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Master's Thesis

On Quantum Random Walks

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Contents

Chapter 1

Introduction

As the title suggests, the following thesis constitutes a thorough yet by no means complete journey through the current and ongoing research into quantum random walks. Classical random walks have been introduced and formalised during the beginning of the 20th century as tools to model and study financial as well as physical or biological phenomena. The well-known Brownian motion was first described by the French mathematician Louis Bachelier in his doctoral thesis *Théorie de la spéculation* in 1900 where he sought to study price changes at the Paris stock exchange. From there on the development of measure theory by Henri Lebesgue, Émile Borel, Paul Lévy and others allowed for a rigorous definition of stochastic processes like the random walk. In short, a random walk is a random path in some mathematical space like a graph, a group or a vector space. Chapter 2 will present the relevant definitions as well as an introduction to the theorems on limit behaviours of random walks, as we are interested in how the classical setting differs from the quantum theoretic one.

Figure 1.1: Illustration of a Brownian motion in the plane

So what is a quantum random walk and in what sense is it "quantum"? In contrast to its classical counterpart, the quantum random walk describes transitions between quantum states which is given by evolution under a unitary operator on a Hilbert space. These operators change the position of the walker – a quantum particle – as well as the so-called spin. The randomness arises in a completely different way. While in the classical case each step involves a "random draw" the quantum random walk is determined by an invertible, unitary operator. The source of randomness lies therefore in the quantum superposition of states as well as the state measurements performed at some random time. Most mathematicians are, if at all, only slightly familiar with terms like *quantum superposition*, *state measurement* and other quantum theoretic jargon. In Chapter 3 we will go over the necessary details from operator theory, present the definitions and axioms of quantum theory and formulate the theorems in order to better understand the evolution of a quantum system.

In the remaining Chapter 4 quantum random walks or QRWs for short are introduced and the current research is reviewed. There exists a plethora of interesting results that show the difference between the classical random walk and the quantum random walk. For example, the "diffusion" speed of a quantum random walker is quadratically faster than that of a random walker. This can already be seen for a (quantum) random walker on the line but holds true in almost all settings. This result is in particular interesting as random walks are used for algorithm design. There exist a hand-full of applications in computer science, among them recommender systems, computer vision and semi-supervised learning where a random walk can help find similarities by discovering an unknown-graph randomly. For the quantum random walk too we have interesting applications in search and page ranking algorithms which would, in addition, benefit from a quadratic speed up compared to the classical counterparts. The application of quantum random walks is itself a fruitful topic with a lot of publications going into the theoretical details and even the concrete details of implementing these algorithms on a quantum computer. We will focus on exploring quantum random walks for their own sake, but one can always keep in the back of one's mind that these constructions are the foundation for a lot of other research.

Chapter 2

Classical Random Walks

The theory of random walks sits somewhere in between the subjects of probability theory, graph theory, analysis and algebra. As such, we will see the application of many techniques when we analyse the behaviour of a random walk. This chapter mainly follows lecture notes from the author's master courses on the topic, as well as the famous book *Markov Chains and Mixing Times* by David Levin and Yuval Peres [1]. We start off with an easy example – the simple random walk on the integers.

Remark/Example 2.1 (Simple random walk on $\mathbb{Z}$)**.** Imagine the integers, i.e. $\{\dots, -2, -1, 0, 1, 2, \dots\}$ and a walker X_n that starts at 0 and within one time step moves to the left or the right with probability $\frac{1}{2}$, i.e.

$$\mathbb{P}\big[X_1 = 1 \,\big|\, X_0 = 0\big] = \mathbb{P}\big[X_1 = -1 \,\big|\, X_0 = 0\big] = \frac{1}{2}.$$

The process is illustrated in Figure 2.1, and we realise that the probability of

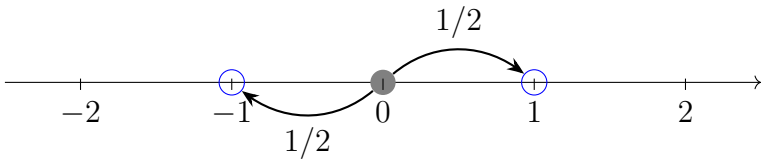


Figure 2.1: Transition probabilities of the random walk at $t = 0$

stepping to the right follows a binomial distribution. Say that at time n the walker took k steps to the right and l to the left so $n = k + l$. Then, the position of the walker at time n is $X_n = k - l$ and the probability of this event is

$$\mathbb{P}\big[X_n = k - l\big] = \binom{n}{k}\left(\frac{1}{2}\right)^k\left(\frac{1}{2}\right)^{n-k} = \binom{k+l}{k}\left(\frac{1}{2}\right)^k\left(\frac{1}{2}\right)^l.$$

Since the single step probabilities to the left and to the right are both one half, we get that the expected step width is $\mathrm{E}\big[X_i - X_{i-1}\big] = \frac{1}{2}\,1 + \frac{1}{2}\,(-1) = 0$ and therefore

$$\mathrm{E}\big[X_n\big] = \mathrm{E}\bigg[\sum_{i=1}^{n}(X_i - X_{i-1})\bigg] = \sum_{i=1}^{n}\mathrm{E}\big[X_i - X_{i-1}\big] = 0.$$

Furthermore, we may ask how far does this process on average propagate. Let us denote the i-th step by $Y_i := X_i - X_{i-1}$. As we have seen above $\mathrm{E}\big[Y_i\big] = 0$. By $\mathrm{Var}\big[X\big] = \mathrm{E}\big[X^2\big] - \mathrm{E}\big[X\big]^2$ for any random variable X, we have that

$$\mathrm{Var}\big[X_n\big] = \mathrm{E}\big[X_n^2\big] = \mathrm{E}\bigg[\sum_{i=1}^{n} Y_i^2 + \sum_{i\neq j} Y_i\,Y_j\bigg] = \mathrm{E}\bigg[\sum_{i=1}^{n} 1\bigg] = n.$$

Finally, do we expect the walker to return to the origin infinitely many times? For the walker to return means that we take k steps to the right and k steps to the left, i.e. $n = 2k$. Then

$$\mathbb{P}\big[X_n = 0\big] = \binom{2k}{k}\frac{1}{2^{2k}} = \frac{2k!}{(k!)^2\,2^{2k}}.$$

We use Stirling's approximation formula

$$n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n, \quad n \to \infty$$

to arrive at

$$\lim_{n\to\infty}\mathbb{P}\big[X_n = 0\big] = \lim_{n\to\infty}\frac{1}{\sqrt{\pi n}} = 0.$$

We count the average number of returns by taking the indicator functions on sets of the form $\{X_k = 0\}$. So, let $J_k := \mathbb{1}_{\{X_k=0\}}$, then we get the average number of returns to the origin by

$$\mathrm{E}\bigg[\sum_{k=1}^{\infty} J_{2k}\bigg] = \sum_{k=1}^{\infty}\mathbb{P}\big[X_{2k} = 0\big] = \infty.$$

That this series diverges can for example be seen by the p-series test. The divergence tells us that the walker will return infinitely many times and will not start to "get away" from the origin at some point. △

2.1 Markov Chains

In the previous example we have seen common properties for random walks such as the variance and the expected number of returns to the start. Now, it is time to make these notions precise for a family of random walks – Markov chains.

A Markov chain is a process which moves between elements of some set $\mathcal{X}$ where the next position is given by a probability distribution $P(x, \cdot)$ depending only on the current state x.

Definition 2.2 (Markov chain and stochastic matrix)**.** We call a sequence of random variables $(X_0, X_1, \ldots)$ a *Markov chain with state space $\mathcal{X}$ and transition matrix P* if for all $x, y \in \mathcal{X}$, all $t \geq 1$ and all events $H_{t-1} = \bigcap_{s=0}^{t-1} \{X_s = x_s\}$ satisfying $\mathbb{P}\big(H_{t-1} \cap \{X_t = x\}\big) > 0$, we have

$$\mathbb{P}\big[X_{t+1} = y \,\big|\, H_{t-1} \cap \{X_t = x\}\big] = \mathbb{P}\big[X_{t+1} = y \,\big|\, X_t = x\big] = P(x, y).$$

This property is called the *Markov property*.

Furthermore, we call P a *stochastic matrix* if $\sum_{y \in \mathcal{X}} P(x, y) = 1$, i.e. the rows of the matrix describe a probability distribution. Notice that the term *matrix* must not necessarily refer to a finite one. The state space $\mathcal{X}$ may be infinite. △

From the definition above we see for example that the transition matrix for the simple random walk on $\mathbb{Z}$ is

$$P(j, k) = \begin{cases} \frac{1}{2}, & \text{if } k \in \{j-1, j+1\}, \\ 0, & \text{otherwise.} \end{cases}$$

for $x, y \in \mathbb{Z}$. As we are going to look at quantum random walks on graphs, we also want to define random walks on graphs. Let $G = (V, E)$ be a graph, consisting of a *vertex set* V and an *edge set* E where the edges are unordered pairs of vertices, i.e. $E \subseteq \{\{x, y\} \mid x, y \in V, x \neq y\}$. The usual illustration is that of a network of nodes connected by lines. If $\{x, y\} \in E$, we also write $x \sim y$ and call x a *neighbour* of y. The degree $\deg(x)$ of a vertex x is the number of neighbours of x.

