An Insight Into:
Quantum Random Walks

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Abstract

We shall review both the discrete and continuous time quantum walks on the line and on graphs, and then compare them to their classical analogues. Where we see that the quantum walks have a standard deviation of t, as compared to the classical case of $\sqrt{t}$, where t represents the number of steps taken by the walker. This means that the quantum walker travels much further on average, than their classical counterpart. This is because the quantum walker can be in a superposition of multiple positions at any one time; this property of quantum systems offers great rewards for quantum algorithmic development. Taking advantage of this property we introduce one simple, but very important quantum database search algorithm, Grover's algorithm. The algorithm can find an element in a random database of N elements in a computational time of $t = \mathcal{O}(\sqrt{N})$, which is much faster than the equivalent classical algorithm of $t = \mathcal{O}(N)$. Where t still represents the number of steps (or iterations). We then use the discrete quantum walk to adapt Grover's algorithm, so that we can use it for the spatial search algorithm in N-dimensions, without losing any quantum speed up. We finally discuss how to experimentally implement the discrete walk via trapped ions.

Contents

1 Introduction

Although quantum random walks is a relatively new field, much has happened since the inception of the 1993 paper by Aharonov *et al.* [42], which was the first paper to official coin the term quantum random walk, but was not necessarily the first to introduce the concept of the quantum walk. That was actually done by Mr Feynman in the 1940's [16], who discussed a checkerboard which described the way a spin-$\frac{1}{2}$ particle moved through 1 spatial dimension in discrete time steps. Although, Feynmans definition of the discrete quantum walk is rather different to how the walk is defined in literature today.

To begin our journey of discovery, we begin in section 2 by exploring the basic notions of quantum mechanics. Although Section 2 does not contain all the introductory information to the subject, I have simply sought to give you the key concepts that will be used throughout this paper and a little extra. In section 3 we shall briefly discuss the basic properties of both the classical discrete and the classical continuous versions of the random walks , which were first introduced by Karl Pearson in 1905 [31] . We see that for both the discrete and continuous walks, that we have a Gaussian probability distribution, with a width of $\sqrt{n} \equiv \sqrt{t}$, where n just represents the discrete time case, rather than the continuous time step t. This then allows us to progress on to section 4, where we begin our discussion of the discrete quantum random walks, which were the first of the walks to be discussed [42] and developed on the line and the graph [13] . We find that the dynamics of the discrete walk can be easily manipulated, depending on the coin operator $\hat{C}$ that we use [20]. In looking at the evolution of the walks, we see that the probability distribution of the discrete quantum walk on the line is not Gaussian. In fact, it does not satisfy the central limit theorem [21] and so to calculate the statistical measures analytically is rather difficult to do. So we merely quote the results that have been found after many years of extensive research [21] [6]. Which have found that both the discrete and continuous [2] quantum walks on the line have distributions of width t. This means that a walker carrying out a quantum walk on the line travels much further than their classical counterpart.

This property of the walks has spurred many to research how to implement both versions of the quantum walks on graphs [13] [2] [30] [4] , so that they are poised for algorithmic development. As if we can develop a truly quantum computer, being able to implement these quantum algorithms would allow us to greatly enhance even the most simplest of classical search algorithms [33] [27]. We shall also include a discussion in section 4 on how to implement discrete quantum walks on the undirected graph $G(V, E)$ and go through the example of a discrete quantum walk on a hypercube, which can be reduced to just a walk on the line [20] [32]. From this, follows the discussion of the continuous quantum walks, which are very different in construction as compared to the discrete walks. They were first developed and discussed by Childs *et al.* [2]in 2002, who showed for certain problems on graphs, specifically glued trees, that we can actually get an exponential speed up in computational time. We then go through the example of the continuous quantum walk on the line. We see that the continuous quantum random walk on the line has essentially the same global distribution as the discrete case, even though it is formulated very differently. We then move on to section 5, to discuss a simple, but incredibly important database quantum search algorithm for N items, called Grover's algorithm, which was introduced by Grover in 1996/1997 [18] [22]. The algorithm only has to search through $\sqrt{N}$ items on average to find our required element,or correctly stated has a computational time of $t = \mathcal{O}(\sqrt{N})$, which is much faster than its classical counterpart of $\mathcal{O}(N)$ [22] [12]. After discussing the algorithm, we then see how we can modify Grover's algorithm for a spatial search algorithm via discrete quantum random walks [4]. As if we try and use the standard Grover algorithm for the spatial search, we revert back to the classical computation time $\mathcal{O}(N)$ [30], which is not what we want. In using the the discrete quantum walks, we state that for 2-dimensions the computation time is $\mathcal{O}(\sqrt{N} \log N)$ and for 3 or more dimensions we get a computational time of $\mathcal{O}(\sqrt{N})$ [4]. In the final section, section 6, we discuss one method for experimentally implementing the discrete quantum walk on a quantum computer via trapped ions [8] [36], which was introduced in 1996 by Monroe *et al.* [10]. It should however be noted, that this is just one of many current ideas for how to

experimentally construct a quantum computer [7] [3] [23] [24]. The reason we have chosen to specifically focus on the trapped ion's approach, is due to its recent successes [39] and its analogies with the discrete quantum walk.

2 An Introduction To Quantum Mechanics

In this section we will discuss the various background knowledge that is required, in order to understand this review project and appreciate some of the wonders of quantum mechanics. We shall explore first the basic mathematical structure of quantum mechanics, which shall allow us to describe the postulates. I would have liked to of given you the postulates first and then the mathematical structure, but it leads to problems as key definitions are left out and it becomes a maze for the reader.

I hope that the below suffices for the given reader, if unfortunately it does not, then a list of the resources used for this section are given in the bibliography [19] [41] [25] [40] [7], which dive in to much more detail than I am able to give here.

2.1 The Hilbert Space

The mathematical framework of the quantum world takes place inside a Hilbert space $\mathcal{H}$, where the Hilbert space is, if you like the scene in which all the action takes place. However, the Hilbert space does not describe the action happening in that scene, it only gives us the framework, which allows us to introduce the mathematical concepts so that we can then explain the dynamics and the properties of quantum systems.

But what exactly constitutes a Hilbert space? A finite dimensional Hilbert space $\mathcal{H}$, is equivalent to a complex inner product space with an additional property of a complete normed space. Using Dirac notation we represent the state of a physical system by the state vectors of a Hilbert space $\mathcal{H}$, represented by the "kets" $|\psi\rangle$. Where if $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ are possible states, then by the principle of superposition $|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle \ \forall \alpha, \beta \ \epsilon \ \mathbb{C}$ is also a state of the system. This is a very profound statement and is a very interesting property of quantum systems, as it means physical states can be in a superposition of one another, which is the meaning behind the famous Schödinger statement "Is the cat dead

or alive?" . The principle of superposition allows us to define the qubit[1]

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \tag{2.1}$$

where $|0\rangle$ and $|1\rangle$ are the standard basis vectors and can be represented by the spin up $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and spin down $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ of a spin-$\frac{1}{2}$ particle[2]. The use of Dirac notation shall become clearer along the way, for now you will just have to trust the judgement of those who formulated the subject.

Definition 2.1. *: Let $\mathcal{H}$ be a finite dimensional complex Hilbert space. An inner product on $\mathcal{H}$ is a map $\langle .|. \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ satisfying the following conditions for all $|\phi\rangle, |\psi\rangle$ and $|\mu\rangle \in \mathcal{H}$, $\alpha \in \mathbb{C}$*

1. Positivity $\langle \psi | \psi \rangle \geq 0, \forall |\psi\rangle \in \mathcal{H}$

2. Definiteness $\langle \psi | \psi \rangle = 0$ if and only if $|\psi\rangle = 0$

3. Additivity $\langle \psi | \phi + \mu \rangle = \langle \psi | \phi \rangle + \langle \psi | \mu \rangle \; \forall |\psi\rangle, |\phi\rangle, |\mu\rangle \in \mathcal{H}$

4. Homogeneity $\langle \psi | \alpha \phi \rangle = \alpha \langle \psi | \phi \rangle$

5. Conjugate symmetry $\langle \psi | \phi \rangle = \overline{\langle \phi | \psi \rangle}$

and in addition to the above, a Hilbert space requires the additional structure

Definition 2.2. *: Let $(\mathcal{H}, \langle .|. \rangle)$ be an inner product space. $\mathcal{H}$ is called a Hilbert space if it is complete as a normed space with norm $\|.\|$*

where a complete normed space is defined as follows

Definition 2.3. *: A normed space $(V, \|.\|)$ is called complete if and only if any Cauchy sequence in V is convergent, i.e. If u_n is a sequence in V such that $\|u_n - u_m\| \to 0$ as $n, m \to \infty$ then there exists $u \in V$ such that $\lim_{n \to \infty} \|u_n - u\| = 0$*

With the framework now in place, let us introduce Dirac notation, which is a vital tool for quantum theorists and is used throughout quantum mechanics.

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[1]More shall be said about the qubit later on

[2]$|0\rangle$ and $|1\rangle$ are also called the computational basis states, see Appendix 1

2.2 Dirac Notation

Dirac bra-ket notation is a very useful tool to both the physicist and the mathematical physicist,but is something of an annoyance to the pure mathematician, as it prevents them from making distinctions that they find important. Dirac notation enables quicker calculation as it makes the structure of quantum states clearer, as vectors represent the states of physical systems in quantum mechanics. We begin by starting in a complex finite dimensional Hilbert space $\mathcal{H} = \mathbb{C}^d$. Within this space we introduce the $ket's\,|.\rangle$, where the ket's have a similar structure to the d-dimensional row vectors

$$\boldsymbol{\psi} = |\psi\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix}$$

and if $|\psi\rangle$, $|\psi_1\rangle$ and $|\psi_2\rangle \in \mathcal{H}$ then following linearity property holds

$$|\psi\rangle = \alpha\,|\psi_1\rangle + \beta\,|\psi_2\rangle \in \mathcal{H} \tag{2.2}$$

Before we discuss the other properties of the ket's let us introduce the dual space $\mathcal{H}^*$, which is the space of all continuous linear functionals on $\mathcal{H}$

$$f : \psi \to f(\psi) \in \mathbb{C} \tag{2.3}$$

$$f(\alpha\psi_1 + \beta\psi_2) = \alpha f(\psi_1) + \beta f(\psi_2) \tag{2.4}$$

where $f \in \mathcal{H}^*$. Within this space we introduce the $bra's\,\langle.|$, where the bra has a similar structure to the transposed d-dimensional row vector

$$\boldsymbol{\psi}^\dagger = \langle\psi| = \begin{pmatrix} \bar{a}_1 & \dots & \bar{a}_d \end{pmatrix}$$

where $\bar{a}_d$ represents the conjugate to a_d. Thus for any $|\psi\rangle \in \mathcal{H}$ we can construct $f_\psi = \langle\psi|.\rangle$ such that

$$f_\psi(\phi) = \langle\psi|\phi\rangle \in \mathbb{C} \tag{2.5}$$

where we call $\langle\psi|\phi\rangle$ the "bra-ket". With the above now in place let us state the other properties of the ket's and the bra's, which are just that of a Hilbert space. The inner

product is defined by equation (2.5), combining this with the linearity condition (2.2) we have

$$\langle \psi | \alpha \phi_1 + \beta \psi_2 \rangle = \alpha \langle \psi | \phi_1 \rangle + \beta \langle \psi | \phi_2 \rangle \tag{2.6}$$

we also have conjugate symmetry

$$\langle \psi | \phi \rangle = \overline{\langle \phi | \psi \rangle} \tag{2.7}$$

and thus if $|\phi\rangle = |\psi\rangle$ we define the norm as follows $\langle \psi | \psi \rangle = \sqrt{\|\psi\|}$. We may also define the completeness relation for the braket notation as follows

Definition 2.4. *For any cauchy sequence $\{|\psi_d\rangle\}$ there exists $|\psi\rangle \in \mathcal{H}$ such that $\lim_{d\to\infty} |\psi_d\rangle = |\psi\rangle$*

which is analogous to definition 2.3. If we were dealing with an infinite Hilbert space there would be an additional requirement, that is, a Hilbert space is separable if and only if it admits a countable orthonormal basis, which we also find is true.

Another nice property of Dirac notation is how we may express matrices M_{nm}, which represent the operators $\hat{O}$ in quantum mechanics. We may express M_{nm} as follows

$$M_{nm} = |\psi\rangle\langle\phi|$$

where $[|\psi\rangle][\langle\phi|] = (n \times 1)(1 \times m) = n$ by m matrix This notation is incredibly useful for all realms of quantum mechanics, and is especially useful for when we discuss projector operators and spectral decomposition . This is because it allows us to quickly identify orthonormal states and allows us to determine the structure of an object. Where if two states $|\psi\rangle$ and $|\phi\rangle$ are orthogonal we have the following relation, $\langle \psi | \phi \rangle = 0 = \langle \phi | \psi \rangle$. In quantum mechanics we like to ensure that we are dealing with states that are both orthogonal and normalised to unity.

Since we have now seen that the bra's and ket's satisfy the properties of a Hilbert space, let us introduce two key theorems *The Cauchy-Schwarz* and *The Triangle inequality* . These inequalities stem directly from the properties of a Hilbert space and are used in several areas of quantum mechanics, although in this review we will not require their services .

Theorem 2.1. : *Let $(\mathcal{H}, \langle .|. \rangle)$ be a Hilbert space and let $|\psi\rangle , |\phi\rangle$ be arbitrary vectors in V then the following hold:*

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle \langle\phi|\phi\rangle \tag{2.8}$$

$$||\psi\rangle + |\phi\rangle| \leq \sqrt{\langle\psi|\psi\rangle} + \sqrt{\langle\phi|\phi\rangle} \tag{2.9}$$

where (2.8) is the Cauchy-Schwarz inequality and (2.9) is the Triangle inequality .

Let us now prove the Cauchy-Schwarz inequality, from which we can then prove the triangle inequality.

Proof. Let $|\psi\rangle , |\phi\rangle \in \mathcal{H}$. If $|\psi\rangle = \mathbf{0}$ then the inequality is automatically satisfied. For when this is not the case we construct an orthogonal decomposition via the Gram-Schmidt procedure

$$|\psi\rangle = \frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle} |\phi\rangle + |\mu\rangle$$

where $|\mu\rangle$ is orthogonal to $|\phi\rangle$. Now setting $X = \frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle}$ and re-writing the above as follows $|\mu\rangle = |\psi\rangle - X |\phi\rangle$, we take the inner product of $|\mu\rangle$ with itself to get the following

$$\langle\mu|\mu\rangle = \langle\psi|\psi\rangle - \bar{X} \langle\phi|\psi\rangle - X \langle\psi|\phi\rangle + |X|^2 \langle\phi|\phi\rangle \geq 0$$

where $\bar{X}$ is the complex conjugate to X. We then substitute X back in to the equation and simplify

$$\langle\psi|\psi\rangle - \frac{\langle\psi|\phi\rangle}{\langle\phi|\psi\rangle} \langle\phi|\phi\rangle \geq 0$$

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle \langle\phi|\phi\rangle$$

$\square$

With the Cauchy-Schwarz inequality proven, let us use it to prove the triangle inequality (2.9)

Proof. Let us begin by squaring $|| |\psi\rangle + |\phi\rangle ||^2$ to get the following

$$|| |\psi\rangle + |\phi\rangle ||^2 = \langle\psi + \phi|\psi + \phi\rangle$$

$$= \langle\psi|\psi\rangle + \langle\phi|\phi\rangle + \langle\psi|\phi\rangle + \overline{\langle\psi|\phi\rangle}$$

$$= \langle\psi|\psi\rangle + \langle\phi|\phi\rangle + 2\mathbf{Re} \langle\psi|\phi\rangle$$

and in using 2.8 we get the following

$$\leq \langle\psi|\psi\rangle + \langle\phi|\phi\rangle + 2\sqrt{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}$$

$$= (\langle\psi|\psi\rangle + \langle\phi|\phi\rangle)^2$$

thus taking the square root as both sides are positive, we get the triangle inequality (2.9) $\square$

It is now wise to introduce an important example of a Hilbert space that is of great use throughout quantum mechanics, especially in the physical sense. That is the space of square integrable functions $L^2(\mathbb{C})$.

Definition 2.5. *Let A be an open set in $\mathbb{C}$. Then the space $L^2(A)$ is the set of complex valued functions such that*

1. *$\langle f|g\rangle = \int_{-\infty}^{\infty} \|f(x)\|^2\, dx < \infty$*

2. *$\langle f|g\rangle = \int_A \overline{f(x)}g(x)\, dx$*

where $f, g : A \to \mathbb{C}$ are continuous functions

The space of square integrable functions satisfy all the properties of a complex inner product space, with the added complete normed space property. In quantum mechanics f is the conjugate function to g, where g is represented by the wavefunction $\psi(\mathbf{x}, t)$.

