Understanding Quantum Teleportation via SIMPS formalism of Tensor Networks

by

Rahul Pal
18111003

A thesis submitted to the Department of Mathematics and Natural Sciences
in partial fulfillment of the requirements for the degree of
B.Sc. in Physics

Department of Mathematics and Natural Sciences
BRAC University
August 2025

Declaration

It is hereby declared that

1. The thesis submitted is my own original work while completing degree at BRAC University.
2. The thesis does not contain material previously published or written by a third party, except where this is appropriately cited through full and accurate referencing.
3. The thesis does not contain material which has been accepted, or submitted, for any other degree or diploma at a university or other institution.
4. I have acknowledged all main sources of help.

Student's Full Name & Signature:

Rahul Pal
18111003

Approval

The thesis titled "Understanding Quantum Teleportation via SIMPS Formalism of Tensor Networks" submitted by

1. Rahul Pal (18111003)

Of Summer, 2025 has been accepted as satisfactory in partial fulfillment of the requirement for the degree of B.Sc. in Physics on August 19th, 2025.

Examining Committee:

Supervisor:
(Associate Dean)

Tibra Ali, PhD
Professor & Associate Dean
Department of Mathematics & Natural Sciences
School of Data & Sciences
BRAC University

Program Coordinator:
(Member)

Md. Lutfor Rahman
Assistant Professor & Program Coordinator
Department of Mathematics & Natural Sciences
BRAC University

Head of Department:
(Chair)

Md. Firoze H. Haque, PhD
Associate Professor & Chairperson
Department of Mathematics & Natural Sciences
BRAC University

Abstract

The goal of this thesis is to explore a new formalism of Tensor Networks called SIMPS and review its feasibility at tackling the computational challenges posed by many-body systems. We will start this thesis with the review of some foundational concepts of quantum mechanics and quantum information, and we review the existing formalism of TNs. Afterwards, we will review the literature by David. T. Stephen [27] [26] which introduces the SIMPS formalism and proceed to investigating the cases where SIMPS provides obvious computational advantages over existing formalisms.

KEYWORDS:

Quantum Teleportation, Long-range Quantum Teleportation, Tensor Networks, MPS, SIMPS, Non-Onsite Symmetries, Quantum Wire.

Acknowledgement

I am grateful to my supervisor, Tibra Ali (Professor and Associate Dean), for assigning me this research topic and for his feedback and support throughout the process. Over the past years, his role in shaping my academic perspective, especially my interest in quantum theory, has been significant, and his trust in my independent approach allowed this work to develop in its own course.

My deepest thanks go to Nazmoon Falgunee Moon, who patiently helped rebuild my grasp of the core concepts and offered valuable feedback throughout the thesis. This thesis would have taken a very different shape without her.

I also acknowledge BRAC University for providing the institutional framework and resources within which this research was completed, especially Dr.Firoz H. Haque (Professor and Chairperson) and Md. Lutfor Rahman (Assistant Professor and Coordinator) who helped me learn the basics of physics during my first year in BRAC and also supported me at various times all throughout my undergrad. I would also like to acknowledge Prof. Syed M. Hashemi, under whose guidance I deepened my understanding of socio-economic concepts and learned to challenge my limits and expand my perspectives.

Finally, I thank my parents and grandmother for granting me the autonomy to pursue my studies without hindrance, which proved indispensable in bringing this work to completion.

Table of Contents

List of Figures

Nomenclature

The next list describes several symbols & abbreviation that will be later used within the body of the document

GHZ Greenberger–Horne–Zeilinger

MBQC Measurement Based Quantum Computation

MPS Matrix Product State

OBC Open Boundary Conditions

PBC Periodic Boundary Conditions

SIMPS Split Index Matrix Product State

SPT Symmetry Protected Topology

SVD Singular Value Decomposition

TN Tensor Network

EPR Einstein, Podolsky, Rosen

Chapter 1

Introduction

Quantum information is the study of finite dimensional quantum systems, where the abstractions are given a more quantitative representation so that they allow for easier computations. This enables us to have more insight of how information is stored, modified or transferred at the quantum scale.

A natural complication that arises when studying quantum systems like this is the more than exponential increase in computational complexity as the number of particles in the system increases. This is due to the exponential increase of the possible degrees of freedom that each new particle added to the system causes. For example, if we were to perform some quantum measurement on a system with 1 mole particles having spin degree of freedom, there would be a total of $2 \times (6.022 \times 10^{23})$ possible degrees of freedom. In other words, we would have to deal with $2 \times (6.022 \times 10^{23})$ variables in our calculation, which would be incalculable. In fact, we know through experiments that as the number of particles in a quantum system approaches 8, 9 or 10, the number of possible degrees of freedom quickly approaches incalculable territory. So we cannot get remotely close to the 1 mole particle mark before the calculations get impossible to solve. This can be referred to as the many-body problem.

In this thesis we will take a look at an algebra known as tensor networks, which help us more efficiently mitigate this many-body problem by taking advantage of the fact that in real systems, ground states have low entanglement. We will focus on analysing a new formalism of TNs, called SIMPS. This was suggested by David. T. Stephen in his recently published paper, "Non-onsite symmetries and quantum teleportation in split-index matrix product states" [27]. We will further explore how this new formalism is better suited to capturing certain symmetries of quantum systems, and how it enables more efficient computation of quantum information transfer (quantum teleportation).

To begin our analysis, we will first lay some groundwork by reviewing the foundations of quantum mechanics and quantum information in chapter 2. We will review some

relevant language and the density operator formalism of quantum mechanics. Then we will introduce some special states that are widely used in quantum information and have a look at some operators (gates) relevant to it. Finally, we will wrap up our foundation by reviewing quantum entanglement and its quantization.

In chapter 3 we will look at how quantum systems behave. We will look at the randomness of measurement outcomes that are inherent to quantum systems. We will see how information is transferred (teleportation) and the interactions of spin systems.

After that, in chapter 4 we will introduce TNs. We will see what they are and why they work in detail. Then we will move on to defining the existing formalism of TNs known as MPS, both mathematically and graphically. We will then do the same for SIMPS. Throughout this chapter we will focus on the algebra, how it works, how we convert from one formalism to another, and also some example calculations of what certain well known states look like under each formalism.

Finally, in chapter 5, we will review the advantages of the SIMPS formalism that Stephen found in his paper. We will start by exploring how certain physical symmetries are represented in both the MPS and SIMPS formalisms, and how SIMPS are able to better capture these symmetries under certain conditions. Next we will look at how teleportation is computed for many-body systems in each formalism, where we will see that SIMPS enable us to more efficiently compute something called the byproduct operator - something that is challenging to do in the MPS formalism.

Chapter 2

Background Material

In this chapter we will start by looking at some foundational concepts of finite dimensional quantum theory, like unitary transformations and measurements, etc. which are tools that will constantly be used to describe and decode quantum systems. We will explore the geometric representation of qubits through the use of Bloch spheres and also look at the density matrix formalism of quantum mechanics and see how the postulates of quantum mechanics are affected by it. As we move along, we will start to shift our focus to topics that make up the foundations of quantum information theory. We will look at some special states that are heavily made use of in quantum information, and look at gates, which is how operators are generally applied to systems in quantum computation. And finally to finish off the chapter we will explore quantum entanglement. This will serve as the core idea behind the topics we will handle in the next chapter - no-cloning, teleportation and spin chains. These topics were explored with the help of foundational literature like [3], [23], [17], [9], and [28]. Some well established papers like [6], [8], [10], and [15], were also studied.

2.1 Some Relevant Languange

These are some core concepts that are relevant to understanding quantum systems, entanglement, and teleportation.

2.1.1 Unitary Transformation

Unitary transformations[3], are linear transformations which satisfies the following,

$$U^\dagger U = UU^\dagger = \mathbb{I},$$

where, U is a linear operator (called unitary operator), $U^\dagger$ is the Hermitian adjoint of U, and $\mathbb{I}$ is the identity matrix. As we move forward, we will see logical operators called gates. These are all unitary operators and hence will be reversible via unitary transformation, i.e. preserve inner products, and therefore probabilities.

2.1.2 Measurement

Unlike classical mechanics, in quantum physics, measurement is not a simple process of observation where we reveal pre-existing properties of the system. Rather, in quantum physics, measurements have the ability to change the system[28], a phenomenon which is sometimes known as quantum collapse.

Let us take some quantum system with state $|\psi\rangle$, and say that we want to measure it via some operator $\hat{O}$ (which is a Hermitian operator we call the observable) that has the following eigenvalue equation,

$$\hat{O}\,|\phi_n\rangle = \lambda_n\,|\phi_n\rangle\,.$$

Decomposing the state $|\psi\rangle$ in terms of the orthonormal eigenstates of $\hat{O}$,

$$|\psi\rangle = \sum_n a_n\,|\phi_n\rangle\,.$$

If the eigenvalue spectrum for this state is non-degenerate, by the Born rule we get the following probability,

$$\begin{aligned} &\text{Prob}(\lambda_n) = |a_n|^2, \\ \&\quad &\sum_n \text{Prob}(\lambda_n) = 1. \end{aligned}$$

Now that we have gotten this result λ_n, our wavefunction collapses like so,

$$|\psi\rangle \longrightarrow |\phi_n\rangle\,,$$

with probability $|a_n|^2$ and consecutive measurements of the system for the same λ_n will yield the same collapsed state $|\phi_n\rangle$ with a probability of 1. When the eigenvalue spectrum is degenerate, we will see the following,

$$\begin{aligned} &\text{Prob}(\lambda) = \sum_{n|\lambda_n=\lambda} |a_n|^2, \\ \&\quad &|\psi\rangle \longrightarrow C \sum_{n|\lambda_n=\lambda} a_n\,|\phi_n\rangle\,, \end{aligned}$$

where C is some normalization factor and n is just one of the possible outcomes (eigenvalue) of the measurement.

2.1.3 Bloch Sphere

The Bloch sphere is a fundamental tool used in quantum mechanics that allows us to visualize the state space of a single qubit by providing a geometric representation of all its possible mixed and pure states[17]. It is constructed around the Pauli matrices and has X, Y, and Z bases corresponding to the Pauli matrix directions,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

as shown in Fig.2.1.

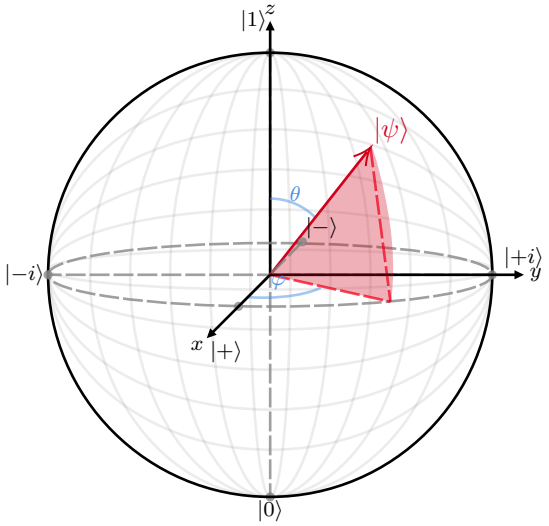


Figure 2.1: Single qubit in Bloch sphere representation

X-Basis

This basis comprises of the states $|+\rangle$ in the x_+ direction and $|-\rangle$ in the x_- direction,

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \quad \text{and} \quad |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}.$$

This basis is useful when representing superpositions.

Y-Basis

This basis comprises of the states $|+i\rangle$ in the y_+ direction and $|-i\rangle$ in the y_- direction,

$$|+i\rangle = \frac{|0\rangle + i\,|1\rangle}{\sqrt{2}} \quad \text{and} \quad |-i\rangle = \frac{|0\rangle - i\,|1\rangle}{\sqrt{2}}.$$

This basis is useful when showing relative phase.

Z-Basis (Computational Basis)

This basis comprises of the states $|0\rangle$ in the z_+ direction and $|1\rangle$ in the z_- direction,

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Mathematically, a qubit can be represented as a linear combination of basis states $|0\rangle$ and $|1\rangle$ as follows,

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \quad \& \quad |\alpha|^2 + |\beta|^2 = 1,$$

where α and β are complex numbers. We can rewrite this qubit with the help of trigonometric functions as,

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle\,. \tag{2.1}$$

This θ and φ allows us to show the state of a qubit as a point on the Bloch sphere as shown in Fig.2.1. Of these two parameters, the polar angle has some additional significance than just showing the position of the qubit. Especially the fact that this parameter is always written as $\theta/2$ in Eqn.2.1. A qubit lives in a 2D $\mathcal{H}$-space. When we then express this on a unit sphere like the Bloch sphere, its degrees of freedom is reduced from 4 real parameters (in the $\mathcal{H}$-space) to 2 for convenient visualization. This change in parameter causes the polar angle in the unit sphere to always be double that of the projective $\mathcal{H}$-space, i.e., a full rotation of θ on the Bloch sphere corresponds to half a rotation in the $\mathcal{H}$-space. Thus we always have to correct the polar angle by dividing it by half to get the correct amplitudes.
This graphical visualization for a qubit is quite useful, however it is limited in that there exists no such graphical generalization for higher dimensional qubits.

2.2 Density Operator

The density operator (or density matrix) is a way to formulate quantum mechanics that makes it more convenient to describe a system with an unknown state[17]. It is a more generalized form of the state vector formalism. While the state vector formalism can only be used to describe pure states, the density operator formalism can also be used to describe mixed states. This comes in very handy when dealing with quantum teleportation, which is a significant part of this paper.

Let us say, we have a quantum system which could be in any of the state $|\psi_i\rangle$. Each state has the respective probabilities p_i. The density operator (or matrix) of the system can be then defined as,

$$\rho \equiv \sum_i p_i\,|\psi_i\rangle\,\langle\psi_i| \quad \{\text{where } \rho^\dagger = \rho\}.$$

It will satisfy the following properties,

1. The matrices are Hermitian, $\rho = \rho^\dagger$,
2. The trace of the matrices will be, $\mathrm{Tr}(\rho) = 1$,
3. All eigenvalues of ρ must be ≥ 0.

For example, let us take the pure state,

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$
$$\therefore \langle\psi|^* = \alpha^*\,\langle 0| + \beta^*\,\langle 1|\,.$$

Its density operator would be given by,

$$\begin{aligned}\rho &= |\psi_i\rangle\,\langle\psi_i| \\ &= (\alpha\,|0\rangle + \beta\,|1\rangle)(\alpha^*\,\langle 0| + \beta^*\,\langle 1|) \\ &= \alpha\alpha^*\,|0\rangle\,\langle 0| + \alpha\beta^*\,|0\rangle\,\langle 1| + \beta\alpha^*\,|1\rangle\,\langle 0| + \beta\beta^*\,|1\rangle\,\langle 1| \\ \therefore \rho &= \begin{bmatrix} \alpha\alpha^* & \alpha\beta^* \\ \beta\alpha^* & \beta\beta^* \end{bmatrix}\end{aligned}$$

2.2.1 Postulates of Quantum Mechanics Under the Density Operator Formalism

Using this density operator ρ we just defined, we can make the following changes to the postulates of quantum mechanics to fit the density operator formalism[17].

Postulate 1 *Any and all isolated physical systems will have a state space (Hilbert space) associated to it. The density operator acting on the state space of the said system will be able to fully describe it and can be expressed as,*

$$\rho = \sum_i p_i\rho_i \quad \{\rho = \rho^\dagger; \lambda \text{ of } \rho \geq 0; Tr(\rho) = 1\},$$

where, ρ_i is the state the system is in, and p_i is the probability associated with it. [17]

Postulate 2 *A unitary transformation can be used to describe the evolution of a closed quantum system, i.e.,*

$$\rho' = U\rho U^\dagger,$$

where, ρ is the state of the system at t_1 and ρ' is the state of the system at t_2. [17]

Postulate 3 *Measurements taken of a quantum system are expressed as a collection of measurement operators $\{M_m\}$, which act on the state space of the system that is being measured - m refers to the measurement outcomes that may occur during measurement. So for a state ρ, the probability of getting result m will be given by,*

$$p(m) = \mathrm{tr}\left(M_m^\dagger M_m\rho\right),$$

and the state immediately after the measurement will be,

$$\rho' = \frac{M_m\rho M_m^\dagger}{\mathrm{tr}\left(M_m^\dagger M_m\rho\right)}.$$

Furthermore, the measurement outcomes will have to satisfy the following,

$$\sum_m M_m^\dagger M_m = I.$$

[17]

Postulate 4 *The tensor product of the state spaces of the individual physical systems makes up the state space of a composite physical system. Additionally, if systems* 1 *through* n *are present and system* i *is equipped in state* ρ_i*, the joint state of the entire system is given by,*

$$\rho_1 \otimes \rho_2 \otimes \dots \rho_n.$$

[17]

2.2.2 Pure States Vs Mixed States

A quantum system for which we know the state $|\psi\rangle$ exactly is called a pure state. Let us consider some observable $\mathbf{A}$ with eigenvalue λ_n and eigenvector $|\lambda_n^i\rangle$ where $i = 1, 2, 3, \dots, g_n$. We can define the following,

1. **Normalization Condition:**

$$\mathrm{Tr}(\rho) = 1. \tag{2.2}$$

2. **Expectation Values:**

$$\langle \mathbf{A} \rangle = \mathrm{Tr}(\rho \mathbf{A}). \tag{2.3}$$

3. **Probability of Measurement Outcome:**

$$P(\lambda_n) = \mathrm{Tr}(\rho P_n), \tag{2.4}$$

   where $P_n = \sum_{i=1}^{g_n} |\lambda_n^i\rangle \langle \lambda_n^i|$ is the projection operator.

4. **Time Evolution:**

$$\frac{d}{dt}\rho_i(t) = \frac{1}{i\hbar}[H(t), \rho(t)]. \tag{2.5}$$

When we do not know the state $|\psi\rangle$ of our quantum system exactly, we call it a mixed state. It is a statistical mixture of different pure states. Each $|\psi\rangle$ will have probability p_i associated to it, s.t $\sum_i p_i = 1$. Here our density matrix, ρ, can be denoted by,

$$\rho = \sum_i p_i \rho_i. \tag{2.6}$$

For mixed states we can define the quantities in equations 2.2, 2.3, 2.4 and 2.5 by simply substituting the density operator for pure states, ρ, with Eqn.2.6

Pure or Mixed State?