Definition 2.3 (Simple random walk on a graph)**.** Given a graph $G = (V, E)$, we define a *simple random walk on G* to be the Markov chain with state space V and transition matrix

$$P(x, y) = \begin{cases} \dfrac{1}{\deg(x)}, & \text{if } x \sim y, \\ 0, & \text{otherwise.} \end{cases}$$

So, the Markov chain moves from a state to all its neighbours with equal probability. △

Remark/Example 2.4. (i) This justifies why we called the random walk on $\mathbb{Z}$ simple in case that we move to the left or the right with probability $\frac{1}{2}$.
(ii) Another common example is that of the simple random walk on the n-cycle with state space $\mathcal{X} = \mathbb{Z}/n\mathbb{Z}$ and transition matrix

$$P(j,k) = \begin{cases} \frac{1}{2}, \text{ if } k \equiv j+1 \pmod{n}, \\ \frac{1}{2}, \text{ if } k \equiv j-1 \pmod{n}, \\ 0, \text{ otherwise.} \end{cases}$$

The case $n = 5$ is illustrated in Figure 2.2. △

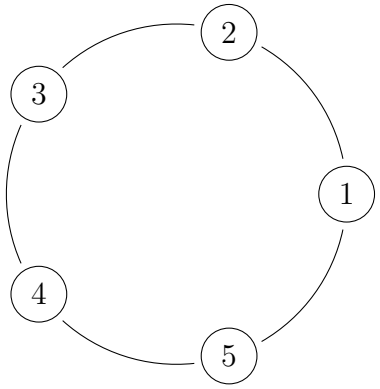


Figure 2.2: Illustration of the 5-cycle

One might wonder if there exists a distribution on the set $\mathcal{X}$ that is invariant under a random walk, i.e. evolving the walk for another time step results in exactly the same distribution.

Definition 2.5 (Stationary distribution)**.** We call a probability distribution π on $\mathcal{X}$ *stationary* if for all $y \in \mathcal{X}$

$$\pi(y) = \sum_{x \in \mathcal{X}} \pi(x) P(x,y).$$

In case that $\mathcal{X}$ is finite, we may write $\pi = \pi P$. △

Remark/Example 2.6. Consider the simple random walk on the finite graph $G = (V, E)$. By the definition of a *simple* random walk it holds that

$$\sum_{x \in V} \deg(x) P(x,y) = \sum_{x \in V,\, x \sim y} \frac{\deg(x)}{\deg(x)} = \deg(y).$$

To get a probability distribution on V we normalise by $\sum_{y \in V} \deg(y) = 2|E|$ and therefore

$$\pi(y) = \frac{\deg(y)}{2|E|}$$

is always a stationary distribution for a random walk on a finite graph. If G has the property of being d-regular, i.e. every vertex has the same degree d, then the stationary distribution is the uniform distribution since $2|E| = d|V|$ and therefore $\pi(y) = 1/|V|$. △

2.2 Properties of Markov Chains

Important properties of quantum random walks are *hitting times*, *return times* and *mixing times*. We will therefore take the time to introduce the concepts for classical random walks as well.

Definition 2.7 (Hitting time and return time)**.** Given a Markov chain (X_t) on a state space $\mathcal{X}$, we call

$$\tau_A := \min\{t \geq 0 \mid X_t \in A\}$$

the *hitting time of a subset* $A \subseteq \mathcal{X}$. In addition, by

$$\tau_x^+ := \min\{t \geq 1 \mid X_t = x\}$$

we denote the so-called *first return time* if $X_0 = x$. △

Mixing times describe the required time for a Markov chain's current distribution to get close to the stationary distribution. To describe this behaviour, we first need to introduce the *total variation distance*.

Definition 2.8 (Total variation distance)**.** Given two probability distributions μ and ν on $\mathcal{X}$, we define the *total variation distance* by

$$\|\mu - \nu\|_{TV} := \max_{A \subseteq \mathcal{X}} |\mu(A) - \nu(A)|,$$

where $A \subseteq \mathcal{X}$ is a measurable set. So, the distance between μ and ν is the maximum difference between the probabilities assigned to a single event by the two distributions. Because we will later investigate the distance between $P^t(x, \cdot)$ and the stationary distribution π, we set

$$d(t) := \max_{x \in \mathcal{X}} \|P^t(x, \cdot) - \pi\|_{TV}$$

and

$$\bar{d}(t) := \max_{x,y\in\mathcal{X}} \|P^t(x,\cdot) - P^t(y,\cdot)\|_{TV}.$$

△

One can prove the following lemma.

Lemma 2.9. *For the distance to stationarity, the following inequalities hold.*

$$d(t) \le \bar{d}(t) \le 2d(t).$$

Proof. From the triangle inequality of the total variation distance

$$\begin{aligned}\max_{x,y\in\mathcal{X}} \|P^t(x,\cdot) - P^t(y,\cdot)\|_{TV} &= \max_{x,y\in\mathcal{X}} \|P^t(x,\cdot) - P^t(y,\cdot) + \pi - \pi\|_{TV} \\ &\le \max_{x\in\mathcal{X}} \|P^t(x,\cdot) - \pi\|_{TV} + \max_{y\in\mathcal{X}} \|P^t(y,\cdot) - \pi\|_{TV} \\ &= 2d(t).\end{aligned}$$

If π is stationary, then it holds that

$$\pi(A) = \sum_{y\in\mathcal{X}} \pi(y) P^t(x,A)$$

by the definition of stationarity. Using this equality we get

$$\begin{aligned}|P^t(x,A) - \pi(A)| &= \left| \sum_{y\in\mathcal{X}} \pi(y) \Big[P^t(x,A) - P^t(y,A) \Big] \right| \\ &\le \sum_{y\in\mathcal{X}} \pi(y) \|P^t(x,\cdot) - P^t(y,\cdot)\|_{TV} \le \bar{d}(t).\end{aligned}$$

By maximising both sides over all measurable $A \subseteq \mathcal{X}$ we get the desired result. □

Definition 2.10 (Mixing time)**.** The *mixing time* is defined by

$$t_{\text{mix}}(\varepsilon) := \min\big\{ t \mid d(t) \le \varepsilon \big\}.$$

It can be shown that $\bar{d}$ is submultiplicative, thus for a positive integer ℓ

$$d(\ell t_{\text{mix}}(\varepsilon)) \le \bar{d}(t_{\text{mix}}(\varepsilon))^\ell \le (2\varepsilon)^\ell.$$

In particular, for $\varepsilon = 1/4$

$$d(\ell t_{\text{mix}}(1/4)) \le 2^{-\ell}$$

or

$$t_{\text{mix}}(\varepsilon) \le \lceil \log_2 \varepsilon^{-1} \rceil t_{\text{mix}}(1/4).$$

We can therefore set $t_{\text{mix}} := t_{\text{mix}}(1/4)$. △

2.3 Examples and Applications

On the following pages, we want to apply these definitions to a couple of canonical examples.

Theorem 2.11. *Let (X_t) be the simple random walk on $\mathbb{Z}$ and let*

$$\tau_0 = \min\{t \geq 0 \mid X_t = 0\}$$

be the first hitting time for 0. We write $\mathbb{P}_k[\,\cdot\,] := \mathbb{P}[\,\cdot \mid X_0 = k]$. Then

$$\mathbb{P}_k[\tau_0 > r] \leq \frac{6k}{\sqrt{r}}.$$

We need a couple of lemmas to prove this result.

Lemma 2.12 (Reflection Principle)**.** *Let (X_t) be the simple random walk on $\mathbb{Z}$. For any positive integers j, k, and r it holds that*

(i)
$$\mathbb{P}_k[\tau_0 < r, X_r = j] = \mathbb{P}_k[X_r = -j],$$

(ii)
$$\mathbb{P}_k[\tau_0 < r, X_r > 0] = \mathbb{P}_k[X_r < 0].$$

Proof. If the walk visits 0 at time s, then from time s onwards, the walk has the same distribution as the walk that originated at 0 and is independent of the history of the walk up until the time s by the Markov property. Hence, for $s < r$ and $j > 0$

$$\mathbb{P}_k[\tau_0 = s, X_r = j] = \mathbb{P}_k[\tau_0 = s]\mathbb{P}_0[X_{r-s} = j].$$

We have seen that the distribution of X_t is symmetric when starting at 0, so the right-hand side is equal to

$$\mathbb{P}_k[\tau_0 = s]\mathbb{P}_0[X_{r-s} = -j] = \mathbb{P}_k[\tau_0 = s, X_r = -j].$$

Summing over all $s < r$, we obtain

$$\mathbb{P}_k[\tau_0 < r, X_r = j] = \mathbb{P}_k[\tau_0 < r, X_r = -j].$$

Since a random walk starting at $k > 0$ must necessarily pass through 0 if the walk is at $-j$ at time r, it holds that

$$\mathbb{P}_k[\tau_0 < r, X_r = -j] = \mathbb{P}_k[X_r = -j],$$

proving the first statement. If we now sum over all $j > 0$, we get the second statement. □

Lemma 2.13. *For the simple random walk (X_t) on $\mathbb{Z}$, we have*

$$\mathbb{P}_k\big[\tau_0 > r\big] = \mathbb{P}_0\big[-k < X_r \leq k\big]$$

for any $k > 0$.

Proof. First, one sees that

$$\begin{aligned}\mathbb{P}_k\big[X_r > 0\big] &= \mathbb{P}_k\big[X_r > 0, \tau_0 \leq r\big] + \mathbb{P}_k\big[X_r > 0, \tau_0 > r\big] \\ &= \mathbb{P}_k\big[X_r > 0, \tau_0 \leq r\big] + \mathbb{P}_k\big[\tau_0 > r\big].\end{aligned}$$

Then by the previous Lemma 2.12 and $\mathbb{P}_k\big[X_r > 0, \tau_0 = r\big] = 0$ we have

$$\mathbb{P}_k\big[X_r > 0\big] = \mathbb{P}_k\big[X_r < 0\big] + \mathbb{P}_k\big[\tau_0 > r\big].$$

Since the simple random walk on $\mathbb{Z}$ is symmetric with respect to the starting point k, we obtain

$$\mathbb{P}_k\big[X_r < 0\big] = \mathbb{P}_k\big[X_r > 2k\big],$$

and using this together with the equation above yields

$$\begin{aligned}\mathbb{P}_k\big[\tau_0 > r\big] &= \mathbb{P}_k\big[X_r > 0\big] - \mathbb{P}_k\big[X_r > 2k\big] \\ &= \mathbb{P}_k\big[0 < X_r \leq 2k\big] = \mathbb{P}_0\big[-k < X_r \leq k\big],\end{aligned}$$

which concludes the proof. □

With the following lemma, we want to find an upper bound for the probability of the walker being at a point k.