2.3   Orthonomal basis

As briefly mentioned above, in quantum mechanics we like to deal with orthonormal states as they highlight the mathematical structure of an object. But what exactly is a basis? A basis is set of vectors that are linearly independent and span a d-dimensional space, in our case the Hilbert space $\mathcal{H}$. This means that any vector $|\psi\rangle$ has a unique decomposition such that it can be written as a linear combination of the basis vectors $|\psi\rangle = \sum_{i=1}^{d} c_i |e_i\rangle$, where the c_i are unique complex coefficients $c_i, \ldots, c_d$ and the $|e_i\rangle$ are the basis vectors that span d.

Definition 2.6. *Let $\mathcal{H}$ be a Hilbert space. A basis $\{|e_1\rangle \ldots |e_d\rangle\}$ of $\mathcal{H}$ is called orthonormal if and only if*

$$\langle e_i | e_j \rangle = \delta_i j = \begin{cases} 1, & \text{if } i = j. \\ 0, & \text{if } i \neq j \end{cases} \tag{2.10}$$

$\forall i, j = 1, \ldots, d$

In the case that our set of vectors is not orthonomal , we can make them orthonormal by use of the Gram-Schmidt procedure. It is important to add, that as an immediate consequence of this definition we can write the following Fourier decomposition of a state $|\psi\rangle$ as follows

$$|\psi\rangle = \sum_{i=1}^{d} \langle e_i | \psi \rangle |e_i\rangle$$

where $\langle e_i | \psi \rangle$ are the Fourier coefficients of $|\psi\rangle$. This condition can easily be proved by taking the inner product of each side with $|e_i\rangle$ and then using definition 2.6.

So we have now have a good feel for the framework in which the quantum mechanics takes place, but what about the action and the dynamics ? In order to describe this, we will require linear operators.

2.4 Linear operators

Within quantum mechanics linear operators play a vital role as they actually give a meaning to the seemingly abstract mathematical structure. They allow us to define measurements and give a description of the dynamics taking place among a particular quantum system . Aside from that, any linear operator on a d-dimensional Hilbert space $\mathcal{H}$ may be represented as a matrix and so follows the mathematical laws associated with matrices.

Definition 2.7. *: Let $(\mathcal{H}, \langle .|.\rangle)$ be a Hilbert space. A linear operator on $\mathcal{H}$ is a map $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$ satisfying the linearity condition $\hat{A}(\alpha |\phi\rangle + \beta |\psi\rangle) = \alpha \hat{A} |\psi\rangle + \beta \hat{A} |\phi\rangle . \; \forall |\psi\rangle , |\phi\rangle \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C}$*

With the matrix structure of operators in mind, let us now introduce a very important concept that is crucial in our definition of postulate 2, and is how we define operators that represent observable quantities in quantum mechanics. Recall from basic linear algebra that the adjoint of a matrix $A = A_{ij}$ is A^*. Where A^* is found by taking the transpose of matrix $A^T = A_{ji}$ and then taking the conjugate of the transposed matrix $\overline{A_{ji}}$. A matrix A_{ij} that is equal to its adjoint is called self-adjoint and has real eigenvalues. It is important that our operators have real eigenvalues, as the eigenvalues tell us what measurement we are to expect from a given observable. It would not make sense to have a "complex" physical quantity and it is for this reason that all observable quantities in quantum mechanics are represented by self-adjoint operators. Four important linear operators that are used through out quantum mechanics and quantum information theory are the Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.11}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2.12}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{2.13}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.14}$$

you will quite commonly see the $1, 2$ and 3 replaced with x, y and z as they represent the components of spin of a spin-$\frac{1}{2}$ particle, along the respective directions for angular momentum.

2.5 Trace

An important matrix function is the trace and has a whole variety of uses throughout quantum mechanics. The trace of a matrix $A \in M_d$ is defined as follows

$$Tr(A) = \sum_i A_{ii}$$

Definition 2.8. *Suppose $\{|\phi_i\rangle\}$ is a complete orthonormal basis set in $\mathcal{H}$. Since a linear operator on a d-dimensional Hilbert space can be represented as a matrix with elements $A_{ij} = \langle\phi_i|\hat{A}|\phi_j\rangle$, we can define the trace of an operator as follows*

$$Tr(\hat{A}) = \sum_{i=1}^{d} \langle\phi_i|\hat{A}|\phi_i\rangle \tag{2.15}$$

Let us now give some basic properties of the trace

1. Linearity : $Tr(\alpha\hat{A} + \beta\hat{B}) = \alpha Tr(\hat{A}) + \beta Tr(\hat{B})$

2. Cyclicity : $Tr(\hat{A}\hat{B}) = Tr(\hat{B}\hat{A})$

3. Basis free representation: If $\{|\mu_1\rangle, \ldots, |\mu_d\rangle\}$ is another complete orthonormal basis in $\mathcal{H}$ then

$$Tr(\hat{A}) = \sum_{i=1}^{d} \langle\phi_i|\hat{A}|\phi_i\rangle = \sum_{i=1}^{d} \langle\mu_i|\hat{A}|\mu_i\rangle$$

4. $Tr(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$ for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$

2.6 Normal and Unitary Operators

Let us introduce a very important type of linear operator, the unitary operator $\hat{U}$. The unitary operator is a special type of normal operator that enables us to describe the evolution of a quantum system, from one state $|\psi\rangle$ to some output state $\hat{U}|\psi\rangle$

Definition 2.9. *Let $\mathcal{H}$ be a Hilbert space. An operator $\hat{N}$ on $\mathcal{H}$ is called normal if $\hat{N}\hat{N}^\dagger = \hat{N}^\dagger\hat{N}$.*

where a unitary operator is defined as

Definition 2.10. : *A operator $\hat{U}$ is unitary if and only if the following holds $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$ where $\hat{U}^\dagger$ is the adjoint of $\hat{U}$. Unitary operators have the following interesting properties:*

1. *The rows and columns of $\hat{U}$ form an orthonormal basis*

2. *$\hat{U}$ preserves inner products $\left\langle \psi\hat{U} \middle| \hat{U}\phi \right\rangle = \langle \psi | \hat{U}^\dagger\hat{U} | \phi \rangle = \langle \psi | \phi \rangle$ which implies $\hat{U}$ preserves norms and angles up to some phase*

3. *The eigenvalues of $\hat{U}$ are all of the form $\exp(i\theta)$*

4. *Which means $\hat{U}$ can be diagonalized in the following way*

$$\hat{U} = \begin{pmatrix} e^{i\theta_1} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & e^{i\theta_d} \end{pmatrix}$$

A nice property of unitary dynamics is that it is fully reversible for an isolated system, in the same sense as classical Newtonian dynamics [3]. An important example of a unitary operator is the Hadamard, which we will see much of throughout this review. We can define the Hadamard as follows

$$\hat{H} = |+\rangle\langle 0| + |-\rangle\langle 1| \tag{2.16}$$

where $|0\rangle$ and $|1\rangle$ represent the basis states and $|+\rangle$ and $|-\rangle$ are the Hadamard basis states. Which are defined as

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{2.17}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{2.18}$$

this means that we may write $\hat{H}$ in following matrix form

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2.19}$$

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[3]The irreversible element comes from quantum measurements

We also see that the Hadamard acts on the two basis states $|0\rangle$ and $|1\rangle$ in the following way; $\hat{H}|0\rangle = |+\rangle$ and $\hat{H}|1\rangle = |-\rangle$. If we then make a measurement on one of the Hadamard basis states we find that it collapses to either $|0\rangle$ or $|1\rangle$ with a probability of $\frac{1}{2}$. This means that the Hadamard is a balanced coin, in the context of the discrete quantum walks. We shall discuss other types of 'coins' in section 4 that are not balanced.

2.7   Projectors

Projectors play a key role in quantum mechanics, especially in the role of measurement. Suppose U is a k-dimensional subspace of the Hilbert space $\mathcal{H}$, it can be shown that there exists a unique decomposition of a vector $|\psi\rangle$ in to its component in U and $U^\perp$, where $U^\perp$ is the subspace orthogonal to U, so that we have

$$|\psi\rangle = |\psi_U\rangle + |\psi_{U^\perp}\rangle$$

where $|\psi_U\rangle \in U$ and $|\psi_{U^\perp}\rangle \in U^\perp$.

Thus we define the orthogonal projection onto U by

$$\boldsymbol{P}_U : |\psi\rangle \mapsto |\psi_U\rangle$$

we can see that $\boldsymbol{P}_U$ has the following properties; $\boldsymbol{P}_U \cdot \boldsymbol{P}_U = \boldsymbol{P}_U^2 = \boldsymbol{P}_U$ and $\boldsymbol{P}_U = \boldsymbol{P}_U^*$ so the projector is self adjoint.

Definition 2.11. *Let $\mathcal{H}$ be a Hilbert space. A projection operator $\hat{P}$ is a linear operator on $\mathcal{H}$ satisfying*

1. *$\hat{P} = \hat{P}^*$ self-adjoint*

2. *$\hat{P}^2 = \hat{P} \cdot \hat{P} = \hat{P}$ thus the projector is orthogonal if and only if it is self-adjoint*

In the general case where $U := Range(\hat{P})$ is multidimensional, we can choose an arbitrary orthonormal basis $\{|e_1\rangle, \ldots, |e_k\rangle\} \in U$ and express $\hat{P}$ as the sum of one-dimensional

projectors onto these vectors

$$\hat{P} = \sum_{i=1}^{k} |e_i\rangle\langle e_i| \tag{2.20}$$

As a final point, the trace acts on projectors in the following way, if $\hat{P}_\psi = |\psi\rangle\langle\psi|$ and $\hat{P}_\phi = |\phi\rangle\langle\phi|$ are two 1-dimensional projectors, then $Tr(\hat{P}_\psi \hat{P}_\phi) = |\langle\psi|\phi\rangle|^2$, provided $\|\psi\| = \|\phi\| = 1$.

2.8 Spectral Decomposition

Before we actually introduce the definition of the spectral theorem remember that eigenvalues λ and the eigenvectors $|i\rangle$ can be found by solving the following equation

$$\hat{A}|i\rangle = \lambda|i\rangle$$

$(\hat{A} - \lambda\hat{I})|i\rangle = \mathbf{0}$ As $|i\rangle \neq \mathbf{0}$ we have

$$\det\left|\hat{A} - \lambda\hat{I}\right| = \mathbf{0} \tag{2.21}$$

where the set of all possible eigenvalues of $\hat{A}$ is called the spectrum of $\hat{A}$ and is denoted by $\sigma(\hat{A})$. The linear subspace spanned by the eigenvectors with eigenvalue λ is called the eigenspace, and its dimension is called the multiplicity of λ.

Spectral decomposition is an extremely useful representation theorem for normal operators, as any normal operator may be characterised completely in terms of their eigenvalues and eigenvectors (their spectral data)

Theorem 2.2. *Let $\hat{A}$ be a normal operator on a d-dimensional Hilbert space $\mathcal{H}$. Then there exists an orthonormal basis $\{|\psi_1\rangle, \ldots, |\psi_d\rangle\}$ and a sequence of complex eigenvalues $\{\lambda_1, \ldots, \lambda_d\}$ such that*

$$\hat{A} = \sum_{i=1}^{d} \lambda_i |\psi_i\rangle\langle\psi_i| \tag{2.22}$$

We shall now see an example that connects the ideas of the projector operator and spectral decomposition to quantum mechanics.

Example: We refer back to the Pauli matrix that represents the spin component of angular momentum of a spin 1/2 particle in the x-direction, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Finding the eigenvalues is incredibly simple since the matrix is symmetric and so we have $\lambda_{1,2} = \pm 1$. Solving equation (2.21) for λ_1 we find the components of the eigenvector $|+\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ equal one another, $a = b$, so normalising and setting $a = 1$ we get the following eigenvector $|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. Likewise for λ_2, we find $a = -b$ and so in doing the same as before, normalising and setting $a = 1$ we get the following eigenvector $|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. In order to construct the projectors onto $|+\rangle$ and $|-\rangle$ we use equation (2.20) and define

$$\hat{P}_+ = |+\rangle\langle+| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\hat{P}_- = |-\rangle\langle-| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

thus we see that the completeness relation is satisfied $\hat{P}_+ + \hat{P}_- = \hat{I}$ and that the projectors are orthogonal $\hat{P}_+\hat{P}_- = 0$ and thus the spectral decomposition of σ_1 is given as

$$\sigma_1 = \lambda_1 \hat{P}_+ + \lambda_2 \hat{P}_- = \hat{P}_+ - \hat{P}_- \tag{2.23}$$

where we have used the spectral theorem (2.22).

2.9 Tensor products

In quantum mechanics we like to deal with several different systems which are part of several different Hilbert spaces. In order to connect these systems we introduce the tensor product, which in one sense acts as our glue to join the different systems together. Let us first define the tensor product for matrices

Definition 2.12. *Let $A \in M_{n,m}$ and $B \in M_{k,p}$ be two complex matrices. The tensor product $A \otimes B$ is the $mk \times np$ matrix with the following block structure*

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{pmatrix} \tag{2.24}$$

as an example let us take the tensor product of two 2×1 vectors

$$\begin{pmatrix} 2 \\ 8 \end{pmatrix} \times \begin{pmatrix} 3 \\ 5 \end{pmatrix} = \begin{pmatrix} 6 \\ 10 \\ 24 \\ 40 \end{pmatrix} \tag{2.25}$$

The properties of the tensor product on Hilbert spaces are defined as follows

Definition 2.13. *Let U and V be two linear vector spaces. The tensor product $U \otimes V$ is the linear space spanned by elements of the form $|\psi\rangle \otimes |\phi\rangle$, where $|\psi\rangle \in U$ and $|\phi\rangle \in V$ such that the following relations hold*

1. $(|\psi\rangle + |\psi'\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes |\phi\rangle + |\psi'\rangle \otimes |\phi\rangle$

2. $|\psi\rangle \otimes (|\phi\rangle + |\phi'\rangle) = |\psi\rangle \otimes |\phi\rangle + |\psi\rangle \otimes |\phi'\rangle$

3. $(\alpha |\psi\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes (\alpha |\phi\rangle) = \alpha(|\psi\rangle \otimes |\phi\rangle)$

where $\alpha \in \mathbb{C}$ and $u' \in U$ and $v' \in V$ are arbitrary vectors.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. The tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ becomes a Hilbert space when endowed with the inner product

$$\langle \psi \otimes \phi | \psi' \otimes \phi' \rangle = \langle \psi | \psi' \rangle \langle \phi | \phi' \rangle$$

to a sesquilinear form $\langle \cdot | \cdot \rangle : \mathcal{H}_1 \otimes \mathcal{H}_2 \times \mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathbb{C}$

To finish our discussion on tensor products let us see how the tensor product acts on linear operators. So as before let $|\psi\rangle \in U$ and $|\phi\rangle \in V$ and let $\hat{A} : \mathcal{H}_1 \to \mathcal{H}_1$ and

$\hat{B} : \mathcal{H}_2 \to \mathcal{H}_2$ be linear operators. Then we can define a linear operator $\hat{A} \otimes \hat{B}$ on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ as follows

$$(\hat{A} \otimes \hat{B})(\ket{\psi} \otimes \ket{\phi}) = \hat{A}\ket{\psi} \otimes \hat{B}\ket{\phi} \tag{2.26}$$

2.10　The Postulates

Let us now discuss the so called "loose" axioms of quantum mechanics, that being the postulates. The postulate should be seen as a rough guide on which we construct our mathematical framework, they are by no means "rigourous" laws in the mathematical sense , but are analogous to the axioms of analysis except based on a more physical footing.

It can vary between texts on how many such postulates there are, it tends to range between 4 and 5 postulates, depending on whether the observables postulate has been absorbed into the measurement postulate, as it can be deduced as a consequence of the measurement postulate. In this review we shall look at 5 postulates, those being "States, Observables, Unitary Evolution, Measurement and Composite Systems ". It should be noted that although we shall discuss all 5 postulates, we shall only do so briefly since there are many technicalities and subtle points that we are simply not able to discuss here. For a more complete picture, I strongly recommend that the reader view the references stated at the beginning of this chapter.

Postulate 1: State The state space of each quantum system is a Hilbert space $\mathcal{H}$. A state is a normalised vector $\ket{\psi}$ up to a constant phase factor. Equivalently, the state may be described by a one dimensional projection $\ket{\psi}\bra{\psi}$. The state vector $\ket{\psi}$ contains all the information we would ever need to know regarding that quantum system.