The above mentioned definitions for pure and mixed states look very similar, but there are two very fundamental relations which hold true for one and not the other.

For pure states, we can show that they are idempotent, i.e.,

$$\rho^2 = |\psi_i\rangle \underbrace{\langle\psi_i|\psi_i\rangle}_{\mathbb{I}} \langle\psi_i| = |\psi_i\rangle \langle\psi_i| = \rho.$$

From this we can say,

$$\mathrm{Tr}(\rho^2) = \mathrm{Tr}(\rho) = 1.$$

For mixed states we have defined,

$$\rho = \sum_i p_i \rho_i = \sum_i p_i |\psi_i\rangle \langle\psi_i| .$$

When we try to check for idempotency, we will see that,

$$\rho^2 = \sum_i p_i^2 |\psi_i\rangle \langle\psi_i| \neq \rho.$$

Ofcourse, what will follow is that,

$$\mathrm{Tr}(\rho^2) \neq \mathrm{Tr}(\rho).$$

2.3 Some Special States

2.3.1 Bell State

The Bell States[2], also known as the EPR pairs[1], are one of the most important two qubit states in quantum computation. They form the fundamentals of quantum teleportation - used as shared entangled pairs between qubits. The states are[17],

$$\begin{aligned}
|\beta_{00}\rangle &= \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) , \\
|\beta_{01}\rangle &= \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) , \\
|\beta_{10}\rangle &= \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) , \\
|\beta_{11}\rangle &= \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) .
\end{aligned}$$

This can be written in a more generalized form as,

$$|\beta_{ij}\rangle = \frac{1}{\sqrt{2}} (|0, j\rangle + (-1)^x |1, \bar{j}\rangle) . \tag{2.7}$$

These states can be creating using a circuit that utilizes the Hadamard and C-**NOT** gates as shown below,

Input	Output
$\|00\rangle$	$\frac{1}{\sqrt{2}}(\|00\rangle + \|11\rangle) \equiv \|\beta_{00}\rangle$
$\|01\rangle$	$\frac{1}{\sqrt{2}}(\|01\rangle + \|10\rangle) \equiv \|\beta_{01}\rangle$
$\|10\rangle$	$\frac{1}{\sqrt{2}}(\|00\rangle - \|11\rangle) \equiv \|\beta_{10}\rangle$
$\|11\rangle$	$\frac{1}{\sqrt{2}}(\|01\rangle - \|10\rangle) \equiv \|\beta_{11}\rangle$

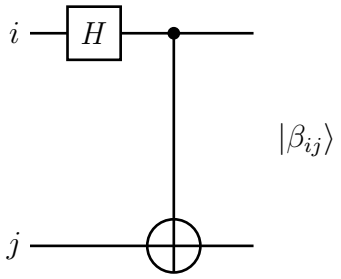


Figure 2.2: Creating Bell States

Finally, these states can be proven to have the four following properties[17],

1. They are maximally entangled states.
2. The states are orthogonal with each other and form the basis for a $\mathcal{H}^{\otimes 4} \cong \mathcal{H}^{\otimes 2} \otimes \mathcal{H}^{\otimes 2}$ Hilbert space,
3. $|\beta_{00}\rangle$ and $|\beta_{01}\rangle$ are symmetric while $|\beta_{10}\rangle$ and $|\beta_{11}\rangle$ are asymmetric.

Eqn.2.7 can be further generalized for D-dimensional $\mathcal{H}$-spaces as,

$$\left|\psi_D^+\right\rangle = \frac{1}{D}\sum_{a=0}^{D-1}|aa\rangle\,, \tag{2.8}$$

where $|a\rangle$ are the computational basis states of the system.

2.3.2 GHZ State

The GHZ state[12] is a maximally entangled state that builds on the Bell states and extends it to three or more qubits,

$$|GHZ\rangle = \tfrac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$

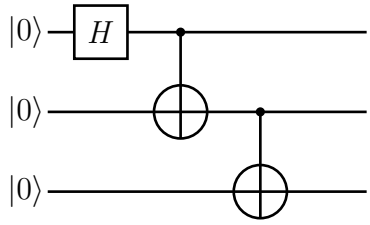


Figure 2.3: Smallest GHZ State

It can be expressed more generally for up to n-qubits as the following tensor product,

$$\begin{aligned}|\text{GHZ}\rangle &= \frac{1}{\sqrt{d}}\sum_{i=0}^{d-1}|i\rangle \otimes \cdots \otimes |i\rangle \\ &= \frac{1}{\sqrt{d}}(|0\rangle \otimes \cdots \otimes |0\rangle + \cdots + |d-1\rangle \otimes \cdots \otimes |d-1\rangle).\end{aligned}$$

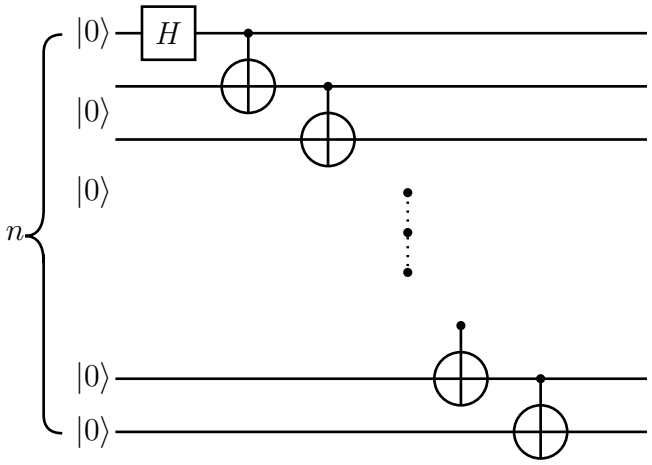


Figure 2.4: GHZ State of n-Qubits

It has the following properties,

1. All qubits in a GHZ state are entangled together - there are no subsets of entangled qubits.

2. Taking a partial trace (measurement) over any one of the states will lead to the whole system collapsing into an unentangled mixed state.

2.4 Gates

When building a classical device (circuit/algorithm), we use different kind of logical devices/arguments that manipulate the signals/classical bits to build up to different functions. Some common examples are **AND**, **OR**, **XOR**, **NOT**, etc. These logical devices are essentially the building blocks of our classical device.

Gates are the quantum analog of these logical arguments, defined to take advantage of superposition and entanglement so that they work on qubits in a quantum circuit. All quantum gates have these general properties,

1. They are unitary operators so they are reversible.

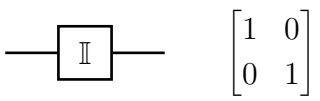
2. Their action on qubits are linear.

3. They will not clone a qubit except for basis states(we will see this in more detail in Sec.3.1).

Let us take a look at some common gates which we will need for the later parts of this paper.

2.4.1 Identity Gate

The identity gate is quite simply the identity matrix acting on a single qubit. The application of this will not modify the quantum state of the qubit. It is usually used to compliment the mathematical representation of the results of other gate operations.



$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

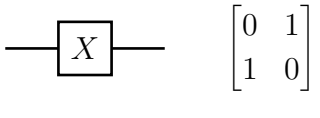
Figure 2.5: Identity Gate

2.4.2 Pauli Gates

These gates are the Pauli matrices σ_x, σ_y and σ_z respectively. When applied to a single qubit, they generate rotations around the X, Y and Z axis of the Bloch sphere.

X Gate

The X gate (also known as the quantum **NOT** or bit-flip gate) when applied to the qubit $|0\rangle$, maps it to $|1\rangle$, and vice versa, i.e. it flips the qubit.



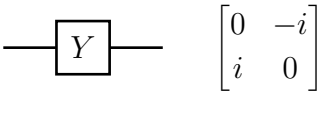
$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Figure 2.6: X Gate

On the Bloch sphere, the action of this gate can be shown with a rotation of π around the x-axis.

Y Gate

The Y gate combines a flip with a phase when applied to a qubit - a $|0\rangle$ is mapped to $i\,|1\rangle$ and a $|1\rangle$ is mapped to $-i\,|0\rangle$.



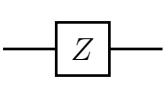
$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

Figure 2.7: Y Gate

On the Bloch sphere, the action of this gate can be shown with a rotation of π around the y-axis.

Z Gate

The Z gate (also known as phase-flip) when applied to a single qubit, does not change $|0\rangle$. However, it maps $|1\rangle$ to $-|1\rangle$.



$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

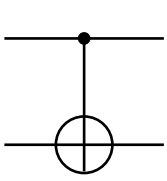
Figure 2.8: Z Gate

On the Bloch sphere, the action of this gate can be shown with a rotation of π around the z-axis.

We will sometimes see these Pauli gates/operators being refered to as "byproduct" operators. Essentially, when we are taking measurements of a system of entangled qubits, due to the randomness of measurement outcome, unitary operators will arise. These are just the the Pauli matrices, which then needs to be corrected for (Hermitian transpose (†) of said matrices need to be applied) to successfully perform the teleportation. This process is also termed the Pauli correction.

2.4.3 Control-NOT Gate

The Control-**NOT** or C-**NOT** gate acts on two qubits. When applied, one qubit acts as the control qubit (• on Fig.2.9) and the other as the target qubit ($\bigoplus$ on Fig.2.9).



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Figure 2.9: C-**NOT** Gate

When the control qubit is $|0\rangle$ then the target qubit remains unchanged. If the control qubit is $|1\rangle$ then the target qubit is flipped. The operation on the four basis states is as shown,

$$|00\rangle \mapsto |00\rangle \quad |10\rangle \mapsto |11\rangle \quad |01\rangle \mapsto |01\rangle \quad |11\rangle \mapsto |10\rangle .$$

This can be further generalized into,

$$|i\rangle\,|j\rangle \mapsto |i\rangle\,|i \oplus j\rangle\,, \tag{2.9}$$

where $\oplus$ is the binary addition.

This flip arises as a result of the Pauli X operator,

$$\mathrm{C-NOT} = |0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes X,$$

which is why it is also referred to as the control-X gate. Mathematically, the operation on a qubit will be as follows,

$$\begin{aligned}
|0\rangle|0\rangle &\longrightarrow |0\rangle \underbrace{\langle 0|0\rangle}_{\delta_{ij}=1} \otimes \mathbb{I}|0\rangle + |1\rangle \underbrace{\langle 1|0\rangle}_{\delta_{ij}=0} \otimes X|0\rangle \longrightarrow |0\rangle|0\rangle \\
|0\rangle|1\rangle &\longrightarrow |0\rangle \underbrace{\langle 0|0\rangle}_{\delta_{ij}=1} \otimes \mathbb{I}|1\rangle + |1\rangle \underbrace{\langle 1|0\rangle}_{\delta_{ij}=0} \otimes X|1\rangle \longrightarrow |0\rangle|1\rangle \\
|1\rangle|0\rangle &\longrightarrow |0\rangle \underbrace{\langle 0|1\rangle}_{\delta_{ij}=0} \otimes \mathbb{I}|0\rangle + |1\rangle \underbrace{\langle 1|1\rangle}_{\delta_{ij}=1} \otimes X|0\rangle \longrightarrow |1\rangle|1\rangle \\
|1\rangle|1\rangle &\longrightarrow |0\rangle \underbrace{\langle 0|1\rangle}_{\delta_{ij}=0} \otimes \mathbb{I}|1\rangle + |1\rangle \underbrace{\langle 1|1\rangle}_{\delta_{ij}=1} \otimes X|1\rangle \longrightarrow |1\rangle|0\rangle
\end{aligned}$$

The control gate can be similarly defined for the Pauli-Y and Z operators in the following way,

$$\begin{aligned}
\mathrm{Control-Y\ (CY)} &= |0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes Y, \\
\&\ \mathrm{Control-Z\ (CZ)} &= |0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes Z.
\end{aligned}$$

The operation of the CY gate produces a bit-flip like the C-**NOT** with an added phase, e.g.,

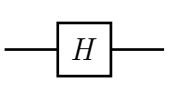
$$\begin{aligned}
|0\rangle|0\rangle &\longrightarrow |0\rangle|0\rangle, \\
|0\rangle|1\rangle &\longrightarrow |0\rangle|1\rangle, \\
|1\rangle|0\rangle &\longrightarrow i|1\rangle|1\rangle, \\
\&\ |1\rangle|1\rangle &\longrightarrow -i|1\rangle|0\rangle.
\end{aligned}$$

The operation of CZ produces a phase-flip, e.g.,

$$\begin{aligned}
|0\rangle|0\rangle &\longrightarrow |0\rangle|0\rangle, \\
|0\rangle|1\rangle &\longrightarrow |0\rangle|1\rangle, \\
|1\rangle|0\rangle &\longrightarrow |1\rangle|1\rangle, \\
\&\ |1\rangle|1\rangle &\longrightarrow -|1\rangle|0\rangle.
\end{aligned}$$

2.4.4 Hadamard Gate

The Hadamard gate or H gate acts on a single qubit and generates an equal superposition state of the basis state it is applied on.



$$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Figure 2.10: H Gate

Its operation is as follows,

$$H\left|0\right\rangle = \frac{1}{\sqrt{2}}(\left|0\right\rangle + \left|1\right\rangle) = \left|+\right\rangle, \quad H\left|1\right\rangle = \frac{1}{\sqrt{2}}(\left|0\right\rangle - \left|1\right\rangle) = \left|-\right\rangle. \tag{2.10}$$

On the Bloch sphere, the action of this gate can be shown with a map of $z \leftrightarrow x$.

2.5 Entanglement

In quantum physics, entanglement is used to refer to a particular type of correlation between quantum particles - for example, between qubits. This correlation is such that, if we have two entangled qubits, their states will depend on each other regardless of their physical space seperation, i.e. measuring the state of one qubit will determine the state of the other. This phenomenon can be both a good or a bad thing depending on the behavior. If, say, we have control over the states of both entangled qubits, it would be a good thing. However, if we can only control the state of one qubit and not the other, it is problematic as it leads to things like decoherence and quantum error correction. We will see this in the later part of this paper when we are dealing with teleportation - due to randomness of measurement outcomes, byproduct operators will arise which needs to be corrected for. Most real world quantum system behave like this.

Let us look at a system of two qubits more closely and try to generate entanglement using a circuit comprising of the C-**NOT** and Hadamard gates.

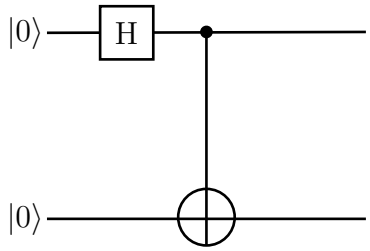


Figure 2.11: Generating Entanglement

We are starting with two qubits in the $\left|0\right\rangle$ state, feeding one to the C-**NOT** gate via the Hadamard gate, and the other to the C-**NOT** gate directly. We know from Eqn.2.10 that the action of the Hadamard gate on $\left|0\right\rangle$ will be,

$$\begin{aligned} H\left|0\right\rangle &= \left(\frac{1}{\sqrt{2}}(\left|0\right\rangle + \left|1\right\rangle)\right)\left|0\right\rangle \\ &= \frac{1}{\sqrt{2}}(\left|0\right\rangle\left|0\right\rangle + \left|1\right\rangle\left|0\right\rangle) \\ &= \frac{1}{\sqrt{2}}(\left|00\right\rangle + \left|10\right\rangle). \end{aligned}$$

So now, we can see that when $\left|00\right\rangle$ goes through the control qubit ($\bullet$), the $\left|0\right\rangle$ going through the target qubit ($\bigoplus$) will remain unchanged. And when $\left|10\right\rangle$ goes through

the control qubit, the $|0\rangle$ going through the target qubit will flip to $|1\rangle$. This will yield us the state,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{2.11}$$

The state we got from this circuit is the Bell state $|\beta_{00}\rangle$. We have already defined in an earlier section that this state is maximally entangled. So why do we call it entangled, and what does the term "maximal" mean in this context?

If we try to assign any particular state to either of the two qubits, i.e., take any state $|0\rangle$ or $|1\rangle$ and try to factor it out of eqn.2.11, we can clearly see that it is not possible to do so. Such states are called non-separable and hence entangled. A seperable state would be something like,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |01\rangle) = \frac{1}{\sqrt{2}}\,|0\rangle\,(|0\rangle + |1\rangle).$$

We could easily factor out (seperate) the $|0\rangle$ state, giving a tensor product between $|0\rangle$ and the equally likely superposition of $|0\rangle + |1\rangle$.

Again, we can see that the qubit configurations $|00\rangle$ and $|11\rangle$ both have a probability amplitude $\frac{1}{\sqrt{2}}$. We know from the Born rule that the sum of probabilities of all states in a system must be equal to 1. Since the qubits in this system also follow this rule, we can intuitively see that each state having the same probability amplitude means that the total probability is evenly distributed $(50:50)$, i.e., each state is completely dependent on the other (measurement of the state of one qubit would give the state for the other). If the distribution of probability were not so even, the state would still be entangled, but not maximally. When more than two states are involved, this becomes more apparent as not having an even probability distribution would create more randomness in measurement outcomes, so we would not necessarily be able to fully measure the other states just by measuring one of them. And the more skewed this probability distribution gets, the lower and lower the entanglement would get, eventually leading to no entanglement when the probability amplitude of one state goes to 0 and the other goes to 1. This is the significance of calling eqn.2.11 maximally entangled.

Coming back to the circuit in Fig.2.11, if we repeat the experiment with the qubits $|01\rangle$, $|10\rangle$, and $|11\rangle$, we will get the other bell states $|\beta_{01}\rangle$, $|\beta_{10}\rangle$, and $|\beta_{11}\rangle$, respectively.

2.6 Measure of Entanglement & Separability of States

Entanglement is mathematically quantifiable. Under this quantification, two or more states in a composite system can be split into three categories, which carries

information about how they decompose or fail to. The categories are:

1. Separable,
2. Entangled, and
3. Maximally Entangled.

Before we go into how we define these categories, we need to take a look at how we can quantify entanglement. We will focus on pure states as there is no exact way to quantify how entangled a mixed state is.