Lemma 2.14. *For the simple random walk (X_t) on $\mathbb{Z}$, it holds that*

$$\mathbb{P}_0\big[X_t = k\big] \leq \frac{3}{\sqrt{t}}.$$

Proof. If the walker ends up at $2k$ after $2r$ time steps, i.e. $X_{2r} = 2k$, there have been $r + k$ moves to the right and $r - k$ moves to the left. The probability of this event is $\binom{2r}{r+k}2^{-2r}$. The binomial coefficient is maximised at $k = 0$, so we have that

$$\mathbb{P}_0\big[X_{2r} = 2k\big] \leq \binom{2r}{r}2^{-2r} = \frac{(2r)!}{(r!)^2 2^{2r}}.$$

Using Stirling's approximation, we obtain

$$\sqrt{2\pi n}\left(\frac{n}{e}\right)^n e^{\frac{1}{12n+1}} < n! < \sqrt{2\pi n}\left(\frac{n}{e}\right)^n e^{\frac{1}{12n}},$$

and this yields

$$\mathbb{P}_0\big[X_{2r} = 2k\big] \leq \sqrt{\frac{8}{\pi}}\frac{1}{\sqrt{2r}}.$$

By some more tedious calculations and estimations one can show that

$$\mathbb{P}_0\big[X_{2r+1} = 2k+1\big] \leq \frac{4}{\sqrt{\pi}}\frac{1}{\sqrt{2r+1}}.$$

Since $\sqrt{\frac{8}{\pi}} \leq \frac{4}{\sqrt{\pi}} \leq 3$, we get that $\mathbb{P}_0\big[X_t = k\big] \leq \frac{3}{\sqrt{t}}$ □

Proof of Theorem 2.11. Lemma 2.13 implies

$$\mathbb{P}_k\big[\tau_0 > r\big] = \mathbb{P}_0\big[k < X_r \leq k\big],$$

which together with Lemma 2.14 implies

$$\mathbb{P}_k\big[\tau_0 > r\big] \leq \frac{6k}{\sqrt{r}}.$$

This proves the desired result. □

We go on proving that the random walk on the n-cycle mixes in quadratic time. First, we need some more definitions.

Definition 2.15 (Coupling (of Markov chains))**.** A *coupling of two probability distributions* μ and ν is a pair of random variables (X, Y) defined on a single probability space such that the marginal distribution of X is μ and the marginal distribution of Y is ν. That is, a coupling (X, Y) satisfies $\mathbb{P}\big[X = x\big] = \mu(x)$ and $\mathbb{P}\big[Y = y\big] = \nu(y)$.

Furthermore, we define a *coupling of Markov chains* with transition matrix P to be a process (X_t, Y_t) with the property that both (X_t) and (Y_t) are Markov chains with transition matrix P, although the two chains may have different starting distributions. △

Theorem 2.16. *Let (X_t, Y_t) be a coupling such that if $X_s = Y_s$ for some $s \in \mathbb{N}$, then $X_t = Y_t$ for all $t \geq s$. Furthermore $X_0 = x$ and $Y_0 = y$. Let τ_{couple} denote the first time the two Markov chains meet, i.e.*

$$\tau_{couple} := \min\big\{t \mid X_s = Y_s \text{ for all } s \geq t\big\}.$$

Then, it holds that

$$\|P^t(x,\cdot) - P^t(y,\cdot)\|_{TV} \leq \mathbb{P}_{x,y}\big[\tau_{couple} > t\big].$$

Proof. It can be shown that for two probability distributions μ and ν

$$\|\mu - \nu\|_{TV} = \inf\{\mathbb{P}[X \neq Y] \mid (X, Y) \text{ is a coupling of } \mu \text{ and } \nu\}.$$

Since $P^t(x, z) = \mathbb{P}_{x,y}[X_t = z]$ and $P^t(y, z) = \mathbb{P}_{x,y}[Y_t = z]$, we have that

$$\|P^t(x, \cdot) - P^t(y, \cdot)\|_{TV} \leq \mathbb{P}_{x,y}[X_t \neq Y_t].$$

By the definition of our coupling, i.e. if the chains meet they will not separate again, the statement follows. □

Corollary 2.17. *Suppose that for each pair of states $x, y \in \mathcal{X}$ there is a coupling (X_t, Y_t) with $X_0 = x$ and $Y_0 = y$. Then*

$$d(t) \leq \max_{x,y \in \mathcal{X}} \mathbb{P}_{x,y}[\tau_{couple} > t].$$

Therefore, $t_{mix} \leq 4 \max_{x,y} \mathrm{E}_{x,y}[\tau_{couple}]$ by Markov's inequality.

Now we are able to prove the following theorem.

Theorem 2.18. *The lazy random walk on $\mathbb{Z}/n\mathbb{Z}$ is defined by*

$$P(j, k) = \begin{cases} \frac{1}{2}, \text{ if } k \equiv j & (\text{mod } n), \\ \frac{p}{2}, \text{ if } k \equiv j + 1 & (\text{mod } n), \\ \frac{q}{2}, \text{ if } k \equiv j - 1 & (\text{mod } n), \\ 0, \text{ otherwise}, & \end{cases}$$

where $p + q = 1$ and $p, q > 0$. For this random walk it holds that

$$\frac{1}{32} n^2 \leq t_{mix} \leq n^2.$$

Proof. Let us start with the upper bound. We construct a coupling of two walkers performing the lazy random walk on $\mathbb{Z}/n\mathbb{Z}$. One starts at x and the other starts at y. We do not want to move the walkers simultaneously to avoid them jumping over each other if they are within unit distance. Until the two meet a fair coin is tossed to determine which of the two walkers will move. The walker that is selected makes a clockwise increment with probability p and an anticlockwise increment with probability q.

Once the two collide, they will make identical moves. Let D_t be the clockwise distance from X_t to Y_t and note that this process is a simple random walk on the vertices $\{1, \ldots, n-1\}$ and gets absorbed either at 0 or n. One can verify that

$\mathrm{E}_{x,y}\big[\tau\big] = k(n-k)$ where $\tau := \min\big\{t \geq 0 \mid D_t \in \{0,\dots,n\}\big\}$ and k is the clockwise distance between x and y. Since $\tau = \tau_{\text{couple}}$, we have

$$d(t) \leq \max_{x,y} \mathbb{P}_{x,y}\big[\tau > t\big] \leq \frac{\max_{x,y} \mathrm{E}_{x,y}\big[\tau > t\big]}{t} \leq \frac{n^2}{4t}$$

by Markov's inequality. The right-hand side equals $1/4$ for $t = n^2$, so $t_{\text{mix}} \leq n^2$.

Now, let us look at the lower bound. Let (S_t) be the lazy p-q-biased random walk on $\mathbb{Z}$, i.e.

$$P(j,k) = \begin{cases} \frac{1}{2}, \text{ if } k = j, \\ \frac{p}{2}, \text{ if } k = j+1, \\ \frac{q}{2}, \text{ if } k = j-1, \\ 0, \text{ otherwise} \end{cases}$$

and $X_0 = x_0$. Then $X_t \equiv S_t \bmod n$. Let ρ denote the clockwise distance on the circle. If $\mu_t = t(p-q)/2$, set

$$A_t := \big\{k \mid \rho(k, \lfloor x_0 + \mu_t \rfloor \bmod n) \geq n/4\big\}.$$

We have seen in Example 2.6 that the stationary distribution of a simple random walk on a d-regular graph is the uniform distribution. In a similar fashion one can also argue that the *lazy* random walk on a d-regular graph admits the uniform distribution as a stationary one. Therefore, $\pi(A_t) \geq 1/2$. Using Chebyshev's inequality and since $\mathrm{Var}\big[S_t\big] = t(1/4 + pq) \leq t/2$ we get

$$\mathbb{P}\big[X_t \in A_t\big] \leq \mathbb{P}\big[|S_t - \mu_t| \geq n/4\big] \leq \frac{8t}{n^2} < \frac{1}{4}$$

if $t < n^2/32$. For such a t we have that

$$d(t) \geq \pi(A_t) - \mathbb{P}\big[X_t \in A_t\big] > \frac{1}{2} - \frac{1}{4},$$

i.e. $t_{\text{mix}} \geq n^2/32$. □

This concludes our examples. We have seen important characteristics of classical random walks such as hitting times and mixing times which describe the time it takes for a node to get visited for the first time and the closeness of the distribution to stationarity respectively. There exists a myriad of techniques that we have not yet seen. Analysing hitting times and return times can be done using generating functions which involves a fair bit of analysis and power series. In short, a Markov chain's generating function is a power series in one variable where the coefficients depend on the transition matrix. Coupling techniques, as we have seen in the proof of Theorem 2.18, are powerful instruments for bounding the mixing time and studying other phenomena.

Chapter 3

Quantum Theory for Mathematicians

This chapter is meant as an introduction to quantum theory from the point of view of a mathematician. Physics notation is just the tip of the iceberg when it comes to possible sources of confusion and misunderstanding. That the terminology of quantum mechanics has evolved out of and was motivated by classical mechanics is evident to most physicists yet from a mathematician's point of view this is not at all the case. This is why we will follow the book *Quantum Theory for Mathematicians* by Brian Hall [2] for the most part – a mathematician writing for mathematicians.

In classical mechanics one might be interested in the momentum or the energy of a given system. In order to determine quantities like these, one needs to take a measurement at some space in time. For example, one should think about measuring the speed of a car at a certain time. This would result in a real number. By the nature of quantum mechanics particles do not behave deterministically. For example, throughout the 19th century light was thought to behave like a wave but in the beginning of the 20th century its particle-like behaviour was observed. In the double-slit experiment the probabilistic behaviour of quantum particles was demonstrated. It is impossible to predict the outcome of an experiment ahead of time. Only the probabilities for the outcome of an experiment can be. These probabilities are encoded in what is called the *wave function* which is a function dependent on a position in space $\mathbf{x} \in \mathbb{R}^n$. The square of the absolute value of this wave function, for example, is then the probability of the particle being at some position in space or the frequency of the oscillation of the wave function describes the probability for some momentum. The wave function and its evolution in time can be deterministically calculated which does not imply that the position or the momentum of a particle are determined. Only the probability distribution

for these quantities are known.