Postulate 2: Observables As discussed before, the observables of a system with a state space $\mathcal{H}$ are each represented by self-adjoint operators. This is because all self-adjoint operators have real eigenvalues, which means any observable that is represented by an

operator $\hat{O}$ may be decomposed and written in terms of its spectral data. In general, operators do not commute like there classical counterparts, that is $\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0$. This is due to the fact that observables are represented by operators, which are matrices, which in general do not commute, where as the classical observables are well defined objects.

Postulate 3: Unitary Evolution(The Dynamics) In order to understand how a state evolves in time (the dynamics) we say that the evolution of a closed quantum system is described by a unitary transformation of the state space. More precisely, the time dependent state $|\psi(t')\rangle$ of the system at t' is related to the state of the system at an earlier time t by the unitary operator $\hat{U}(t', t)$

$$|\psi(t')\rangle = \hat{U}(t', t) |\psi(t)\rangle \tag{2.27}$$

In general the evolution of an isolated system is described by the **Schrödinger Equation**

$$E |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \tag{2.28}$$

$$\frac{\partial}{\partial t} |\psi(t)\rangle = -\frac{i}{\hbar} \hat{H} |\psi(t)\rangle$$

$$\frac{\partial}{\partial t} \hat{U}(t', t) = -\frac{i}{\hbar} \hat{H} \hat{U}(t', t) \tag{2.29}$$

where $\hat{H} = \sum_i E_i |E_i\rangle\langle E_i|$ is the self-adjoint Hamiltonian operator of the system with eigenvalues E_i, which represent energy levels and $\hbar$ is planks reduced constant, which is commonly set to $\hbar = 1$ in mathematical contexts. In solving the time dependent Schrödinger equation, we are able to find the state at t' if at time t the state $|\psi(t)\rangle = |E_i\rangle$

$$\psi(t') = \exp\left(\frac{i}{\hbar}(t' - t)E_i\right) |E_i\rangle \tag{2.30}$$

in solving (2.29), provided $\hat{H}$ is not time dependent we gain the following

$$\hat{U}(t', t) = \exp\left(-\frac{i}{\hbar}\hat{H}(t' - t)\right)$$

which is the unitary that describes the transformation from t to t'. Obviously when $\hat{H}$ is time dependent we will get a different unitary.

For the measurement postulate we shall go in to a bit more depth , as although measurement may seem like a rather minor topic, it is of great importance. It is what makes the quantum world quantum and the classical world classical.

Before we actually fully define the postulate let first define the projection valued measure

Definition 2.14. *Let $\mathcal{H}$ be the state space of a quantum system. A projection valued measure over a set $\{\lambda_1, \ldots, \lambda_k\}$ is given by a collection of orthogonal projections $\{\hat{P}_{\lambda_1}, \ldots, \hat{P}_{\lambda_k}\}$ on subspaces of $\mathcal{H}$, with the following properties:*

1. *Orthogonality $\hat{P}_{\lambda_i}\hat{P}_{\lambda_j} = \delta_{ij}\hat{P}_{\lambda_i}$*

2. *Completeness $\sum_{i=1}^{k} \hat{P}_{\lambda_i} = \hat{I}$*

For each subset $E \in \{\lambda_1, \ldots, \lambda_k\}$ we define

$$P(E) = \sum_{\lambda_i \in E} \hat{P}_{\lambda_i}$$

where the projection $P(E)$ will be used to define probability that an event E will occur.

It should also be noted that the set of elements λ_i only play the role of labels for the projections and nothing more.

With projection value measure now defined let us formally state the measurement postulate

Postulate 4: Measurement

1. A quantum measurement with outcomes $\{\lambda_1, \ldots, \lambda_k\}$ on a system with state space $\mathcal{H}$, is described by a projection valued measure $\{\hat{P}_{\lambda_1}, \ldots, \hat{P}_{\lambda_k}\}$ on $\mathcal{H}$

2. The result of the measurement is random and forms the probability distribution

$$P(\lambda_i) = \|\hat{P}_{\lambda_i} |\psi\rangle\|^2 = \langle\psi|\hat{P}_{\lambda_i}|\psi\rangle = Tr(|\psi\rangle\langle\psi| \hat{P}_{\lambda_i})$$

where $|\psi\rangle$ is the state of the system before the measurement

3. If the measurement outcome is λ_i, then the state of the system immediately after the measurement is

$$|\psi'\rangle = \frac{1}{\sqrt{P(\lambda_i)}}\hat{P}_{\lambda_i}|\psi\rangle = \frac{\hat{P}_{\lambda_i}|\psi\rangle}{\|\hat{P}_{\lambda_i}|\psi\rangle\|}$$

The measurement postulate is one of the wonders of quantum mechanics, it tells us that world is not all that it may seem, that is we live in a probabilistic world and not a deterministic world. As a by product of the the measurement postulate we gain Heisenberg's uncertainty principle

$$\sigma_A\sigma_B \geq \frac{1}{2}\left|\left\langle\left[\hat{A}, \hat{B}\right]\right\rangle_\psi\right| \tag{2.31}$$

where $\hat{A}$ and $\hat{B}$ are two observable, σ_A, σ_B are the standard deviations $\sigma_O = \sqrt{\left\langle\hat{O}_\psi^2\right\rangle - \langle O\rangle_\psi^2}$, and $\left\langle\hat{O}\right\rangle_\psi = \langle\psi|\hat{O}|\psi\rangle$ is the expectation value of some observable with respect to some quantum state $|\psi\rangle$. What the uncertainty principle tells us, is that regardless of how precise we measure one observable, uncertainty in the measurement of the other observable will ensure that we can not measure the other observable precisely, this is a rather profound statement. However, if two observables commute, that is $\left[\hat{A}, \hat{B}\right] = 0$, then we can measure both observables precisely and simultaneously.

As an example of the measurement process, let us prepare a qubit in the state $|\psi\rangle = C_+|0\rangle + C_-|1\rangle$. If we measure in the standard basis $\{|0\rangle, |1\rangle\}$ then we obtain two possible outcomes C_+ and C_-, with respective probabilities $|\langle 0|\psi\rangle|^2 = |C_+|^2$ and $|\langle 1|\psi\rangle|^2 = |C_-|^2$. Once we have carried out the measurement, we cannot gain any more information about the state $|\psi\rangle$ as it has collapsed(projected) on to one of the basis states $|0\rangle$ or $|1\rangle$.

For postulate 5, we refer back to the tensor product as discussed in the pervious section.

Postulate 5 : Composite Systems The state space of a composite system is the tensor product of the state spaces of the component systems. If the components are numbered

1 through to N, and the system number i is prepared in the state $|\psi_i\rangle$ in isolation from others, then the joint state of the total system is

$$|\psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_N\rangle \tag{2.32}$$

2.11 Qubits, Entanglement and Decoherence

Let us now introduce three concepts; qubits, entanglement and decoherence. These aspects of quantum information theory all have incredibly interesting properties, that make the world of quantum mechanics and quantum information such an interesting place.

2.11.1 Qubits

We did briefly encounter the qubit at the begin of this section (equation 2.1), but what exactly is a qubit? A qubit is the quantum equivalent of the classical bits 0 and 1. The qubit makes use of one of the most fundamental properties of quantum mechanics, that being the linear superposition of states. Because of this quantum property qubits can be in a superposition of both the 0 bit and the 1 bit at the same time

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \tag{2.33}$$

where $\alpha, \beta \in \mathbb{C}$ and $|0\rangle$ and $|1\rangle$ are our quantum analogues to the classical bit. Since the qubit can be in a superposition of the 0 and 1 bits, if we have N qubits, this is equivalent to 2^N classical bits, which is remarkable. If you consider the bog standard, 32-bit classical home computer, the quantum equivalent would contain 2^32 classical bits, which is a truly bewildering number. This is just another reason why so many are working on developing quantum computers.

Figure 1: A comparison of the classical bits 0 and 1, to the qubit, which is in a superposition of those states. Which means for N qubits, we have 2^N classical bits [28]

If we refer back to the 3 Pauli matrices(2.12-2.14), we find that they are incredibly useful for representing our qubit. We find that the corresponding eigenvalues of (2.12-2.14) are $\lambda_{1,2} = \pm 1$ and the corresponding eigenvectors for $\lambda_{1,2}$ are; $|\chi_{x_1,x_2}\rangle = \frac{(|0\rangle \pm |1\rangle)}{\sqrt{2}}$ for σ_1, $|\chi_{y_1,y_2}\rangle = \frac{(|0\rangle \pm i|1\rangle)}{\sqrt{2}}$ for σ_2 and $|\chi_{z_1}\rangle = |0\rangle$ and $|\chi_{z_2}\rangle = |1\rangle$ for σ_3. This is very convenient for us, as the eigenvectors of the Pauli operators represent the state of a qubit. In combining the information of the eigenvectors we are able to construct the Bloch sphere. The Bloch sphere has a unit radius , with each point on the sphere representing a different pure state. Opposite points represent a pair of mutually orthogonal states and we can express generally a qubit's state on the sphere as follows

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{2.34}$$

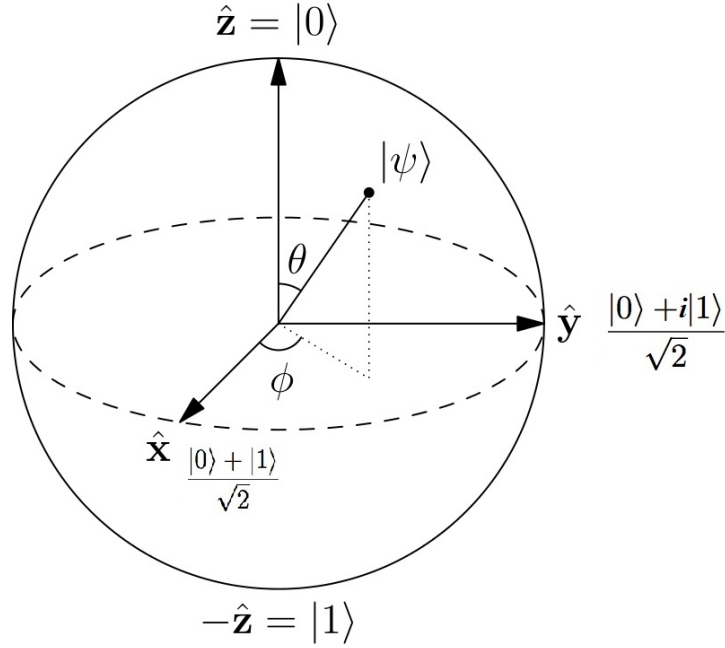where θ and ϕ are the angles in spherical coordinates.

Figure 2: The Bloch sphere, is a very useful representation for 1-qubit. It can be completely characterised by the state $|\psi\rangle$ as defined by equation (2.34)

2.11.2 Entanglement

Entanglement is a the heart of many processes in quantum information, yet it is very difficult to give a precise definition of entanglement , other than it is a property of an entangled state. It does not have a classical analogue and Einstein labelled it "spooky action at a distance". A state that is entangled essentially corresponds to the correlations between two or more quantum systems, in the most simplest of definitions a state is entangled if we are not able to take the product of two or more states and decompose it in to the original products, if we are able to do this then the state is not entangled. As an example consider a system of 2 qubit state on the Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$,

$$|\psi_{ent}\rangle = \frac{(|0 \otimes 0\rangle + |1 \otimes 1\rangle)}{\sqrt{2}}$$

, is it possible to decompose this product in to two separate systems? The answer is no, we could try and decompose it in the following way $|\psi_1\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and $|\psi_2\rangle = \frac{|0\rangle-|1\rangle}{\sqrt{2}}$, but

in taking the tensor product of $|\psi_1\rangle \otimes |\psi_2\rangle$ we have the additional terms $-|0 \otimes 1\rangle + |1 \otimes 0\rangle$ which do not cancel and so our state $|\psi_{ent}\rangle$ is indeed entangled. For a more interesting view of entanglement , without any mathematics please read [5].

2.11.3   Decoherence

Decoherence is like the marmite of the quantum world, you either love it or you hate it. It is essentially an effect that occurs when an isolated quantum system begins to be effected by the outside world, it begins to lose information. As the system becomes nosier, the coherent quantum state stops being coherent. Eventually after enough noise is introduced into the system, i.e. as the system gets larger and larger, it begins to quickly revert back to the classical system and all the quantum properties and effects disappear. Decoherence in one sense bridges the gap between the quantum and classical world, and in one sense is just a manifestation of the second law of thermodynamics. However, decoherence can be huge problem in quantum information, as experimentally we want to keep all the quantum properties of the system in tact for long periods of time, we also want to be able to combine several different systems together, which is incredibly difficult due to decoherence. For this reason decoherence is a topic of intense study and research, and although I give no mathematics of decoherence here I strongly recommend that the reader read about the property of decoherence as it is incredibly interesting [7].

3 The Classical Random Walk

Let us begin with a brief introduction of both the discrete and continuous classical random walks, from which the story of the quantum random walks began. The classical random walk is what is classed as a Markov process, where a Markov process is a simple stochastic process, which is either discrete in time $X(n)$ or continuous in time $X(t)$. In a Markov process the distribution of future states, depends only on the present state and not on how it arrived in the present state.

3.1 The Classical Discrete Random Walk

We first introduce the Bernoulli random walk [34], which will make as an interesting comparison with the equivalent discrete quantum walk. The Bernoulli walk is an unbiased walk that takes place on a line and moves in discrete time steps $t \equiv n \in \mathbb{Z}$. It is a stochastic process that is described by the random variables $\mathbf{X}(n) = \{X(1), \ldots, X(n)\}$. The walker begins at the centered position $X(0) = 0$ and depending on some coin flip jumps in each time step, to either the left or the right, with a probability of $\frac{1}{2}$ and so we would expect the probabilities of being in a particular position to be distributed in the following way

$X(n)$ $\diagdown$ n	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{3}{8}$		$\frac{3}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{1}{4}$		$\frac{3}{8}$		$\frac{1}{4}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{5}{32}$		$\frac{5}{16}$		$\frac{5}{16}$		$\frac{5}{32}$		$\frac{1}{32}$

Table 1: Table of classical probabilities for the unbiased discrete random walk on the line. Where n represents the discrete time step and $X(n)$ represents the position of the walker.

Since repeated coin flips are assumed to be statistically independent of one another, let us introduce the identical, independently distributed (i.i.d) random numbers $Z(n) \in \{-1, 1\}$,which represent our steps to the right $Z(n) = 1$ for a heads and our steps to the

left $Z(n) = -1$ for a tails. We can describe the probability distribution of the Bernoulli walk as follows

$$P(z;n) = \frac{1}{2}(\delta(z-1) + \delta(z+1)) \tag{3.1}$$

Since it is assumed that all the $Z(n)$ at different time steps are independent , it means we can construct the following joint probability density function [34], via multiplication

$$P(z_n, z_{n+l}; n, n+l) = P(z_n; n)P(z_{n+l}; n+l) \tag{3.2}$$

where $l > 0$. We then have the discrete time random process with position $X(n) \in \mathbb{Z}$, where $X(n) = X(n-1) + Z(n) = \sum_{m=1}^{n} Z(m)$.

In defining $X(n)$ we can now calculate the mean and the variance , and thus the width of the distribution. For the nth time step we have

$$\mathbb{E}[X(n)] = \sum_{m=1}^{n} \mathbb{E}[Z(m)] = \sum_{m=0}^{n} zP(z;n) = -1\frac{1}{2} + 1\frac{1}{2} = 0 \tag{3.3}$$

which is exactly what we'd expect for a centred process. Calculating the variance we find

$$Var[X(n)] = \sum_{m=1}^{n} Var[Z(m)] = nVar[Z] = n \tag{3.4}$$

as $Var[Z] = \mathbb{E}[Z^2] - \mathbb{E}[Z]^2 = 1 - 0 = 1$ and so the width of the distribution is $\sigma = \sqrt{Var[Z]} = \sqrt{n}$. Next we aim to calculate the probability distribution for $P(z;n)$. In using the characteristic function, we find $\chi_{X(n)}(s) = (\mathbb{E}[e^{isz}])^n = \chi_Z(s)^n$ from which we can deduce [34]

$$P(x;n) = \sum_{l=-\infty}^{\infty} p_l(n)\delta(x-l) \tag{3.5}$$

where $l = n - 2m$ for some integer $0 \le m \le n$. Thus the probability of being at a particular position $X(n) = l$ at a discrete time step n is

$$p(n) = \frac{1}{2^n}\binom{n}{m} \tag{3.6}$$

where $\binom{a}{b} = \frac{a!}{(a-b)!b!}$ is the binomial coefficient. What is interesting about equations (3.5) and (3.6) is that they satisfy the central limit theorem, and so we should expect as n tends

to a large number that we get a Gaussian distribution. In rescaling $X(n) = \sqrt{n}\tilde{X}(n)$ and taking the limit as $n \to \infty$ we find

$$\lim_{n \to \infty} P(\tilde{x}; n) = \sqrt{2\pi}e^{-\frac{\tilde{x}^2}{2}} \tag{3.7}$$

However, as 3.5 is defined in terms of Dirac delta functions, this means that we are summing over Dirac delta functions and so we could have some problems with convergence [34]. Also, as we are taking the limit as $n \to \infty$, what about for large, but finite n? Thankfully as all expectation values are sufficiently nice functions, which means they converge absolutely, we do not have to worry about the fact that we are summing over dirac delta functions. Also if we do have a large, but finite n we find that we get the following asymptotic probability distribution

$$P(x; n) \sim \frac{1}{\sqrt{2\pi n}}e^{-\frac{\tilde{x}^2}{2n}} \tag{3.8}$$

which is a probability distribution in the form of a centered Gaussian, which is exactly what we should get.

