{\sigma_l})_P(A^{\sigma_{l+1}}...A^{\sigma_L})_Q \times \\
&\quad (A^{\sigma_L'^{\dagger}}...A^{\sigma_{l+1}'^{\dagger}})_Q(A^{\sigma_l'^{\dagger}}...A^{\sigma_1'^{\dagger}})_P|\sigma_1...\sigma_l\rangle_P|\sigma_{l+1}...\sigma_L\rangle_Q\langle\sigma_1'...\sigma_l'|_P\langle\sigma_{l+1}'...\sigma_L'|_Q.
\end{aligned}$$

Taking out the degrees of freedom of Q, we obtain the reduced density operator $\rho_P^{[l]}$.

$$\begin{aligned}
\hat{\rho}_P^{[l]} &= tr_Q(|\psi\rangle\langle\psi|), \\
&= \sum_{\sigma_{l+1}''...\sigma_L''\in Q}\langle\sigma_{l+1}''...\sigma_L''|\psi\rangle\langle\psi|\sigma_{l+1}''...\sigma_L''\rangle, \\
&= \sum_{\sigma_{l+1}''...\sigma_L''\in Q}\sum_{\sigma_1...\sigma_l\in P}\sum_{\sigma_1'...\sigma_l'\in P}\sum_{\sigma_{l+1}...\sigma_L\in Q}\sum_{\sigma_{l+1}'...\sigma_L'\in Q} \\
&\quad (A^{\sigma_1}...A^{\sigma_l})_P(A^{\sigma_{l+1}}...A^{\sigma_L})_Q(A^{\sigma_L'^{\dagger}}...A^{\sigma_{l+1}'^{\dagger}})_Q(A^{\sigma_l'^{\dagger}}...A^{\sigma_1'^{\dagger}})_P \times \\
&\quad \langle\sigma_{l+1}''...\sigma_L''|_Q\ |\sigma_1...\sigma_l\rangle_P\ |\sigma_{l+1}...\sigma_L\rangle_Q\ \langle\sigma_1'...\sigma_l'|_P\ \langle\sigma_{l+1}'...\sigma_L'|_Q\ |\sigma_{l+1}''...\sigma_L''\rangle_Q, \\
&= \sum_{\sigma_{l+1}''...\sigma_L''\in Q}\sum_{\sigma_1...\sigma_l\in P}\sum_{\sigma_1'...\sigma_l'\in P}(A^{\sigma_1}...A^{\sigma_l})_P(A^{\sigma_{l+1}''}...A^{\sigma_L''})_Q \times \\
&\quad (A^{\sigma_L''^{\dagger}}...A^{\sigma_{l+1}''^{\dagger}})_Q(A^{\sigma_l'^{\dagger}}...A^{\sigma_1'^{\dagger}})_P\ |\sigma_1...\sigma_l\rangle_P\ \langle\sigma_1'...\sigma_l'|_P, \\
\hat{\rho}_P^{[l]} &= \sum_{\sigma_1...\sigma_l\in P}\sum_{\sigma_1'...\sigma_l'\in P}(A^{\sigma_1}...A^{\sigma_l})_P\left[\sum_{\sigma_{l+1}''...\sigma_L''\in Q}(A^{\sigma_{l+1}''}...A^{\sigma_L''})_Q(A^{\sigma_L''^{\dagger}}...A^{\sigma_{l+1}''^{\dagger}})_Q\right]\times \\
&\quad (A^{\sigma_l'^{\dagger}}...A^{\sigma_1'^{\dagger}})_P|\sigma_1...\sigma_l\rangle_P\ \langle\sigma_1'...\sigma_l'|_P.
\end{aligned}$$

$$\hat{\rho}_P^{[l]} = \sum_{\sigma,\sigma' \in P} A^{\sigma_1}...A^{\sigma_l}\ \rho_P^{[l]}\ A^{\sigma_l'^\dagger}...A^{\sigma_1'^\dagger}|\sigma\rangle\langle\sigma'|. \tag{7.2}$$

where,

$$\rho_P^{[l]} = \sum_{\sigma'' \in Q} A^{\sigma''_{l+1}}...A^{\sigma''_L}A^{\sigma''^\dagger_L}...A^{\sigma''^\dagger_{l+1}}. \tag{7.3}$$

$\hat{\rho}_P^{[l]}$ is the reduced density operator of P.