So let us start with some pure state $|\psi_{AB}\rangle$ which contains two qubits A and B, and is in a 4-dimensional $\mathcal{H}$-space,

$$\mathrm{Dim}(\mathcal{H}^{|A\rangle\otimes|B\rangle}) = 4,$$

since each qubit is in a $\mathcal{H}$-space of 2-dimensions. We can define the following density operator to describe the state,

$$\rho_{AB} = |\psi_{AB}\rangle \langle\psi_{AB}| .$$

We then do a partial trace for any one of the qubits,

$$\rho_A = \mathrm{Tr}_B(\rho_{AB}) \quad \text{or} \quad \rho_B = \mathrm{Tr}_A(\rho_{AB}).$$

Then we check the purity of either one of the qubits,

$$\mathrm{Tr}(\rho_A^2) \quad \text{or} \quad \mathrm{Tr}(\rho_B^2).$$

This will give us some value,

$$\frac{1}{\mathrm{Dim}(\mathcal{H}^{|A\rangle})} \text{ or } \frac{1}{\mathrm{Dim}(\mathcal{H}^{|B\rangle})} \leq \mathrm{Tr}(\rho^2) \leq 1.$$

This result can then be interpreted in the following ways:

- $\mathrm{Tr}(\rho^2) = 1$:

  The reduced states of $|\psi_{AB}\rangle$ are pure, which implies that there are no quantum correlations and the state is **separable**,

  $$|\psi_{AB}\rangle = |A\rangle \otimes |B\rangle .$$

  We can also say that $|\psi_{AB}\rangle$ can be expressed as a product of its reduced states.

- $\frac{1}{\mathrm{Dim}(\mathcal{H}^{|A\rangle})}$ or $\frac{1}{\mathrm{Dim}(\mathcal{H}^{|B\rangle})} < \mathrm{Tr}(\rho^2) < 1$:

  This implies that the reduced states of $|\psi_{AB}\rangle$ are in some probabilistic mixture, that is, there is some quantum correlation. As a result, it is not possible to express it as a simple product of reduced states - we call this an **entangled** state.

- $\mathrm{Tr}(\rho^2) = \frac{1}{\mathrm{Dim}(\mathcal{H}^{|A\rangle})}$ or $\frac{1}{\mathrm{Dim}(\mathcal{H}^{|B\rangle})}$:

  This tells us that the reduced states of $|\psi_{AB}\rangle$ are as mixed as they can be, which means that there is a very strong quantum correlation between them. We call this a **maximally entangled** state.

Chapter 3

Cloning, Teleportation & Spin-Chains

Continuing from the last chapter where we discussed entanglement, now we will build up on it and study the interactions in multi-particle systems. We will start with a look at cloning which is a common misinterpretation that arises from preconceived notions of classical computation. Then we will move on to quantum teleportation where entanglement plays a heavy role. From that, we will move on to spin-chains which deal with very large quantum systems. There we will see the complications that arise from having large multi-particle systems. This will serve as a gateway to the next chapter where we will discuss very specific algebras that help us deal with these complications. For this chapter the resources used were mostly well documented articles like [14], [7], [5], [4], [11], popular lecture material [28], and a pre-print book [25].

3.1 Quantum Cloning[25]

When applying the gates discussed above, under certain configurations, it may look like the original qubit we start with is being cloned. For example, if we fix the basis state $|0\rangle$ as input to the target qubit as shown in the following diagram,

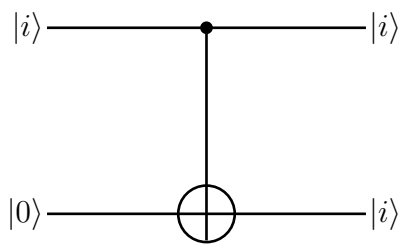


Figure 3.1: C-**NOT** circuit setup that seems to clone qubits

it will look like, for whatever qubit we input to the control qubit, it will get cloned

and we will have two of them,

$$|i\rangle\,|0\rangle \longrightarrow |i\rangle\,|i\rangle\,.$$

However, we can very easily see that this illusion of cloning falls apart when we input anything a little more complicated than the basis states. Let us take the following superposition of states and run it through the circuit in Fig.3.1,

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle\,.$$

On the LHS of the circuit we will have,

$$\begin{aligned}
&|\psi\rangle\,|0\rangle \\
&= (\alpha\,|0\rangle + \beta\,|1\rangle)\,|0\rangle \\
&= \alpha\,|00\rangle + \beta\,|10\rangle \\
&= \alpha\,|00\rangle + \beta\,|11\rangle\,.
\end{aligned}$$

And on the RHS of the circuit we will have,

$$\begin{aligned}
&|\psi\rangle\,|\psi\rangle \\
&= (\alpha\,|0\rangle + \beta\,|1\rangle)(\alpha\,|0\rangle + \beta\,|1\rangle) \\
&= \alpha^2\,|00\rangle + \alpha\beta\,|01\rangle + \beta\alpha\,|10\rangle + \beta^2\,|11\rangle\,.
\end{aligned}$$

It should be very clear by now that the C-**NOT** gate is not capable of doing any kind of cloning. In this case, it only generated some entanglement. Although this was a very specific example, it can be shown that regardless of what approach we take, it is impossible to do anything that can be called quantum cloning, except maybe creating the illusion of it.

3.2 Shared Randomness[25]

Let us again look at two observers, A and B, who are very far apart. And let us give them some qubit pairs from some maximally entangled state,

$$|\Omega\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

As shown in Fig.3.2, when A performs a measurement and determines the state of the qubit it is observing, we know B will observe the same state in its qubit, i.e., if A observes $|0\rangle$ B will also observe $|0\rangle$, and if A observes $|1\rangle$ B will also observe $|1\rangle$. This is due to the phenomenon known as quantum collapse which was discussed near the beginning of this chapter - by performing a measurement the observer causes the superposition to collapse into the state that was observed first.

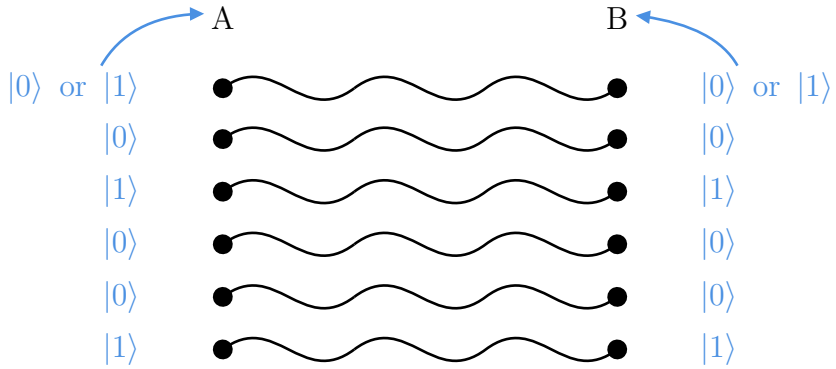


Figure 3.2: Qubit Pairs

This simplification may create the misconception that A can influence its measurement outcome. It also looks like A is using this "prior knowledge" of its measurement outcomes and instantly communicating it with B. However, neither is possible, as A only knows the probability of the state collapsing into either $|0\rangle$ or $|1\rangle$ and cannot influence it, meaning it does not have any "prior knowledge" that it can communicate to B. In actuality, both observers get a random probabilistic outcome from measurement, i.e., A, the moment it decides to take a measurement, is generating a perfectly correlated pair with B that is randomly chosen to be either $|0\rangle$ or $|1\rangle$.

While this lack of control of measurement outcomes and inability to predetermine bit values is a challenge, the ability of entangled qubits to generate this shared randomness at two very distant locations is quite useful!

3.3 What is Quantum Teleportation?[25]

Quantum teleportation is the name given to the method where a state can be transported from one observer to another by the classical transfer of quantum information rather than physically transporting the state itself. For a more technical look at this method, we can look at the following scenario.

Let us take two observers, A and B as shown in the figure. They share two qubits (2 and 3) with the maximally entangled state $|\Omega\rangle$. Now, let us bring the state $|\psi\rangle$ (qubit 1), over to observer A. And let us also assume that A does not really know about the state $|\psi\rangle$, rather, it just knows about qubit 1 and would like to somehow send it over to B. However, A cannot physically send over the qubit to B.

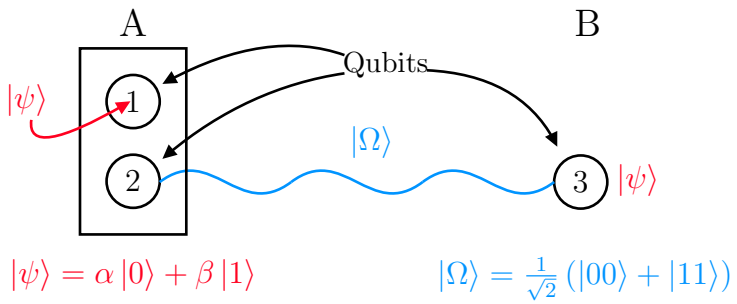


Figure 3.3: Quantum Teleportation

This is where we can apply the method called Quantum Teleportation. What A will do now, is take both the qubits it has (1 and 2) and perform a Bell measurement on it using quantum collapse. This will give 4 possible outcomes. A will now communicate the information of these outcomes to B using some classical communication channel. To clean up the byproduct operator which arises from measurement, B will then apply some unitary operation on its qubit (3) with the information it received from A, leading to the reconstruction of the state $|\psi\rangle$. The algebra can be shown as follows,

$$
\begin{aligned}
|\psi\rangle|\Omega\rangle =& (\alpha|0\rangle + \beta|1\rangle)\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\
=& \underbrace{\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)(\alpha|0\rangle + \beta|1\rangle)}_{\mathbb{I}} + \underbrace{\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)(\alpha|0\rangle - \beta|1\rangle)}_{Z} \\
&+ \underbrace{\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)(\alpha|1\rangle + \beta|0\rangle)}_{X} + \underbrace{\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)(\alpha|1\rangle - \beta|0\rangle)}_{XZ}.
\end{aligned}
$$

The first term here is unchanged from before, so we can put the identity operator $\mathbb{I}$ there which leaves everything unchanged. The second term has had its sign flipped, so we can apply the sigma operator Z. The the third term has had its bits flipped, so we apply the bit flip operation X over there. And finally, for the fourth term, we can see both a sign change and a bit flip, so we apply both Z and X. We can further illustrate this using the following graphical representation of the quantum circuit,

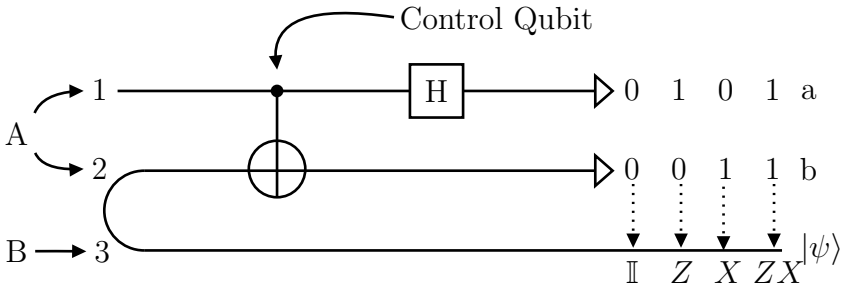


Figure 3.4: Quantum Teleportation Circuit

So in summary, we are destroying qubit 1 while A does the Bell measurement by utilizing the Hadamard and C-Not gates as shown in Fig.3.4, which is just a unitary transformation.This gives A the information on state $|\psi\rangle$ which is then transferred via some classical medium to B, who then reconstructs $|\psi\rangle$ at qubit 3 by reverting the unitary transformation, essentially performing a teleportation.

3.4 Spin Chains

3.4.1 What is Spin?

Quantum particles have an intrinsic quantity known as spin. We call it intrinsic because there are no classical analogs of it. Rather, it is an inherent property of quantum particles. We describe it in terms of the spin operator,

$$S = (S_x, S_y, S_z)\,,$$

and satisfies the following angular momentum commutation relation,

$$[S_i, S_j] = i\hbar\epsilon_{isk}S_k.$$

We also define the following for S:

1. Total spin magnitude of a system,

$$S^2 = S_x^2 + S_y^2 + S_z^2.$$

2. Eigenvalues,

$$\begin{aligned} S^2\,|s,m\rangle &= \hbar^2 s(s+1)\,|s,m\rangle\,, \\ \&\quad S_z\,|s,m\rangle &= \hbar m\,|s,m\rangle\,. \end{aligned}$$

   Here $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ is known as the spin quantum number(which is a fixed value depending on the particle), and $m = -s, -s+1, \ldots, s$ is the magnetic quantum number. These are both eigenvalues of the corresponding eigenvectors $|s\rangle$ and $|m\rangle$.

This spin exists in some Hilbert space $\mathcal{H}$ of dimension,

$$\mathrm{Dim}(\mathcal{H}) = 2s + 1.$$

For a spin-$\frac{1}{2}$ particle, this total spin magnitude can be also expressed using σ^2 which is the sum of the Pauli spin matrices, or the generator of SU(2) times the identity matrix,

$$\sigma^2 = \sum_{a=1}^{3}\sigma_a^2 = \frac{1}{4}\times 3\times\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = s(s+1)\mathbb{I},$$

where σ are the Pauli matrices,

$$\sigma_a = \frac{1}{2}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_x, \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}_y, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_z\right).$$

A possible Hamiltonian with only spin-degree-of-freedom for a single particle can be of the form,

$$H = \mu\sigma_z.$$

This says that if the spin is up, the magnetic moment is μ, and if it is down, the magnetic moment is $-\mu$.

3.4.2 Spin Addition

One of the more important interactions we need to understand for a quantum system is spin addition or coupling - since most quantum systems we deal with involve more than one quantum particle. This is especially true for teleportation and quantum computation.

To understand how coupling works we can define a very simple system involving two spin-$\frac{1}{2}$ particles (electrons) as shown in Fig.3.5,

$$S = S_1 + S_2,$$

where S_1 will have components $(S_{x_1}, S_{y_1}, S_{z_1})$ and S_2 will have components $(S_{x_2}, S_{y_2}, S_{z_2})$. This will let us eventually work out some interaction energy which is responsible for coupling them.

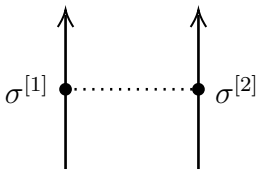


Figure 3.5: Interaction Between 2 Spin-$\frac{1}{2}$'s

Each spin will have two possible states which can be expressed as the superposition,

$$|\psi\rangle = \alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle\,.$$

where up would be a clockwise spinning electron and down would be the converse - spinning counter-clockwise. Therefore, the total system will be described by a 4D Hilbert space,

$$\mathrm{Dim}(\mathcal{H}) = \mathrm{Dim}(\mathcal{H}_1 \otimes \mathcal{H}_2) = \mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4,$$
$$\text{where, } \mathrm{Dim}(\mathcal{H}_1) = \mathrm{Dim}(\mathcal{H}_2) = 2s + 1 = 2\left(\frac{1}{2}\right) + 1 = 2 \text{ or } \mathbb{C}^2.$$

To find the combined spin states of this system we start with the total spin magnitude,

$$\begin{aligned} S^2 &= (S_1 + S_2)^2, \\ &= S_1^2 + S_2^2 + 2S_1 \cdot S_2, \\ &= S_1^2 + S_2^2 + 2(S_{x_1}S_{x_2} + S_{y_1}S_{y_2} + S_{z_1}S_{z_2}), \\ &= S_1^2 + S_2^2 + 2(S_{z_1}S_{z_2}) + S_1^+S_2^- + S_1^-S_2^+. \end{aligned}$$

Here the $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$ operators are known as the raising and lowering operators. Solving for the eigenvalues for the total spin will give us four states, which we group into the singlet state ($S^2 = 0$) and the triplet states ($S^2 = 1$),

$$\begin{aligned} \text{Singlet State } S^2 = 0 : &\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}, \\ \text{Triplet States } S^2 = 1 : &\frac{|\uparrow\uparrow\rangle}{\sqrt{2}}, \frac{|\downarrow\downarrow\rangle}{\sqrt{2}}, \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}. \end{aligned}$$

The interaction between these two spins can be explained by writing the total spin magnitude as,

$$\lambda\left(\sigma^{[1]} + \sigma^{[2]}\right)^2 = \frac{3}{4}\lambda\mathbb{I} \times 2 + 2\lambda\underbrace{\sigma^{[1]} \cdot \sigma^{[2]}}_{\text{spin-spin coupling}}. \tag{3.1}$$

We can express this spin-spin coupling term in Eqn.3.1 as,

$$\begin{aligned} \lambda\sigma^{[1]} \cdot \sigma^{[2]} &= -\frac{3}{4}\lambda\mathbb{I} + \frac{\lambda}{2} \times \begin{cases} 0(0+1) \longrightarrow \text{for the singlet} \\ 1(1+1) \longrightarrow \text{for the triplet} \end{cases} \\ \therefore \lambda\sigma^{[1]} \cdot \sigma^{[2]} &= \frac{\lambda}{4}P_{triplet} - \frac{3\lambda}{4}P_{singlet}. \end{aligned}$$

Here, P are projectors which satisfy,

$$P_{triplet} + P_{singlet} = \mathbb{I}.$$

The λ in Eqn.3.1 are some constants which measure the interaction strength of the coupling - we can call them coupling constants. The value of this constant tells us if there exists any ground state entanglement in the spin chains.

When $\lambda < 0$, the spins like to align. We call such a ground state the ferromagnetic vacuum and it may look something like,

$$|\psi_{GS}\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle \otimes \cdots .$$

A state like this can be factored out into a product, i.e. if we have a chain of L spins, we can break it into two parts, the first part containing n spins, and the second part containing $L - n$ spins, and then express the $|\psi_{GS}\rangle$ as a product of these two parts. This means that $|\psi_{GS}\rangle$ is separable, therefore there is no entanglement.

When $\lambda > 0$, the spins do not want to align. We call a $|\psi_{GS}\rangle$ like this the anti-ferromagnetic vacuum,

$$|\psi_{GS}\rangle = |\uparrow\downarrow\uparrow\downarrow\cdots\rangle + |\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots\rangle + \cdots .$$

This $|\psi_{GS}\rangle$ is a complicated linear combination of singlets, and it can in no way be factored out into some product of states. So it is not separable, meaning there is entanglement in this state.