3.2 Classical Discrete Time Markov Chains

We say a collection of possible values that a random variable $X(n)$ can be is described by the state space S, which in the discrete case shall refer to $\mathbb{Z}$.

Definition 3.1. *A stochastic process $\boldsymbol{X}(n)$ is called a Markov chain, if for all times $n \geq 0$ and all states $i_0, \ldots, i_n, i_{n+1} = j \in S$,*

$$P(X(n+1) = i_{n+1} = j | X(n) = i_n, X_{n-1} = i_{n-1}, \ldots, X(0) = i_0) = P(X(n+1) = j | X(n) = i)$$
$$= p_{i,j}(n, n+1)$$

where $p_{i,j}(n, n+1)$ is the probability of going from state i to a state j in one unit of time, such that for each $i \in S$ the $\sum_{j \in S} p_{i,j} = 1$. Thus we can define

$$\mathbf{P} = (p_{i,j})_{i,j \in S} \tag{3.9}$$

this is the discrete time transition matrix, which describes how all states evolve and represents a probability distribution, as the entries in the rows of $\mathbf{P}$ sum to 1 . Thus we introduce the row vector $\mathbf{p}(n+1)$,which denotes a row vector of probabilities, where $\mathbf{p}_j(n+1) = P(X(n+1) = j)$. Where the row vector of probabilities evolves according to

$$\mathbf{p}(n+1) = \mathbf{p}(n)\mathbf{P} \tag{3.10}$$

which means in order to determine all future states , we only require $\mathbf{p}(0)$ and $\mathbf{P}$.

3.3   The Continuous Time Random Walk

The continuous time random walk is typically described as Brownian motion, which was brought to fame by Albert Einstein in 1905. Now, we shall not go in to detail on Brownian motion, we aim only to discuss it briefly, as we are only interested in the statistical measures that we find from the walk and not how it is constructed. We begin by modifying our original walk, by assuming that each step has the same time duration τ and associate times $t_n = n\tau$ to the nth step of the random walk. In doing this we get Brownian motion, that is the probability distribution $P(x;t)$ obeys the partial differential equation known as the diffusion equation

$$\frac{\partial}{\partial t}P(x;t) = \frac{D}{2}\frac{\partial}{\partial x^2}^2 P(x;t) \tag{3.11}$$

where D is know as the diffusion constant $D = \frac{\sigma^2}{\tau}$. In solving the diffusion equation for a centred walk, with initial condition $P(x;0) = \delta(x-0)$ we get the following Gaussian

$$P(x;t) = \frac{1}{\sqrt{2\pi Dt}}e^{-\frac{(x^2)}{2Dt}} \tag{3.12}$$

and since it is a Gaussian distribution we can directly read off the standard deviation and the mean. As it is a centred Gaussian the mean is 0, but the width of the distribution is $\sigma = \sqrt{Dt}$ and so on average we would expect our walker undergoing Brownian motion to spread out a distance $\sqrt{Dt}$ from the origin. Which is of course very similar to the discrete case of $\sigma = \sqrt{n}$, up to a constant factor.

3.4 Classical Continuous Time Markov Chain

Let us introduce the graph $G(V, E)$, where V represents a set of vertices $\{1, \dots, v\}$ and the edges E specify which pairs of vertices are connected. In order to describe how the walker moves between connected vertices we must define our transition matrix, which is no longer discrete in time. We introduce the jumping rate γ, where if we start at any vertex the probability of jumping to any connected vertex in a time ϵ, where $\epsilon \to 0$, is $p_{jump} = \gamma\epsilon$. Thus our infinitesimal transition matrix is a $d \times d$ matrix M defined as follows

$$M_{ij} = \begin{cases} k\gamma, & i = j \text{ and } k \text{ is the degree of vertex } i \\ -\gamma, & i \neq j, \ i \text{ and } j \text{ are connected by an edge} \\ 0, & i \neq j, \ i \text{ and } j \text{ are not connected} \end{cases} \tag{3.13}$$

thus following [2] the probability of being at vertex i at time t is given by

$$\frac{\mathrm{d}p_i(t)}{\mathrm{d}t} = -\sum_j M_{ij} p_j(t) \tag{3.14}$$

solving this would give us our probability distribution of being at vertex i. Where

$$\sum_i p_i(t) = 1 \tag{3.15}$$

ensures probability is conserved. This construction of the walk will draw many parallels to the construction of the continuous time quantum walk.

4 Quantum random walks

Now that we have covered all the background material and have seen an introduction to the classical random walk in both the discrete and continuous case, we are now in a position to discuss the quantum random walks. We will begin by looking at the discrete case, in which our walker moves from position i to $i \pm 1$ on a line via a unitary coin operator $\hat{C}$, followed by a translational shift operator $\hat{S}$. We will then see how to define the discrete quantum random walk on the undirected graph $G(V, E)$. This will allow us to gain further insight in to how we construct quantum algorithms. After we have covered the discrete case we shall move on to the continuous quantum random walk, which is described by the Schrödinger equation. We see that the introduction of the complex variable i leads to something very interesting. We will finally conclude this section, by comparing the two quantum walks on the line to their classical analogues. For this section we will be using a combination of the following sources [20] [2] [35] [32] [27] .

4.1 Discrete Quantum Random Walk on The Line

The framework for the discrete quantum walk on the line , is described by the Hilbert space $\mathcal{H}$, which is the tensor product of the coin space $\mathcal{H}_c$ and the position space $\mathcal{H}_p$. Thus the total space is

$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p \tag{4.1}$$

The position space $\mathcal{H}_p$, is the Hilbert space spanned by the position states $\{|i\rangle : i \in \mathbb{Z}\}$ and is augmented by the coin space $\mathcal{H}_c$, which is spanned by the basis vectors $\{|\uparrow\rangle, |\downarrow\rangle\}$. As discussed previously, These basis vectors represent the state of a spin-$\frac{1}{2}$ particle, where spin up is $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and spin down is $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and so they act like the "flipping" of the coin. We then introduce a unitary shift operator, which enables us to transition

between different position states. The shift operator acts on $\mathcal{H}$ in the following way

$$\hat{S} : |\uparrow\rangle \otimes |i\rangle \to |\uparrow\rangle \otimes |i + 1\rangle \tag{4.2}$$

$$\hat{S} : |\downarrow\rangle \otimes |i\rangle \to |\downarrow\rangle \otimes |i - 1\rangle \tag{4.3}$$

we can see that the shift operator does not affect the coin space and that it only affects the position space. For the entire walk, we define the shift operator formally as

$$\hat{S} = |\uparrow\rangle\langle\uparrow| \otimes \sum_i |i + 1\rangle\langle i| + |\downarrow\rangle\langle\downarrow| \otimes \sum_i |i - 1\rangle\langle i| \tag{4.4}$$

which has the properties of (4.2) and (4.3) built into it and i runs over all of $\mathbb{Z}$. With the shift operator defined, let us discuss what kind of "coin flip", a rotation of the coin space, we require. Interestingly, it turns out that there is a whole family of unitary coin operators $\hat{C}$ that we can use, which one we use will depend on the behaviour we want to observe. Whether that be symmetrical (unbiased walk) or asymmetrical distributions (biased walk).

Next we construct a unitary operator $\hat{U}$, that acts upon the whole of $\mathcal{H}$ and describes the evolution of the walk

$$\hat{U} = \hat{S} \cdot (\hat{C} \otimes \hat{I}) \tag{4.5}$$

To carry out multiple steps of the discrete quantum walk, we must apply $\hat{U}$ t times to some initial state $|\psi(0)\rangle \in \mathcal{H}$, where t represents the number of steps or iterations .

$$|\psi(t + 1)\rangle = \hat{U}^t |\psi(t)\rangle \tag{4.6}$$

after applying the unitary for t steps, we make a measurement $|\psi(t + 1)\rangle$ in order to determine the state of the system, as the walk can in a superposition of lots of different position states.

In order to see some connection to the classical walk on the line, let us introduce the Hadamard coin, which we briefly saw back in section 2

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{4.7}$$

Since the Hadamard coin is balanced, we see that it can provide us with the classical random walk on the line, provided we measure the final state after every application of $\hat{U}$. Preparing the walk in an initial state $|\psi(0)\rangle = |\uparrow\rangle \otimes |0\rangle$ and acting upon this with $\hat{U}$ we get the following

$$
\begin{aligned}
|\psi(1)\rangle &= \hat{U}^1 |\psi(0)\rangle \\
&= \hat{S}\hat{H}(|\uparrow\rangle \otimes |0\rangle) \\
&= \hat{S}(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle) \text{ using eq.(2.16)} \\
&= (|\uparrow\rangle\langle\uparrow| \otimes \sum_i |i+1\rangle\langle i|)(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle) + \\
&\quad (|\downarrow\rangle\langle\downarrow| \otimes \sum_i |i-1\rangle\langle i|)(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle) \\
&= \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle + |\downarrow\rangle \otimes |-1\rangle) \quad (4.8)
\end{aligned}
$$

now performing a measurement on $|\psi(1)\rangle$, we find $a_{left} = \langle\downarrow|\psi(1)\rangle = \frac{1}{\sqrt{2}}$ and $a_{right} = \langle\uparrow|\psi(1)\rangle = \frac{1}{\sqrt{2}}$, thus the probability $P(a_{left}) = \frac{1}{2}$ and $P(a_{right}) = \frac{1}{2}$. In continuing this process of applying the unitary and then measuring, we will of course get the discrete classical random walk on a line, which is not very interesting. In order to see the quantum processes at work, let us carry out the process as before , still with the Hadamard coin, except this time we shall not measure after each iteration. Let our initial state this time be $|\psi(0)\rangle = |\downarrow\rangle \otimes |0\rangle$ and let us perform the first 3 iterations. As the Hadamard is a balanced coin, for our first iteration we get

$$
|\psi(1)\rangle = \hat{U}^1 |\psi(0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle + |\downarrow\rangle \otimes |-1\rangle)
$$

which is the same as before. Carrying out the 2nd iteration we get

$$
\begin{aligned}
|\psi(2)\rangle &= \hat{S}(\hat{H}|\psi(1)\rangle) \\
&= \frac{1}{2}[|\uparrow\rangle \otimes |2\rangle - (|\uparrow\rangle - |\downarrow\rangle) \otimes |0\rangle + |\downarrow\rangle \otimes |-2\rangle] \quad (4.9)
\end{aligned}
$$

and for the third iteration we have

$$
\begin{aligned}
|\psi(3)\rangle &= \hat{S}(\hat{H}\,|\psi(2)\rangle) \\
&= \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |3\rangle + |\downarrow\rangle \otimes |1\rangle + |\uparrow\rangle \otimes |-1\rangle - \\
&\quad\; 2\,|\downarrow\rangle \otimes |-1\rangle - |\downarrow\rangle \otimes |-3\rangle)
\end{aligned}
\tag{4.10}
$$

In analysing equation (4.10) we find that the walker can be in multiple positions, each with its own probability. The probability that the walker is in particular position is given by the following table

t \ i	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{17}{32}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{5}{32}$		$\frac{1}{32}$

Table 2: The probability of being found at position i after t steps of the quantum random walk on the line, with the initial state $|\psi(0)\rangle = |\downarrow\rangle \otimes |0\rangle$.

From table (2) we see that the quantum walk is asymmetric with a drift to the left. This is because we have begun in the initial state $|\psi(0)\rangle = |\downarrow\rangle \otimes |0\rangle$ with a balanced coin. If we had started in the state $|\psi(0)\rangle = |\uparrow\rangle \otimes |0\rangle$ with a balanced coin, then we would observe a skew to the right. However, if we had chosen a different (unbalanced) coin this would have not been the case.
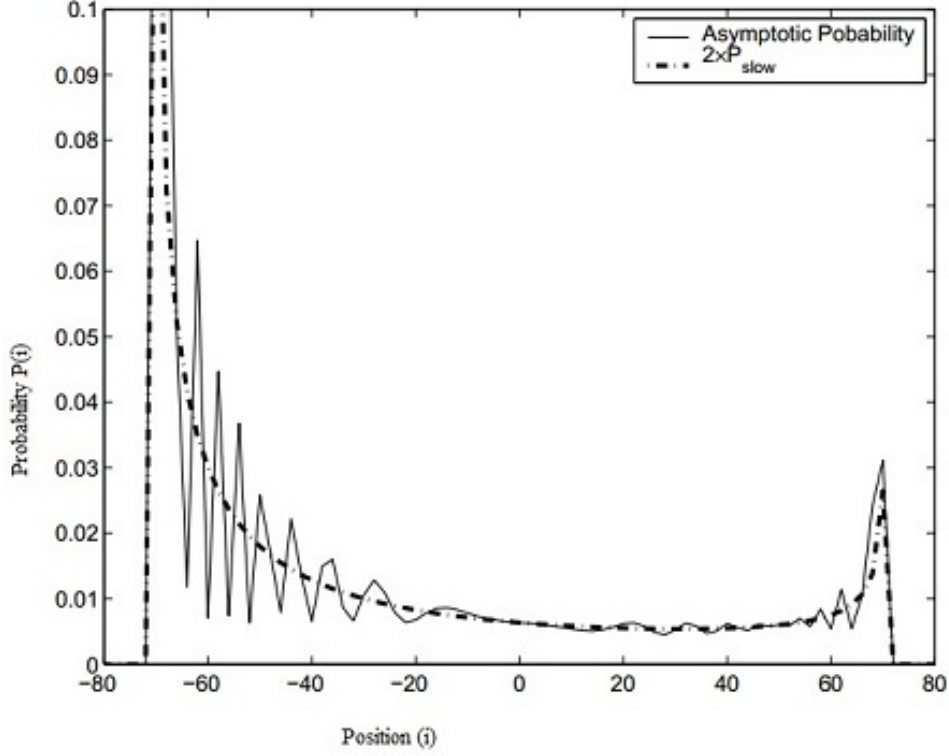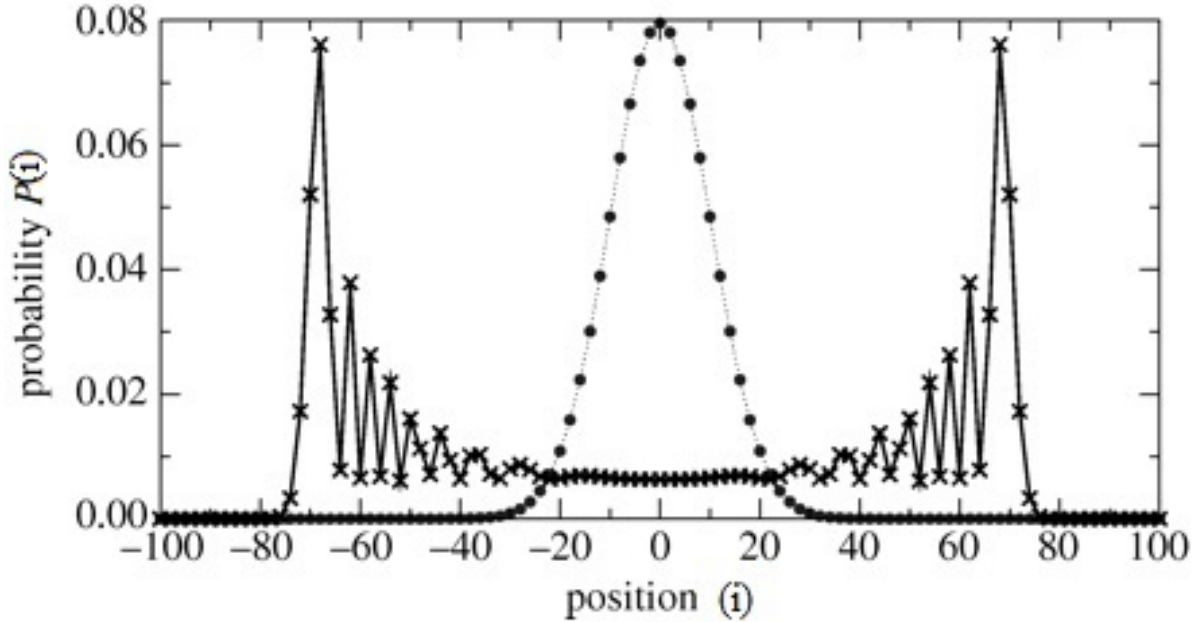
Figure 3: The probability distribution for after t = 100 steps, for the initial state $|\psi(0)\rangle = |\downarrow\rangle \otimes |0\rangle$. Only the probability at the even points is plotted, since the odd points have probability zero. The dotted line gives a long-wavelength approximation [20]

In order to get a more symmetrical distribution we can either; prepare our initial state in the following way $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle) \otimes |0\rangle$ and use the Hadamard coin, or we can introduce another coin. One such coin operator is $\hat{M}$, which is defined as follows

$$\hat{M} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{4.11}$$

In using this particular coin, the walk is not biased and is independent of the initial state of the system .