7.2 Reduced density operator for subsystem Q

To get reduced density operator $\hat{\rho}_Q^{[l]}$, we express the state in terms of the $B-$matrices,

$$|\psi\rangle = \sum_{\sigma} B^{\sigma_1}...B^{\sigma_L}|\sigma\rangle.$$

Now find,

$$|\psi\rangle\langle\psi| \ = \ \sum_{\sigma,\sigma'} B^{\sigma_1}...B^{\sigma_L}B^{\sigma_L'^\dagger}...B^{\sigma_1'^\dagger}|\sigma\rangle\langle\sigma'|.$$

The products $(B^{\sigma_1}...B^{\sigma_L})$ and $(B^{\sigma_L'^\dagger}...B^{\sigma_1'^\dagger})$ are just numbers. So we can write,

$$\begin{aligned}
|\psi\rangle\langle\psi| &= \sum_{\sigma,\sigma'} B^{\sigma_L'^\dagger}...B^{\sigma_1'^\dagger}B^{\sigma_1}...B^{\sigma_L}|\sigma\rangle\langle\sigma'|, \\
&= \sum_{\sigma_1...\sigma_L}\sum_{\sigma_1'...\sigma_L'} B^{\sigma_L'^\dagger}...B^{\sigma_{l+1}'^\dagger}B^{\sigma_l'^\dagger}...B^{\sigma_1'^\dagger}B^{\sigma_1}...B^{\sigma_l}B^{\sigma_{l+1}}...B^{\sigma_L} \times \\
&\quad |\sigma_1...\sigma_l\sigma_{l+1}...\sigma_L\rangle\langle\sigma_1'...\sigma_l'\sigma_{l+1}'...\sigma_L'|.
\end{aligned}$$

$$\begin{aligned}
|\psi\rangle\langle\psi| \ = \ & \sum_{\sigma_1...\sigma_l\in P}\sum_{\sigma_1'...\sigma_l'\in P}\sum_{\sigma_{l+1}...\sigma_L\in Q}\sum_{\sigma_{l+1}'...\sigma_L'\in Q}(B^{\sigma_L'^\dagger}...B^{\sigma_{l+1}'^\dagger})_Q(B^{\sigma_l'^\dagger}...B^{\sigma_1'^\dagger})_P \times \\
& (B^{\sigma_1}...B^{\sigma_l})_P(B^{\sigma_{l+1}}...B^{\sigma_L})_Q\ |\sigma_1...\sigma_l\rangle_P\ |\sigma_{l+1}...\sigma_L\rangle_Q\ \langle\sigma_1'...\sigma_l'|_P\ \langle\sigma_{l+1}'...\sigma_L'|_Q.
\end{aligned}$$

Taking out the degrees of freedom of P, we obtain the reduced density operator $\rho_Q^{[l]}$.

$$\begin{aligned}
\hat{\rho}_Q^{[l]} &= tr_P(|\psi\rangle\langle\psi|), \\
&= \sum_{\sigma_1''...\sigma_l'' \in P}\langle\sigma_1''...\sigma_l''|\psi\rangle\langle\psi|\sigma_1''...\sigma_l''\rangle,
\end{aligned}$$

$$\hat{\rho}_Q^{[l]} = \sum_{\sigma_1^{''}...\sigma_l^{''}\in P} \sum_{\sigma_1...\sigma_l\in P} \sum_{\sigma_1^{'}...\sigma_l^{'}\in P} \sum_{\sigma_{l+1}...\sigma_L\in Q} \sum_{\sigma_{l+1}^{'}...\sigma_L^{'}\in Q}$$
$$(B^{\sigma_L^{'\dagger}}...B^{\sigma_{l+1}^{'\dagger}})_Q (B^{\sigma_l^{'\dagger}}...B^{\sigma_1^{'\dagger}})_P (B^{\sigma_1}...B^{\sigma_l})_P (B^{\sigma_{l+1}}...B^{\sigma_L})_Q \times$$
$$\langle\sigma_1^{''}...\sigma_l^{''}|_P \, |\sigma_1...\sigma_l\rangle_P \, |\sigma_{l+1}...\sigma_L\rangle_Q \, \langle\sigma_1^{'}...\sigma_l^{'}|_P \, \langle\sigma_{l+1}^{'}...\sigma_L^{'}|_Q \, |\sigma_1^{''}...\sigma_l^{''}\rangle_P,$$