3.4.3 Chained Spin-Spin Interaction

We can build upon the interaction between two spins in Sec.3.4.2 and form a spin chain, which is a collection of spins that are coupled to both neighboring spins all the way around, forming a chain.

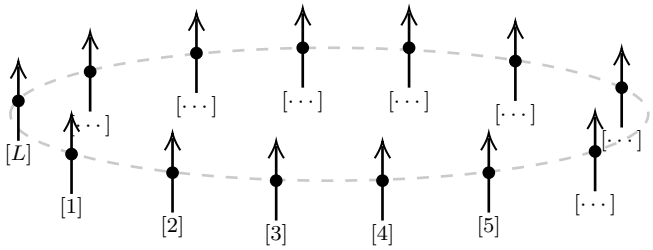


Figure 3.6: Spin Chain

A chain interaction like this is usually called the nearest neighbor interaction and its Hamiltonian, H, will be given by a sum, going from the first spin ($i = 1$) all the way to the last ($i = L$), of some Hamiltonian density, $H_{i,i+1}$, defined by the interaction at each site,

$$H = \sum_{i=1}^{L} H_{i,i+1} \quad \& \quad H_{i,i+1} = \sum_{\tilde{s}} C_{\tilde{s}} P_{\tilde{s}}. \tag{3.2}$$

Here the Hamiltonian density is defined in a way that protects the symmetry of the group we are representing in, and C_j are just some numbers. The example we showed in Sec.3.4.2 dealt with two spin-$\frac{1}{2}$ particles and preserved the symmetry of the SU(2) representation.

The Hamiltonian in Eqn.3.2 hold true for any group G in any representation, provided that they are nearest neighbors and the symmetry of the group is being protected. And we can summarize our example,

$$G = \mathrm{SU}(2),\ s = \mathrm{spin}-\frac{1}{2},\ H = \sum \lambda \sigma^{[i]} \cdot \sigma^{[i+1]}.$$

Another example we can do is the for interaction between spin-1 particles under the

SU(2) representation,

$$G = \mathrm{SU}(2),\ s = \text{spin} - 1,\ \mathrm{Dim}(\mathcal{H}) = (\mathbb{C}^3)^{\otimes L}$$

$$H = \sum_i \left[\sum_{s=0,1,2} C_j P_j^{i,i+1} \right] = a\mathbb{I} + b\left(s^{[i]} \cdot s^{[i+1]}\right) + c\left(s^{[i]} \cdot s^{[i+1]}\right)^2.$$

The constant a is not that important as it just scales all the energies by a fixed amount. What really matters in these expressions are the constants b and c as it lets us express the ratio between the two couplings, $\frac{c}{b}$, which lets us differentiate between different Hamiltonians. We call this ratio λ and it allows us to determine things like, is our vacuum gap or not-gap, etc.

Another thing to take away from all this is that we are working with very large $\mathcal{H}$-spaces! Even in our example which is the simplest of such representations in the smallest group, SU(2), the dimension of our $\mathcal{H}$-space is 2^L. So our spin chain Hamiltonian would be a matrix of dimension $2^L \times 2^L$. This imposes a computational restriction on us - we can only realistically compute systems that have $L \leq 10$. Anything more is just physically impossible to compute.

This latter problem means that questions like, "what is the $|\psi\rangle_{GS}$?" are often open problems - meaning we can not say for certain if they are solvable or not. Some are, like the spin-$\frac{1}{2}$ example we have been discussing throughout this section. However the spin-1 example is only solvable under very specific conditions - in this case, for it to be solvable, we need $b = -c$. Solvable, in this context means two things,

1. the ability to extract various energy levels from these systems, i.e., the ground state energy, the first excited state energy, etc.

2. the ability to compute the expectation value of the energy state of the interaction between two spins at different locations, e.g, $\langle E_{GS}| \sigma_n \cdot \sigma_{n+k} |E_{GS}\rangle$.

We will explore in Sec.4.2 and 4.3, certain algebras that can be used to make these higher dimension systems more solvable with varying degrees of success (Chap.5).

Chapter 4

Tensor Networks & its Formalisms

We saw in the previous chapter that as the number of particles in a quantum system increases, the computational complexity increases more than exponentially. Dealing with this complexity using traditional means (like the Schrödinger Equation) becomes almost impossible for systems with 10 particles or more. To circumvent this complexity, in this chapter we will explore an algebra called tensor networks and its different formalisms. These algebra inherently contain the capability to efficiently deal with low-entanglement many-body systems. We will explore how the different formalisms (MPS and SIMPS) deal with symmetries, boundary conditions, etc. and help with the efficient computation of observables. This will set the stage for the next chapter where we will discuss how the SIMPS formalism is more suitable to compute systems with certain symmetries. The sources used for this chapter were [20], [13], [18], [22].

4.1 What are Tensor Networks?

It is a generally accepted fact that as the number of particles in a quantum system increases, it becomes more than exponentially complex and difficult to solve, and once a system crosses ten particles it becomes impossible to solve it with current computational technology. This is due to the increasing number of entanglements and hence possibilities that arise with an increase in the number of particles. However, this complexity is somewhat of an illusion as nature does not explore all possibilities. In real systems, ground states have low entanglement, so it should not be too difficult to solve such a system if we can account for this. Tensor networks are a language that lets us do just that - it lets us directly work with the states that have low entanglement, something we cannot do with regular quantum mechanics.

There are many different kinds of TNs depending on the different geometries of

entanglement. They are generally expressed as,

$$|\psi\rangle = \sum_{n_1 n_2 n_3} \overbrace{\psi^{n_1 n_2 n_3}}^{\text{set of amplitides}} \underbrace{|n_1 n_2 n_3\rangle}_{\text{basis states}}.$$

Here, a wave function is represented by tensors that do not have any fancy mathematical properties attached to them. They are simply mathematical objects with several indices. They can be visualized graphically as shown below.

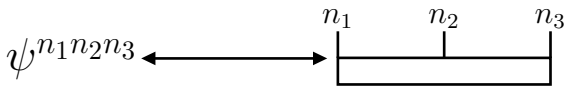


Figure 4.1: Graphical representation of a TN

And operators are expressed as a set of amplitudes in a set of basis states,

$$O = \sum_{nn'} O^{n_1 n_2 n_3}_{n'_1 n'_2 n'_3} |n_1 n_2 n_3\rangle \langle n'_1 n'_2 n'_3|$$

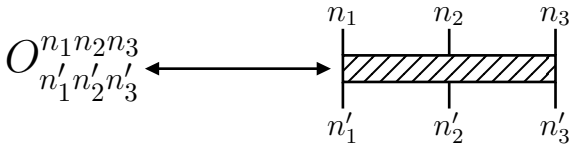


Figure 4.2: Graphical representation of an operator as a TN

Some Example Operations

1.

$$\langle\psi|\phi\rangle = \textstyle\sum_n \psi_{n_1 n_2 n_3} \phi^{n_1 n_2 n_3}$$

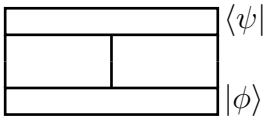


Figure 4.3: Inner Product of Two States

2.

$$\langle\psi| O |\psi\rangle = \textstyle\sum_{nn'} \psi_{n_1 n_2 n_3} O^{n_1 n_2 n_3}_{n'_1 n'_2 n'_3} \psi^{n_1 n_2 n_3}$$

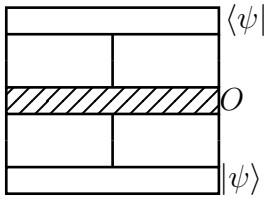


Figure 4.4: Expectation Value of An Operator

Going forward, we will be using these tools to deal with spin systems. Therefore, we will make some changes to the notation to make things less confusing. We will

be using i_N instead of n_i to represent our basis vectors as our basis will now be formed with spins. We will be using C instead of ψ to write out the amplitudes so as to not mix it up with the state $|\psi\rangle$. And finally we will be using A instead of O to represent operators as from here on their significance as matrices will be more important to us.

4.2 MPS Formalism

MPS are the simplest and most popular form of TN states as they are very useful when trying to simulate 1D many-body systems in quantum mechanics. They are a 1D array of tensors where there is one tensor per site in a many-body system. If we have a state,

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_N} c_{i_1,i_2,\ldots,i_N} |i_1, i_2, \ldots, i_N\rangle ,$$

The corresponding MPS will be written as a product of matrices,

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_N} A^{[1]}_{i_1} A^{[2]}_{i_2} A^{[3]}_{i_3} \ldots A^{[N-1]}_{i_{N-1}} A^{[N]}_{i_N} |i_1, i_2, \ldots, i_N\rangle . \tag{4.1}$$

And the graphical representation of MPS is as shown,

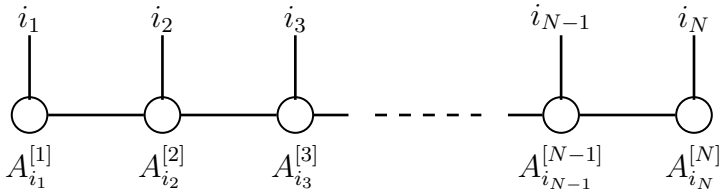


Figure 4.5: Graphical representation of a MPS

A few things to note here:

1. The summed over indices represent entanglement between sites. These are represented by the lines in Fig.4.5. Depending on the context, they might be called bonds (as in chemical bonds), auxiliary dimensions, etc. However, they all mean the same thing.

2. In addition to the first and last A, which are vectors, the rest are square matrices - this depends on the boundary conditions which we will see in the next section.

3. The upper index $[k]$ is used to denote the site number (there can be different A at each site).

4. For a given state, A are not unique, as they can be replaced by some invertible matrix X s.t. $A^{[k]}A^{[k+1]} \to (A^{[k]}X)(X^{-1}A^{[k+1]})$. This will be explored further in the normalization and canonical forms section.

4.2.1 Boundary Conditions

If we take a system with N qubits, the general wavefunction will be,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} c_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle \,. \tag{4.2}$$

When we use the MPS formalism, we rewrite the coefficients $c_{i_1 \ldots i_N}$ as a product of matrices,

$$c_{i_1 \ldots i_N} = A^{[1]}_{i_1} A^{[2]}_{i_2} \ldots A^{[N]}_{i_N},$$

where each $A^{[k]}_{i_k}$ is a $\mathbb{C}^{D_{k-1} \times D_k}$ matrix, D_k being the bond dimension at site k. So the wavefunction written as a MPS will look like,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} A^{[1]}_{i_1} A^{[2]}_{i_2} \ldots A^{[N]}_{i_N} |i_1 i_2 \ldots i_N\rangle \,.$$

In this context, boundary conditions describe how the ends of these 1D systems are treated. For this system with N qubits, which is just a chain of N qubits, the boundary conditions tell us if the ends of the chain are connected or disconnected. This information has both physical and mathematical significance.

Open Boundary Conditions (OBC)

When the ends of the qubit chain are disconnected, we call it an open boundary condition (OBC) — this chain has a natural start and end. So the wavefunction we just saw in Eqn.4.2 would have the following MPS form,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} A^{[1]}_{i_1} A^{[2]}_{i_2} \ldots A^{[N]}_{i_N} |i_1 i_2 \ldots i_N\rangle \,, \tag{4.3}$$

which would have the following matrices:

- $A^{[1]}_{i_1} \in \mathbb{C}^{1 \times D_1}$ {A row matrix},
- $A^{[k]}_{i_k} \in \mathbb{C}^{D_{k-1} \times D_k}$ {A square matrix},
- $A^{[N]}_{i_N} \in \mathbb{C}^{D_{N-1} \times 1}$ {A column matrix}.

This means that the product of all these matrices would be a scalar — which is what we started with ($c_{i_1 \ldots i_N}$). This would be represented by the following diagram:

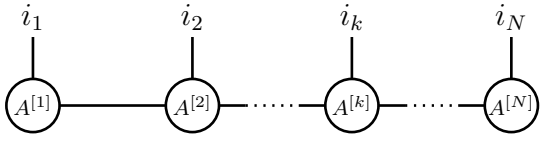


Figure 4.6: MPS Under OBC

Here, each node is a tensor $A^{[k]}$ with one physical leg i_k and two virtual legs (called bonds) — except for the first and last tensors, which will only have one virtual leg each.

Periodic Boundary Condition (PBC)

When the first and last qubit of our chain is also connected, i.e., the chain is a loop, it is called a periodic boundary condition (PBC). In such cases, the wavefunction written as a MPS will have the following form,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{Tr}\left(A^{[1]}_{i_1} A^{[2]}_{i_2} \ldots A^{[N]}_{i_N}\right) |i_1 i_2 \ldots i_N\rangle \,. \tag{4.4}$$

Here, every matrix would be a square matrix of the form $A^{[k]}_{i_k} \in \mathbb{C}^{D_{k-1}\times D_k}$. The graphical representation for it would be the following:

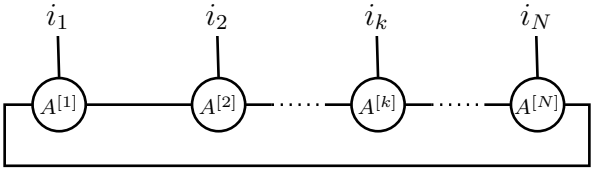


Figure 4.7: MPS Under PBC

In this case, every node $A^{[k]}$ will have one physical leg and two virtual legs (bonds).

The important distinction to make note of here is that, unlike in OBC where the product of the matrices (representing the expectation value of a state) is a scalar quantity, for PBC the product will be a $\mathbb{C}^{D_{k-1}\times D_k}$ matrix. To extract the expectation value from this, we need to perform a trace on the product matrix. This distinction is why Eqn.4.4 is just Eqn.4.3 with a trace added to it.

A Small Example

Let us consider a spin chain with 3 qubits, where each qubit has states $|0\rangle$ and $|1\rangle$, and bond dimension $D_k = 2$.

If it were under OBC, we would have the following:

$$A^{[1]}_{i_1} \in \mathbb{C}^{1\times 2}, \quad \text{i.e.} \quad A^{[1]}_0 = [\alpha_1, \alpha_2] \quad \& \quad A^{[1]}_1 = [\alpha_3, \alpha_4],$$
$$A^{[2]}_{i_2} \in \mathbb{C}^{2\times 2}, \quad \text{i.e.} \quad A^{[2]}_0 = \begin{bmatrix} \alpha_5 & \alpha_6 \\ \alpha_7 & \alpha_8 \end{bmatrix} \quad \& \quad A^{[2]}_1 = \begin{bmatrix} \alpha_9 & \alpha_{10} \\ \alpha_{11} & \alpha_{12} \end{bmatrix},$$
$$A^{[3]}_{i_3} \in \mathbb{C}^{2\times 1}, \quad \text{i.e.} \quad A^{[3]}_0 = \begin{bmatrix} \alpha_{13} \\ \alpha_{14} \end{bmatrix} \quad \& \quad A^{[3]}_1 = \begin{bmatrix} \alpha_{15} \\ \alpha_{16} \end{bmatrix},$$

where $\alpha_j \in \mathbb{C}$. The expectation value is given by,

$$c_{i_1 i_2 i_3} = A^{[1]}_{i_1} A^{[2]}_{i_2} A^{[3]}_{i_3}.$$

And if it were under PBC, we would have,

$$A^{[k]}_{i_k} \in \mathbb{C}^{2\times 2}, \quad \text{i.e.} \quad A^{[k]}_0 = \begin{bmatrix} \alpha_1 & \alpha_2 \\ \alpha_3 & \alpha_4 \end{bmatrix} \quad \& \quad A^{[k]}_1 = \begin{bmatrix} \alpha_5 & \alpha_6 \\ \alpha_7 & \alpha_8 \end{bmatrix},$$

for all tensors. So the expectation value is given by,

$$c_{i_1 i_2 i_3} = \mathrm{Tr}\left(A^{[1]}_{i_1} A^{[2]}_{i_2} A^{[3]}_{i_3}\right).$$

4.2.2 Canonical Forms & Normal MPS

MPS are not unique — if we insert some invertible matrix X and its inverse in between the A matrices, the state $|\psi\rangle$ will remain unchanged. Let us take this invertible matrix to be X and its inverse to be X^{-1}, s.t. $XX^{-1} = X^{-1}X = \mathbb{I}$. If we were to insert these X matrices in between the A matrices in Eqn. 4.5, we would observe the following:

$$\begin{aligned} A^{[k]}_{i_k} &= A^{[k]}_{i_k} X, \\ A^{[k+1]}_{i_{k+1}} &= X^{-1} A^{[k+1]}_{i_{k+1}}, \end{aligned} \tag{4.5}$$

which clearly illustrates that performing this operation would leave the state $|\psi\rangle$ unchanged. These X matrices are referred to as *gauge matrices* and have the following graphical representation, as shown in Fig.4.8:

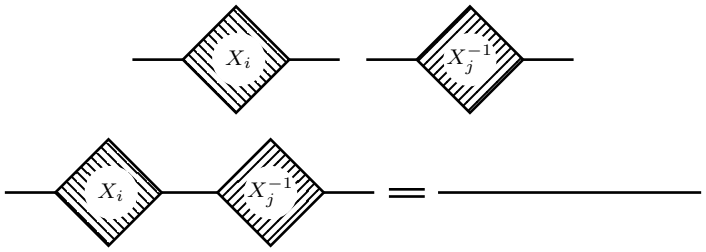


Figure 4.8: Gauge matrices

The figure below illustrates what happens when these matrices are applied to an MPS.

Figure 4.9: Applying gauge matrices to MPS

We can utilize these gauge matrices to give our A matrices nicer mathematical forms which allow us to compute quantities, like the inner product, more efficiently. These forms are referred to as 'normal' or 'canonical'. There are three such forms.

Left-Normalized (Left-Canonical) Form

The left canonical form allows us to maintain orthonormality when contracting the A matrices from left to right. The matrix at each site k needs to maintain the condition,

$$\sum_{i_k} \left(A_{i_k}^{[k]}\right)^\dagger A_{i_k}^{[k]} = \mathbb{I} \tag{4.6}$$

where the identity matrix $\mathbb{I}$ will have dimension D_k, the bond dimension at the right of site k.