[27]

Figure 4: The probability distribution for both the classical and symmetrical quantum walk on the line, after t = 100 steps. Where we have used $\hat{M}$ to create the symmetrical quantum walk

From figures 3 and 4 we can clearly see that the discrete quantum walk on the line has no Gaussian properties , unlike that of the classical case. This makes the statistical analysis of the discrete quantum random walk much harder. This is because calculating the long term behaviour of the walk cannot be done by standard means, since quantum walks do not converge to any stationary distribution. Despite this, it has been shown analytically that the width (standard deviation) of the distribution is t [21], as compared to the classical case of $\sqrt{t}$. This means that the walker carrying out a discrete quantum random walk travels much further than their classical counterpart. We shall give a very basic mathematical argument for how this is calculated at the end of this section. This is quite remarkable and is why there has been so much research in developing quantum algorithms for quantum computers. As we shall see later, even for simple spatial search algorithms, the use of the discrete walk leads to a significant speed up.

4.2   Discrete Quantum Walks on Graphs

The discrete random walk on a graph is of course very similar to that of a walk on a line, except it takes place on a graph $G(V, E)$. Implementng the walks on graphs is vital, if we want to construct quantum algorithms.

In order to construct our discrete quantum walk on the graph we follow the approach of Kempe [20]and Portugal [32]. We begin by starting on a undirected d-regular graph, which is a graph where each vertex has the same number of neighbours (outgoing edges). As before our Hilbert space $\mathcal{H}$ is defined as $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$, where $\mathcal{H}_c$ is of dimension d and $\mathcal{H}_p$ contains the vertices of $G(V, E)$. Next we label each edge of the graph with a distinct label $j \in \{1, \ldots, d\}$, where an edge from some vertex v to a vertex w is labelled by $e(v, w)$. The edge coming from v's end is labelled by j and the edge on w's side is labelled by another j, which may or may not be equal to j on v's side, see figure 6. The state associated with the edge $e(v, w)$ is $|j\rangle \otimes |v\rangle$, which is analogous to the way we defined our initial state for the line , that being $|\uparrow\rangle \otimes |i\rangle$.
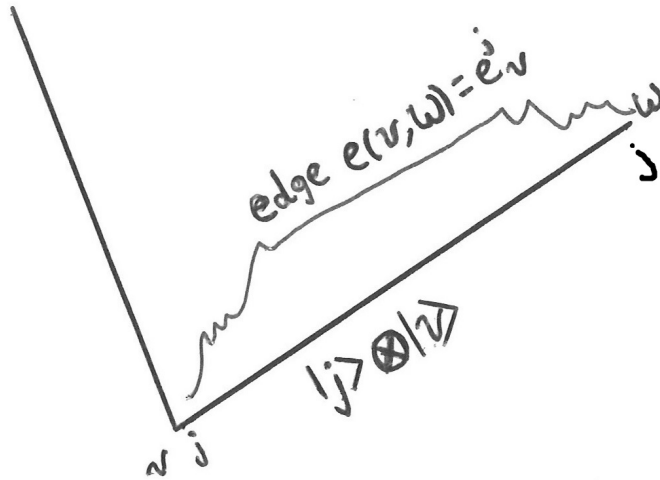

Figure 5: Here is pictorial representation of the edge $e(v, w)$ and the labelling system, where j at v's end does not have to equal j at w's end

As before we introduce a shift operator

$$\hat{S}\left|j\right\rangle \begin{cases} \left|j\right\rangle \otimes \left|v\right\rangle, & \text{if } e = (v,w) \\ \\ 0, & \text{otherwise} \end{cases} \tag{4.12}$$

which just moves the walker from vertex v to vertex w if both edges are labelled with the same j, see figure 6. Due to the set up of the graph G, we have a coin-flip $\hat{C}$ that is a d-dimensional unitary transformation and so we have even more freedom in the way we choose our coin operator. Again $\hat{C}$ will be devised depending on the specifics of the problem at hand. As discussed in the previous subsection 4.1, the choice of the coin operator $\hat{C}$ can drastically change the way a walk evolves, which is only amplified in higher dimensions [38]. In the case that the walk is not d-regular, such that the vertices have a varying numbers of edges that is less than d, we are able to modify the graph by adding self loops to those particular vertices, see figure 6. Which means we may still apply our coin operator $\hat{C}$, to create the quantum random walk.
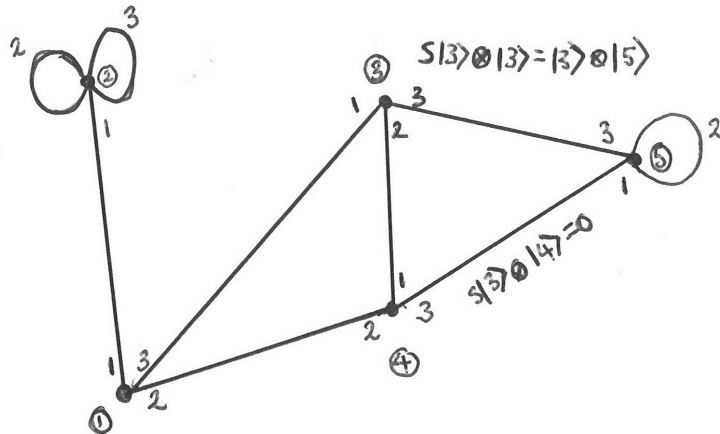

Figure 6: An example of an undirected regular graph, that has been made regular by the added self loops to the vertices that had a degree less than d. If the j's are not the same on vertices v and w, then the walker stays at there current vertex. If they are the same, then the shift operator moves the walker to vertex w.

We may also take a different approach, rather than adding self loops to our irregular graphs to make them regular, we can keep there irregularity but define the coin operator to be $\hat{C}'$, which is of dimension d' , where $d' \leq d$. However, in defining a new coin operator we can no longer use equation(4.5) and so in this case the coin-operation has to be conditioned on the position of the walker. But, we want to be able to define a coin that is balanced. The reason being is that when we are able to define the classical random walk we can then define our quantum random walk via the balanced coin and thus implement it efficiently on a quantum computer. In order to retain this property for general graphs we introduce the discrete fourier transform (DFT) matrix, which is our d-dimensional Hadamard operator. We define the (DFT) as follows

$$
DFT = \frac{1}{\sqrt{d}}
\begin{pmatrix}
1 & 1 & 1 & \dots & 1 \\
1 & \omega & \omega^2 & \dots & \omega^{d-1} \\
\vdots & & & \dots & \\
1 & \omega^{d-1} & \omega^{2(d-1)} & \dots & \omega^{(d-1)(d-1)}
\end{pmatrix}
\tag{4.13}
$$

where $\omega_d = \exp\left(\frac{2\pi i}{d}\right)$ is a dth-root of unity. The (DFT) may also be represented in the following way

$$
|F_k\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} \omega_d^{jk} |j\rangle
\tag{4.14}
$$

where the Fourier transform defines a new orthonormal basis $\{|F_k\rangle : 0 \leq k \leq d-1\}$ called the Fourier basis. We can see from (DFT) that after a measurement each direction is equally probable with a probability $P = \frac{1}{d}$ and so this coin is balanced.

But what about the case when we have a non-balanced coin ? A common example used throughout many research papers is the d-dimensional hypercube,
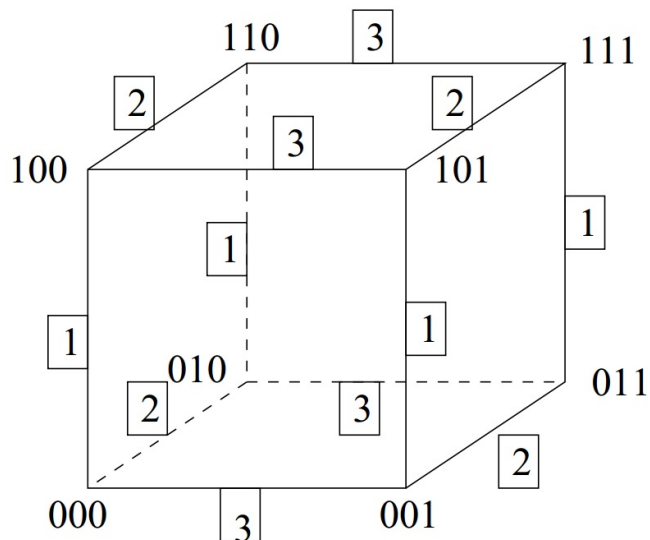
Figure 7: A picture of a hypercube with d=3. The vertices are labelled with bit strings and the edges are labelled according to which bit in the string, 1,2 or 3, needs to be flipped to a 1.

which links in very nicely to Grover's algorithm, which will be discussed in detail in the next section. A hypercube is d-dimensional regular graph of degree d, with $N = 2^d$ vertices. The labels of the vertices are represented by d-strings of binary bits. For example, if $d = 3$ we could have 000, 101 etc as our vertex label, see figure 7. We say that two vertices are adjacent if there binary strings differ only by one bit, that is their Hamming distance $d_H = 1$. We also label the edges according to which bit on the vertex the walker begins on, differs as compared to the vertex the walker is going to. For example, in the d=3 case, let the walker start at the vertex 000 and travel to 001, this means that the edge connecting them is labelled by 3, as it is the third bit that differs. The Hilbert space associated with the quantum walk on the hypercube is

$$\mathcal{H} = \mathcal{H}^d \otimes \mathcal{H}^{2^d} \tag{4.15}$$

where $|e\rangle \in \mathcal{H}_d$ is the coin state associated with the edge label $1 \leq e \leq d$ and specifies the direction of movement. Contained within the position space $\mathcal{H}^{2^d}$ are the computational

basis states $|\mathbf{v}\rangle$, where $\mathbf{v}$ represents a d-string of binary bits that specifies the state 'vertex' the walker is in. Thus vectors of the form $|e\rangle \otimes |\mathbf{v}\rangle$, form the computational basis of $\mathcal{H}$.

Before we introduce the shift operator , let us introduce the Grover coin [4] $\hat{G} = 2|D\rangle\langle D| - \hat{I}$, where $|D\rangle$ is the diagonal state of the coin space . We can represent $\hat{G}$ as the following matrix

$$\hat{G} = \begin{pmatrix} \frac{2}{d} - 1 & \frac{2}{d} & \cdots & \frac{2}{n} \\ \frac{2}{d} & \ddots & \cdots & \frac{2}{d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d} & \cdots & \cdots & \frac{2}{d} - 1 \end{pmatrix} \tag{4.16}$$

where the entries of $\hat{G}$ are determined by $G_{ij} = \frac{2}{d} - \delta_{ij}$.

We require the shift operator to move the walker from $|e\rangle \otimes |\mathbf{v}\rangle$ to $|e\rangle \otimes |\mathbf{v} \oplus \mathbf{e}_a\rangle$ [32] [15], where $\mathbf{e}_a$ represents the binary string with all zero entries except the ath entry, thus the ath entry is 1 and the $\oplus$ represents the bitwise xor (binary sum) [5].
This means that if the coin value is e and the walkers position is $\mathbf{v}$, the walker will move through edge e to the adjacent vertex $|\mathbf{v} \oplus \mathbf{e}_a\rangle$. We can formally define the shift operator $\hat{S}$ as follows

$$\hat{S} : |e\rangle \otimes |\mathbf{v}\rangle \rightarrow |e\rangle \otimes |\mathbf{v} \oplus \mathbf{e}_a\rangle \tag{4.17}$$

$$\equiv \sum_{e=1}^{d} \sum_{\mathbf{v}=1}^{N} |e, \mathbf{v} \oplus \mathbf{e}_a\rangle\langle e, \mathbf{v}| \tag{4.18}$$

where combining everything together we state that our unitary operator is described as

$$\hat{U} = \hat{S}(\hat{G} \otimes \hat{I}) \tag{4.19}$$

and thus the quantum walk on the hypercube maybe written as

$$|\psi(t)\rangle = \hat{U}^t |\psi(0)\rangle = [\hat{S}(\hat{G} \otimes \hat{I})]^t |\psi(0)\rangle \tag{4.20}$$

---

[4]A more detailed analysis of the Grover "coin" operator will be given in the next section

[5]Please see Appendix 1 to for a definition of the bitwise xor

This equation can be solved analytically although it requires numerous pages of working out, to see a full analytical derivation please see **pp** 105-112 [32].

What is nice about the quantum walk on the hypercube, is that the hypercube can be reduced to a walk on the line due to the symmetry of the Grover coin [20]. Since the quantum random walk on the line can be directly related to the classical walk via a balanced coin, it means that we can implement this walk efficiently on a quantum computer. Which is good for us, since the hypercube is very useful for network routing, i.e. in the $d = 3$ case, we want to route a string of binary bits from one corner of the hypercube (000) to another corner (111). When then let the walker move approximately d-steps and then measure to see where the string of binary bits is. The reason the hypercube is so useful for network routing is that it is noise resistant, in the sense that deleting edges will only slightly effect the walk and requires less hardware to implement [11]

4.3   Continuous Quantum walks on Graphs

Let us now discuss the construction of continuous quantum random walks, which are discrete in space but continuous in time. The continuous walks are fundamentally different from the discrete walks, as continuous quantum random walks only take place in the position space $\mathcal{H}_p$, as there is no coin space required, as no coin flip takes place. Which means [32] all we have to do is convert the classical vector that describes the probability distribution to a state vector and the transition matrix (equation (3.13)) to an equivalent unitary operator. However, the transition matrix M, representing the transition probabilities, is not unitary. In order to make it unitary we essentially just times the transition matrix M (equation (3.13)) by i, the imaginary number [2]. The transition matrix in the quantum picture is essentially our Hamiltonian $\hat{H}$.

Given the outline above, let us see how to implement the continuous walk on the graph $G(V, E)$. In order to describe the quantum evolution of the walk in a d-dimensional

Hilbert space $\mathcal{H}_p$, according to a given Hamiltonian $\hat{H}$ with matrix elements

$$\langle a|\hat{H}|b\rangle = M_{ab}{}^6 \tag{4.21}$$

we require the Schrödinger equation for some state $|\psi(t)\rangle$

$$i\frac{\mathrm{d}}{\mathrm{d}t}\langle a|\psi(t)\rangle = \sum_b \langle a|\hat{H}|b\rangle \langle b|\psi(t)\rangle \tag{4.22}$$

where equation (4.22) is written in terms of the computational basis $|1\rangle, \ldots, |v\rangle$ and $|a\rangle$ and $|b\rangle$ represent vertices of the graph. The Schrödinger equation in this form is almost parallel to equation(3.14). Equation (4.22) also conserves probability in the same sense as equation (3.15)

$$\sum_a |\langle a|\psi(t)\rangle|^2 = 1 \tag{4.23}$$

except the probabilities are now determined via the projection valued measure. It should also be noted to the reader that [2] in some sense, *any* evolution in a finite-dimensional Hilbert space can be thought of as a "quantum random walk". However, the analogy is clearest when the Hamiltonian has an obvious local structure. In using (4.21) and solving the Schrödinger equation we gain the following time evolution unitary operator

$$\hat{U}(t) = e^{-i\hat{H}t} \tag{4.24}$$

where the time evolution of the walk is defined as

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle \tag{4.25}$$

and the probability distribution is given by

$$P(t) = \left| \langle a|\hat{U}(t,0)|\psi(0)\rangle \right|^2 \tag{4.26}$$

4.4 Continuous Quantum Random Walk on the Line

With the definitions that we have in place, let us consider the example of applying the continuous time quantum walk on the line $k = 2$ (equation (3.13)). This means that our

---

[6]This is the transistion matrix from section 3, where i is now a , and j is now b. The variables have been changed to avoid confusion with the imaginary number$i$

Hamiltonian "transition matrix" is defined as

$$\hat{H}\ket{i} = -\gamma\ket{a-1} + 2\gamma\ket{a} - \gamma\ket{a+1} \tag{4.27}$$

Beginning the walk in some initial state $\ket{\psi(0)} = \ket{0}$ and setting $\gamma = \frac{1}{2\sqrt{2}}$ we get the following probability distribution.