Before we dive into the mathematical machinery of quantum theory, making precise the notion of a wave function and the time evolution, we look at the classical world. The time evolution of a system in classical mechanics is described by Newton's law

$$\frac{d\mathbf{p}}{dt} = m\frac{d^2\mathbf{x}}{dt^2} = F,$$

where $\mathbf{p} \in \mathbb{R}^n$ is the momentum of a particle and $\mathbf{x} \in \mathbb{R}^n$ its position. This translates to "the force is the rate of change of the momentum". The key point is a reformulation of this law in terms of the total energy of the system. This is called the Hamiltonian approach defining an energy function called the *Hamiltonian*

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m}\sum_{j=1} p_j^2 + V(\mathbf{x}),$$

consisting of the kinetic energy and the potential energy of a particle, where $-\nabla V = F$. Now, one can express Newton's law in terms of the Hamiltonian as

$$\frac{dx_j}{dt} = \frac{\partial H}{\partial p_j},$$
$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial x_j},$$

since the first equation tells us that $dx_j/dt = p_j/m$ and the second that $dp_j/dt = -\partial V/\partial x_j = F_j$ which together state the famous law. We will come back to the time evolution of a quantum system at a later time and we will see that the involved partial differential equation is very much motivated by Hamilton's equations.

3.1 Operators and Adjoints

In the realm of quantum mechanics the physical quantities like position, momentum and energy are represented by operators on a Hilbert space $\mathbf{H}$. These operators are unbounded which represents the fact that these quantities are in theory unbounded. We will now look at the definitions regarding unbounded operators and their adjoints.

$\mathbf{H}$ is going to denote a separable Hilbert space over $\mathbb{C}$. In the physics literature the convention is that the inner product on $\mathbf{H}$ is linear in the second factor, i.e.

$$\langle \phi, \lambda\psi \rangle = \lambda\langle \phi, \psi \rangle \quad \text{and} \quad \langle \lambda\phi, \psi \rangle = \overline{\lambda}\langle \phi, \psi \rangle$$

for all $\phi, \psi \in \mathbf{H}$ and $\lambda \in \mathbb{C}$.

Definition 3.1 (Bounded linear operator)**.** Let $\mathbf{H}$ be a complex separable Hilbert space. A map $A : \mathbf{H} \to \mathbf{H}$ is called a *linear operator* if $A(\lambda\phi + \psi) = \lambda A\phi + A\psi$ for all $\phi, \psi \in \mathbf{H}$ and $\lambda \in \mathbb{C}$. A linear operator is *bounded* if there exists a constant C such that $\|A\psi\| \leq C\|\psi\|$ for all $\psi \in \mathbf{H}$. △

First, we are going to define the adjoint for bounded operators and we will address the issue that our operators are generally unbounded in a moment.

Definition 3.2 (Adjoint of a bounded operator)**.** By Riesz representation theorem, for any bounded operator A there exists a unique bounded operator A^* called the *adjoint* of A, such that

$$\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$$

for all $\phi, \psi \in \mathbf{H}$. To see this, observe that for a fixed $\phi \in \mathbf{H}$ the map $\psi \mapsto \langle \phi, A\psi \rangle$ is a bounded linear functional on $\mathbf{H}$. Riesz representation theorem guarantees the existence of a unique χ_ϕ such that

$$\langle \phi, A\psi \rangle = \langle \chi_\phi, \psi \rangle$$

for all $\psi \in \mathbf{H}$. We simply define A^* pointwise via $A^*\phi := \chi_\phi$ which defines the adjoint uniquely. A bounded operator is said to be *self-adjoint* if $A^* = A$. △

Operators in quantum mechanics are self-adjoint. This guarantees that the quantities described by the operator are real. We will see the position and momentum operators later on and observe that they are not bounded. Yet, if A is an operator defined on all of $\mathbf{H}$ and has the property that $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\phi, \psi \in \mathbf{H}$, then A is automatically bounded. Thus, an unbounded, self-adjoint operator cannot be defined on all of $\mathbf{H}$. For this reason we introduce the *domain* of A.

Definition 3.3 (Unbounded linear operator)**.** An *unbounded linear operator* A on $\mathbf{H}$ is a linear map from a dense subspace $\mathrm{Dom}(A) \subseteq \mathbf{H}$ into $\mathbf{H}$. △

The definition does not exclude bounded operators since $\mathrm{Dom}(A)$ could be all of $\mathbf{H}$. In contrast to bounded operators we cannot use the Riesz representation theorem to define A^* since $\langle \phi, A\cdot \rangle$ might not be bounded. Thus, we change the definition accordingly.

Definition 3.4 (Adjoint of an unbounded operator)**.** For an unbounded operator A on $\mathbf{H}$, the *adjoint* A^* of A is defined as follows. A vector $\phi \in \mathbf{H}$ belongs to the domain $\mathrm{Dom}(A^*)$ of A^* if the linear functional

$$\psi \mapsto \langle \phi, A\psi \rangle,$$

defined on $\mathrm{Dom}(A)$ is bounded. For $\phi \in \mathrm{Dom}(A^*)$, let $A^*\phi$ be the unique vector χ such that

$$\langle \chi, \psi \rangle = \langle \phi, A\psi \rangle$$

for all $\psi \in \mathrm{Dom}(A)$. △

For the linear functional $\langle \phi, A\,\cdot \rangle$ to be bounded means that there exists a constant C such that $|\langle \phi, A\psi \rangle| \leq C\|\psi\|$ for all $\psi \in \mathrm{Dom}(A)$. We required $\mathrm{Dom}(A)$ to be a dense subspace of $\mathbf{H}$ so every completion of $\mathrm{Dom}(A)$ is all of $\mathbf{H}$. This allows us to use another theorem from functional analysis. If $\langle \phi, A\,\cdot \rangle$ is bounded on $\mathrm{Dom}(A)$, then it has a unique bounded extension on all of $\mathbf{H}$. We can apply Riesz theorem again for this unique extension and get that the adjoint of an unbounded operator is a linear operator on its domain.

Definition 3.5. An unbounded operator A on $\mathbf{H}$ is called *symmetric* if

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$$

for all $\phi, \psi \in \mathrm{Dom}(A)$. The operator A is *self-adjoint* if $\mathrm{Dom}(A^*) = \mathrm{Dom}(A)$ and $A^*\phi = A\phi$ for all $\phi \in \mathrm{Dom}(A)$. Finally, A is called *essentially self-adjoint* if the closure in $\mathbf{H} \times \mathbf{H}$ of the graph of A is the graph of a self-adjoint operator. △

Remark/Example 3.6. (i) So, an operator A is self-adjoint if A^* and A are the same operator with the same domain.
(ii) Every self-adjoint or essentially self-adjoint operator is symmetric, yet, not every symmetric operator needs to be essentially self-adjoint. For a symmetric operator it holds true that $\mathrm{Dom}(A) \subseteq \mathrm{Dom}(A^*)$ and A^* agrees with A on $\mathrm{Dom}(A)$. So, $\mathrm{Dom}(A^*)$ might be strictly larger than $\mathrm{Dom}(A)$.
(iii) The relevant definition for quantum theory is the one of self-adjointness. Especially, the spectral theorem does only apply to self-adjoint operators. In many cases essentially self-adjoint is enough since we always obtain a self-adjoint operator by simply taking the closure and applying the relevant theorems to this operator instead. △

We start with a theorem justifying the definitions above.

Theorem 3.7. *Suppose A is a symmetric operator on $\mathbf{H}$.*

(i) For all $\psi \in \mathrm{Dom}(A)$, $\langle \psi, A\psi \rangle$ is real. More generally, if $\psi, A\psi, A^{m-1}\psi$ for some $m \in \mathbb{N}$ all belong to $\mathrm{Dom}(A)$, then $\langle \psi, A^m\psi \rangle$ is real.

(ii) Suppose λ is an eigenvector for A, meaning that $A\psi = \lambda\psi$ for some nonzero $\psi \in \mathrm{Dom}(A)$. Then $\lambda \in \mathbb{R}$.

Proof. Since A is symmetric, we have

$$\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle = \overline{\langle \psi, A\psi \rangle}$$

for all $\psi \in \mathrm{Dom}(A)$. If $\psi, A\psi, A^{m-1}\psi$ all belong to the domain of A, we can use the symmetry of A repeatedly to show that

$$\langle \psi, A^m\psi \rangle = \langle A^m\psi, \psi \rangle = \overline{\langle \psi, A^m\psi \rangle}.$$

Meanwhile, if $\psi \neq 0$ is an eigenvector for A with eigenvalue λ, then it holds that

$$\lambda\langle \psi, \psi \rangle = \langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle = \overline{\lambda}\langle \psi, \psi \rangle.$$

This proves that the relevant quantities are all real. □

We will later see that $\langle \psi, A\psi \rangle$ represents the expected value for the measurement of A in state ψ, where A will be the operator determining for example position or momentum. Furthermore, the eigenvalue λ is one of the possible values for that measurement. This is also why we want this numbers to be real as they represent physical quantities.

3.2 Position and Momentum Operators

We begin by considering a single particle moving on the real line. The wave function is $\psi : \mathbb{R} \to \mathbb{C}$. Later on we will see how such a particle evolves in time but for now consider time fixed. Taking the absolute value squared is supposed to produce the probability density for the position of the particle. So, the probability of the particle being in some region $E \subseteq \mathbb{R}$ is given by

$$\int_E |\psi(x)|^2 \, dx$$

where in order to have a probability distribution we normalise ψ in such a way that

$$\int_{\mathbb{R}} |\psi(x)|^2 \, dx = 1.$$

This means that ψ should be a unit vector in $L^2(\mathbb{R})$. Using this definition we can also talk about the expected value simply by defining

$$\mathrm{E}(x) := \int_{\mathbb{R}} x|\psi(x)|^2 \, dx,$$

and assuming that the integral is absolutely convergent. Generally, we can define

$$\mathrm{E}(x^m) := \int_{\mathbb{R}} x^m |\psi(x)|^2 \, dx.$$

Now, we want to formalise these definitions to get operators on a Hilbert space, in this case $L^2(\mathbb{R})$, where the inner product is the usual one

$$\langle \phi, \psi \rangle = \int_{\mathbb{R}} \overline{\phi(x)} \psi(x) \, dx.$$

Then, the position operator X is "the multiplication by x", i.e.

$$(X\psi)(x) := x\psi(x)$$

and the expected value of the position can be written as $\langle \psi, E\psi \rangle$. Therefore, we introduce the shorthand notation

$$\langle X \rangle_\psi := \langle \psi, X\psi \rangle$$

for the expected value of the operator X in the state ψ. Clearly, for $\psi \in L^2(\mathbb{R})$ it might not be the case that $X\psi$ is in $L^2(\mathbb{R})$. Thus, we cannot define X on all of $L^2(\mathbb{R})$ hinting at the unboundedness of the operator. Nevertheless, for any unit vector ψ in $L^2(\mathbb{R})$ we have a well-defined probability density on $\mathbb{R}$, given by $|\psi(x)|^2$.