Right-Normalized (Right-Canonical) Form

This form allows us to maintain orthonormality when contracting from right to left. Here the matrices at each site need to maintain the condition,

$$\sum_{i_k} A_{i_k}^{[k]} \left(A_{i_k}^{[k]}\right)^\dagger = \mathbb{I} \tag{4.7}$$

Here, the dimension D_k of $\mathbb{I}$ will be the bond dimension at the left of site k.

Mixed-Canonical Form

In this form we leave one A matrix unnormalized, while all the matrices to its left are left-normalized according to Eqn.4.6, and all the matrices to its right are right-normalized according to Eqn.4.7. The unnormalized matrix is denoted by some unique symbol (say Λ) and contains all the entanglement between the left and right parts. We will call this the Schmidt coefficent - shown in more detail in Sec.4.2.3. The wavefunction $|\psi\rangle$, written as an MPS in mixed-canonical form is given by,

$$|\psi\rangle = \sum_{\alpha}^{\chi} \Lambda_\alpha \left|\phi_\alpha^{[L]}\right\rangle \otimes \left|\phi_\alpha^{[R]}\right\rangle$$

where,

$$\begin{aligned}
\left|\phi_\alpha^{[L]}\right\rangle &= \sum_{i_1,\ldots,i_k} L_{i_1}^{[1]} \cdots L_{i_k,\alpha}^{[k]} \left|i_1 \cdots i_k\right\rangle, \\
\left|\phi_\alpha^{[R]}\right\rangle &= \sum_{i_{k+1},\ldots,i_N} R_{i_{k+1},\alpha}^{[k+1]} \cdots R_{i_N}^{[N]} \left|i_{k+1} \cdots i_N\right\rangle,
\end{aligned}$$

and $\alpha = 1, \ldots, \chi$ is the Schmidt index. The Schmidt coefficient and index together tell us how entangled two parts of our system is. If $\Lambda_\alpha = 1$, there is no entanglement. And if $\Lambda_\alpha = \frac{1}{\sqrt{\chi}}$, the two parts are maximally entangled - shown in more detail in Sec.2.6.

Fundamental Theorem of MPS

The interaction of these gauge matrices X with the MPS matrices can be formalized in the following way:

Theorem 1 (Fundamental Theorem of MPS) *If we have the normal matrices A_i and B_i which generate the same MPS, then there exists invertible matrices X that can relate the two via a process called "gauge transformation",*

$$A_i = XB_iX^{-1}.$$

[14]

4.2.3 MPS Algebra

Singular Value Decomposition

SVD is a mathematical technique that factors a matrix into three components enabling better insight into its properties of orthogonality, symmetry, optimization, etc. It is a widely used tool in computation, especially signal and image processing. For physics and mathematics, a related tool called eigenvalue decomposition is more widely used, however, for our purposes in this paper, SVD is the superior tool due to its robustness. To be specific, SVD is not limited to square matrices and does not have any symmetry requirement, properties that are important when dealing with MBQC. We will see these benefits in more detail later. For now we will define it and go into some technical details as it is a necessary tool to derive the MPS for a wavefunction.

Let us say we have some matrix A and we want to find an orthogonal set of vectors v_1 and v_2, which when transformed by A will remain orthogonal. To do this, we could start with a v_1 and v_2 that are orthogonal, and then use some brute force algorithm to map out all their rotations and corresponding transformations after applying A till we find another set of vectors v_1' and v_2' that satisfy our requirement,

$$Av_1 = v_1' \quad \& \quad Av_2 = v_2'.$$

This new set of vectors v_1' and v_2' is what defines the SVD or A - we have factorized A into a set of rotations and a rescaling. If we wanted to repeat this exercise in higher dimensions, the computational complexity would increase significantly with each increase in dimension and at some point become impractical to brute force. So let us find a generalization for higher dimensions.

Starting again, we want,

$$Av_1 = v_1' \quad \& \quad Av_2 = v_2',$$

where v_1 and v_2 are orthogonal and v_1' and v_2' are orthogonal as well. We now split the transformed vectors into some magnitude u and direction σ,

$$Av_1 = \sigma_1 u_1 \quad \& \quad Av_2 = \sigma_2 u_2,$$

where u_1 and u_2 are unit vectors. We can rewrite all this in matrix form as,

$$\begin{aligned} A(v_1\ v_2) &= (\sigma_1 u_1 \quad \sigma_2 u_2), \\ \Rightarrow A(v_1\ v_2) &= (u_1\ u_2)\begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}, \\ \Rightarrow AV &= U\Sigma, \\ \therefore A &= U\Sigma V^\dagger. \end{aligned}$$

Now, instead to having to do some very intensive brute force computation, we just need to solve this matrix equation for a U and V that are orthogonal ($U^\dagger U = \mathbb{I}$ and $V^\dagger V = \mathbb{I}$). Here, the matrix Σ is a diagonal matrix that comprises only positive real numbers called the singular values of A,

$$\Sigma = \begin{pmatrix} \Sigma_1 & & & & & \\ & \ddots & & & & \\ & & \Sigma_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix},$$

where,$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > \lambda_{r+1} = \cdots = \lambda_N = 0$.

To find the values of V and U we just need to compute the eigen-decomposition. For V we do the eigen-decomposition of $A^\dagger A$,

$$\begin{aligned} A^\dagger A &= \left(U\Sigma V^\dagger\right)^\dagger U\Sigma V^\dagger, \\ &= V\Sigma U^\dagger U\Sigma V^\dagger, \{U \text{ is orthogonal}\} \\ &= V\Sigma\Sigma V^\dagger, \{\Sigma \text{ is diagonal}\} \\ \therefore A^\dagger A &= V\Sigma^2 V^\dagger. \end{aligned}$$

And for U we do the eigen-decomposition of $AA^\dagger$,

$$\begin{aligned} AA^\dagger &= U\Sigma V^\dagger \left(U\Sigma V^\dagger\right)^\dagger, \\ &= U\Sigma V^\dagger V\Sigma U^\dagger, \\ &= U\Sigma\Sigma U, \\ \therefore AA^\dagger &= U\Sigma^2 U^\dagger. \end{aligned}$$

The SVD of matrix A can also be expressed as a sum of outer products as,

$$M_{ij} = \sum_k \lambda_k U_{ik} \left(V^\dagger\right)_{kj} = \sum_k \lambda_k u_i^{(k)} v_j^{(k)},$$

where, $u_i^{(k)} = U_{ik}$, $v_i^{(k)} = V_{ik}$, $i = 1, \ldots, m$, $k = 1, \ldots, N$ and $N = \min(m, n)$ are the column vectors of U and V.

Schmidt Decomposition

This is another important tool we need to explore to calculate the MPS of a wavefunction. Let us consider a system with two subsystems $A,\ B$, and their basis states be $|j\rangle_A$ and $|k\rangle_B$ respectively (the basis are orthonormal). We can then express the state as,

$$|\psi\rangle = \sum_{j,k} c_{jk} |j\rangle_A |k\rangle_B .$$

Here, c_{jk} are coefficients which we can regard as a matrix and perform SVD on,

$$c_{jk} = U\Sigma V^\dagger. \quad \{U \text{ and } V \text{ are unitary}\}$$

Rewriting this as a sum of outer products,

$$c_{jk} = \sum_{\alpha=1}^{\chi} \Lambda_\alpha U_{j\alpha} \left(V_{\alpha k}\right)^\dagger .$$

Here χ is the rank of the matrix c_{jk} and is known as the Schmidt-rank. Since U and V are unitary, we can perform the following basis transformations,

$$|A\rangle_\alpha := \sum_j U_{j\alpha} |j\rangle_A \text{ and } |B\rangle_\alpha := \sum_k \left(V^\dagger\right)_{\alpha k} |k\rangle_B .$$

Finally we can express $|\psi\rangle$ in terms of the new basis we just derived,

$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \Lambda_\alpha |A\rangle_\alpha |B\rangle_\alpha .$$

This is the Schmidt decomposition and it always exists for a general state $|\psi\rangle$.

4.2.4 Deriving the MPS

Let us start with some pure state $|\psi\rangle$,

$$|\psi\rangle = \sum_{i_1 \ldots i_N} c_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle .$$

To write it out as a MPS we need to go through the system and perform Schmidt decompositions to each individual site. We start with writing out the c coefficients as a matrix $c_{i_1,(i_2 \ldots i_N)}$, where i_1 is the row index and the rest is the column index. Performing the SVD will give us,

$$c_{i_1,(i_2 \ldots i_N)} = \sum_{\alpha_1=1}^{2} U^{[1]}_{i_1\alpha_1} \Sigma^{[1]}_{\alpha_1} V^\dagger_{\alpha_1(i_2 \ldots i_N)}.$$

The upper index [1] means we are dealing with the first lattice site. The matrix U will be unitary and of dimension (2×2) as i_1 has only two values, $\uparrow$ & $\downarrow$. We

can split this into two (1×2) matrices, $A^{[1]\uparrow}$ and $A^{[1]\downarrow}$ for the corresponding spin components of i_1. We can simplify the indices a little and rewrite,

$$c_{i_1,(i_2 \ldots i_N)} = \sum_{i_1 \ldots i_N} A^{[1]}_{i_1 \alpha_1} \Sigma^{[1]}_{\alpha_1} V^{\dagger}_{\alpha_1 (i_2 \ldots i_N)}.$$

Now we move on to the second site and consider $\Sigma_{\alpha_1} V^{\dagger}_{\alpha_1 (i_2 \ldots i_N)}$ as a matrix with row index $(\alpha_1 i_2)$ and column index $(i_3 \ldots i_N)$ and decompose it further,

$$\Sigma_{\alpha_1} V^{\dagger}_{\alpha_1 (i_2 \ldots i_N)} = \sum_{\alpha_2 = 1}^{4} U^{[2]}_{(\alpha_1 i_2) \alpha_2} \Sigma^{[2]}_{\alpha_2} V^{\dagger}_{\alpha_2 (i_3 \ldots i_N)}.$$

Matrix $U^{[2]}$ will be unitary and have a dimension of (4×4) due to the summation index α_2 having 4 indices (possible combinations of $\alpha_1 = \{1, 2\}$ and $i_2 = \{\uparrow, \downarrow\}$). Again, we split this (4×4) matrix into two (2×4) matrices $A^{[2]\uparrow}$ and $A^{[2]\downarrow}$. Rewriting everything,

$$c_{i_1,(i_2 \ldots i_N)} = \sum_{i_1 \ldots i_N} A^{[1]}_{i_1 \alpha_1} A^{[2]}_{i_2 \alpha_1 \alpha_2} \cdots .$$

After iterating up-to the last site k in a similar manner we will get,

$$|\psi\rangle = \sum_{i_1 \ldots i_N} \sum_{\alpha_1}^{2} \sum_{\alpha_2}^{4} \sum_{\alpha_3}^{8} \ldots U^{[1]}_{i_1 \alpha_1} U^{[2]}_{(\alpha_1 i_2) \alpha_2} \ldots U^{[k]}_{(\alpha_{k-1} i_k) \alpha_k} \Sigma^{[k]}_{\alpha_k} V^{\dagger}_{\alpha_k (i_{k+1} \ldots i_N)} |i_1 \ldots i_N\rangle ,$$

which, when represented using the split matrices A will give us the following MPS,

$$|\psi\rangle = \sum_{i_1 \ldots i_N} \sum_{\{\alpha_i\}} A^{[1]}_{i_1 \alpha_1} A^{[2]}_{i_2 \alpha_1 \alpha_2} A^{[3]}_{i_3 \alpha_2 \alpha_3} \ldots A^{[N-1]}_{i_{N-1} \alpha_{N-2} \alpha_{N-1}} A^{[N] i_N}_{i_N \alpha_{N-1}} |i_1 \ldots\rangle ,$$

as we saw in Eqn.4.1, the graphical representation of which was shown in Fig.4.5.

Example - Expressing the GHZ state as MPS

$$|\mathrm{GHZ}_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$

We can first write out the computational basis in order,

$$|000\rangle , |001\rangle , |010\rangle , |011\rangle , |100\rangle , |101\rangle , |110\rangle , |111\rangle .$$

We can expand out the GHZ state,

$$\begin{aligned} |\psi\rangle &= |\mathrm{GHZ}_3\rangle , \\ &= \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle), \\ &= \frac{1}{\sqrt{2}} |000\rangle + \frac{1}{\sqrt{2}} |111\rangle , \\ &= \frac{1}{\sqrt{2}}[1\ 0\ 0\ 0\ 0\ 0\ 0\ 1]^{\dagger}, \end{aligned}$$

which, as we can see, is an 8-dimensional vector. To be able to perform SVD, we need to reorganize this vector as a matrix of the same dimension. We will go with a 2×4 configuration, as having two rows of elements will make it mathematically easier for us to iteratively strip off qubits site-by-site using SVD. So we group the elements as shown,

- Qubit 1 (site 1), $i_1 \in (0, 1)$ {row index},
- Remaining qubits (sites 2 & 3), $i_2 i_3 \in (00, 01, 10, 11)$ {column index}.

This allows us to construct the following matrix,

$$\psi_{i_1,i_2 i_3} = \begin{bmatrix} \langle 000\rangle & \langle 001\rangle & \langle 010\rangle & \langle 011\rangle \\ \langle 100\rangle & \langle 101\rangle & \langle 110\rangle & \langle 111\rangle \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Now we can apply SVD to the first site,

$$\psi^{[1]} = U^{[1]} \Sigma^{[1]} V^{[1]\dagger}.$$

To find $U^{[1]}$, we will do the following eigen-decomposition,

$$\begin{aligned} \psi^{[1]}\psi^{[1]\dagger} &= U^{[1]}\Sigma^{[1]2}U^{[1]\dagger}, \\ &= \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \\ &= \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}. \end{aligned}$$

For this resulting matrix, we can use the eigenvector equation to find the eigenvalues and eigenvectors. Since the matrix is just an identity matrix with a factor of $\frac{1}{2}$, the calculation is very simple,

$$\begin{aligned} (\psi^{[1]}\psi^{[1]\dagger})X &= \lambda X, \\ \Rightarrow \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} &= \lambda \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}, \\ \Rightarrow \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} &= \lambda \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}, \\ \Rightarrow \frac{1}{2} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} &= \lambda \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}, \\ \therefore \lambda &= \frac{1}{2}. \end{aligned}$$

Furthermore, we know that for an identity matrix, any non-zero vector can be the eigenvector. For our purposes, here we will go with perpendicular unit vectors,

$$X_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \& \quad X_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

This will let us construct the following $U^{[1]}$,

$$U^{[1]} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Now for the $V^{[1]\dagger}$ matrix, we do the following eigen-decomposition,

$$\begin{aligned} \psi^{[1]\dagger}\psi^{[1]} &= V^{[1]}\Sigma^{[1]2}V^{[1]\dagger} \\ &= \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \\ &= \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}. \end{aligned}$$

Solving for the eigenvalues gives us,

$$\lambda = 0 \quad \& \quad \frac{1}{2},$$

and the corresponding eigenvectors,

$$X_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \& \quad X_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \{\text{for } \lambda = 0\},$$

$$X_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \& \quad X_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \{\text{for } \lambda = \frac{1}{2}\}.$$

Since we know unitarity has to be preserved for our calculations, we will only use X_3 and X_4 to form the matrix $V^{[1]}$,

$$V^{[1]} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix},$$

$$\therefore V^{[1]\dagger} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Finally, for our singular value matrix Σ,

$$\Sigma^2 = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix},$$

$$\therefore \Sigma^{[1]^2} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix},$$

$$\Rightarrow \Sigma^{[1]} = \begin{bmatrix} \sqrt{\lambda_1} & 0 \\ 0 & \sqrt{\lambda_2} \end{bmatrix},$$

$$= \begin{bmatrix} \sqrt{\frac{1}{2}} & 0 \\ 0 & \sqrt{\frac{1}{2}} \end{bmatrix},$$

$$\therefore \Sigma^{[1]} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

All of this can be put together for the first site,

$$\psi^{[1]} = U^{[1]}\Sigma^{[1]}V^{[1]\dagger},$$

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

To produce the split matrices for site 1, we take the product $U^{[1]} \times \Sigma^{[1]}$ and define two row matrices $A^{[1]}_{i_1} \in \mathbb{C}^{1\times 2}$, where $i_1 = 0,\ 1$,

$$A^{[1]}_0 = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad \& \quad A^{[1]}_1 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Moving on to site 2, we define,

$$\Sigma^{[1]}V^{[1]\dagger} = \psi^{[2]},$$

$$\therefore \psi^{[2]} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

We will rewrite this as a 2×2 matrix $\psi^{[2]}_{i_2,\beta_2}$,

$$\psi^{[2]} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix},$$

and perform SVD again,

$$\psi^{[2]} = U^{[2]}\Sigma^{[2]}V^{[2]\dagger},$$

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

This time we produce the split matrices for site 2 by defining $A^{[2]}_{i_2} \in \mathbb{C}^{2\times 2}$ where $i_2 = 0,\ 1$,

$$A^{[2]}_0 = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \end{bmatrix} \quad \& \quad A^{[2]}_1 = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Now all that is left is site 3, the split matrices for which can be defined as $A^{[3]}_{i_3} \in \mathbb{C}^{2\times 1}$ where $i_3 = 0,\ 1$,

$$A^{[3]}_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \& \quad A^{[3]}_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Finally we can put all these parts together to express the GHZ state as an MPS,

$$\begin{aligned} |GHZ_3\rangle &= \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \\ &\equiv |\psi\rangle = \sum_{i_1,i_2,i_3=0}^{1} A^{[1]}_{i_1} A^{[2]}_{i_2} A^{[3]}_{i_3} |i_1 i_2 i_3\rangle . \end{aligned}$$

We can show that one can easily go back to the original state just by multiplying the matrices - it will give us the un-normalized expectation value of each configuration the state can be in. When $(i_1, i_2, i_3) = (0, 0, 0)$,

$$A^{[1]}_0 A^{[2]}_0 A^{[3]}_0 = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{2}.$$

And when $(i_1, i_2, i_3) = (1, 1, 1)$,

$$A^{[1]}_1 A^{[2]}_1 A^{[3]}_1 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{2}.$$

When (i_1, i_2, i_3) are any in any other configuration, the corresponding matrix multiplications will all yield 0, meaning the expectation value of the state being in those configurations is zero - just how we defined it in the first place. This allows us to reconstruct the un-normalized GHZ state,

$$|GHZ_3\rangle = \frac{1}{2}|000\rangle + \frac{1}{2}|111\rangle ,$$

which is equivalent to the normalized GHZ state we started with. A little side note here - this system was converted to MPS under OBC.

