Mathematics of Quantum Computing

(Tentative Title)

A report submitted in partial fulfillment
of the requirement for the degree of

MASTER OF SCIENCE
IN
MATHEMATICS

by

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22MMT002

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Abstract

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CERTIFICATE

This is to certify that the dissertation entitled **Mathematics of Quantum Computing (Tentative Title)** submitted by **Pranay Raja Krishnan** (22MMT002) towards the partial fulfillment of the requirement for the degree of Master of Science (M.Sc) is a bonafide record of work carried out by him at the Department of Mathematics, The LNM Institute of Information Technology, Jaipur, (Rajasthan) India, during the academic session 2018-2019 under my supervision and guidance.

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Acknowledgements

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Date: August 28, 2023 Pranay Raja Krishnan

List of Notations

Unless explicitly defined the following notations are used.
TODO: Add Required Notation

Symbol	Meaning
$\subseteq$	subset or equal to
$\not\subset$	not subset
$\supseteq$	superset or equal to
$\emptyset$	empty set
$\in$	belongs to
$\notin$	does not belong to
$\prod_{i \in I}$	product over index set I
$\mathbb{C}$	the set of real numbers
$\mathbb{R}$	the set of real numbers
$\mathbb{N}$	the set of natural numbers

Contents

Chapter 1

A brief history of Quantum Computing

In the last decades of the twentieth century, certain scientists sought to combine two recent theories that were highly influential: **Information Theory** and **Quantum Mechanics**.

- **1984:** Charles Bennet and Gilles Brassad published a quantum key distribution protocol now called **BB84**, allowing two parties to establish an absolutely secure secret key.

- **1980s:** Feynman recognized that a system of n-particle quantum systems could not be simulated efficiently by a Turing machine, seemingly requiring time/space that is exponential in n. He proposed that computers based on quantum systems could simulate quantum processes with more efficiency. This led to the question: If simluating quantum problems was more efficient on a quantum computer, would there be other problems that would run more efficiently on a quantum computer?

- **1994:** Peter Shor found the famous **Shor's Algorithm** for a quantum computer which could factors n-digit integers into primes with n^2 efficiency (with high probability). The fastest known algorithm for factoring n-digit integers in classical computing is of efficiency around $2^{n^{1/3}}$

Chapter 2

Qubits

The computers we use today rely on classical information theory, which are based on **bits** (binary digits) which can represents a 0 or 1 state. These **classical computers**) are equivalent to a Turing Machine in computational efficiency.
On a quantum computer the **qubit** (quantum bit) is the basic unit of information.

On a real-life quantum computer, a qubit can be implemented using a variety of quantum phenomena. In labs, qubits have been implemented using photon polarization, electron spin, the ground/excited state of an atom in a cavity, and even defect centers in a diamond. While there could be many such real-life realizations of qubits, in this text, we are not concerned with the specific implementation as long as they follow certain abstract rules.

Definition 2.0.1 (Qubit)**.** *A **qubit** is any quantum mechanical system which is associated with* 2*-dimensional complex Hilbert space* $\mathcal{H}$ *(known as the **state space** and follows the below principles:*

- *Principle of Superposition*
- *Principle of Measurement*
- *Principle of Projection 'TODO: Refer Scherer, P37'*
- *Principle of Entanglement*
- *Principle of Transformation*

A given state of the system is completely described by a unit vector $|\psi\rangle$*, which is called the **state vector** (or wave function) on the Hilbert Space*

The principles in the above definition will be elaborated on in the upcoming sections.

Notation 2.0.2. *Observe above that we have written the vector* $\vec{\psi} \in \mathcal{H}$ *as* $|\psi\rangle$*. This is the notation for a vector in* Dirac's bra/ket notation*, and is read **ket psi***

Lemma 2.0.3 (Principle of Superposition)**.** *Suppose* $|\psi\rangle$ *and* $|\sigma\rangle$ *are two perfectly distinguishable quantum states of a quantum system, and* $\alpha, \beta \in \mathbb{C}$ *with* $\alpha^2 + \beta^2 = 1$*. Then* $\alpha |\psi\rangle + \beta |\sigma\rangle$ *is a valid state of the quantum system.*

The principle of superposition says that the state of a qubit can be modelled with a 2-dimensional Hilbert space. This leads to qubits being referred to as **two-state** quantum systems. This does not mean that this system has only two states, but rather that all possible states exist as a linear combination of just two states.
When working with Hilbert spaces associated with quantum systems, we normally use *orthonormal bases.*

Definition 2.0.4. *The **computational basis** of the two dimensional complex vector space $\mathcal{H}$ is $\{|0\rangle, |1\rangle\}$ where $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$ and $|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$*

With respect to the computational basis $\{|0\rangle, |1\rangle\}$, the state of the qubit can be described as
$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix}a\\0\end{bmatrix} + \begin{bmatrix}0\\b\end{bmatrix} = \begin{bmatrix}a\\b\end{bmatrix}$ where $a, b \in \mathbb{C}$ and $a^2 + b^2 = 1$.
Another commonly used orthonormal basis for the Hilbert space $\mathcal{H}$ modelling a qubit is the Hadamard Basis.