Now, we turn our attention to momentum. We have seen that the probabilities for the position of a particle are encoded in $|\psi(x)|^2$. The momentum on the other hand is encoded in the oscillations of the wave function ψ. An important idea in quantum physics is the *de Broglie*[1] *hypothesis* which proposes a particular relationship between the frequency of the oscillation of the wave function and its momentum.

Theorem 3.8 (de Broglie hypothesis)**.** *If the wave function of a particle has a spatial frequency k, then the momentum p of a particle is*

$$p = \hbar k,$$

where $\hbar$ is Planck's constant.

Theorem 3.8 is meant in the following way. If the wave function is of the form $\psi(x) = e^{ikx}$, then it represents a particle with momentum $p = \hbar k$. Now, this function is not square integrable so it fails to meet the requirement of being a unit

[1] Louis de Broglie (* 15 August 1892, Dieppe; † 19 March 1987, Louveciennes) French physicist.

element in the L^2 sense. For the moment, let us switch to a particle on a circle, avoiding some difficulties like integrability. The wave function for such a particle is a 2π-periodic function on $\mathbb{R}$ such that

$$\int_0^{2\pi} |\psi(x)|^2 \, dx = 1.$$

For any integer k we can say that a particle with the normalised wave function $\psi(x) = e^{ikx}/\sqrt{2\pi}$ has momentum $p = \hbar k$. Such a particle has a definite momentum and there is no randomness. So, a measurement of the particle's momentum should with probability 1 give the value $\hbar k$.

One can verify that the functions $e^{ikx}/\sqrt{2\pi}$ with $k \in \mathbb{Z}$ form an orthonormal basis of the Hilbert space of 2π-periodic, square-integrable functions denoted $L^2([0, 2\pi])$. Therefore, a wave function for a particle on a circle is

$$\psi(x) = \sum_{k=-\infty}^{\infty} a_k \frac{e^{ikx}}{\sqrt{2\pi}},$$

where the series is convergent in $L^2([0, 2\pi])$. If ψ is normalised to be a unit vector, then we have

$$\sum_{k=-\infty}^{\infty} |a_k|^2 = \|\psi\|^2_{L^2([0,2\pi])} = 1.$$

For a wave function of this form the momentum is no longer uniquely determined. Now, when we take a measurement, we expect one of the values $\hbar k$, $k \in \mathbb{Z}$, with probability $|a_k|^2$. Again we can write

$$\mathrm{E}(p) = \sum_{k=-\infty}^{\infty} \hbar k |a_k|^2,$$

and for the higher moments

$$\mathrm{E}(p^m) = \sum_{k=-\infty}^{\infty} (\hbar k)^m |a_k|^2$$

respectively, where we assume that the series actually converges. Again, we would like to encode the information in a *momentum operator* P such that

$$\mathrm{E}(p^m) = \langle \psi, P^m \psi \rangle.$$

We can achieve this relation if P satisfies

$$P e^{ikx} = \hbar k e^{ikx},$$

since then we would have

$$\langle \psi, P^m \psi \rangle = \sum_{k=-\infty}^{\infty} (\hbar k)^m |a_k|^2 = \mathrm{E}(p^m).$$

The choice for P is thus

$$P = -i\hbar \frac{d}{dx}.$$

Let us return to the particle on the real line. Somehow we want to avoid the problem of square-integrability. For this, we use the fact that the Fourier transform allows us to build up any square-integrable function out of functions of the form e^{ikx}. Physicists call a linear combination or the continuous analogue, i.e. an integral, of such functions *superpositions* of functions of the form e^{ikx}. This means that

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \hat{\psi}(k)\, dk,$$

where $\hat{\psi}(k)$ is the Fourier transform of ψ, defined by

$$\hat{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \psi(x)\, dx.$$

Furthermore, the Plancherel theorem tells us that the Fourier transform is a unitary map of $L^2(\mathbb{R})$ onto $L^2(\mathbb{R})$. Thus, for any unit vector $\psi \in L^2(\mathbb{R})$ we obtain

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{\infty} \left|\hat{\psi}(k)\right|^2\, dk = 1.$$

So, it is natural to think that $|\hat{\psi}(k)|^2$ is essentially the probability density for the momentum of the particle. We can now summarise this in a theorem, expressing the properties of the momentum operator without explicit reference to the non-square-integrable function e^{ikx}.

Theorem 3.9. *Define the momentum operator P by*

$$P = -i\hbar \frac{d}{dx}.$$

Then for all "sufficiently nice" unit vectors ψ in $L^2(\mathbb{R})$, we have

$$\langle \psi, P^m \psi \rangle = \int_{-\infty}^{\infty} (\hbar k)^m \left|\hat{\psi}(k)\right|^2\, dk,$$

for all positive integers m. The quantity is interpreted as the expected value of the mth power of the momentum $\mathrm{E}(p^m)$.

To end this section, we want to summarise properties of these two important operators.

Definition 3.10. For a particle moving on $\mathbb{R}$, let the quantum Hilbert space be $L^2(\mathbb{R})$ and define the position and momentum operators X and P by

$$X\psi(x) = x\psi(x)$$
$$P\psi(x) = -i\hbar\frac{d\psi}{dx}.$$

Importantly, these two operators are not defined on the entire space $L^2(\mathbb{R})$ but on a dense subspace. △

Theorem 3.11. *The position and momentum operators X and P do not commute, but satisfy the relation*

$$XP - PX = i\hbar I.$$

This relation is known as the canonical commutation relation.

Proof. Using the product rule, we obtain that

$$\begin{aligned} PX\psi &= -i\hbar\frac{d}{dx}(x\psi(x)) \\ &= -i\hbar\psi(x) - i\hbar x\frac{d\psi}{dx} \\ &= -i\hbar\psi(x) + XP\psi(x). \end{aligned}$$

This concludes the proof. □

Theorem 3.12. *For all sufficiently nice functions ϕ and ψ in $L^2(\mathbb{R})$ we have*

$$\langle\phi, X\psi\rangle = \langle X\phi, \psi\rangle$$

and

$$\langle\phi, P\psi\rangle = \langle P\phi, \psi\rangle.$$

Proof. Suppose that ϕ and ψ both belong to $L^2(\mathbb{R})$ and that the functions $x\phi(x)$ and $x\psi(x)$ also belong to $L^2(\mathbb{R})$. Then since x is real, we have

$$\int_{-\infty}^{\infty} \overline{\phi(x)}x\psi(x)\,dx = \int_{-\infty}^{\infty} \overline{x\phi(x)}\psi(x)\,dx,$$

where both integrals are convergent because they are both integrals of the product of two L^2 functions.

For the second statement, let us assume that ϕ and ψ are continuously differentiable and that $\phi(x)$ and $\psi(x)$ tend to zero as x tends to $\pm\infty$. Let us also assume that ϕ, ψ, $d\phi/dx$ and $d\psi/dx$ belong to $L^2(\mathbb{R})$. We note that $d\overline{\phi}/dx$ is the same as $\overline{d\phi/dx}$. Thus, using integration by parts, we obtain

$$-i\hbar \int_{-A}^{A} \overline{\phi(x)} \frac{d\psi}{dx}\, dx = -i\hbar\, \overline{\phi(x)}\psi(x)\Big|_{-A}^{A} + i\hbar \int_{-A}^{A} \overline{\frac{d\phi}{dx}}\psi(x)\, dx.$$

Under the assumptions above, as A tends to infinity, the boundary terms will vanish and the remaining integral will tend to

$$\int_{-\infty}^{\infty} \overline{\phi(x)} \left(-i\hbar \frac{d\psi}{dx}\right)\, dx = \int_{-\infty}^{\infty} \overline{\left(-i\hbar \frac{d\phi}{dx}\right)}\psi(x)\, dx,$$

by dominated convergence. □

The preceding theorem shows that X and P are symmetric operators on certain dense subspaces of $L^2(\mathbb{R})$, i.e. the space of function for which the theorem was proven. One can actually show that X and P are essentially self-adjoint on these domains.

3.3 The Axioms of Quantum Mechanics

The following section deals with the fundamental principles of quantum mechanics. These so-called axioms are not to be understood in a mathematical sense as the foundation from which all other results are deduced logically. We will look at "kinematic" axioms first, those that apply at one fixed time, and in the next section we will consider the axiom that governs evolution in time.

Axiom 1. *The state of the system is represented by a unit vector ψ in an appropriate Hilbert space* $\mathbf{H}$*. If ψ_1 and ψ_2 are two unit vectors in* $\mathbf{H}$ *with $\psi_2 = c\psi_1$ for some constant $c \in \mathbb{C}$, then ψ_1 and ψ_2 represent the same physical state.*

Sometimes the Hilbert space $\mathbf{H}$ is called "quantum Hilbert space". This does not mean that the space is mathematically different from a generic Hilbert space. It only signifies that there is a quantum system associated with that space. Furthermore, elements of $\mathbf{H}$ are so-called "pure states". There is a more general notion of a "mixed state" which we will not concern ourselves with in this work.