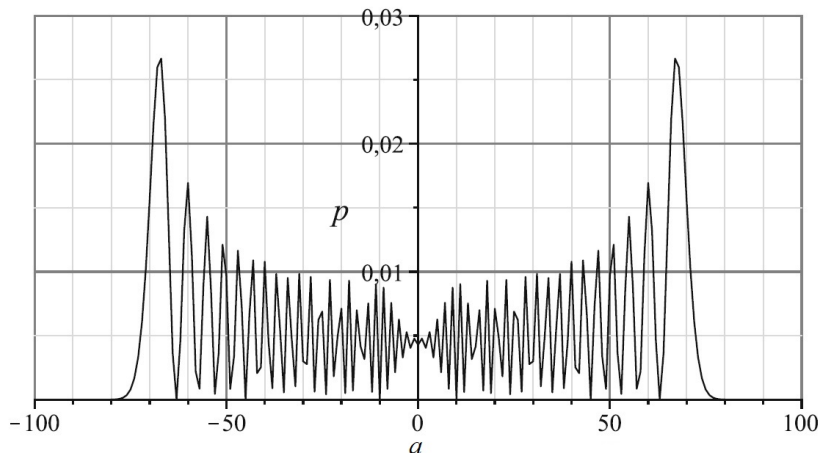
Figure 8: Starting in the initial state $\ket{\psi(0)} = \ket{0}$ and setting the jumping rate $\gamma = \frac{1}{2\sqrt{2}}$, we get the following probability distribution for a continuous time random walk on the line for $t = 100$. Plotted with mathematica (source code given in [32])

In comparing figure 8 to the discrete probability distribution figure 4 we see both similarities and differences. Obviously on a global picture they have fairly similar distributions, but how they are formed is very different. The distribution in the discrete case is controlled by the choice of the coin operator $\hat{C}$ or the initial condition. Whereas in the continuous case the dispersion is controlled by our jumping rate γ, and so if we shrink γ our distribution shrinks around the origin.

In order to find the state of the walk at any time t, we must use the above information to find the state vector $\ket{\psi(t)}$. Using the initial state of the walker $\ket{\psi(0)} = \ket{0}$ we write

$$\hat{H}\ket{0} = -\gamma(\ket{-1} - 2\ket{0} + 0\ket{1}) \tag{4.28}$$

now for some time t we have the following

$$\hat{H}^t \left|0\right\rangle = \gamma^t \sum_{a=-t}^{t} (-1)^a \begin{pmatrix} 2t \\ t-a \end{pmatrix} \left|a\right\rangle \tag{4.29}$$

where $\begin{pmatrix} 2t \\ t-a \end{pmatrix}$ is the binomial coefficient. From this expression we can compute $\hat{U}(t,0)\left|0\right\rangle$ in terms of two nested sums [32] . We then invert the sums and use the following identity [29]

$$\exp(-2i\gamma t) J_{|a|}(2\gamma t) = \exp\left(\frac{\pi i}{2}|a|\right) \sum_{j=|a|}^{\infty} \frac{(-i\gamma t)^j}{j!} \begin{pmatrix} 2j \\ j-a \end{pmatrix} \tag{4.30}$$

where J is the Bessel function of the first kind with integer a [7]. In doing this we find our state $\left|\psi(t)\right\rangle$ for the continuous quantum random walk on the line for any time t to be

$$\left|\psi(t)\right\rangle = \sum_{a=-\infty}^{\infty} \exp\left(\frac{\pi i}{2}|a| - 2i\gamma t\right) J_{|a|}(2\gamma t) \left|a\right\rangle \tag{4.31}$$

from which we can deduce what the probability distribution is

$$P(t) = \left\langle a|\hat{U}(t,0)|\langle\psi(0)|\psi(0)\rangle\right\rangle^2 = |J_a(2\gamma t)|^2 \tag{4.32}$$

where (4.32) describes figure 8. It is also worth noting that we can deduce this probability distribution via Laplace transforms as shown in [14] which for some is easier.

4.5   Comparison of the Quantum and Classical Walks

In calculating the asymptotic behaviour of both the continuous and discrete quantum walks [1] [6] [21] we find that we have ballistic spreading in both cases, as the standard deviation of both quantum walks on the line is found to be t, as compared to diffusive spreading in the classical case of $\sqrt{t}$. So the walker in the quantum walk travels much further. The reason we have to calculate the behaviour of the walks asymptotically is because the unitary operators preserve the norm of $\left|\psi(t+1)\right\rangle - \hat{U}\left|\psi(t)\right\rangle$. This means in

---

[7]For more information on Bessel functions of the first kind please see `http://mathworld.wolfram.com/BesselFunctionoftheFirstKind.html`

general, that the limit as $\lim_{t\to\infty}|\psi(t+1)\rangle$ does not exist and has to be found asymptotically [21].

Returning to the walker, why does the quantum walker travel so much further? We can think about this in two ways, mathematically and in a physical sense. Mathematical speaking, in order to get the standard deviation of t, it was shown by Konno [21] and Grimmett *et al.* [17] that by modifying the central limit theorem, so that instead of

$$\lim_{n\to\infty}\frac{X(n)-n\mathbb{E}[X(n)]}{\sigma\sqrt{n}}\to\mathcal{N}(0,1) \tag{4.33}$$

where $\mathcal{N}(0,1)$ represents a centered Gaussian with variance 1 . We normalize by n, rather than $\sqrt{n}$. We do this as we think of the central limit theorem as a result about weak limits of measures [17], rather than about the stochastic process $X(n)$ and we can show that this converges weakly as $n\to\infty$ to a certain distribution which is absolutely continuous and of bounded support. From a physically perspective it can be summed up in four words, "the protocol of measurement". As the walker is in a superposition of many different states at any one time t, in order to gain any information about the system , we must make a measurement on the position of the walker. It is only then, that the system is projected on to some state $|i\rangle$, but prior to this observation our walker was in all those states at once. This is a very strange, but wonderful property of quantum systems.

5 Grovers Algorithm and The Discrete Quantum Random Walk

In this section we will discuss a very useful property of the discrete quantum random walk, in regards to computer science and the development of quantum algorithms . We shall begin by introducing Grover's algorithm, a simple database search algorithm that takes place on a N-dimensional Hilbert space. At the heart of Grover's algorithm lies amplitude amplification , a technique which paved the way for the development of quantum algorithms. We then go on to modify Grover's algorithm for the spatial search in $d \geq 2$ dimensions. Where a spatial search has N items that are stored in N different locations and so there is an additional time cost in moving from different locations. Due to this, if we try and apply Grover's original algorithm to the spatial search , we revert back to the classical computation time of $\mathcal{O}(N)$ [30] which is not what we want. But in using the coin space and discrete the quantum random walk we are able to modify Grovers algorithm, to regain the quantum speed up of $\mathcal{O}(\sqrt{N})$.

5.1 An Introduction to The Grover Algorithm

Imagine a phone book directory [22] containing N names in a completely random order, where we only want one name , or a part completed crossword puzzle where we want to find the missing letter. A classical algorithm would have to search through each of these elements one at a time, which would be incredibly time consuming, as if we have N data points, on average we would expect to look through at least $N/2$ data points to find our required result, or at the very worst we would have to look through all N data points and so this would take a time of at least $\mathcal{O}(N)$ to complete. Which as you can imagine with a $1,000,000$ data-points, would take on average $500,000$ time steps, which depending on processing power would take a very long time.

However, Grover managed to create an algorithm that took advantage of the quantum

mechanical property of the linear superposition of states and at the very heart of Grover's algorithm is the method of amplitude amplification , which paved the way for many other quantum algorithms. By using these methods Grover was able to reduce the computation time of the data base problem down to $\mathcal{O}(\sqrt{N})$, which can be proved to be optimal [12] [8] up to a multiplicative constant.

5.1.1 Grover's Search Algorithm

It is first wise to see how we would solve this problem classically, from which we in essence 'quantize' the classical formulation in terms of unitary operators. There are many approaches we can follow to derive Grover's algorithm such as [22] and [32] , but I will follow that of Vedral [41] and Barnett [25] as it is my preference. So let us begin, *classically* the search problem may be formulated as:

Definition 5.1. *Suppose that f is a function with domain $\mathcal{D} := \{1, \ldots, N = 2^n\}$, and the image is defined as*

$$f(i) = \begin{cases} 0, & \text{if } i \neq x \text{ and } 1 \leq i < N, \\ 1, & \text{if } i = x \end{cases} \tag{5.1}$$

where the $i's$ are the database elements and our required element is $i = x$. All of the elements are represented by a string of n bits, where $n \in \mathbb{Z}^{+,0}$.

If we can arrange for the image $f(i)$ to be computed by an oracle [9] (or blackbox) then we can take our classical algorithm and ' quantize ' it to gain the quantum speed up we want. This means that we can implement the unitary transform

$$|i\rangle \otimes |B\rangle \rightarrow |i\rangle \otimes |B \oplus f(i)\rangle \tag{5.2}$$

where $|i\rangle$ is our first register and stores the domain points and $|B\rangle$ is the second register[10] of a single qubit, that stores the image points of f . The $\oplus$ represents modulo arithmetic

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[8]This simply put means that this algorithm cannot reduce the number of time steps any further

[9]Where an oracle is a formal way of describing how many time steps an algorithm takes

[10]See Appendix 1 for definitions of a register and the computational basis

in base 2. If we prepare $|B\rangle$ in the Hadamard basis state $|-\rangle$ [11], so that $f(i)$ appears as a phase factor, this implies

$$|i\rangle \otimes \frac{1}{\sqrt{2}}(|-\rangle) \rightarrow (-1)^{f(i)} |i\rangle \otimes |-\rangle \tag{5.3}$$

which means that the oracle is shifting the phase of our required state $|x\rangle$ by π, while all other elements remain unchanged. Thus the oracle induces a reflection in our required state(data-point).
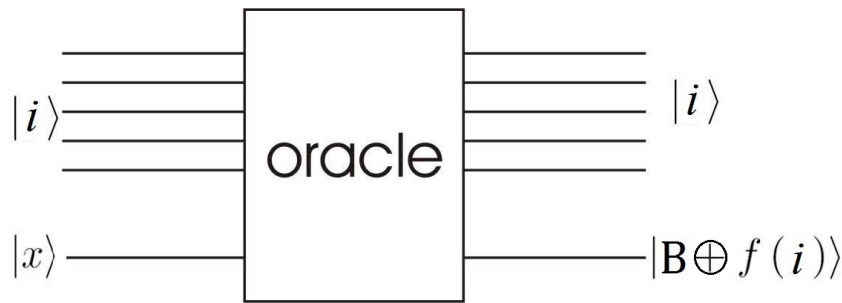

Figure 9: The Oracle. The oracle is unitary operator, that acts like a black box, for which the states $|i\rangle$ and $|x\rangle$ are inputted. If the oracle recongises $|x\rangle$ it applys the unitary 5.2 which flips the phase of $|x\rangle$. If the oracle recongonises $|i\rangle$, it does nothing and continues to search for $|x\rangle$.

thus the oracle acts on the state vectors $|i\rangle$ and $|x\rangle$ in the following way

$$\hat{O} |x\rangle = - |x\rangle \tag{5.4}$$

$$\hat{O} |i\rangle = |i\rangle \tag{5.5}$$

Since the oracle represents a reflection we may write the oracle as a householder transformation

$$\hat{O} = \hat{I}^{\otimes n} - 2 |x\rangle\langle x| \tag{5.6}$$

to see the effect of this phase shift, we initially prepare the input(our first register) in an equal superposition of all states

$$|\psi\rangle = \sum_{i=1}^{N} \frac{1}{\sqrt{N}} |i\rangle \tag{5.7}$$

---

[11]Where $|-\rangle$ is the Hadamard basis state seen in section 2

which is very much like our (DFT) in section 4. After preparing our state, we then apply the oracle $\hat{O}$ [12] , as defined in (5.3), to our state $|\psi\rangle$

$$\hat{O} |\psi\rangle \otimes |-\rangle = \sum_{i=1}^{N} \frac{1}{\sqrt{N}} (-1)^{f(i)} |i\rangle \otimes |-\rangle$$

For the next step we ponder in to the heart of Grover's algorithm and introduce the diffusion transform $\hat{D}$, an n-bit unitary operator, which increases the probability of our required state being found after the first iteration. Without the diffusion operator this would not be the case as all entries are equally probable, the diffusion transform changes this.

We formally define the diffusion transform $\hat{D}$ [22] as

$$\hat{D} = 2 |\psi\rangle\langle\psi| - \hat{I}^{\otimes n} \tag{5.8}$$

where $|\psi\rangle$ is the superposition state as defined in (5.7)and $\hat{I}^{\otimes n}$ is the n-qubit identity operator.

With both the oracle and diffusion transform defined, let us introduce Grover's unitary operator [22]

$$\hat{G} = \hat{D}\hat{O} \tag{5.9}$$

which acts on a subspace of the Hilbert space $\mathcal{H}^2 N$. In order to perform the algorithm we continually apply the Grover operator for a number of time steps t, make a measurement and repeat until we have found our required element. The longer we delay measurement, the greater the probability of finding our required state.

Let us now carry out the first iteration and see how the amplitude of our desired state $|x\rangle$ is increased , in comparison to the classical case. We begin by applying $\hat{G}$ to the state $|\psi\rangle$ and then take a measurement $\langle x|$, from which we are able to deduce the amplitude.

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[12]Where the oracle itself is a unitary

We will make use of the following results; $\langle\psi|\psi\rangle = 1$ and $\langle\psi|x\rangle = \frac{1}{\sqrt{N}}$. Thus

$$\hat{G}\,|\psi\rangle \otimes |-\rangle$$

$$= ((2\,|\psi\rangle\langle\psi| - \hat{I}^{\otimes n})(\hat{I}^{\otimes n} - 2\,|x\rangle\langle x|)\,|\psi\rangle) \otimes |-\rangle$$

$$= ((2\,|\psi\rangle\langle\psi| - \hat{I}^{\otimes n})(|\psi\rangle - \frac{2}{\sqrt{N}}\,|x\rangle)) \otimes |-\rangle$$

$$= (|\psi\rangle - \frac{4}{N}\,|\psi\rangle + \frac{2}{\sqrt{N}}\,|x\rangle) \otimes |-\rangle$$

$$= [(1 - \frac{4}{N})\,|\psi\rangle + \frac{2}{\sqrt{N}}\,|x\rangle] \otimes |-\rangle \tag{5.10}$$

and now we make a measurement $\langle x|$ on 5.10 to find that the amplitude is

$$a = \frac{1}{\sqrt{N}}(3 - \frac{4}{N}) \tag{5.11}$$

which means that the probability is approximately 9 times greater than if we had not used the diffusion transform!
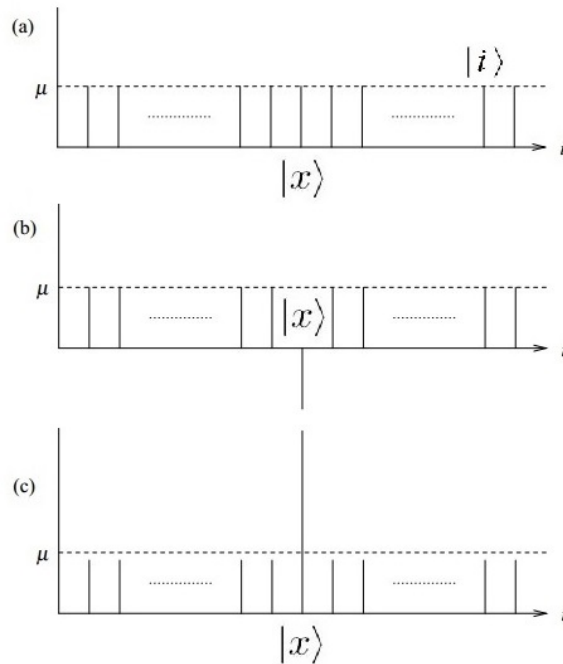

Figure 10: Amplitude amplification, μ represents the mean , $|x\rangle$ is the state "element" that we are looking for and $|i\rangle$ represents all other elements. (a) represents the uniform superposition of all states, (b) represents what happens after we apply the oracle and (c) is what happens after we have applied the diffusion operator $\hat{D}$

This is amplitude amplification and is why Grover's algorithm gives us such a speed up .