Definition 2.0.5. *The **Hadamard Basis** $\{|+\rangle, |-\rangle\}$ is given by*
$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ *and* $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

The principle of superposition says that the state of a qubit is a continuum which might indicate that we can use a single qubit to store an infinite amount of information. However, a principal of quantum mechanics states that we cannot interact with the qubit without fundamentally altering its state. To work with the state stored in a qubit, we must perform a measurement which forces the state of the qubit to "collapse" into one of two *preferred states.*

Lemma 2.0.6 (Principle of Measurement)**.** *Any measurement device that interacts with the qubit will be calibrated with a pair of orthonormal vectors called the **preferred basis**, say $\{|u\rangle, |v\rangle\}$. If the state of the qubit with respect to the preferred basis is $|\psi\rangle = a|u\rangle + b|v\rangle$, then measurement of the qubit will yield either $|u\rangle$ with a probability of $|a|^2$ or $|v\rangle$ with a probability $|b|^2$.*
After measurement, the state of the qubit itself will be changed to the output of the measurement. 'TODO Formalize'

This behaviour is an axiom of quantum mechanics substantiated by empirical observations from experiments over the last hundred years.
'From Scherer'

Definition 2.0.7. *An **observable** is a physically measurable quantity of a quantum system which is represented by a self-adjoint operator on a Hilbert space*

Lemma 2.0.8. *In a qubit represented by Hilbert space $\mathcal{H}$, the possible measurement values of an observable are given by the spectrum $\sigma(A)$ of the self adjoint operator A representing the observable. The probability $p_\psi(\lambda)$ that a quantum system in the pure state $|\psi\rangle \in \mathcal{H}$ yields the eigenvalue λ of A upon measurement is given by the projection P_λ onto the eigenspace $Eig(A, \lambda)$ of λ as $p_\psi(\lambda) = ||P_\lambda |\psi\rangle ||^2$*

Definition 2.0.9. *Let $\mathcal{H}$ be a Hilbert space. We call states $|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_n\rangle \in \mathcal{H}$ perfectly distinguishable if there exists a measurement system $\{M_i\}_{i=1}^m$ with $m \geq n$ such that $||M_j |\psi_1\rangle ||^2 = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$*

Here *perfectly distinguishable* means that there is some experiment or experimental setup that can distinguish between these two states, atleast in theory.

Result 2.0.10. *The states $|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_n\rangle$ are perfectly distinguishable if and only if they are orthogonal. This result is the reason we use orthogonal basis in quantum computing.*

‘TODO: Refer Nielsen, Chuang
This property limits the amount of information that can be extracted from a qubit: a measurment yields atmost a single classical bit worth of information. In most cases, we also cannot make more than one measurement of original state of the qubit. On measurement, we have two possibilities, each corresponding to a probability of $|a|^2$ and $|b|^2$, then the total probability of the whole space will be $|a|^2 + |b|^2 = 1$, which is valid for unit vectors $|\psi\rangle = a|0\rangle + b|1\rangle$.

Notation 2.0.11. *When $|\psi\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$, then $\langle\psi|$ is the conjugate transpose of $|\psi\rangle$ and is read as **bra psi**, $\langle\psi| = \begin{bmatrix} \overline{a} & \overline{b} \end{bmatrix}$*

This lets us write the inner product for $\mathcal{H}$ as: For any $|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, |w\rangle = \begin{bmatrix} c \\ d \end{bmatrix} \in \mathcal{H}$, the operation $\langle v|w\rangle = \langle v| |w\rangle = \begin{bmatrix} \overline{a} & \overline{b} \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} = \overline{a}c + \overline{b}d$
We will consider the inner product as being linear in the second variable and conjugate-linear in the first variable.

Remark 2.0.12. *If* $|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$, *then we can show* $\langle 0|\psi\rangle = a$, $\langle 1|\psi\rangle = b$. *Therefore we can write* $|\psi\rangle = a\,|0\rangle + b\,|1\rangle = \langle 0|\psi\rangle\,|0\rangle + \langle 1|\psi\rangle\,|1\rangle$.