$$= \sum_{\sigma_1^{''}...\sigma_l^{''}\in P} \sum_{\sigma_{l+1}...\sigma_L\in Q} \sum_{\sigma_{l+1}^{'}...\sigma_L^{'}\in Q} (B^{\sigma_L^{'\dagger}}...B^{\sigma_{l+1}^{'\dagger}})_Q (B^{\sigma_l^{''\dagger}}...B^{\sigma_1^{''\dagger}})_P \times$$
$$(B^{\sigma_1^{''}}...B^{\sigma_l^{''}})_P (B^{\sigma_{l+1}}...B^{\sigma_L})_Q \, |\sigma_{l+1}...\sigma_L\rangle_Q \, \langle\sigma_{l+1}^{'}...\sigma_L^{'}|_Q,$$

$$= \sum_{\sigma_{l+1}...\sigma_L\in Q} \sum_{\sigma_{l+1}^{'}...\sigma_L^{'}\in Q} (B^{\sigma_L^{'\dagger}}...B^{\sigma_{l+1}^{'\dagger}})_Q \left[\sum_{\sigma_1^{''}...\sigma_l^{''}\in P} (B^{\sigma_l^{''\dagger}}...B^{\sigma_1^{''\dagger}})_P (B^{\sigma_1^{''}}...B^{\sigma_l^{''}})_P\right] \times$$
$$(B^{\sigma_{l+1}}...B^{\sigma_L})_Q \, |\sigma_{l+1}...\sigma_L\rangle_Q \, \langle\sigma_{l+1}^{'}...\sigma_L^{'}|_Q,$$

$$\hat{\rho}_Q^{[l]} = \sum_{\sigma,\sigma^{'}\in Q} B^{\sigma_L^{'\dagger}}...B^{\sigma_{l+1}^{'\dagger}} \, \rho_Q^{[l]} \, B^{\sigma_{l+1}}...B^{\sigma_L}|\sigma\rangle\langle\sigma^{'}|, \tag{7.4}$$

where,

$$\rho_Q^{[l]} = \sum_{\sigma^{''}\in P} B^{\sigma_l^{''\dagger}}...B^{\sigma_1^{''\dagger}} B^{\sigma_1^{''}}...B^{\sigma_l^{''}}, \tag{7.5}$$

$\hat{\rho}_Q^{[l]}$ is the reduced density operator of Q subsystem.

7.3 Analytical calculation and discussion with one example

Consider the 2 qubit Bell state, for partition $\underbrace{[1]}_{P} : \underbrace{[2]}_{Q}$.

$$|\psi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

For reduced density operator of P, we find the $A-$matrices using LCMPS as,

$$A^{[1]0} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad A^{[1]1} = \begin{pmatrix} 0 & 1 \end{pmatrix},$$

$$A^{[1]0} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}, \qquad A^{[2]1} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

Further,

$$\begin{aligned}
\rho_P^{[1]} &= \sum_{\sigma_2 \in Q} A^{\sigma_2} A^{\sigma_2^\dagger}, \\
&= A^{[2]0} A^{[2]0^\dagger} + A^{[2]1} A^{[2]1^\dagger}, \\
&= \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \\
&= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}.
\end{aligned}$$