With some further calculation it is possible to derive a general MPS for a GHZ state of n-qubits,

$$\begin{aligned} |GHZ_n\rangle &= \frac{1}{\sqrt{2}}\left(|0\rangle^{\otimes n} + |1\rangle^{\otimes n}\right), \\ &= \frac{1}{\sqrt{2}}\left(|00\cdots 0\rangle + |11\cdots 1\rangle\right), \\ &= \sum_{i_1\cdots i_n} A^{[1]}_{i_1} A^{[k]}_{i_k} \cdots A^{[n]}_{i_n} |i_1 i_2 \cdots i_n\rangle . \end{aligned}$$

where,

$$A^{[1]}_{i_1} \in \mathbb{C}^{1\times 2},$$
$$A^{[k]}_{i_k} \in \mathbb{C}^{2\times 2},$$
$$A^{[n]}_{i_n} \in \mathbb{C}^{2\times 1}.$$

4.3 Split Index Matrix Product States (SIMPS)

SIMPS are TNs, and they are similar to MPS as they both are matrix product states. The key physical difference between them is that when we calculate the A matrices (tensors) for a MPS, they only carry one index, i.e., the information of one state is carried by one matrix. Meanwhile, when we convert a wavefunction to SIMPS, the matrices will be determined by two neighboring states, i.e., the information of two states will be carried by one matrix. Mathematically, this means that the SIMPS representation is very dependent on the choice of physical basis, which is not something we consider while creating a MPS. Its construction is similar to that of double-line TNs, where a given degree of freedom is shared by more than one tensor in the network. Fig.4.10 is what a SIMPS matrix looks like graphically compared to a MPS matrix.

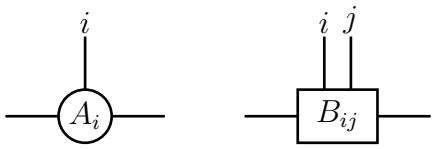


Figure 4.10: SIMPS vs MPS Matrices (Tensors)[26]

Similar to MPS, SIMPS can be defined under both PBC and OBC. Under PBC, we define SIMPS in terms of a trace of a product of matrices, same as MPS,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{Tr}\left(B^{[1]}_{i_1 i_2} B^{[2]}_{i_2 i_3} \cdots B^{[N-1]}_{i_{N-1} i_N} B^{[N]}_{i_N i_1}\right) |i_1 i_2 \cdots i_N\rangle\,. \tag{4.8}$$

Here, B matrix is an $\eta_i \times \eta_j$ matrix, where η is the SIMPS bond dimension. This bond dimension is not the same as D which we used for MPS - we will see why later. Also, we can see from the indices on the B matrix that our system is periodic - the index i_1 is overlapping between the first and last B, signifying that the system is a ring, i.e., periodic. We can represent this graphically using Fig.4.11.

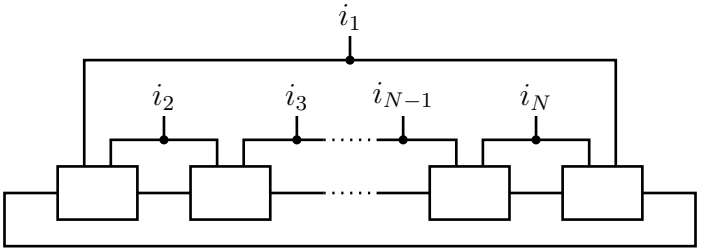


Figure 4.11: SIMPS under PBC

Here, we can see some additional nodes. These are called δ tensors and their purpose is to take a state coming in from the top and copying it left and right, i.e, splitting the index. Fig.4.12 shows what they look like.

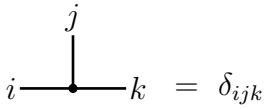


Figure 4.12: δ Tensor

Since each B matrix is connected to two such δ tensors, they are 4-index tensors which take two inputs and puts out a matrix.

Similarly, we can define SIMPS under OBC in the following way,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \sum_{\alpha,\beta} \langle\alpha| B^{[1]}_{i_1 i_2} \cdots B^{[N]}_{i_{N-1} i_N} |\beta\rangle \, |\alpha, i_1 \cdots i_N, \beta\rangle \,. \tag{4.9}$$

Here, α and β are η-dimensional spins and have values $0, \ldots, \eta - 1$. And the lack of overlap between the first and last matrix shows that this system does not form a loop, i.e., open boundaries. The graphical representation will be as shown in Fig.4.13.

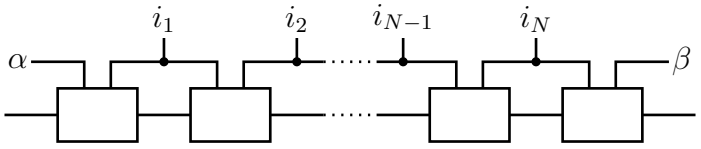


Figure 4.13: SIMPS under OBC

Another thing that we can carry over from MPS to SIMPS is the idea of canonical/normal forms. A SIMPS is defined to be normal when,

$$\text{span}\{B_{s_1 i_1} B_{i_2 i_2} \cdots B_{i_{L_1} s_2}\}_{i_1,\ldots,i_{L_1}} = M_{\eta_{s_1},\eta_{s_2}}.$$

Here $M_{\eta_{s_1},\eta_{s_2}}$ is the space of all $\eta_{s_1} \times \eta_{s_2}$ matrices, and L_1 is a finite length called the injectivity length[27, p3, e6]. When $L_1 = 1$, the SIMPS matrix is injective. And like for MPS, this property is stable - if it is true for some length L, then it will be true for $L + 1$, and by extension all lengths greater than L.

4.3.1 SIMPS Algebra

The SIMPS algebra is just a continuation of MPS algebra and utilizes similar tools as the MPS algebra. Both these representations are fundamentally different only when we have non-full-rank A_i matrices for some basis $\{i\}$.

When we have a standard SIMPS,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{Tr}\left(B^{[1]}_{i_1 i_2} B^{[2]}_{i_2 i_3} \cdots B^{[N]}_{i_N i_1}\right) |i_1 i_2 \cdots i_N\rangle \,,$$

we can convert the B_{ij} matrices to A_i matrices of MPS via SVD. In the case of a SIMPS under PBC, no special preparation is necessary. However, for a SIMPS under OBC, due to the addition of the η-dimensional spins (α and β) at the boundaries, we need to first flatten the B matrix:

$$\mathbb{B} = \sum_{i,j,\alpha,\beta} B^{\alpha\beta}_{ij} \, |i\alpha\rangle \langle j\beta| \,.$$

Now B has a dimension of $\eta \times \eta$ and we can move forward with performing SVD,

$$\mathbb{B} = U \Sigma V^\dagger.$$

Like before, the U matrix will have dimension $\eta \times D$, Σ will be a diagonal matrix with dimension $D \times D$, and V will have dimension $\eta \times D$ as well. The U and V matrices must also follow,

$$U^\dagger U = V^\dagger V = \mathbb{I}.$$

Here, the dimension D is found using,

$$\mathrm{Dim}(D) = \mathrm{Rank}(B).$$

Now we can absorb V into Σ for compactness, defining,

$$W^\dagger = \Sigma V^\dagger.$$

Finally, our corresponding A_i matrix can be expressed as,

$$A_i = W^\dagger (|i\rangle \langle i| \otimes \mathbb{I}) U.$$

Repeating this procedure on every B_{ij} in a SIMPS will give us every A_i matrix we would need to construct the MPS that will give us the same state.

To go from MPS to SIMPS, we may naively claim,

$$A_i = B_{ij}.$$

And, this would be correct for full-rank matrices ($\eta = D$) - we will see why in a bit. However, for non-full-rank A_i matrices, making this generalization would lead to a drop in bond dimension in the SIMPS representation for the same state. To avoid this problem, we write A_i in terms of some projectors,

$$A_i = A_i P_i P_i^\dagger. \tag{4.10}$$

Here $P_i P_i^\dagger$ is a projector onto the domain of A_i [27], and $P_i : \mathbb{C}^{\eta_i} \to \mathbb{C}^D$, where η_i is the rank of A_i, such that, $P_i^\dagger P_i = \mathbb{I}_{\eta_i}$. Now we can define the matrix for the SIMPS representation as,

$$B_{ij} = P_i^\dagger A_j P_j.$$

For a full-rank matrix, $P_i = \mathbb{I}$, this causes the equation to simplify to,

$$B_{ij} = A_i.$$

This whole operation can be shown graphically as in Fig.4.14.

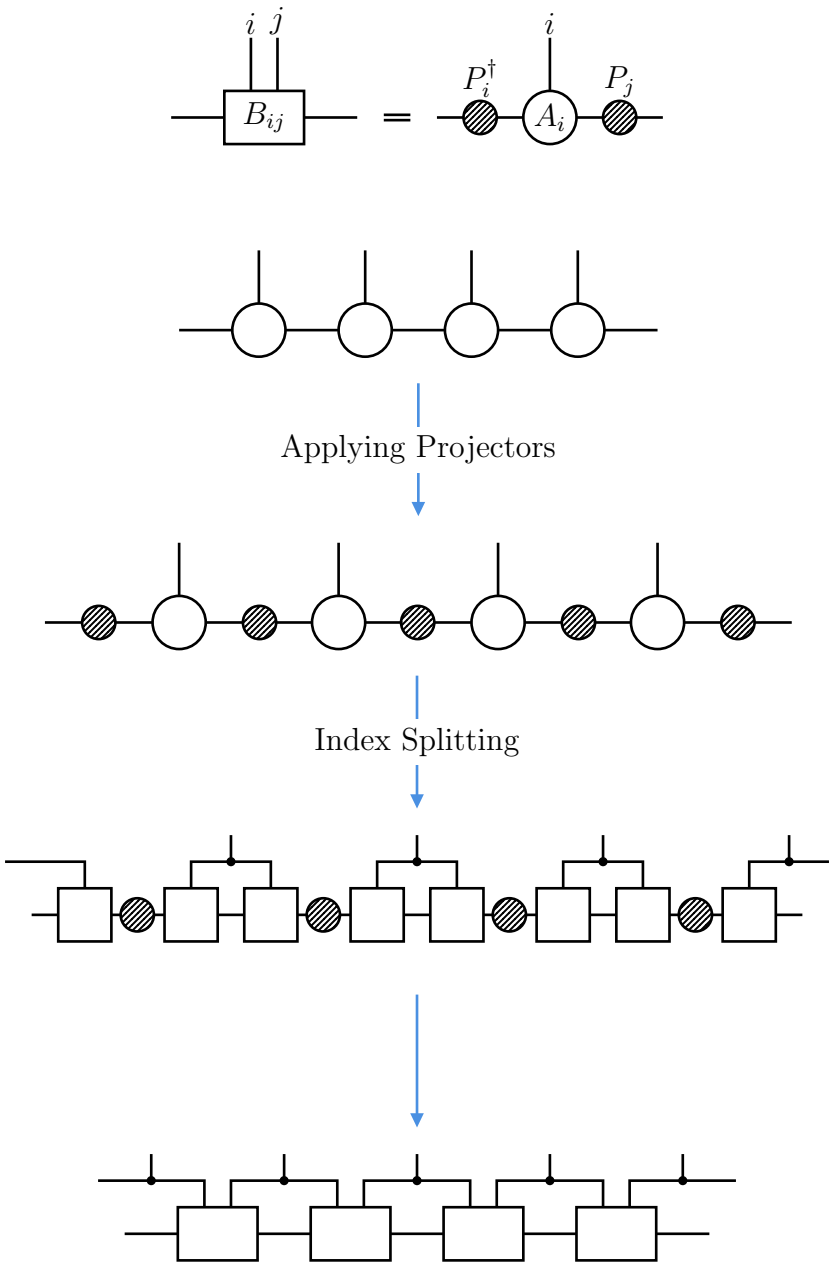


Figure 4.14: MPS to SIMPS Conversion

This means that going from the MPS representation to the SIMPS representation only makes sense when the A matrices of a MPS are non-full-rank, because only then will we have a SIMPS that is distinct from the MPS representation of the state we are working with. This allows us to define the following:

Definition 1 (Good SIMPS[27]) *A normal(canonical) MPS makes for a good SIMPS when the A matrices are non-full-rank for some i.*

In the later sections we will explore some condition like enforcing non-onsite symmetries, which will give us MPS representations that will lead to good SIMPS.

The general MPS to SIMPS conversion we did was an optimal one. This means that

the SIMPS we calculated had the minimal possible bond dimension. This can be declared as the following:

Proposition 1 (Optimal Conversion) *If we have a SIMPS matrix B_{ij} which is normal and has injectivity length L_1, the MPS we calculate from it will have injectivity length $L_0 \leq L_1 + 2$. Similarly, if we have a MPS matrix A_i which is normal and has injectivity length L_0, the SIMPS we calculate from it will have injectivity length $L_1 \leq L_0$.[27]*

4.3.2 Fundamental Theorem of SIMPS

We will now have a look at a fundamental interaction between two normal SIMPS matrices, where, when the SIMPS are injective, gauge transformations can be still used to obtain new tensors generating the same state,

$$B_{ij} \rightarrow X B_{ij} X^{-1}.$$

Similar to what we did with MPS, we can define the following theorem:

Theorem 2 (Fundamental Theorem of SIMPS) *Let us assume C_{ij} and B_{ij} are two normal SIMPS tensors, and they generate the same state for all system sizes. We will then have a set of invertible matrices X_i such that,*

$$C_{ij} = X_i B_{ij} X_j^{-1},$$

where $i = 0, \ldots, d-1$. [27]

The theorem can be represented graphically as in Fig.4.15.

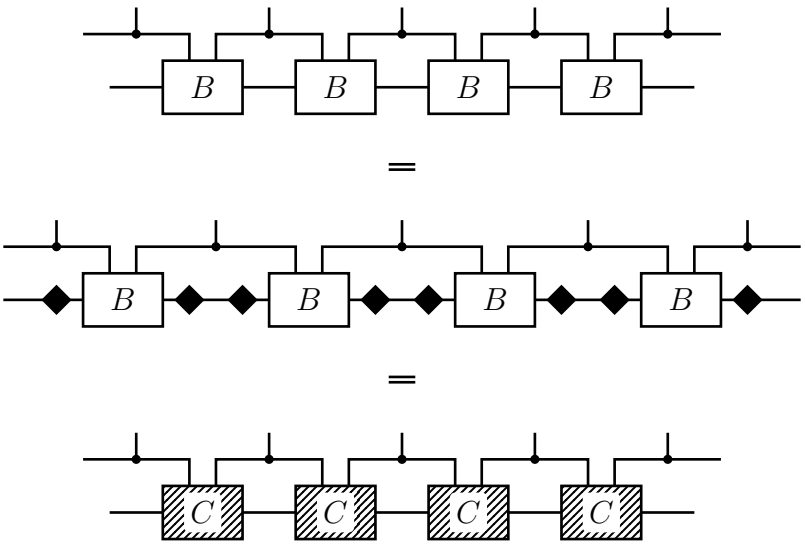


Figure 4.15: Fundamental Theorem of SIMPS[26]

This theorem tells us that the bond dimension of all normal SIMPS representations of a state will be the same for any particular basis of physical spins. So for a

given physical basis, it is well defined to refer to the SIMPS bond dimension. This theorem will be essential to understanding the non-onsite symmetries in SIMPS representations.

Example - Expressing the GHZ state as SIMPS

Now let us revisit the example calculation we did to convert a GHZ state to MPS, and build upon it to express it in the SIMPS representation.

We have seen that the GHZ state,

$$|\mathrm{GHZ}_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle),$$

can be represented using MPS (for PBC) as,

$$|\mathrm{GHZ}_3\rangle = \sum_{i_1,i_2,i_3=0}^{1} A^{[1]}_{i_1} A^{[2]}_{i_2} A^{[3]}_{i_3} |i_1 i_2 i_3\rangle \,.$$

This state gives us a non-normal MPS of bond dimension, $D = 2$. Furthermore, if we analyze the ranks of the MPS matrices, A_i, we will see,

$$\mathrm{Rank}(A_i) = 1.$$

And this will cause A_i to be non-full-rank for some i. As per our definition of the projectors for non-full-rank A_i (Eqn.4.10), the bond dimension for the corresponding SIMPS matrices B_{ij} will be,

$$\mathrm{Dim}(B_{ij}) = \eta = \mathrm{Rank}(A_i) = 1.$$

Therefore, the SIMPS matrices B_{ij} will have dimension 1, which will just be some number that we can express as,

$$B_{ij} = \delta_{ij}.$$

Here, if $i = j$, $B_{ij} = 1$ and if $i \neq j$, $B_{ij} = 0$.

Chapter 5

SIMPS vs MPS for Quantum Teleportation

Now that we have seen what TNs are, and how its different formalisms can be used to represent the same system, and how those representations capture important physical and virtual aspects of the system, we can move on to more focused comparison between the two formalisms. We will focus on two main aspects of quantum systems — symmetry and quantum information transfer (teleportation). The analysis of both these aspects will visualize clearly how the SIMPS formalism is more suitable at handling symmetries of certain phases of matter, and how it is less computationally taxing when dealing with teleportation, while simultaneously being more accurate. This analysis is mostly a review of [27], [24], and [26], supported by some fairly modern papers like [19], [16] and [21], which formalizes some of the recent developments in our understanding of symmetries and entanglement.

5.1 Non-Onsite Symmetries & SPT Phases

We will start our analysis of the two formalisms by seeing how effective they are at describing some physical properties of systems. We will start by introducing the properties (Sec.5.2.2 and Sec.5.1.2), then move on to how it is described by the MPS formalism (Sec.5.1.3), and finally see how the SIMPS formalism better captures the intricacies of these properties (Sec. 5.1.4).