Axiom 2. *To each real-valued function f on the classical phase space there is associated a self-adjoint operator $\hat{f}$ on the quantum Hilbert space.*

This operator $\hat{f}$ is almost always unbounded, as we have seen with the position and the momentum operator X and P respectively. Furthermore, we have seen that self-adjointness is a rather technical property when the operator is unbounded. Thankfully, some basic functions are enough most of the time, among them position, momentum, energy and angular momentum. For these one can individually convince oneself that they are indeed (essentially) self-adjoint.

For a particle moving in $\mathbb{R}^1$, the classical phase space is $\mathbb{R}^2$ which is a pair (x, p) consisting of a particle's position and its momentum. The quantum Hilbert space in that case is usually taken to be $L^2(\mathbb{R})$. If the function in Axiom 2 is the position function $f(x, p) = x$, then $\hat{f}$ is the position operator X and if $f(x, p) = p$, then $\hat{f} = P$. The function f is often called a *classical observable*, whereas the operator $\hat{f}$ is called a *quantum observable*.

Axiom 3. *If a quantum system is in a state described by a unit vector $\psi \in \mathbf{H}$, the probability distribution for the measurement of some observable f satisfies*

$$\mathrm{E}(f^m) = \left\langle \psi, (\hat{f})^m \psi \right\rangle .$$

In particular, the expected value for a measurement of f is given by

$$\left\langle \psi, \hat{f}\psi \right\rangle .$$

So, we still measure a classical observable f but this observable does not have a definite value any longer. The probabilities for measuring a certain value are encoded in the operator $\hat{f}$ and the state $\psi \in \mathbf{H}$.

If ψ is a nonzero vector in $\mathbf{H}$ but not a unit vector we can always write

$$\left\langle \tilde{\psi}, \hat{f}\tilde{\psi} \right\rangle = \frac{\langle \psi, \hat{f}\psi \rangle}{\langle \psi, \psi \rangle}.$$

So we can assume ψ to be of unit length from the start.

Furthermore, $\hat{f}$ is assumed to be self-adjoint and every self-adjoint operator is symmetric. By Theorem 3.7 we know that $\mathrm{E}(f)$ and $\mathrm{E}(f^m)$ are real. Additionally, for self-adjoint operators one could even construct a probability measure $\mu_{\hat{f},\psi}$ on $\mathbb{R}$ which we will skip as a technicality.

Axiom 3 also motivates why two states that differ by a constant $c \in \mathbb{C}$, with $|c| = 1$ describe the same physical state. For if $\psi_2 = c\psi_1$ for any operator A, then we have that

$$\langle \psi_2, A\psi_2 \rangle = \langle c\psi_1, Ac\psi_1 \rangle = |c|^2 \langle \psi_1, A\psi_1 \rangle = \langle \psi_1, A\psi_1 \rangle$$

We recall the notation introduced in a previous section.

Remark/Example 3.13. If A is a self-adjoint operator on $\mathbf{H}$ and $\psi \in \mathbf{H}$ is a unit vector, the expected value of A in the state ψ is denoted $\langle A \rangle_\psi$ and is defined as in Axiom 3 by

$$\langle A \rangle_\psi := \langle \psi, A\psi \rangle. \qquad \triangle$$

Theorem 3.14 (Eigenvectors)**.** *If a quantum system is in a state described by a unit vector $\psi \in \mathbf{H}$ and for some observable $\hat{f}$ we have that $\hat{f}\psi = \lambda\psi$ for some $\lambda \in \mathbb{R}$, then*

$$\mathrm{E}(f^m) = \left\langle (\hat{f})^m \right\rangle_\psi = \lambda^m$$

for all positive integers m. The unique probability distribution measure consistent with this condition is the one in which f has the definite value λ with probability one.

This means that if ψ is an eigenvector of $\hat{f}$, then the measurement of f for a particle in state ψ is not random but determined uniquely by λ. We want to find a probability measure μ on $\mathbb{R}$ such that

$$\int_{\mathbb{R}} x^m \, d\mu = \lambda^m.$$

The theorem claims that there exists only one such measure, namely the Dirac measure at the point λ, i.e.

$$\delta_\lambda(A) := \begin{cases} 0, & \lambda \notin A, \\ 1, & \lambda \in A. \end{cases}$$

If, more generally, the state of the system is a linear combination of eigenvectors for $\hat{f}$, measurements of f will no longer be deterministic.

Remark/Example 3.15. Suppose $\hat{f}$ has an orthonormal basis $\{e_j\}$ of eigenvectors with distinct (real) eigenvalues λ_j. Suppose also that ψ is a unit vector in $\mathbf{H}$ with the expansion

$$\psi = \sum_{j=1}^{\infty} a_j e_j.$$

Then for a measurement in the state ψ of the observable f, the observed value of f will always be one of the numbers λ_j. Furthermore, the probability of observing the value λ_j is given by

$$\mathbb{P}\big[f = \lambda_j\big] = |a_j|^2. \qquad \triangle$$

The next axiom is the final kinematic axiom.

Axiom 4. *Suppose a quantum system is initially in a state ψ and that a measurement of an observable f is performed. If the result of the measurement is the number $\lambda \in \mathbb{R}$, then immediately after the measurement, the system will be in a state ψ' that satisfies*

$$\hat{f}\psi' = \lambda\psi'.$$

The passage from ψ to ψ' is called the collapse of the wave function. Here $\hat{f}$ is the self-adjoint operator associated with f by Axiom 2.

If we assume that $\hat{f}$ has an orthonormal basis of eigenvectors $\{e_j\}$ with distinct eigenvalues λ_j, then we can say that if we observe the value λ_j in a measurement of $\hat{f}$, then $\psi' = e_j$. That is, the measurement "collapses" the wave function. We loose all the components of ψ in the direction of the e_k except the one where $k = j$. In a sense the collapse of the wave function behaves like conditional probability. Directly after we measured the observable we know the state of the system. The state may of course change over time according to a law that we will get to know in just a bit. In any case, Axiom 4 guarantees that if we measure f and then measure f again a very short time later, the two results will agree. So, immediately after the first measurement, the probabilities for a second measurement of f are not based on ψ but rather on ψ' and since ψ' is an eigenvector for $\hat{f}$ with eigenvalue λ, Proposition 3.14 tells us that this gives the value λ.

Before we look at the time evolution we want to define one last concept. For a random variable Y the variance is usually computed by

$$\sigma^2 = \mathrm{E}\left[(Y - \mathrm{E}(Y))^2\right] = \mathrm{E}(Y^2) - \mathrm{E}(Y)^2.$$

This motivates the following definition.

Definition 3.16 (Uncertainty)**.** If A is a self-adjoint operator on a Hilbert space $\mathbf{H}$ and ψ is a unit vector in $\mathbf{H}$, let $\Delta_\psi A$ denote the standard deviation associated with measurements of A in the state ψ, which is computed as

$$(\Delta_\psi A)^2 = \left\langle (A - \langle A\rangle_\psi\, I)^2 \right\rangle_\psi = \left\langle A^2 \right\rangle_\psi - \left(\langle A\rangle_\psi\right)^2.$$

We refer to $\Delta_\psi A$ as the uncertainty of A in the state ψ. △

For any observable A one can always choose ψ such that $\Delta_\psi A$ becomes arbitrarily small. Though, it can be shown that in case that two observables A, B do not commute one cannot minimise both $\Delta_\psi A$ and $\Delta_\psi B$ at the same time. We have seen that the position operator X and the momentum operator P do not commute. From this, one can deduce *Heisenberg's uncertainty principle*, i.e.

$$(\Delta_\psi X)(\Delta_\psi P) \geq \frac{\hbar}{2},$$

for all ψ for which $\Delta_\psi X$ and $\Delta_\psi P$ are defined.

3.4 Time Evolution in Quantum Theory

In the preceding section we have always assumed that ψ is the wave function of a particle for a fixed time. In this section we want to describe how a quantum system evolves in time. We have seen that in the Hamiltonian formulation of classical mechanics the time evolution is governed by Hamilton's equations and the Hamiltonian which basically encodes conservation of energy. According to Axiom 2 there must exist a corresponding self-adjoint operator $\hat{H}$ on the quantum Hilbert space $\mathbf{H}$ which we call the *Hamiltonian operator* for the system.

Before, we formulated the *de Broglie hypothesis*, $p = \hbar k$, where k is the spacial frequency of the wave function. Similarly, we motivate the time evolution by a relation between the energy and the temporal frequency of the wave function

$$E = \hbar\omega.$$

This relationship was proposed by Max Planck[2] in his model of blackbody radiation. Suppose now that a wave function ψ_0 has a definite energy E meaning that ψ_0 is an eigenvector for $\hat{H}$ with eigenvalue E. Then, the relationship tells us that the time dependency should be purely at frequency $\omega = E/\hbar$. So, if the state of the system at $t = 0$ is ψ_0, then the state of the system at some other time t should be

$$\psi(t) = e^{-i\omega t}\psi_0 = e^{-iEt/\hbar}\psi_0.$$

This can be written as a differential equation

$$\frac{d\psi}{dt} = -\frac{iE}{\hbar}\psi = \frac{E}{i\hbar}\psi.$$

It is a useful convention that the temporal frequency ω leads to a time dependence of the form $e^{-i\omega t}$ and the spatial frequency k to e^{ikx}. Exponential solutions to the differential equation are then of the form $e^{i(kx-\omega t)}$ which describes a solution moving to the right with speed ω/k.

We see that if ψ_0 is an eigenvector of $\hat{H}$, ψ is just a multiple of ψ_0 and thus still an eigenvector of $\hat{H}$ to the eigenvalue E. So, E in the equation can be replaced by $\hat{H}$. This motivates the following axiom.

Axiom 5. *The time evolution of the wave function ψ in a quantum system is given by the Schrödinger equation,*

$$\frac{d\psi}{dt} = \frac{1}{i\hbar}\hat{H}\psi,$$

[2] Max Planck (* 23 April 1858, Kiel; † 4. October 1947, Göttingen) German theoretical physicist

where $\hat{H}$ is the operator corresponding to the classical Hamiltonian H by means of Axiom 2.

Now, we want to see how the expected value of an observable is influenced by evolution in time.