$$\begin{aligned}
\hat{\rho}_P^{[1]} &= \sum_{\sigma_1, \sigma_1^{'} \in P} A^{\sigma_1} \rho_P^{[1]} A^{\sigma_1^{'\dagger}} |\sigma_1\rangle\langle\sigma_1^{'}|, \\
&= A^{[1]0}\ \rho_P^{[1]}\ A^{[1]0^\dagger}\ |0\rangle\langle 0| + A^{[1]0}\ \rho_P^{[1]}\ A^{[1]1^\dagger}\ |0\rangle\langle 1| + \\
&\quad A^{[1]1}\ \rho_P^{[1]}\ A^{[1]0^\dagger}\ |1\rangle\langle 0| + A^{[1]1}\ \rho_P^{[1]}\ A^{[1]1^\dagger}\ |1\rangle\langle 1|, \\
&= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} |0\rangle\langle 0| + \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} |0\rangle\langle 1| + \\
&\quad \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} |1\rangle\langle 0| + \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} |1\rangle\langle 1|, \\
&= \begin{pmatrix} \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} |0\rangle\langle 0| + \begin{pmatrix} \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} |0\rangle\langle 1| + \\
&\quad \begin{pmatrix} 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} |1\rangle\langle 0| + \begin{pmatrix} 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} |1\rangle\langle 1|, \\
&= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \\
&= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \\
&= \frac{I}{2},
\end{aligned}$$

as expected.

Now for reduced density operator of Q, we use RCMPS to find,

$$B^{[1]0} = \begin{pmatrix} 1 & 0 \end{pmatrix}, \qquad B^{[1]1} = \begin{pmatrix} 0 & 1 \end{pmatrix},$$

$$B^{[1]0} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}, \qquad B^{[2]1} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}.$$

$$\begin{aligned} \rho_Q^{[1]} &= \sum_{\sigma_1 \in P} B^{\sigma_1^\dagger} B^{\sigma_1}, \\ &= B^{[1]0^\dagger} B^{[1]0} + B^{[1]1^\dagger} B^{[1]1^\dagger}, \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix}, \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned}$$

Further,

$$\begin{aligned} \hat{\rho}_Q^{[1]} &= \sum_{\sigma_2, \sigma_2^{'} \in Q} B^{\sigma_2^{'\dagger}} \rho_Q^{[1]} B^{\sigma_2} |\sigma_2\rangle\langle\sigma_2^{'}|, \\ &= B^{[2]0^\dagger}\ \rho_Q^{[1]}\ B^{[2]0}\ |0\rangle\langle 0| + B^{[2]0^\dagger}\ \rho_Q^{[1]}\ B^{[2]1}\ |0\rangle\langle 1| + \\ &\quad B^{[2]1^\dagger}\ \rho_Q^{[1]}\ B^{[2]0}\ |1\rangle\langle 0| + B^{[2]1^\dagger}\ \rho_Q^{[1]}\ B^{[2]1}\ |1\rangle\langle 1|, \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} |0\rangle\langle 0| + \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} |0\rangle\langle 1| + \\ &\quad \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} |1\rangle\langle 0| + \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} |1\rangle\langle 1|, \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} |0\rangle\langle 0| + \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} |0\rangle\langle 1| + \\ &\quad \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} |1\rangle\langle 0| + \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} |1\rangle\langle 1|, \\ &= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \end{aligned}$$

$$\hat{\rho}_Q^{[1]} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \\ = \frac{I}{2},$$

as expected.

7.4 Python code for obtaining the reduced density operator of P subsystem for any d and L

```
def rdmP(d, L, z1, l):
    rhol = np.zeros((d,d))
    for i in range (0,d):
        rhol = rhol + np.dot(z1[d*L-i-1], np.transpose(np.conjugate(
   z1[d*L-i-1])))
    for i0 in range (1, L-l):
        x = d**(L-(i0+1))
        if (i0 < L//2):
            x = d**(i0+1)
        elif (L % 2 == 1 and i0 == L//2):
            x = d**(i0)
        d2 = np.zeros((x,x))
        for i in range (0,d):
            d2 = d2 + np.dot(np.dot(z1[d*L-1-i-i0*d], rhol), np.
   transpose(np.conjugate(z1[d*L-1-i-i0*d])))
        rhol = d2
    rangelist = []
    num = 0
    for i in range (1, l+1):
        templist = []
        for j in range (0, d):
            templist.append(num)
            num = num +1
        rangelist.append(templist)
    rdm = []
```

```
    def for_recursive(number_of_loops, range_list, current_index=0, iter_list = []):
        if (iter_list == []):
            iter_list = [0]*number_of_loops
        if current_index == number_of_loops-1:
            for iter_list[current_index] in range_list[current_index]:
                iter_list = np.array(iter_list)
                result = np.identity(1)
                for i in range(0, len(iter_list)):
                    result = np.dot(result, z1[iter_list[i]])
                AmatrixMul.append(result)
        else:
            for iter_list[current_index] in range_list[current_index]:
                for_recursive(number_of_loops, iter_list = iter_list, range_list = range_list,  current_index = current_index+1)
    for_recursive(range_list = rangelist, number_of_loops = l)
    for i in range (0, len(AmatrixMul)):
        for j in range (0, len(AmatrixMul)):
            rdm.append(np.dot(np.dot(AmatrixMul[i], rhol), np.transpose(np.conjugate(AmatrixMul[j])))[0][0])
    rdm = np.array(rdm).reshape((d**l, d**l))
```