5.1.1 On-Site & Non-Onsite Symmetries

An onsite symmetry U_g acts locally and independently on each site,

$$U_g = \bigotimes_{i=1}^{N} u_g^{[k]},$$

where u_g is a linear, local unitary representation of the group $g \in G$ on the physical indices, for example spin flips and spin rotations. For our purposes, unless otherwise

mentioned, the group G will be always assumed to be abelian. This means that it will be assumed to have some commutative operation in it.

A non-onsite symmetry cannot be expressed as a simple tensor product of unitary operators for each site. This is because, while it resembles linear symmetry on the physical degrees of freedom, it acts projectively on the virtual structure responsible for the entanglement. Therefore to express it we need to bring in entangling operators, non-local structures, etc.

5.1.2 Symmetry Protected Topological (SPT) Phases

A good example of a system that shows non-onsite symmetries are SPT phases. They are a phase of matter that has no low energy excitations (gapped) and short-range entanglements only. This short range entanglement arises from the lack of any kind of intrinsic topological order in this phase of matter. This means that if a system in such a phase were to have its symmetry broken, it would become void of any kind of topological features as it does not have any inherent to it. The name "SPT phase" arises from this fact that the topology of these phases are held together by the symmetry of the system.

If the symmetry is broken the ground state would be deformed to a trivial product state. In other words, a system in SPT phase preserves or "orders" itself under symmetry constraints - known as SPT order. Mathematically, this means that SPT phases preserves the global symmetry G by fulfilling,

$$[H, U_g] = 0 \; \forall g \in G \quad \text{and} \quad U_g \left|\psi\right\rangle = \left|\psi\right\rangle .$$

Therefore, the system is forced to be symmetric by making sure its evolution is not arbitrary - the entanglements, correlations, etc. must be controlled during evolution to respect symmetry.

Another thing to make note of here would be that while we are enforcing symmetry, we cannot make the general claim of there being any degeneracy. It is true that if we have some Hamiltonian that respects the symmetry, there will be some boundary degeneracy (near the edges).

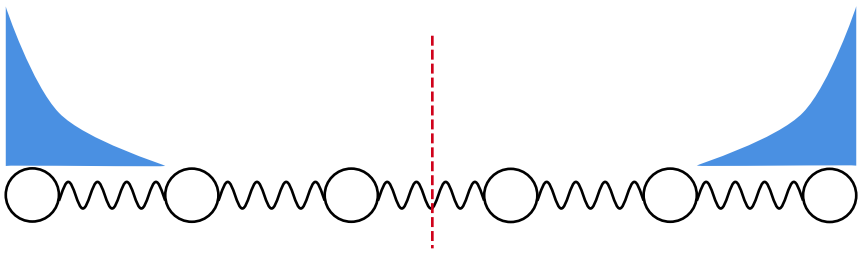


Figure 5.1: Boundary Degeneracy[26]

However, there will be no entanglement spectrum degeneracy, i.e., if we cut our state in half and compute the reduced density matrix, the eigenvalues will not be two-fold degenerate.

5.1.3 Using MPS to Represent Systems in SPT Phases

Now let us look at how we can use MPS to represent systems in SPT phases and their symmetries. Let us start with a symmetrically invariant MPS under PBC for some state $|\psi\rangle$,

$$|\psi\rangle = \sum_{i_1,\cdots,i_N} \mathrm{Tr}(A_{i_1}^{[k]} \cdots A_{i_N}^{[k]}) \, |i_1 \cdots i_N\rangle \, .$$

And let us say that it has some global onsite symmetry of the form,

$$u_g^{\otimes N} \, |\psi\rangle = |\bar{\psi}\rangle = \sum_{i_1,\cdots,i_N} \mathrm{Tr}(\bar{A}_{i_1}^{[k]} \cdots \bar{A}_{i_N}^{[k]}) \, |i_1 \cdots i_N\rangle \, .$$

To show the local symmetry at each site k we will use the relation,

$$\bar{A}_i^{[k]} := \sum_j (u_g)_{ij} A_j = V_g A_i V_g^\dagger, \tag{5.1}$$

where V_g are virtual, unitary matrices and $(u_g)_{ij} = \langle i| \, u_g \, |j\rangle$ is the local unitary representation of whatever group we are in on the physical indices. Through some very trivial algebra [27, p5, e23] we can show,

$$\begin{aligned} |\bar{\psi}\rangle &= \sum_{i_1,\cdots,i_N} \mathrm{Tr}(\bar{A}_{i_1}^{[k]} \cdots \bar{A}_{i_N}^{[k]}) \, |i_1 \cdots i_N\rangle \, , \\ &= \sum_{i_1,\cdots,i_N} \mathrm{Tr}(A_{i_1}^{[k]} \cdots A_{i_N}^{[k]}) \, |i_1 \cdots i_N\rangle \, , \\ &= |\psi\rangle \, . \end{aligned}$$

This can be also replicated for a MPS under OBS as long as Eqn.5.1 is satisfied.

Now if we had a representation of group G formed by a set of u_g such that,

$$u_g u_h = u_{gh},$$

the virtual operators V_g will form a projective representation,

$$V_g V_h = \omega(g,h) V_{gh},$$

where $\omega(g,h)$ are some phase factors. Due to G being abelian, we can rewrite this expression as,

$$V_g V_h = \Omega(g,h) V_h V_g,$$

where $\Omega(g,h) = \omega(g,h)\omega(h,g)^{-1}$. These Ω will represent the SPT phase to which the MPS belongs, and if they all are equal to 1 the phase it belongs to will be trivial and thus have no symmetry. If they all are not equal to 1, the phase will be non-trivial, which would imply that the system has a symmetry protected degeneracy.

An example of a state that belongs to a non-trivial SPT phase is the cluster state generated by,

$$X_A = \prod_{i=1}^{\frac{N}{2}} X_{2i} \quad \text{and} \quad X_B = \prod_{i=1}^{\frac{N}{2}} X_{2i+1}.$$

It is symmetric under a $Z_2 \times Z_2$ symmetry and has the following MPS matrices,

$$\begin{aligned} A_{++} &:= A^+A^+ = \mathbb{I}, \\ A_{+-} &:= A^+A^- = \mathbb{Z}, \\ A_{-+} &:= A^-A^+ = \mathbb{X}, \\ A_{--} &:= A^-A^- = \mathbb{Z}\mathbb{X}. \end{aligned}$$

Under the symmetry constraints, the MPS matrices will be,

$$\sum_{ij} [XI]_{ij,i'j'} A_{i'j'} = ZA_{ij}Z \quad \text{and} \quad \sum_{ij} [IX]_{ij,i'j'} A_{i'j'} = XA_{ij}X.$$

Here, Z and X will not commute, giving us a non-trivial SPT.

5.1.4 Using SIMPS to Represent Systems in SPT Phases

We had seen in Sec.4.3 that the SIMPS formalism for MPS is more desirable, in particular for cases when the MPS matrices are non-full-rank (Def.1). Now we shall explore why exactly SIMPS are better suited than MPS for such cases.

Let us start by defining a non-onsite symmetry operator,

$$\mathcal{U} = \prod_{i=1}^{N} U_{i,i+1},$$

where $U|ij\rangle = e^{i\varphi_{ij}}|ij\rangle$ is a two-body unitary gate for some phases $e^{i\varphi_{ij}}$, and U is also diagonal in the physical basis of the SIMPS. As mentioned in Sec.5.1.1 we are changing up the notations here as the symmetry operator cannot be expressed in terms of simple tensor products anymore.

Now let us define our SIMPS,

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{Tr}\left(B^{[k]}_{i_1 i_2} \cdots B^{[k]}_{i_N i_1}\right) |i_1 \cdots i_N\rangle,$$

which under the symmetry operator $\mathcal{U}$ will be,

$$\mathcal{U}\left|\psi\right\rangle = \left|\tilde{\psi}\right\rangle = \sum_{i_1,\ldots,i_N} \mathrm{Tr}\left(\tilde{B}^{[k]}_{i_1 i_2}\cdots\tilde{B}^{[k]}_{i_N i_1}\right)\left|i_1\cdots i_N\right\rangle, \tag{5.2}$$

where $\tilde{B}^{[k]}_{ij} = e^{i\varphi_{ij}}B^{[k]}_{ij}$. The operator $\mathcal{U}$ acts on the SIMPS matrices without changing the bond dimension which happens due to the split-index structure of the SIMPS - this structure splits the gate U across different matrices. If we now say that our SIMPS is normal and $\mathcal{U}\left|\psi\right\rangle = \left|\tilde{\psi}\right\rangle = \left|\psi\right\rangle$ for all system sizes, according to Theorem.2 there must exist invertible matrices V_i s.t,

$$e^{i\varphi_{ij}}B^{ij} = V_i B^{ij} V_j^{-1}. \tag{5.3}$$

Therefore it is possible to express symmetries in terms of SIMPS gauge transformations as long as the symmetry operators can be split to act on each matrix independently.

These non-onsite symmetries can also be expressed using MPS. However, such symmetries will increase the bond dimension of the MPS meaning they cannot be expressed using simple gauge transformations anymore. Instead we would see the need to bring in 3-index reduction tensors [27, p6] and other conditions which makes the process extremely complicated - these are irrelevant to our topic and outside the scope of the mathematics of this paper, so we can just ignore them. Thus, SIMPS are much more convenient when it comes to capturing the non-onsite symmetries in SPT phases.

Furthermore, we can build a proposition utilizing Eqn.5.3 to show that, the MPS that remains invariant under the action of non-onsite symmetry operators make for good SIMPS (Def.1).

Proposition 2 *Given a non-onsite symmetry operator,*

$$\mathcal{U} = \prod_{i=1}^{N} U_{i,i+1}, \quad \{\textit{where } U \textit{ is diagonal}\}$$

under the action of which a normal MPS remains invariant, then there exists at least one MPS matrix $A^{[k]}_i$ which will not be full rank. [27]

The mathematical proof [27, p6] of this allows us to deduce that MPS do not behave well under non-onsite symmetry operators.

Let us revisit the 1D cluster state in Sec.5.1.3 where we saw using MPS, that under symmetry constraints it exhibits non-trivial SPT. Using the SIMPS formalism, it is possible to show that the SIMPS matrices easily predicts non-onsite symmetries.

We define a SIMPS matrix of bond dimension $\eta = 2$ and some physical onsite dimension d which will generate states $|\psi_{a,b}\rangle$,

$$B_{ij}^{a,b} = X^{a_{ij}} Z^{b_{ij}}, \tag{5.4}$$

where a and b are some $d \times d$ binary matrices, and X and Z are Pauli operators. This SIMPS matrix will satisfy the relations,

$$\begin{aligned} (-1)^{b_{ij}} B_{ij}^{a,b} &= X B_{ij}^{a,b} X, \\ \& \quad (-1)^{a_{ij}} B_{ij}^{a,b} &= Z B_{ij}^{a,b} Z. \end{aligned} \tag{5.5}$$

This will mean the states $|\psi_{a,b}\rangle$ will have non-onsite symmetries of the form,

$$\begin{aligned} U^a &:= \prod_i u_{i,i+1}^a, \\ \& \quad U^b &:= \prod_i u_{i,i+1}^b, \end{aligned}$$

which will form a $Z_2 \times Z_2$ symmetry group $G_{a,b}$, where $u^a |ij\rangle = (-1)^{a_{ij}} |ij\rangle$ and $u^b |ij\rangle = (-1)^{b_{ij}} |ij\rangle$ - diagonal in the physical basis. If (a_{ij} or b_{ij}) $\neq c_i d_j$ (where c snd d are some binary vectors), then U^a and U^b are non-onsite. Furthermore, the relations in Eqn.5.5 will be anti-commutative, signalling non-trivial SPT order in $G_{a,b}$.

5.2 Quantum Teleportation

In the previous section we saw how the SIMPS formalism of TNs is more effective at capturing certain symmetries and phases of a system, which are physical properties. Now we will move on to computational properties. We will review how the MPS and SIMPS formalisms can be used to describe long range quantum teleportation involving many-bodies.

5.2.1 Many-Body Quantum Teleportation

We have already seen quantum teleportation in Sec.3.3 where we illustrate two observers, A and B, with a shared maximally entangled state $|\Omega\rangle$, performing teleportation to transfer information about a state $|\psi\rangle$ from A to B. We saw a very detailed graphical representation of the process which captures both the algebra and what is physically happening. Now we want to expand upon that and perform teleportation at a longer range by using a long chain of entangled qubits.

So let us start by simplifying the graphical representation and leave behind mostly the physical process.

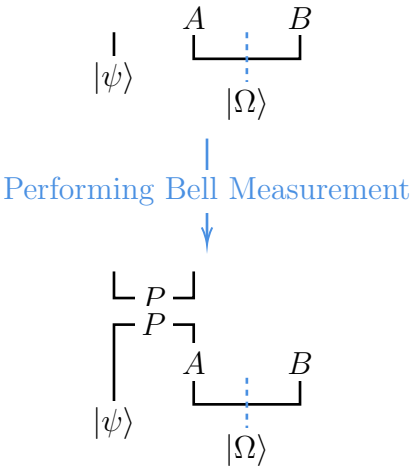


Figure 5.2: Teleportation with 2 Entangled Qubits[26]

Here P are projectors we use to perform the Bell measurement and they are Pauli operators,

$$P = (\mathbb{I} \otimes P) \, |\Omega\rangle \, .$$

Fig.5.2 shows that before measurement B is not connected to $|\psi\rangle$ and has no information of it. After A does the measurement using P, the information of $|\psi\rangle$ is now connected to the circuit and can be transmitted along the shared entanglement to B. B can then recover the information of $|\psi\rangle$ by reverting the unitary transformation caused by P which it has some classical communication channel to.

Now we can extend this representation to a system of more than two qubits where every two qubits are entangled as shown in Fig.5.3. After performing Bell measurements between each qubit pair we can establish some long-range entangled state as shown, where the boundary spins have some direct entanglement.

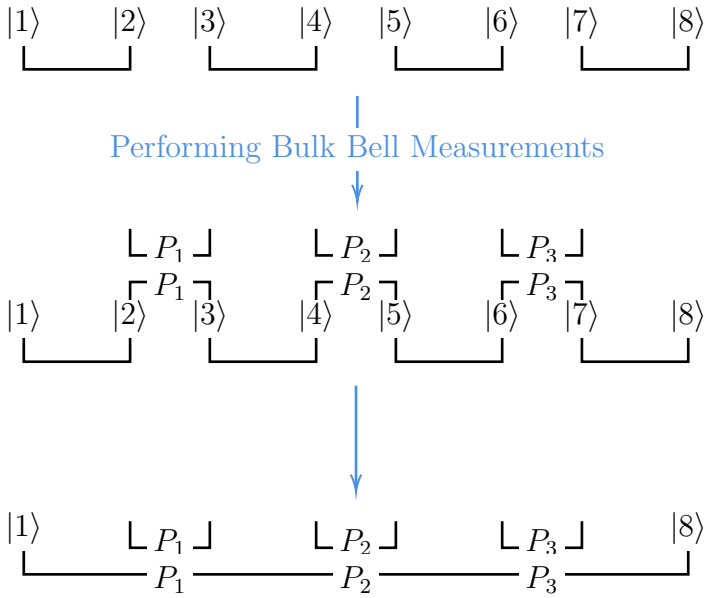


Figure 5.3: Many-Body Quantum Teleportation Circuit[26]

Such circuit setups, where a bunch of nodes(qubits) with some local interaction is measured and some long-range entanglement is established between them, are known as the "Quantum Repeater Architecture"[26]. We can simplify the systems before and after the bulk Bell measurements as in Fig.5.4.

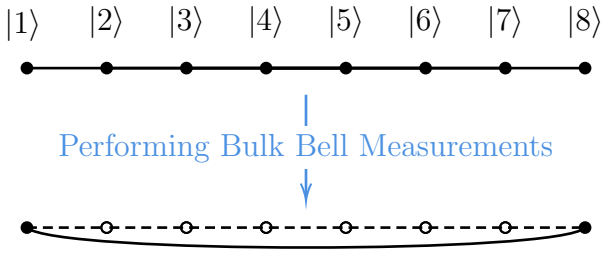


Figure 5.4: MBQT Physical Representation[26]

5.2.2 Quantum Wire

To understand long range quantum teleportation we first need to look at what a quantum wire is. Simply put, it is a tool which allows us to deterministically and efficiently transport quantum information from one end of a system to the other by conducting local measurements . This is similar to localizable entanglement which is the process of concentrating entanglement between two distant spins in a many-body system. A MPS or SIMPS representation of a state is said to be a quantum wire when they satisfy two properties:

- The MPS/SIMPS matrices must allow injective mapping, i.e., allow the reversion of the evolution caused by byproduct operators. This is to ensure quantum information can be recovered at any site of the system.
- The matrices need to obey some global symmetry to ensure quantum states are coherently transformed under symmetry constraints.

5.2.3 Quantum Wire in MPS

To see when a MPS can be regarded as a quantum wire, we will start with a MPS under OBC like the one in Eqn.4.3. Let us say we want to now disentangle the bulk spins from the boundary spins. So we will measure all the bulk spins,

$$|\psi\rangle = \sum_{\substack{i_1,\ldots,i_N \\ a,b}} \langle a|A^{[1]}_{i_1}\ldots A^{[N]}_{i_N}|b\rangle|a,i_1\ldots i_N,b\rangle$$

$$\Rightarrow |\psi'\rangle = \sum_{a,b}\langle a|A^{[1]}_{S_1}\ldots A^{[N]}_{S_N}|b\rangle|a,b\rangle. \quad \{\text{after bulk measurement}\} \tag{5.6}$$

This can also be expressed as,

$$\Rightarrow |\psi'\rangle = (\mathbb{I}\otimes A_{S_1}\ldots A_{S_N})|\psi^+_D\rangle. \tag{5.7}$$

Here, a and b are indices that will have values $0, \ldots, D-1$, to constrain $|\psi'\rangle$ to a $\mathcal{H}$-space of dimension $\mathbb{C}^D \otimes (\mathbb{C}^d)^{\otimes N} \otimes \mathbb{C}^D$, where D is the dimension of the boundary spins and d is the dimension of the bulk spins. $S_1, \ldots, S_N$ are the measurement outcomes for our bulk spin measurements, and $|\psi_D^+\rangle$ is the D-dimensional Bell state (Eqn.2.8). We can also get rid of the site labels, $[k]$, for simplicity.