Theorem 3.17. *Suppose $\psi(t)$ is a solution of the Schrödinger equation and A is a self-adjoint operator on* **H**. *Assuming certain natural domain conditions hold, we have*

$$\frac{d}{dt}\langle A\rangle_{\psi(t)} = \left\langle \frac{1}{i\hbar}[A,\hat{H}] \right\rangle_{\psi(t)},$$

where $[\cdot,\cdot]$ denotes the commutator, defined as

$$[A,B] = AB - BA.$$

Proof. For the following statements to hold it is necessary that the following domain conditions are fulfilled. For every $t \in \mathbb{R}$ we need to have $\psi(t) \in \mathrm{Dom}(A) \cap \mathrm{Dom}(\hat{H})$, $A\psi(t) \in \mathrm{Dom}(\hat{H})$ and $\hat{H}\psi \in \mathrm{Dom}(A)$. Furthermore, $A\psi(t)$ has to be a continuous path in **H**. We use the product rule for the inner product and the self-adjointness of $\hat{H}$ to calculate

$$\begin{aligned}\frac{d}{dt}\langle \psi, A\psi\rangle &= \left\langle \frac{d\psi}{dt}, A\psi \right\rangle + \left\langle \psi, A\frac{d\psi}{dt} \right\rangle \\ &= \frac{i}{\hbar}\left\langle \hat{H}\psi, A\psi \right\rangle - \frac{i}{\hbar}\left\langle \psi, A\hat{H}\psi \right\rangle \\ &= \frac{1}{i\hbar}\left\langle \psi, [A,\hat{H}]\psi \right\rangle.\end{aligned}$$

□

So, interesting behaviour occurs only if A and $\hat{H}$ do not commute, otherwise the expected values would be constant in time. Such quantities are called *conserved quantities* or *constants of motion*. This directly leads us to the following theorem.

Theorem 3.18. *If $\phi(t)$ and $\psi(t)$ are solutions of the Schrödinger equation, the quantity $\langle\phi(t),\psi(t)\rangle$ is independent of t. In particular $\|\psi(t)\|$ is independent of t for any solution $\psi(t)$ of the Schrödinger equation.*

Proof. Using again the product rule, we have

$$\begin{aligned}\frac{d}{dt}\langle\phi(t),\psi(t)\rangle &= \left\langle \frac{1}{i\hbar}\hat{H}\phi(t),\psi(t) \right\rangle + \left\langle \phi(t), \frac{1}{i\hbar}\hat{H}\psi(t) \right\rangle \\ &= -\frac{1}{i\hbar}\left\langle \hat{H}\phi(t),\psi(t) \right\rangle + \frac{1}{i\hbar}\left\langle \phi(t),\hat{H}\psi(t) \right\rangle \\ &= 0,\end{aligned}$$

because $\hat{H}$ is self-adjoint. □

Before introducing quantum random walks we want to tie things together by looking at the time evolution of a particle on the line. First of all, we think about a classical particle on the line. The Hamiltonian which consists of the kinetic energy plus the potential energy is of the form

$$H(x,p) = \frac{p^2}{2m} + V(x),$$

where V is the potential energy function. Thus, we can define the associated operator as

$$\hat{H} = \frac{P^2}{2m} + V(X),$$

where $V(X)$ is the operator that means multiplication by the potential energy, i.e.

$$\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x).$$

Then, the Schrödinger equation takes the form

$$\frac{\partial\psi(x,t)}{dt} = \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} - \frac{i}{\hbar}V(x)\psi(x,t),$$

which is a linear partial differential equation. By applying Theorem 3.17 one can easily arrive at the following statements.

Theorem 3.19. *Suppose $\psi(t)$ is a solution to the Schrödinger equation for a sufficiently nice potential V and for a sufficiently nice initial condition $\psi(0) = \psi_0$. Then the expected position and expected momentum in the state $\psi(t)$ satisfy*

$$\begin{aligned}\frac{d}{dt}\langle X\rangle_{\psi(t)} &= \frac{1}{m}\langle P\rangle_{\psi(t)}\\ \frac{d}{dt}\langle P\rangle_{\psi(t)} &= -\left\langle V'(X)\right\rangle_{\psi(t)}.\end{aligned}$$

Chapter 4

Quantum Random Walks

Quantum walks are a relatively new research topic with the first publications in the early nineties. Up until now, two major models of quantum random walks have been suggested. First, the *discrete-time quantum random walk* consisting of two quantum mechanical systems that are usually called the walker and the coin and an evolution operator which is applied to both systems only at discrete time steps. This means that there exists a unitary operator U such that $\psi_{i+1} = U\psi_i$. The second major model is the *continuous-time quantum random walk*, consisting of a walker and a Hamiltonian operator that can be applied continuously. The governing force is thus the Schrödinger equation that we have seen before.

In both models the underlying sets on which the quantum random walk is usually performed are discrete graphs. This is also why we introduced classical random walks only on graphs since this is where the quantum random walk will live as well. Graphs are widely used in computer science to develop algorithms and trying to achieve the same for quantum algorithms, i.e. algorithms that can be run on a quantum computer, has fuelled a lot of research in the last years. See for example [3].

The idea is to start with a qubit. In contrast to a traditional bit which can only have one of two states, i.e. either a zero or a one, a qubit can be in any superposition of two states. For example, to describe a photon's polarisation we have two eigenstates which in physics notation are written as $|0\rangle$ and $|1\rangle$ which are elements of some Hilbert space $\mathbf{H}$. Then, a qubit is nothing but a linear combination of the eigenstates, i.e.

$$|\psi\rangle = a|0\rangle + b|1\rangle,$$

with $|a|^2 + |b|^2 = 1$. We then apply one or more evolution operators multiple times without making any intermediate measurements or by taking so-called partial measurements.

Let us briefly revisit what a measurement means and also explain what partial measurements are. An observable Q is always connected to some self-adjoint operator $\hat{Q}$ by Axiom 2 having an eigenbasis $\{|q_i\rangle\}$ such that

$$\hat{Q}|q_i\rangle = q_i|q_i\rangle,$$

where we have used the physics notation $|\cdot\rangle$ that represents the eigenvector with respect to the eigenvalue q_i. Axiom 4 tells us that upon measuring a system we get the collapse of the wave function. If a particle has a state $|\psi\rangle$, then this can always be expanded in terms of the eigenbasis of $\hat{Q}$, i.e.

$$|\psi\rangle = \sum_i \psi_i|q_i\rangle,$$

where $\psi_i = \langle q_i|\psi\rangle$, that is the inner product of the eigenvector $|q_i\rangle$ and the state $|\psi\rangle$. We also know that the probability for measuring outcome q_i is $|\psi_i|^2$. Mathematically, the collapse of the wave function is a projection onto one of the eigenstates, that is

$$\hat{\Pi}(q_i) = |q_i\rangle\langle q_i|.$$

If we apply this operator to the state $|\psi\rangle$, we get

$$|\psi'\rangle = |q_i\rangle\langle q_i|\psi\rangle,$$

which is a non-normalised state with outcome probability $\langle\psi'|\psi'\rangle = |\langle q_i|\psi\rangle|^2 = |\psi_i|^2$. The collapsed state is obtained by normalising, i.e. $|\psi'\rangle$ is replaced by $|q_i\rangle$. This is the mathematical way of writing down a measurement. An additional complication arises if we instead consider a multi-particle system. Consider a particle on a Hilbert space $\mathbf{H}_a$ and a particle on a different Hilbert space $\mathbf{H}_b$. The combined system evolves on the space $\mathbf{H}_a \otimes \mathbf{H}_b$. We perform a measurement on the first particle according to a quantum observable $\hat{Q}_a$ that acts on $\mathbf{H}_a$ and has an eigensystem $\{|\mu\rangle \mid \mu = 1, 2, \ldots\}$. We write a state $|\psi\rangle$ using the eigenbasis of $\hat{Q}_a$ and some other basis $\{|\nu\rangle\}$ of $\mathbf{H}_b$ like so

$$\begin{aligned}|\psi\rangle &= \sum_{\mu,\nu} \psi_{\mu,\nu}|\mu\rangle \otimes |\nu\rangle \\ &= \sum_{\mu} |\mu\rangle \otimes |\varphi_\mu\rangle,\end{aligned}$$

where $|\varphi_\mu\rangle = \sum_\nu \psi_{\mu,\nu}|\nu\rangle \in \mathbf{H}_b$. Again, the probability of seeing the outcome labelled by μ should be equal to $\langle\varphi_\mu|\varphi_\mu\rangle$. Let us define the partial projector

$$\hat{\Pi}(\mu) = |\mu\rangle\langle\mu| \otimes \hat{I}.$$

If we apply this projector to the expansion of $|\psi\rangle$ above, we get

$$|\psi'\rangle = |\mu\rangle\langle\mu|\mu\rangle \otimes |\varphi_\mu\rangle = |\mu\rangle \otimes |\varphi_\mu\rangle,$$

since $|\mu\rangle$ is normalised. Then, the probability of the outcome μ is

$$\langle\psi'|\psi'\rangle = \langle\mu|\mu\rangle\langle\varphi_\mu|\varphi_\mu\rangle = \sum_\nu |\psi_{\mu,\nu}|^2,$$

which is exactly what we wanted. Again, the state that the system assumes post-measurement is obtained by normalisation, thus

$$|\psi'\rangle \to \frac{1}{\sqrt{\sum_\nu |\psi_{\mu,\nu}|^2}} \sum_\nu \psi_{\mu,\nu}|\mu\rangle \otimes |\nu\rangle.$$

Performing such partial measurements may have interesting consequences for the long term distribution of the quantum random walk which makes them useful for the application in quantum algorithms.

4.1 The Discrete-time Quantum Random Walk

We are now gonna look at the quantum equivalent of the random walk on the integers. This walk "lives" on a graph where each vertex has two edges and consists of two quantum systems, a *coin* and a *walker* together with a *coin operator* and a *shift operator*. We can really think of the coin operator as "'flipping a coin" and the shift operator as "moving the walker" to the left or to the right according to the state of the coin.