7.5 Python code for obtaining the reduced density operator of Q subsystem for any d and L

```
def rdmB(d, L, z1, l):
    rhol = np.zeros((d,d))
    for i in range (0,d):
        rhol = rhol + np.dot(np.transpose(np.conjugate(z1[d*L-i-1])), z1[d*L-i-1])
    for i0 in range (1, L-l):
        x = d**(L-(i0+1))
        if (i0 < L//2):
            x = d**(i0+1)
        elif (L % 2 == 1 and i0 == L//2):
            x = d**(i0)
```

```
        d2 = np.zeros((x,x))
        for i in range (0,d):
            d2 = d2 + np.dot(np.dot(np.transpose(np.conjugate(z1[d*L
-1-i-i0*d])), rhol), z1[d*L-1-i-i0*d])
        rhol = d2
    def for_recursive(number_of_loops, range_list, current_index=0,
iter_list = []):
        if (iter_list == []):
            iter_list = [0]*number_of_loops
        if current_index == number_of_loops-1:
            for iter_list[current_index] in range_list[current_index
]:
                iter_list = np.array(iter_list)
                result = np.identity(1)
                for i in range(0, len(iter_list)):
                    result = np.dot(result, np.transpose(np.
conjugate(z1[iter_list[i]])))
                BmatrixMul.append(result)
        else:
            for iter_list[current_index] in range_list[current_index
]:
                for_recursive(number_of_loops, iter_list = iter_list
, range_list = range_list,  current_index = current_index+1)
    rangelist = []
    num = 0
    for i in range (1, l+2):
        templist = []
        for j in range (0, d):
            templist.append(num)
            num = num +1
        rangelist.append(templist)
    rdm = []
    for_recursive(range_list = rangelist, number_of_loops = L-l)
    for i in range (0, len(BmatrixMul)):
        for j in range (0, len(BmatrixMul)):
            rdm.append(np.dot(np.dot(BmatrixMul[i], rhol), np.
transpose(np.conjugate(BmatrixMul[j])))[0][0])
    rdm = np.array(rdm).reshape((d**(L-l), d**(L-l)))
```

7.6 Output from the code for reduced density operator of subsystem P and Q for any d and L

Consider the state,

$$|\psi\rangle = \frac{|001\rangle + |010\rangle + |100\rangle}{\sqrt{3}}, \tag{7.6}$$

for the partition $\underbrace{[1]}_{P} : \underbrace{[23]}_{Q}$.

The reduced density operator of P is,

```
[[0.66666667 0.        ]
 [0.         0.33333333]]
```

The reduced density operator of Q is,

```
[[ 3.33333333e-01 -2.61682076e-17 -2.61682076e-17 -2.90525466e-33]
 [-2.61682076e-17  3.33333333e-01  3.33333333e-01  3.70074342e-17]
 [-2.61682076e-17  3.33333333e-01  3.33333333e-01  3.70074342e-17]
 [-2.90525466e-33  3.70074342e-17  3.70074342e-17  4.10865055e-33]]
```

These match exactly with analytical results and we can see that the trace of both the density matrices is unity as the case should be.

7.7 Summary and conclusion

In this chapter the procedure to obtain reduced density operators from MPS representation of any quantum state was discussed in detail. Generalized Python codes were written which can work for any d, L and p, that is for any pure qudit quantum state and for any bipartition. These codes were presented along with examples.

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Visible research output

- *"On the structure and Dynamics of reshaped matrices for effective matrix product state decompositions: M. S. Ramkarthik, Utkarsha Bhute"* (to be sent to Physical Review B, APS) (manuscript under preperation).