Let us now look at the following two questions; what would happen if we were to continue to apply Grover's algorithm? And how many iterations are required to reach a maximum amplitude and thus the greatest probability of finding our required state $|x\rangle$? The first question is easy, the amplitude would continue to increase up to a bound. But what about the second question? We see below, that from the above definitions of the oracle and the diffusion transform that the effects of two reflections caused by the two operators correspond to a rotation in a 2-dimensional sub space.

To see this, we begin by introducing two vectors, $|x\rangle$ and $|y\rangle$ which are orthogonal to each other and span the entire space to form an orthonormal basis. Since $|\psi\rangle$ is a linear superposition of all states, we know that $|\psi\rangle$ will just be a linear combination of the two orthonormal states $|x\rangle$ and $|y\rangle$ as they span the whole search space . Where $|x\rangle$ is the state that we want and $|y\rangle = \frac{1}{\sqrt{N-1}} \sum_{i=1}^{N} |i\rangle$ is the state that we do not.

Therefore from equation (5.7) the initial state can be written as

$$|\psi\rangle = \frac{1}{\sqrt{N}} |x\rangle + \sqrt{\frac{N-1}{N}} |y\rangle \tag{5.12}$$

If we now apply Grover's operator $\hat{G}$ to the state $|\psi\rangle$ we see that we do not move out of this space. For a state $\alpha |x\rangle + \beta |y\rangle$ the act of the oracle reflects the state $|x\rangle$ about $|y\rangle$ and so we get $-\alpha |x\rangle + \beta |y\rangle$. Likewise the diffusion transform is also a reflection, except this time it is about the state $|\psi\rangle$, thus the combination of the diffusion transform $\hat{D}$ and the oracle $\hat{O}$ produces a rotation . As the rotation must be independent of the state, each rotation is by a constant amount. The aim is to rotate the state $|\psi\rangle$ until it is as close as possible to $|x\rangle$.
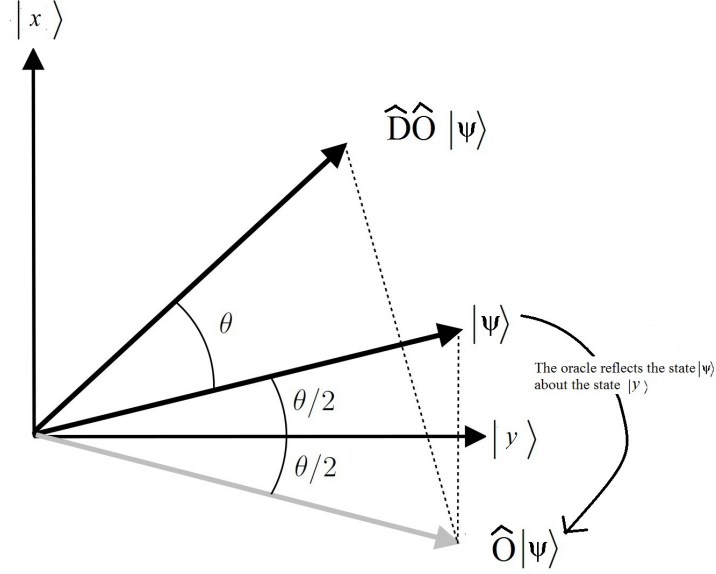
Figure 11: A Geometrical picture of Grover's algorithm. We can see how oracle reflects the initial state about $|y\rangle$ and then the diffusion transform acts as a reflection about $|\psi\rangle$.

We now act the Grover operator on each state $|x\rangle$ and $|y\rangle$

$$\hat{D}\hat{O}|x\rangle$$

$$= (2|\psi\rangle\langle\psi| - \hat{I})(\hat{O}|x\rangle)$$

$$= (2|\psi\rangle\langle\psi| - \hat{I})(-|x\rangle)$$

$$= -2|\psi\rangle\langle\psi|x\rangle + |x\rangle$$

$$= -2(\frac{1}{\sqrt{N}}|x\rangle + \sqrt{\frac{N-1}{N}}|y\rangle)(\frac{1}{\sqrt{N}}) + |x\rangle$$

$$= \frac{N-2}{N}|x\rangle - \sqrt{\frac{N-1}{N}}|y\rangle \tag{5.13}$$

Similarly applying $\hat{G}$ to $|y\rangle$ we get

$$-2\frac{\sqrt{N-1}}{N}|x\rangle + \frac{N-2}{N}|y\rangle \tag{5.14}$$

except this time when the oracle was applied to $\hat{O}|y\rangle = |y\rangle$ it remains in state $|y\rangle$. Now

we see from (5.13) and (5.14) that $\hat{G}$ can be written in the matrix form as follows

$$\hat{G} = \frac{1}{N} \begin{pmatrix} N-2 & 2\sqrt{N-1} \\ -2\sqrt{N-1} & N-2 \end{pmatrix} \tag{5.15}$$

In introducing the angle θ, as shown in figure(11), such that $0 < \theta < \frac{\pi}{2}$, we may represent $\hat{G}$ as a rotation matrix

$$\hat{G} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{5.16}$$

where $\sin\theta = 2\frac{\sqrt{N-1}}{N}$, so that for large N $\theta \simeq 2\frac{1}{\sqrt{N}}$. In defining θ, we can also write the initial state in terms of θ

$$|\psi\rangle = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ \cos\left(\frac{\theta}{2}\right) \end{pmatrix} \tag{5.17}$$

where we see that after applying $\hat{G}$ for k iterations we get

$$\begin{pmatrix} \sin\left(\frac{2k+1}{2}\theta\right) \\ \cos\left(\frac{2k+1}{2}\theta\right) \end{pmatrix} \tag{5.18}$$

Now we need to choose a k such that it is not too large, but is such that $\sin\left(\frac{2k+1}{2}\theta\right)$ is close to unity , which would imply an almost certain probability of finding our state (element) $|x\rangle$. This means that we want $\sin(\phi) \simeq 1$

$$(k + \frac{1}{2})\theta \simeq \frac{\pi}{2} \tag{5.19}$$

which implies that we can find any value of k for any given N, however an approximate solution suffices to determine the way that k scales with N. Recalling that for large N, $\theta \simeq 2\frac{1}{\sqrt{N}}$, this means for large k ,

$$k \simeq \frac{\pi}{4}\sqrt{N} \tag{5.20}$$

which implies the required number of iterations needed to get the maximum amplitude is about $\sqrt{N}$. Thus the second question is answered. This result means that we shall find our required database element using only $\mathcal{O}(\sqrt{N})$ queries of our quantum oracle ; as opposed to $\mathcal{O}(N)$ queries of our classical oracle!

I shall now finish this introduction to Grover's algorithm with how to express the diffusion operator in a way that it may be implemented physically. As stated at the beginning, the system contains $N = 2^n$ elements , where n is the number of qubits. We see that we can generate the state $|\psi\rangle$ from the basis state by applying a Hadamard gate to each qubit on to the n-qubit state $|0\rangle^{\otimes n}$.

$$\hat{H}^{\otimes n} |0\rangle^{\otimes n} = (\hat{H} \otimes \ldots \otimes \hat{H})(|0\rangle \otimes \ldots \otimes |0\rangle)$$

$$= \frac{1}{2^{n/2}}(|0\rangle + |1\rangle) \otimes \ldots \otimes (|0\rangle + |1\rangle)$$

$$= \frac{1}{2^{n/2}} \sum_{i=1}^{2^n} |i\rangle$$

$$= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} |i\rangle = |\psi\rangle \tag{5.21}$$

from this we may write the diffusion operator in terms of the projector $|0\rangle\langle 0|$ as

$$\hat{D} = \hat{H}^{\otimes n}(2 |0\rangle\langle 0| - \hat{I}^{\otimes n})\hat{H}^{\otimes n} \tag{5.22}$$

where $2 |0\rangle\langle 0| - \hat{I}^{\otimes} n$ represents a rotation matrix [22] and $\hat{H}^{\otimes n}$ is the Hadamard transform

$$H^{\otimes n} = (H_n)_{ij} = 2^{-n/2}(-1)^{i \cdot j} \tag{5.23}$$

where is the bitwise dot product of the binary representations.
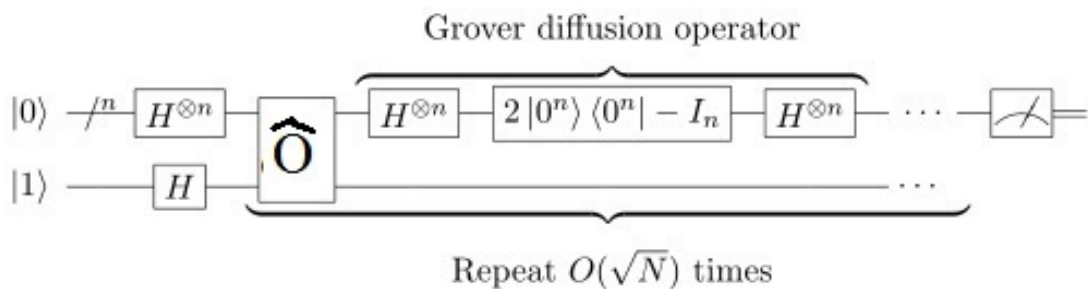

Grover diffusion operator

Repeat $O(\sqrt{N})$ times

Figure 12: A system to physically implement Grover's algorithm. We see that if we choose our marked element to $|1\rangle$ and our unmarked element to be $|0\rangle$, that the algorithm continues to perform until $|1\rangle$ is measured. We would expect to have to apply the algorithm at least $\mathcal{O}(\sqrt{N})$ times

[9]

As a final note, it should be stated that we can actually extend Grover's algorithm to multiple targets, and it is found that with multiple items Grover's algorithm has a computational time of $\mathcal{O}(\sqrt{\frac{N}{m}})$, where m is the number of targets [26]. It is also interesting to note , even if we do not know how many items we are searching for, we still get a computational time of $\mathcal{O}(\sqrt{\frac{N}{m}})$ [26].

5.2 A Modified Version of Grovers Algorithm via Discrete Quantum Random Walk's

In this part we will see how the use of the discrete quantum random walk enables us to modify Grover's algorithm, so that it can perform the spatial search in dimensions $d \geq 2$, without losing the quantum speed up that makes the idea of quantum algorithms for quantum computers so appealing.

5.2.1 The Model

Our framework for the walk is the d-regular and undirected graph $G = (V, E)$ [13], where each vertex v stores a variable $i_v \in \{0, 1\}$.

As with the original algorithm we want to find the element where our oracle (*function*) was equal to 1, in the same sense we now want to find the vertex v for which $a_v = 1$ [4]. These vertices are called the marked vertices, and for the vertices when $a_v = 0$ shall be called unmarked. The algorithm we are going to implement can in one step examine the current vertex or move to another vertex within G. We would like to be able to do this in at least time steps as possible.

What this means is, we shall use a sequence of unitary transformations on a Hilbert space $\mathcal{H} = \mathcal{H}_d \otimes \mathcal{H}_V$, where $\mathcal{H}_V$ is the Hilbert space spanned by the states $\{|1\rangle \dots, |v\rangle\}$, corresponding to the vertices of the graph. Where each state $|v\rangle$ is associated with a label $i \in \{1 \dots d\}$ of the d edges adjacent to it. The coin space (the algorithms internal state)

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[13]An undirected graph is one for which the relations between pairs of vertices are symmetric, so that each edge has no directional character

will be represented by the Hilbert space $\mathcal{H}_d = \{|1\rangle \dots |d\rangle\}$. Where $\mathcal{H}_d$ can be of arbitrary fixed dimension. For our t-step algorithm we shall apply a sequence of unitaries $\hat{U}_1, \dots, \hat{U}_t$, where we want to deduce the computational time t. The $\hat{U}_d$ begin by acting on some fixed starting state $|\psi(0)\rangle$, which allows us to find the final state $|\psi(t)\rangle = \hat{U}_t, \dots, \hat{U}_1 |\psi(0)\rangle$, we then measure $|\psi(0)\rangle$, if we measure the $\mathcal{H}_V$ part of the final state and it gives $|x\rangle$, such that $a_x = 1$, then the algorithm succeeds. The $\hat{U}_d$ are defined to be either a **query** or a **local transformation**. We define a query to consist of two transformations $(\hat{U}_d^0, \hat{U}_d^1)$. For which $\hat{U}_d^0 \otimes \hat{I}$ is applied to all $\mathcal{H}_d \otimes |v\rangle$ for which $a_v = 0$ and $\hat{U}_d^1 \otimes \hat{I}$ is applied to all $\mathcal{H}_d \otimes |v\rangle$ for which $a_v = 1$. For a local transformation $\hat{U}_d$ we define it to be Z - local, which means for any $v \in V$ and $|\psi\rangle \in \mathcal{H}_d$, the state $\hat{U}_d(|\psi\rangle \otimes |v\rangle)$ is contained in the subspace $\mathcal{H}_d \otimes \mathcal{H}_{\Gamma(V)}$, where $\mathcal{H}_{\Gamma(V)} \subset \mathcal{H}_V$ is spanned by the state $|v\rangle$ and the states $|v'\rangle$ for all v' adjacent to v [4] .

Let us now put some fundamental definitions in place which are reminiscent of section 4, that will allow us to combine the discrete random walk with Grover's algorithm.

Definition 5.2. *[Discrete Quantum Walk on G]: The discrete quantum walk is an alternation of a coin flip and moving step: $\hat{U} = \hat{S} \cdot \hat{C}$, where S is a shift controlled by the coin register*

$$\hat{S} : |i\rangle \otimes |x\rangle \rightarrow |\pi(i)\rangle \otimes |\tilde{x}\rangle \tag{5.24}$$

$i = 1, \dots, d$ *and $x, \tilde{x} \in V$, x and $\tilde{x}$ are connected by the edge labelled "i'' on $x's$ side and π is a permutation of the d basis states of the coin space $\mathcal{H}_d$, and the coin is $\hat{C} = \hat{C}_0 \otimes \hat{I}_V$ where $\hat{I}_V$ acts on the identity on $\mathcal{H}_V$ and $\hat{C}_0$ is a "coin flip" acting on $\mathcal{H}_d$*

$$\hat{C}_0 = 2 |s\rangle\langle s| - \hat{I}_d, \text{ where } |s\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle \tag{5.25}$$

Where (5.25) represents (the reflection about the mean) $\hat{D} \rightarrow \hat{C}_0$ and $|\psi\rangle \rightarrow |s\rangle$ represents the superposition of all the states of the graph. We can see that $\hat{C}_0$ is a symmetric coin, as it treats all directions d equally.

For a given i, $\hat{S}$ permutates the vertices of the graph. What is nice about the permutation π is that it allows us to specify shift operators that act differently on coin spaces $\mathcal{H}_d$. The shift operator used for the spatial search, is similar to the one we used in section 4, except this time we introduce the perturbed coin C'

$$\hat{U} = \hat{S} \cdot \hat{C}' \tag{5.26}$$

The is because, if we remain with an unperturbed coin operator, we find that if the walk begins in some initial state $|\psi(0)\rangle = \frac{1}{\sqrt{dN}} \sum_{i=1}^{d} \sum_{x=1}^{N} |i\rangle \otimes |x\rangle$ and it never changes this state. As $|\psi(0)\rangle$ is an eigenvector of $\hat{U}$ with eigenvalue 1, $\hat{U}|\psi(0)\rangle = |\psi(0)\rangle$. Thus in order to perturb the eigenvalue we use a perturbed coin operator to mark a vertex v, which induces a inhomogeneity in to the quantum walk.

Definition 5.3 (*Perturbed Quantum Walk:*). *The perturbed walk with marked vertex v and "marking" coin $\hat{C}_1 = -\hat{I}_d$ is $\hat{U}' = \hat{S} \cdot \hat{C}'$, where*

$$\hat{C}' = \hat{C}_0 \otimes (\hat{I} - |v\rangle\langle v|) + \hat{C}_1 \otimes |v\rangle\langle v| = \hat{C} - (\hat{C}_0 - \hat{C}_1) \otimes |v\rangle\langle v| \tag{5.27}$$

Thus this means that instead of one coin for all nodes $\hat{C}_0 \otimes \hat{I}$, we have a different coin $\hat{C}_1$ on the marked state. Thus we get the following $\hat{C}_0 - \hat{C}_1 = 2|s\rangle\langle s| - \hat{I}_d - (-)\hat{I}_d = 2|s\rangle\langle s|$ and

$$\hat{U}' = \hat{S} \cdot \hat{C} - \hat{S} \cdot (2|s\rangle\langle s| \otimes |v\rangle\langle v|)$$

$$= \hat{U} - \hat{S} \cdot (2|s, v\rangle\langle s, v|)$$

$$= \hat{U}(\hat{I}_{dV} - 2(\hat{C}^{-1} = \hat{C})|s, v\rangle\langle s, v|)$$

thus using the fact that $\hat{C}$ is unitary and $\hat{C}|s\rangle = \hat{C}_0 \otimes \hat{I}_V|s\rangle = |s\rangle$ we have

$$\hat{U} \cdot (\hat{I}_{dV} - 2\hat{S}|s, v\rangle\langle s, v|) \tag{5.28}$$

In order to mark a vertex on the graph, we can set an auxiliary qubit to $|1\rangle$ and the other unmarked vertices will have this qubit set to $|0\rangle$. Then this [4] auxiliary qubit can control the coin to be $\hat{C} = \hat{U}^0$ for the unmarked items and $\hat{C}' = \hat{U}^1$ for the marked item.