Remark 2.0.13. *The standard inner product of the* $|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$ *with itself in the Hilbert space* $\mathcal{H}$ *can therefore be written as* $\langle\psi|\psi\rangle = \langle\psi|\,|\psi\rangle = \begin{bmatrix} \overline{a} & \overline{b} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = |a|^2 + |b|^2 = 1$

Lemma 2.0.14 (Principle of Measurement)**.** *Any physical observable is associated with a self-adjoint operator* $\mathcal{A}$ *on the Hilbert space* $\mathcal{H}_S$. *The possible outcome of a measurement of the observable* $\mathcal{A}$ *is one of the eigenvalues of the operator* $\mathcal{A}$.
Writing the eigenvalues equation, $\mathcal{A}\,|i\rangle = a_i\,|i\rangle$ *where* $|i\rangle$ *is an orthonormal basis of eigenvectors of the operator* $\mathcal{A}$, *and* $|\psi\rangle = \sum_i c_i\,|i\rangle$, *then the probability that a measurement of the observable* $\mathcal{A}$ *results in the outcome* a_i *is given by* $p_i = |\,\langle i|\psi\rangle\,|^2 = |c_i|^2$

'TODO: Proof that self-adjoint matrices represent measurement operators'
'TODO: Relation of POVM and matrices'
Let $\mathcal{H}_1$ be an n-dimensional vector space with basis $\alpha = \{|a_1\rangle, |a_2\rangle, ..., |a_n\rangle\}$ and $\mathcal{H}_2$ be an m-dimensional vector space with basis $\beta = \{|b_1\rangle, |b_2\rangle, ..., |b_n\rangle\}$, then the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is an nm-dimensional space with basis elements of the form $|a_i\rangle \otimes |b_j\rangle$

Notation 2.0.15. *In dirac's bra/ket notation, the tensor product of* $|v\rangle \in \mathcal{H}_2, |w\rangle \in \mathcal{H}_2$ *is* $|vw\rangle = |v\rangle\,|w\rangle = |v\rangle \otimes |w\rangle$

The tensor product is defined to satisfy the following properties:

1. $(|v_1\rangle + |v_2\rangle)\,|w\rangle = |v_1\rangle\,|w\rangle + |v_2\rangle\,|w\rangle$
2. $|v\rangle\,(|w_1\rangle + |w_2\rangle) = |v\rangle\,|w_1\rangle + |v\rangle\,|w_2\rangle$
3. $(a \cdot |v\rangle)\,|w\rangle = |v\rangle\,(a \cdot |w\rangle) = a \cdot (|v\rangle\,|w\rangle)$

Every element $|\sigma\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ can be written as a superposition of elements of the basis $\{|a_i\rangle\,|bj\rangle\}$ as $|\sigma\rangle = \alpha_{11}\,|a_1 b_1\rangle + \alpha_{12}\,|a_1 b2\rangle + ... + \alpha_{nm}\,|a_n b_m\rangle$.
Most elements $|\sigma\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ *cannot* be decomposed to $|\sigma\rangle = |v\rangle\,|w\rangle$ where $v \in \mathcal{H}_1, w \in \mathcal{H}_2$. 'TODO: Check proof'

As we have observed, a single qubit only gives us one classical bit worth of information. This equivalence diverges once we include *multiple* interacting qubits in the system. A system of n classical bits will have one degree of freedom for each bit, resulting in a state-space of n dimensions, i.e. classical systems are linear in n. In quantum systems, however, a system of n qubits will result in a state space of 2^n dimensions. This is because of the quantum property of *entanglement* which describes how quantum systems interact with each other.

Lemma 2.0.16 (Principle of Entanglement)**.** *When we have two qubits being treated as a combined system, the state space of the combined system is the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ of the state spaces $\mathcal{H}_1, \mathcal{H}_2$ of the component qubit subsystems. If the first qubit is in state $|\psi\rangle$ and the second in state $|\sigma\rangle$, then the combined system of two interacting qubits is in state $|\psi\sigma\rangle = |\psi\rangle\,|\sigma\rangle$. Similarly, for a system of n qubits, the state space is the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_n$ of the state spaces of the n independent qubits.*

The most natural basis for $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ is constructed from the tensor products of the basis vectors of $\mathcal{H}_1$ (say $\{|0\rangle_1, |1\rangle_1\}$ and of $\mathcal{H}_2$ (say $\{|0\rangle_2, |1\rangle_2\}$), then a basis for $\mathcal{H}$ is given by $\{|0\rangle_1 |0\rangle_2, |0\rangle_1 |1\rangle_2, |1\rangle_1 |0\rangle_2, |1\rangle_1 |1\rangle_2\}$
$= \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.
We will often this basis as $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ when the context is unambiguous. So an arbitary state $|\psi\rangle \in \mathcal{H}$ can be described as $|\psi\rangle = c_0 |00\rangle + c_1 |01\rangle + c_2 |10\rangle + c_3 |11\rangle = c_0 |0\rangle + c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle$.