We can graphically represent this bulk measurement on a MPS, leading to the formation of a quantum wire, as shown in Fig.5.5.

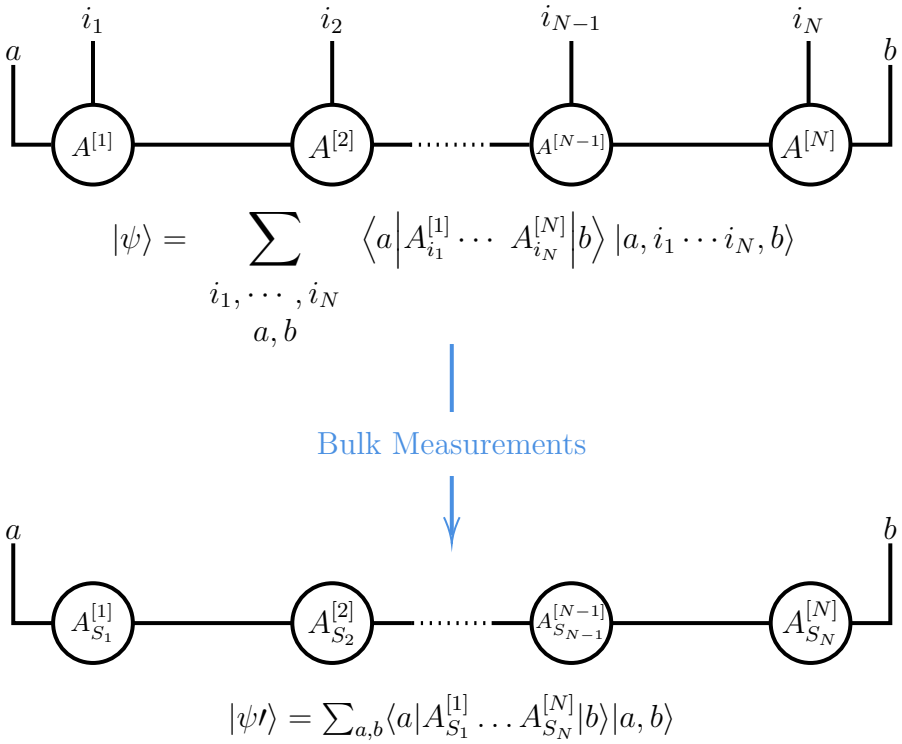


Figure 5.5: Bulk Measurement in MPS Representation

For us to be able to say that $|\psi'\rangle$ has long-range localizable entanglement, the entanglement between the boundary spins in $|\psi'\rangle$ must remain finite as $N \to \infty$. To get this long-range localizable entanglement, we can choose MPS matrices A_i to be unitary for all i, which will mean that the product $A_{S_1} \ldots A_{S_N}$ will also be unitary, implying $|\psi'\rangle$ is maximally entangled.

We can regard Eqn.5.6 as a quantum computation in the virtual $\mathcal{H}$-space. Its action, going from left to right, beginning with state $|a\rangle$, is the application of a series of unitary operations and then measuring $|a\rangle$ by projecting it onto $|b\rangle$. To summarize, this is a unitary evolution where information is being transmitted along the chain via measurement.

To use the state $|\psi'\rangle$ as a tool to perform quantum teleportation, we need to apply a corrective unitary operator (byproduct operator, Sec.2.4.2)on the boundary spins

to map the state to some fixed reference state, e.g., the Bell state. In this case, the product of the unitary operators from measurement, $A_{S_1} \dots A_{S_N}$, will be the byproduct operator. Under ideal conditions, this byproduct operator can be determined by performing some classical side processing on the measurement outcomes.

So we can conclude that if we had a MPS,

- which has long-range localizable entanglement,
- which has some classical side processing algorithm to identify the byproduct operator,
- and finally, allows for injective mapping,

it can be called a quantum wire — it can be used to efficiently and deterministically transmit quantum information from one end of a chain of spins to another.

5.2.4 Quantum Wire in SIMPS

Now we will look at how a SIMPS can be made into a quantum wire. Like before, we will start with a SIMPS under OBC (Eqn.4.9) and perform measurement on the bulk spins, leaving us with,

$$|\psi'\rangle = \sum_{\alpha,\beta} \langle \alpha | B_{S_1 S_2} \cdots B_{S_{N-1} S_N} | \beta \rangle | \alpha, \beta \rangle \tag{5.8}$$

Here α and β are η-dimensional spins at each end of the spin chain and has values $0, \dots, \eta - 1$. And as before, $S_1 \dots S_N$ are the measurement outcomes. Also like before, if the SIMPS matrices B_{ij} are unitary, the product after measurement, $B_{S_1 S_2} \cdots B_{S_{N-1} S_N}$, will also be unitary, thus implying maximal entanglement between the η-dimensional boundary spins.

The graphical representation of this bulk measurement is shown in Fig.5.6

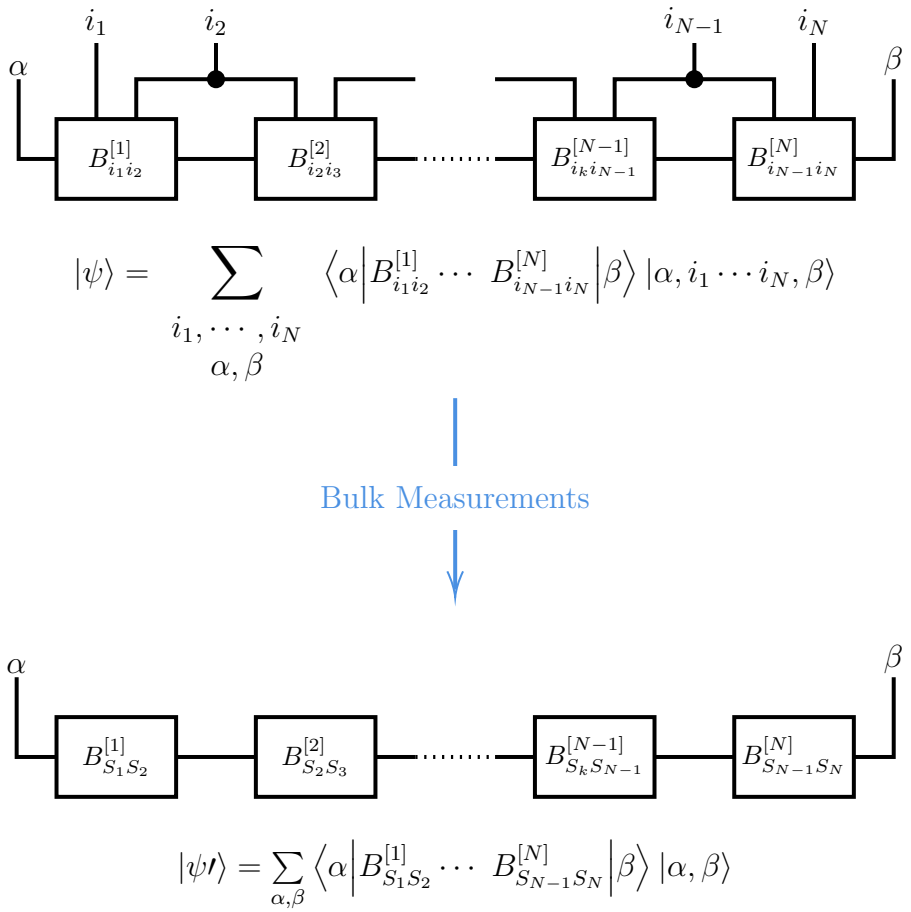


Figure 5.6: Bulk Measurement in SIMPS Representation

This is where we will come across the first advantage of the SIMPS formalism over the MPS formalism. The MPS matrices for a state may not necessarily be unitary, requiring us to choose bases that will cause it to be unitary. SIMPS matrices on the other hand are always unitary. This means that with the SIMPS formalism, it is easier to understand long-range localized entanglement.

Another advantage of the SIMPS representation is the presence of simple classical side-processing to determine the byproduct operator. When we measure the bulk spins of a SIMPS under OBC,

$$B_{S_1 S_2} \cdots B_{S_{N-1} S_N} \propto X_{S_1+S_2+\cdots+S_{N-1}} Z_{S_1 S_2+\cdots+S_{N-1} S_N}$$

where X and Z are the Pauli operators we saw in Sec.2.4.2. This will hold true for every SIMPS in a SPT phase described by Eqn.5.4.

We can visualize how measurement of the bulk spins work for SIMPS using Fig.5.7 which shows what would happen in the case of the 1D cluster state.

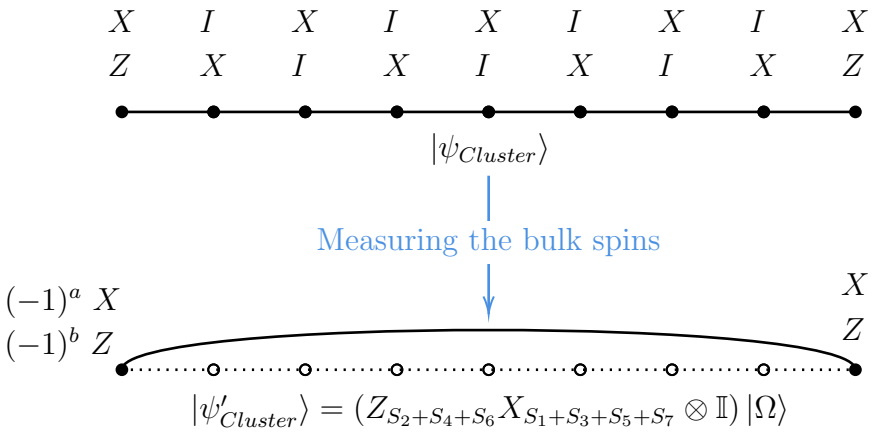


Figure 5.7: Measurement of bulk spins in 1D cluster state[26]

Here, we are applying the Pauli operator X on all the odd/even sites alternatively, with the Pauli operator Z on the endpoints. Since these operators are a symmetry of this state, they will have expectation value 1. We then perform the bulk measurement in the eigenbasis of these local operators, which are acting in the bulk of these symmetry operators. Afterwards, the X operators are replaced with the measured eigenvalue which will be ± 1. This leaves us with a system where the bulk spins have been measured out into some state, with the endpoints satisfying the correlations XX and ZZ up-to some $(-1)^a$ or $(-1)^b$ which are the eigenvalues of the operators we measured in bulk, where,

$$a = S_2 + S_4 + S_6 \quad \& \quad b = S_1 + S_3 + S_5 + S_7.$$

From these two relations we can determine the state of the boundary, which is a Bell state with some Pauli operator applied to it, which in this case is the byproduct operator. This is an example of the simple classical side processing we can do to determine the byproduct operator when we are using the SIMPS formalism, which would not be possible with the MPS formalism.

To sum up, a SIMPS with injective mapping can be shown to have long-range localizable entanglement and shown to have some simple classical side-processing algorithm to determine the byproduct operator, with less effort compared to MPS.

Chapter 6

Conclusion

The primary goal of this thesis was to review the SIMPS formalism of TNs and analyse its computational benefits over the existing MPS formalism, specifically when we are dealing with spin systems that have large degrees of freedom. To accomplish this we started by building a foundation of the core concepts of quantum mechanics und quantum information. We saw what exactly the term "measurement" insinuates. We introduced tools like the Bloch sphere and gates. We defined the postulates of quantum mechanics under the density matrix formalism. We also defined graphical representations to visualize a lot of the processes. Moving on from the foundation, we took a look at some phenomenon native to quantum systems, like entanglement, teleportation and spin interactions, which revolve around the problem we are trying to solve. Afterwards we introduced TNs and did a thorough review of the algebra of both the MPS and SIMPS formalisms. Finally, we conducted deeper analysis of these formalisms, which revealed that the SIMPS formalism does indeed provide some notable advantages over the MPS formalism. It captures the symmetry of certain phases of matter more effectively than MPS, and also provides increased computational efficiency and accuracy during teleportation.

Future Direction

This analysis has some interesting applications that can be explored further. Notably, the application of SIMPS in measurement based quantum computation, where the classical side processing involved in recovering teleported data can be done more efficiently and accurately, compared to existing algorithms built around the MPS formalism. Another benefit that SIMPS may have for measurement based quantum computation comes from its ability to reduce the bond dimension, which may further simplify the algorithms needed to perform teleportation using certain states.

Bibliography

[1] A. Einstein, B. Podolsky, and N. Rosen, "Can quantum-mechanical description of physical reality be considered complete?" *Phys. Rev.*, vol. 47, pp. 777–780, 10 1935. DOI: 10.1103/PhysRev.47.777. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRev.47.777.

[2] J. S. Bell, "On the einstein podolsky rosen paradox," *Physics Physique Fizika*, vol. 1, pp. 195–200, 3 1964. DOI: 10.1103/PhysicsPhysiqueFizika.1.195. [Online]. Available: https://link.aps.org/doi/10.1103/PhysicsPhysiqueFizika.1.195.

[3] R. Shankar, *Principles of quantum mechanics*. New York, NY: Plenum, 1980. [Online]. Available: https://cds.cern.ch/record/102017.

[4] W. K. Wootters and W. H. Zurek, "A single quantum cannot be cloned," *Nature*, vol. 299, no. 5886, pp. 802–803, 1982.

[5] C. H. Bennett, G. Brassard, C. Crépeau, R. Jozsa, A. Peres, and W. K. Wootters, "Teleporting an unknown quantum state via dual classical and einstein-podolsky-rosen channels," *Physical Review Letters*, vol. 70, no. 13, p. 1895, 1993.

[6] A. Barenco, C. H. Bennett, R. Cleve, *et al.*, "Elementary gates for quantum computation," *Physical Review A*, vol. 52, no. 5, pp. 3457–3467, 1995.

[7] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, "Mixed-state entanglement and quantum error correction," *Phys. Rev. A*, vol. 54, pp. 3824–3851, 1996.

[8] A. Peres, "Separability criterion for density matrices," *Phys. Rev. Lett.*, vol. 77, pp. 1413–1415, 1996.

[9] J. Preskill, *Lecture notes for physics 229: Quantum information and computation*, http://theory.caltech.edu/~preskill/ph229/, 1998.

[10] M. Horodecki, P. Horodecki, and R. Horodecki, "Separability of n-particle mixed states: Necessary and sufficient conditions in terms of linear maps," *Physics Letters A*, vol. 283, no. 1, pp. 1–7, 2001, ISSN: 0375-9601. DOI: https://doi.org/10.1016/S0375-9601(01)00142-6. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0375960101001426.

[11] G. Vidal and R. F. Werner, "Computable measure of entanglement," *Phys. Rev. A*, vol. 65, p. 032 314, 2002.

[12] D. M. Greenberger, M. A. Horne, and A. Zeilinger, "Going beyond bell's theorem," 2007. eprint: 0712.0921. [Online]. Available: https://arxiv.org/abs/0712.0921.

[13] D. Pérez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, "Matrix product state representations," *Quantum Information & Computation*, vol. 7, no. 5, pp. 401–430, 2007. eprint: quant-ph/0608197.

[14] D. Pérez-García, M. M. Wolf, M. Sanz, F. Verstraete, and J. I. Cirac, "String order and symmetries in quantum spin lattices," *Physical Review Letters*, vol. 100, no. 16, 2008, ISSN: 1079-7114. DOI: 10.1103/physrevlett.100.167202. [Online]. Available: http://dx.doi.org/10.1103/PhysRevLett.100.167202.

[15] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, "Quantum entanglement," *Reviews of Modern Physics*, vol. 81, no. 2, pp. 865–942, 2009.

[16] X. Chen, Z.-C. Gu, and X.-G. Wen, "Classification of gapped symmetric phases in 1d spin systems," *Physical Review B*, vol. 83, no. 3, p. 035 107, 2011. DOI: 10.1103/PhysRevB.83.035107.

[17] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information: 10th Anniversary Edition*, 10 Anv. Cambridge University Press, 2011, ISBN: 9780511976667.

[18] N. Schuch, D. Perez-Garcia, and J. I. Cirac, "Classifying quantum phases using matrix product states and projected entangled pair states," *Physical Review B*, vol. 84, no. 16, p. 165 139, 2011. DOI: 10.1103/PhysRevB.84.165139.

[19] F. Pollmann, E. Berg, A. M. Turner, and M. Oshikawa, "Symmetry protection of topological phases in one-dimensional quantum spin systems," *Physical Review B*, vol. 85, no. 7, p. 075 125, 2012.

[20] B. Swingle, "Entanglement renormalization and holography," *Phys. Rev. D*, vol. 86, p. 065 007, 6 Sep. 2012. DOI: 10.1103/PhysRevD.86.065007. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevD.86.065007.

[21] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, "Symmetry protected topological orders and the group cohomology of their symmetry group," *Physical Review B*, vol. 87, no. 15, p. 155 114, 2013. DOI: 10.1103/PhysRevB.87.155114.

[22] R. Orús, "A practical introduction to tensor networks: Matrix product states and projected entangled pair states," *Annals of Physics*, vol. 349, pp. 117–158, 2014.

[23] J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, 3rd ed. Cambridge University Press, 2020.

[24] D. T. Stephen and O. Hart, *Preparing matrix product states via fusion: Constraints and extensions*, 2024. arXiv: 2404.16360 [quant-ph]. [Online]. Available: https://arxiv.org/abs/2404.16360.

[25] A. Ekert, T. Hosgood, A. Kay, and C. Macchiavello, *Introduction to Quantum Information Science*, https://qubit.guide, Jul. 24, 2025.

[26] Q. Hannover, *David stephen - on the relationship between quantum teleportation and string order*, YouTube, Feb. 2025. [Online]. Available: https://www.youtube.com/watch?v=LYNV7oZx1cg (visited on 05/20/2025).

[27] D. T. Stephen, "Non-onsite symmetries and quantum teleportation in split-index matrix product states," *Quantum*, vol. 9, p. 1738, 2025, ISSN: 2521-327X. DOI: 10.22331/q-2025-05-12-1738. [Online]. Available: http://dx.doi.org/10.22331/q-2025-05-12-1738.

[28] D. Tong, *Quantum Mechanics: Lectures on Theoretical Physics*. Cambridge University Press, 2025.