5.2.2 Implementing The Model With Grover's Algorithm

In order to view Grover's algorithm as a random walk search algorithm on the complete graph, each vertex must have N edges. We then label both vertices and edges with $\{1, \ldots, N\}$ and so the coin space $\mathcal{H}_c$ and the vertex space $\mathcal{H}_v$ are of dimension N, so the complete space $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_v$ is of dimension $N \times N$. We label the states of the coin space $|i\rangle$, as before, and the states of the vertex space as $|j\rangle$, where the first register is the coin register. We define the shift operation as follows [4]

$$\hat{S} : |i\rangle \otimes |j\rangle \rightarrow |j\rangle \otimes |i\rangle \tag{5.29}$$

so the shift just changes the direction. We then choose the marked coin to be $\hat{C}_1 = -\hat{C}_0$ and the marked state to be $|v\rangle$, thus by equation (5.27) we have

$$\hat{C}' = \hat{C}_0 \otimes (\hat{I}_N - 2|v\rangle\langle v|) \tag{5.30}$$

where $\hat{C}_0$ is just the diffusion transform $\hat{D}$ and $\hat{I}_N - 2|v\rangle\langle v|$ is $\hat{O}$, the oracle, as it flips the phase of the marked element. So we now have both parts of Grover's algorithm $(\hat{G} = (\hat{D}\hat{O})^t |\psi\rangle)$, where $|s\rangle \equiv |\psi\rangle$. We then prepare the initial state of the random walk in the uniform superposition state $|\psi(0)\rangle = |s\rangle \otimes |s\rangle$. Next we introduce our perturbed unitary $\hat{U}'$, thus we have

$$\hat{U}' |\psi_0\rangle$$
$$= \hat{S} \cdot \hat{C}' |\psi(0)\rangle$$
$$= \hat{S} \cdot (\hat{D} \otimes \hat{O}) |\psi(0)\rangle$$
$$= \hat{O} |s\rangle \otimes \hat{D} |s\rangle$$

which is almost Grovers algorithm, in order to get Grovers algorithm we must multiply both sides by the perturbed unitary once more $\hat{U}'$

$$\hat{S}\hat{C}'\hat{U}' |\psi(0)\rangle$$
$$= \hat{S}((\hat{D} \cdot \hat{O}) |\psi(0)\rangle \otimes (\hat{O} \cdot \hat{D}) |\psi(0)\rangle)$$
$$= (\hat{O}\hat{D}) |s\rangle \otimes (\hat{D}\hat{O}) |s\rangle$$
$$= \hat{U}'^2 |\psi(0)\rangle$$

which is precisely Grover's algorithm on both the coin space and the vertex space. This has been derived completely from our discrete random walk, at the expense of having to carry an additional iteration, which in computational terms is not much at all.

5.2.3 Results

In writing Grover's algorithm in terms of the discrete random walk, we are now able to carry out a spatial search without losing the quantum speed up. It is found in [4] that for 2-dimensions we have a computational time of $t = \mathcal{O}(\sqrt{N} \log N)$ and for 3 or more dimensions we have a computational time of $t = \mathcal{O}(\sqrt{N})$, which is much better than $t = \mathcal{O}(N)$ we would have gotten in both the classical scenario ,and if we had not modified Grover's algorithm with the discrete quantum walk. The reason that I have not included the derivations of these results is that they are several pages long proofs, that are not difficult, but hard to condense into the finite space that I have. I do however recommend that the reader look up the paper by [4] and also look up another paper by Aharonov *et al.* [13], which was the first paper published for looking at how to implement quantum walks on graphs for algorithmic development.

As a final point [4] also discuss a rather important point about connecting the discrete quantum walk, to the continuous time quantum random walk. They say that due to the coin space of the discrete quantum random walk, that it may not be possible to get the continuous quantum random walk from the discrete quantum random walk (as the length of the time step approaches 0). This is because the coin space stays with the discrete quantum random walk, even as the time step approaches 0, which is contrary to that of the classical world . It is of great importance to connect the walks as otherwise it would imply that they are two completely different constructions and that would be very strange. Thankfully, it was shown in 2006 by Strauch [37] how to connect the two walks.

6 How To Experimentally Implement a Quantum Random Walk

Actually implementing the walks is of great importance, as if we are to truly harness the power of quantum algorithms, we must be able to implement the mathematical concepts that we have discussed throughout this paper in physical reality. Although there have been many experimental ideas to try and implement the quantum random walks; such as nuclear magnetic resonance(NMR), optical photon computer, harmonic oscillator computer, ion traps and many others [7] [24] [3] [23], we shall only focus on one , that being ion trapping [8]. The reason being ion trapping applies very nicely to the discrete quantum walk on the line and has had some recent successes [39].

6.1 Ion Trapping

I understand that this paper is written for mathematicians, but it is just as important to understand how to use that mathematics in a physical sense as actually deriving the mathematics itself . Before we move on to how to implement the ion trap let us give a brief descriptions of what an trapped ion computer is. It is a type of quantum computer, which uses ions[14], that can be confined and suspended in free space using electromagnetic fields. Qubits are stored in stable electronic states[15] of each ion, and quantum information can be processed and transferred through the collective quantized motion of the ions in the trap, which interact through the Coulomb force. Lasers are then applied to induce coupling between the qubit states for single qubit operations, or coupling between the internal qubit states and the external position states, very much like our coin space and position space. Although we shall only be discussing how to trap one ion. For a more comprehensive review of trapped ion quantum computers see [7] [36]

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[14]atoms which have lost or gained one or more electrons, thus acquiring an electrical charge

[15]The internal (electronic) states are the stable and hyperfine ground states denoted by $|\downarrow\rangle$ and $|\uparrow\rangle$

6.2 The Experimental Set Up

The walk shall be implemented with a single Beryllium ion Be^+, confined in a coaxial resonator radio frequency ion trap [10] . In order to do this we must cool the ion via laser cooling to the electronic ground state $|0\rangle \otimes |\uparrow\rangle \equiv |0\rangle |\uparrow\rangle$ (which is essentially the initial state of our original D.Q.R.W on the line $\mathcal{H}_p \otimes \mathcal{H}_c$) . Our next aim is to simulate the unitary operator as described by equation (4.5), which takes the form

$$\hat{U} = e^{i\hat{p}\sigma_3}\hat{H} \tag{6.1}$$

where $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ is the momentum operator in one-dimension, σ_3 is the Pauli-z operator acting on the qubit and $\hat{H}$ is the Hadamard. In order to simulate this unitary operator we apply a sequence of four Raman beam pulses to our Beryllium ion to create the following state in terms of coherent states $|\alpha\rangle$,

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\alpha\rangle |\downarrow\rangle + |-\alpha\rangle |\uparrow\rangle) \tag{6.2}$$

where the coherent state $|\alpha\rangle$ of the oscillator [16] is defined as [8]

$$|\alpha\rangle = \frac{e^{2Re(\alpha)Im(\alpha)i}}{\pi^{\frac{1}{4}}} \int dx e^{\sqrt{2}iIm(\alpha)x} e^{-\frac{1}{2(x-\sqrt{2}Re(\alpha))^2}} |x\rangle \tag{6.3}$$

where $\alpha = |\alpha|e^{i\theta} \in \mathbb{C}$

The first Raman beam pulse is a $\frac{\pi}{2}$ pulse, which creates an equal superposition of $|0\rangle |\uparrow\rangle$ and $|0\rangle |\downarrow\rangle$. A displacement beam (second pulse) is then applied, this excites the motion correlated to the internal state $|\uparrow\rangle$. The third pulse is a π pulse which exchanges the internal states $|\uparrow\rangle$ and $|\downarrow\rangle$. We then apply another displacement beam (fourth pulse). In performing these four pulses we are essentially performing $\hat{U}$. To produce the full discrete quantum random walk we continue to apply this sequence of 4 pulses for a multiple number of times t.

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[16]As the position states of the ion are characterized by the quantized vibrational harmonic oscillator number states $|n\rangle$, the coherent states are of course a natural basis for representing the Fock states

6.3   Measuring the Walks

We now have our experimental set up for the discrete quantum walk on the line, but this means nothing unless we can take something meaningful away from the experiment , that is we need to measure the current state of the walk after we have applied the sequence of 4 Raman beam pulses t times. We see that when the system inherits enough noise from the pulses, decoherence begins to set in and the system begins to slowly become more and more classical. This leads to a decoupling of the coin space (the internal state ion) and the position space after an appropriate Raman pulse is applied. Now although this may seem like a negative effect, as we are losing the quantum qualities of the system, it is not, as we can actually use this to our advantage [8]. Since we can measure the degree to which the ion is acting as a quantum variable , rather than a classical one, and thus measure the level of decoherence in the ion trap. We can then use the internal state of the ion to tell us about the position state .

Suppose that we have now decoupled the internal state and the position state by measuring whether the ion is in the state $|\uparrow\rangle$ or $|\downarrow\rangle$. We then apply the measurement operator [8]

$$\hat{M} = e^{\pm i\hat{p}\sigma_2} \tag{6.4}$$

where the Hamiltonian $+i\hat{p}\sigma_2$ is applied if the ion is in the state $|\uparrow\rangle$ and the negative Hamiltonian $-i\hat{p}\sigma_2$ otherwise. We then measure the internal state of the ion again. If no decoherence has been measured we shall still remain in the state $|\downarrow\rangle$, if decoherence has completely effected the ion, when we measure $|\downarrow\rangle$, we would just expect the classical probability of $P_\downarrow(t) = \frac{1}{2}$. This is because decoherence causes the system to lose its quantum properties and so we are just observing the classical random walk on the line. Figure 15 [8] shows the probability that we would expect to find the ion in the ground state if no decoherence has effected the ion (it retains it quantumness) or if decoherence has completely effected the ion (it has become a classical system)
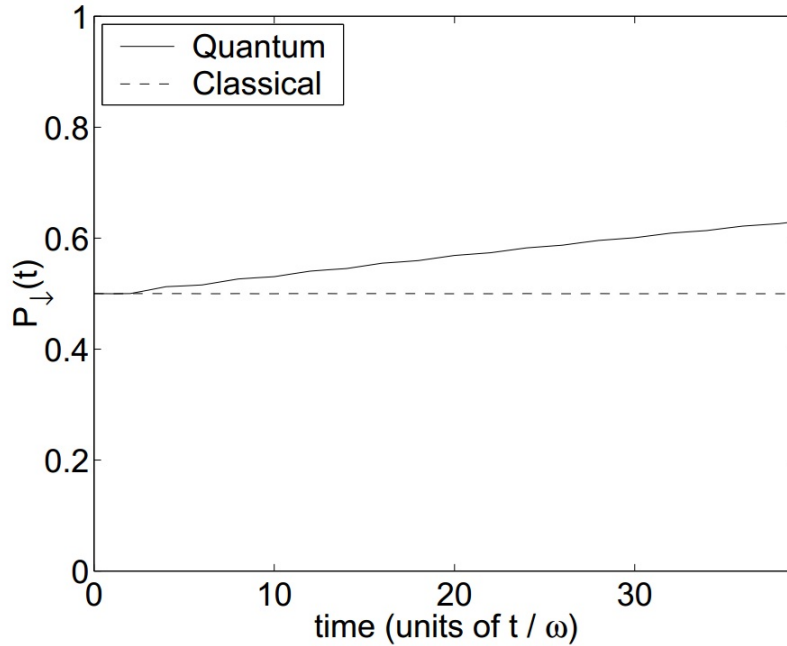
Figure 13: Probability of measuring the ion in the ground state after applying the random walk for a time t/ω, decoupling the coin and position states and then applying the Hamiltonian operator $\hat{H}$

Before we end this discussion, let us briefly discuss the practicalities of the trapped ion experiment. Since this experiment only used one ion , computationally it is not useful at all. However , on the positive side there is a lot of potential to viably extended the process of trapped ions to trapping multiple ions, in fact, in 2011 [39] achieved a system of 14 trapped ions, which is a remarkable improvement from the one trapped ion we were studying. Another problem with the experiment is that it is incredibly difficult to prepare the initial state of the system in $|0\rangle\,|\uparrow\rangle$. However, with new technology being developed and our understanding of the underlying physics continually improving, these type of systems are very slowly, but gradually becoming easier to implement.

7 Conclusion

In this review we have been introduced to the ideas of both the discrete and continuous quantum random walks on the line and on graphs. We have seen how there distributions are not Gaussian, but that they have the interesting property that they travel much further than the classical walk . We have seen how a simple database search algorithm, Grover's algorithm, that enlists the properties of quantum mechanics can offer a significant speed up of $\mathcal{O}(\sqrt{N})$, as compared to its classical counterpart of $\mathcal{O}(N)$. We have seen how modifying Grover'a algorithm for the spatial search via the discrete quantum walk can also offer additional speed ups in multiple dimensions. Finally, we discussed the experimental implementation for conducting the quantum walk on the line via a trapped Beryllium ion, which takes advantage of the quantum property of decoherence. As a final note, the area of quantum random walks is truly one of fascination. I am sorry that I do not have more time and pages to give the reader more information about this every growing and ever more intriguing area of quantum information science. I have only given you a tiny fraction of what is out there. I would have liked to of included how to actually connect the discrete and continuous quantum walks, as was recently shown by Strauch [37] , as this was rather difficult to achieve, but is of great importance. I would have also liked to of discussed the various types of computational problems that these quantum walks have been shown to offer a substantial speed up on, as compared to there classical counterparts. As for particular types of problems, continuous random walks can offer an exponential speed up over there classical counter parts [2]. I would have also of liked to of given more detail on how to calculate the long term asymptotic behaviour of the quantum walks. As calculating the long term behaviour cannot be done by standard means, since quantum walks do not converge to any stationary distribution, as they are unitary and so reversible in closed quantum systems. I hope that the given reader has enjoyed my review, as I have tried to be as broad as possible whilst maintaining some depth to give the reader a small glimpse in to the world of quantum random walks.

A   Appendix 1

A.1   The Computational Basis

The computational basis states of the space $\mathcal{H}^2 = \mathbb{C}^2$ is the set $\{|0\rangle, |1\rangle\}$. Projectors formed of the computational basis states are very useful for writing the spectral decomposition of many useful unitary operators. This has many advantages for when we want to find the possible outcomes of measurement. It also has a resemblance to the classical binary bits 0 and 1. In general for n qubits the computational basis may be written in the following way

Definition A.1. *The computational basis of the Hilbert space of n qubits in decimal notation is the set $\{|0\rangle, \ldots, |2^n - 1\rangle\}$*

where for example if we have 3 qubits ($n = 3$) then for the numbers 3 and 7 we can write

$$|0\rangle \otimes |1\rangle \otimes |1\rangle = |011\rangle = |3\rangle \tag{A.1}$$

$$|1\rangle \otimes |1\rangle \otimes |1\rangle = |111\rangle = |7\rangle \tag{A.2}$$

where if we change the first qubit to be in a superposition of states we get

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |1\rangle \otimes |1\rangle \tag{A.3}$$

$$= \frac{1}{\sqrt{2}}(|3\rangle + |7\rangle) \tag{A.4}$$

where the $\frac{1}{\sqrt{2}}$ is just a normalization factor.

A.1.1   Quantum Register

A quantum register is essentially a set of qubits , which are formed as the CPU memory is divided up.

A mathematical description of a quantum register is achieved by using a tensor product of several qubits. For example, an n qubit quantum register is described by an element

$|\psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_n\rangle$ in the tensor product Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_n$

A.1.2 Binary Sum XOR

A bitwise XOR takes two equal strings of bits 0 and 1, and perform the logical exclusive OR operation on each pair of corresponding bits. The result in each position of the new string is 1, if only the corresponding bit in the first string OR second string is 1, but not both. If the equivalent positioned bit in each string happens to be the same in both bits, then the bit in the resulting position for the new string is 0. For example

$$110(6)$$
$$011(3)$$
$$\text{XOR}$$
$$101(5)$$

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