Definition 2.0.17. *A state $|\psi\rangle$ is said to be* ***entangled*** *if it cannot be written as a simple tensor product of states $|v\rangle \in \mathcal{H}_1$ and $|w\rangle \in \mathcal{H}_2$. If we can write $|\psi\rangle = |v\rangle\,|w\rangle$, the state is said to be* ***seperable****.*

Example 2.0.18. *Consider the state $|\psi_1\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. We can show this is entangled. 'TODO'*

Example 2.0.19. *Consider the state $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |11\rangle)$. We can show this is seperable since we can write $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |1\rangle$*

Chapter 3

Gates

Definition 3.0.1. *An observable is a physically measurable quantity of a quantum system which is represented by a self-adjoint operator on a Hilbert space.*

Definition 3.0.2. *A matrix is said to be* ***unitary*** *if and only if one of the following conditions hold:*

1. $U^\dagger U = I$
2. $UU^\dagger = I$
3. *the columns of* U *are orthonormal vectors*
4. *the rows of* U *are orthonormal vectors*

'Alternate from Scherer'

Definition 3.0.3. *An operator* U *on* H *is called* ***unitary*** *if*
$\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle$ *for all* $|\psi\rangle, |\phi\rangle \in \mathcal{H}$

Proposition 3.0.4. *Gates are described by unitary matrices.*

Proof. Let M be a transformation of a quantum qubit state $|\psi\rangle$. Physics says that the evolution of an isolated quantum system is linear, so the transformation M can be described by a matrix.

For any state $|\psi\rangle$, $M|\psi\rangle$ has to be a unit vector.
If $M|\psi\rangle$ is a unit vector, the inner product with itself is 1.
$\implies \langle\ (M|\psi\rangle) \mid (M|\psi\rangle)\ \rangle = 1$
$\implies \langle\psi| M^\dagger M |\psi\rangle = 1$
$\implies M^\dagger M = I$ where I is the identity matrix
$\implies M$ is unitary

$\square$

Since $UU^\dagger = I$, we can conclude that every unitary matrix is invertible. This leads to the following result:

Result 3.0.5. *Only reversible gates can be implemented in quantum computing and any reversible gate has a quantum analog.*

This shows us that the classical NOT gate has a quantum analog but NAND does not.
Any unitary 2×2 matrix is a valid gate but only a few are used in practice.
'TODO Notation $|\rangle\ \langle|$'

3.1 Gates on a single Qubit

Definition 3.1.1 (Pauli Gates)**.** *I, X, Y, Z are known as the Pauli gates and are defined as:*

1. $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = |0\rangle\langle 0| + |1\rangle\langle 1|$
2. $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = |1\rangle\langle 0| + |0\rangle\langle 1|$
3. $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = i|1\rangle\langle 0| - i|0\rangle\langle 1|$
4. $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$

'TODO: Effect of the Pauli Gates on the Bloch Sphere'

Definition 3.1.2 (Hadamard Gate)**.** *The **Hadamard Gate** is the transformation* $H : \mathcal{H} \to \mathcal{H}$ *such that*
$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$ $H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$. *It is defined by the matrix* $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = |0\rangle\langle +| + |1\rangle\langle -|$

The Hadamard gate allows us to obtain a superposition state.

Remark 3.1.3. *The Hadamard gate is its own inverse.*
$H^2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = I$

Remark 3.1.4. $H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{\sqrt{2}}\left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\right) = \frac{1}{\sqrt{2}}(X + Z)$

Definition 3.1.5. *The **Phase Gate** defines a rotation about the z-axis by an angle* θ *on the Bloch sphere. 'TODO: Bloch Sphere'*
It is given by $R_\phi = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} = |0\rangle\langle 0| + e^{i\phi}|1\rangle\langle 1|$

3.2 Gates on Multiple Qubits

Definition 3.2.1. *The **CNOT gate** is a gate that acts on 2 qubits which flips the second bit if the first bit is in the* $|1\rangle$ *state.*
It is defined by the matrix $CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X$

The CNOT gate allows us to obtain an entangled state.

Definition 3.2.2. *The **Toffoli gate** is a gate that acts on 3 qubits that flips the third bit if the first two are in the* $|1\rangle$ *state.*

Depending on the input the Toffoli gate can function as an AND, NOT and NAND gate. Since the NAND gate is universal, the Toffoli is as well. The Toffoli gate is also unitary which means it is a valid quantum gate. This shows that every classical circuit can be implemented as a quantum circuit.

Bibliography

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