The walker is a quantum system on an infinite Hilbert space $\mathbf{H}_p$ with countable dimension. The position state of the particle is thus an element of this Hilbert space. The canonical basis is denoted by $|i\rangle_p$ and any superposition

$$\sum_i \alpha_i |i\rangle_p,$$

where $\sum_i |\alpha_i|^2 = 1$ is a valid state for the position. Usually, the walker "starts" at zero, i.e. the initial position is $|0\rangle_p$.

The coin, on the other hand, lives on a two-dimensional Hilbert space $\mathbf{H}_c$ where the basis is usually denoted by $|0\rangle_c$ and $|1\rangle_c$ and a valid coin state is any superposition of these two base states

$$a|0\rangle_c + b|1\rangle_c,$$

where $|a|^2 + |b|^2 = 1$. The total system is in that sense a two particle system on $\mathbf{H}_c \otimes \mathbf{H}_p$.

Next, we define an evolution operator which is divided into two parts – the evolution of the coin and the evolution of the walker. In order to change the state of the coin, we define the Hadamard[1] operator which tries to mimic the random behaviour of the simple random walk. In the classical case it's up to chance in which direction the walker will move, in the quantum case this is done by applying a coin operator first and shifting afterwards. The purpose is to get the coin state into a superposition and the randomness comes into the mix if we take a measurement after we have applied the coin and the shift operator a couple of times. The Hadamard coin operator is usually denoted by $\hat{H}$ and defined by

$$\hat{H} = \frac{1}{\sqrt{2}}(|0\rangle_c\langle 0| + |0\rangle_c\langle 1| + |1\rangle_c\langle 0| - |1\rangle_c\langle 1|).$$

The second operator is the shift operator which allows the walker to move one step to the right if the basis state is $|0\rangle_c$ or move on step to the left if the basis state is $|1\rangle_c$. The definition is

$$\hat{S} = |0\rangle_c\langle 0| \otimes \sum_i |i+1\rangle_p\langle i| + |1\rangle_c\langle 1| \otimes \sum_i |i-1\rangle_p\langle i|.$$

To bring these two operators together in one step, we write the operator on the Hilbert space $\mathbf{H}_p \otimes \mathbf{H}_c$ as

$$\hat{U} = \hat{S}\,(\hat{H} \otimes \hat{I}_p).$$

Therefore, the quantum systems at time t are computed by simply applying the operator t times

$$|\psi\rangle_t = \hat{U}^t|\psi_0\rangle,$$

where $|\psi_0\rangle = |c_0\rangle \otimes |p_0\rangle$ is the initial state of the two particle system. One can easily verify that $\hat{U}$ is a unitary operator since $(vv^*)^* = vv^*$.

In the previous chapter we have talked about quantum observables which in a sense are the ways we can extract information out of the system. There are multiple ways we might want to extract such information. For example, a measurement on the coin can be performed using the observable

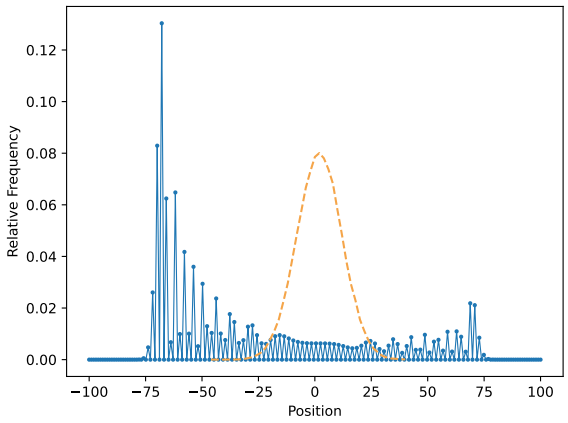
$$\hat{M}_c = \alpha_0|0\rangle_c\langle 0| + \alpha_1|1\rangle_c\langle 1|.$$

[1] Jacques Hadamard (* 8 December 1865, Versailles; † 17 October 1963, Paris) French mathematician

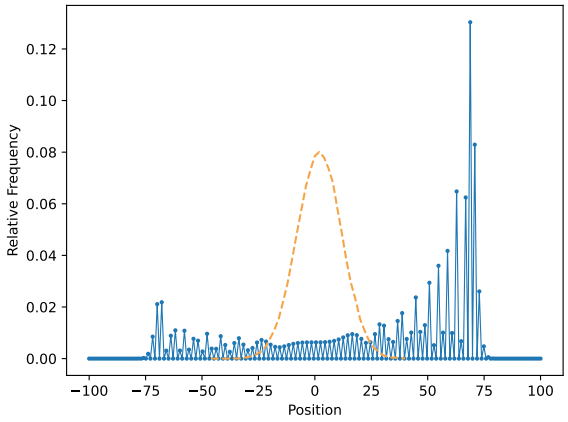
In the same way a measurement on the walker is achieved by the observable

$$\hat{M}_p = \sum_i a_i |i\rangle_p \langle i|.$$

A remarkable fact is the distribution for the position of such a particle. If we simulate say the first 100 steps of such a system, the distribution looks like in Figure 4.1 where the distribution for the first 100 steps of a classical random walk are overlaid. Interestingly, the distribution of the quantum random walk is skewed



(a) Initial state: $|1\rangle_c \otimes |0\rangle_p$



(b) Initial state: $|0\rangle_c \otimes |0\rangle_p$

Figure 4.1: Quantum Random Walk vs. Classical Random Walk

to the left or to the right depending on whether the starting state is $|1\rangle_c \otimes |0\rangle_p$ or $|0\rangle_c \otimes |0\rangle_p$ respectively. Furthermore, one can discern a near uniform distribution emerging around 0. The skewness of the distribution can be remedied by choosing

a balanced initial state like $\frac{1}{\sqrt{2}}(|0\rangle_c + i|1\rangle_c) \otimes |0\rangle_p$ or switching to a different (balanced) coin like

$$\hat{C} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}.$$

To study the long term behaviour of quantum random walks, two approaches are commonly considered. The first one is an approach based on path-integrals which is often referred to as the *Schrödinger approach* and the second one is a *combinatorial approach* using recursions and path-counting methods. The Schrödinger approach is based on the following observation. The quantum walk on a line at time t can be thought of as $|\psi\rangle_t = \hat{U}^t|\psi_0\rangle$ or alternatively

$$\sum_k (a_k|0\rangle_c + b_k|1\rangle_c) \otimes |k\rangle_p.$$

Suppose we have $|\psi_0\rangle = |0\rangle_c \otimes |0\rangle_p$ as the walk's initial state. Then, the first three steps of the walk can be written as

$$|\psi\rangle_1 = \left[\frac{1}{\sqrt{2}}|0\rangle_c \otimes |1\rangle_p\right] + \left[\frac{1}{\sqrt{2}}|1\rangle_c \otimes |-1\rangle_p\right],$$

$$|\psi\rangle_2 = \left[\frac{1}{2}|0\rangle_c \otimes |2\rangle_p\right] + \left[\left(\frac{1}{2}|0\rangle_c + \frac{1}{2}|1\rangle_c\right) \otimes |0\rangle_p\right] - \left[\frac{1}{2}|1\rangle_c \otimes |-2\rangle_p\right]$$

and

$$\begin{aligned} |\psi\rangle_3 = &\left[\frac{1}{2\sqrt{2}}|0\rangle_c \otimes |3\rangle_p\right] + \left[\left(\frac{1}{\sqrt{2}}|0\rangle_c + \frac{1}{2\sqrt{2}}|1\rangle_c\right) \otimes |1\rangle_p\right] \\ &- \left[\frac{1}{2\sqrt{2}}|0\rangle_c \otimes |-1\rangle_p\right] + \left[\frac{1}{2\sqrt{2}}|1\rangle_c \otimes |-3\rangle_p\right]. \end{aligned}$$

So instead of evolving $|\psi\rangle$, we can also try to evolve the coefficients of the coin states. We write

$$\Psi(n,t) = \begin{pmatrix} \Psi_L(n,t) \\ \Psi_R(n,t) \end{pmatrix}$$

for the vector that contains the coefficients of $|0\rangle_c$ and $|1\rangle_c$ at position $|n\rangle_p$ respectively, i.e.

$$|\psi\rangle_t = \sum_n \big(\Psi_R(n,t)|0\rangle_c + \Psi_L(n,t)|1\rangle_c\big) \otimes |n\rangle_p.$$

We will write

$$|\Psi(n,t)\rangle = \Psi_R(n,t)|0\rangle_c + \Psi_L(n,t)|1\rangle_c$$

for the coin part of the n-th summand. Let us analyse the behaviour of such a quantum random walk at point n. We begin by applying the Hadamard coin to the states in position $n-1$, n and $n+1$ and get

$$\begin{aligned}\hat{H}\big(|\Psi(n-1,t)\rangle + |\Psi(n,t)\rangle + |\Psi(n+1,t)\rangle\big) = \frac{1}{\sqrt{2}}\times \\ \times \big(|\Psi_L(n-1,t)\rangle|0\rangle_c + |\Psi_R(n-1,t)\rangle|0\rangle_c \\ - |\Psi_L(n+1,t)\rangle|1\rangle_c + |\Psi_R(n+1,t)\rangle|1\rangle_c \\ - |\Psi_L(n-1,t)\rangle|1\rangle_c + |\Psi_R(n-1,t)\rangle|1\rangle_c \\ + |\Psi_L(n+1,t)\rangle|0\rangle_c + |\Psi_R(n+1,t)\rangle|0\rangle_c \\ + |\Psi_L(n,t)\rangle|0\rangle_c + |\Psi_R(n,t)\rangle|0\rangle_c \\ - |\Psi_L(n,t)\rangle|1\rangle_c + |\Psi_R(n,t)\rangle|1\rangle_c\big).\end{aligned}$$

If we apply the shift operator $\hat{S}$, this transforms into

$$\begin{aligned}\hat{S}(\hat{H}\big(|\Psi(n-1,t)\rangle + |\Psi(n,t)\rangle + |\Psi(n+1,t)\rangle\big)) = \frac{1}{\sqrt{2}}\times \\ \times \big(|\Psi_L(n,t)\rangle|0\rangle_c + |\Psi_R(n,t)\rangle|0\rangle_c \\ - |\Psi_L(n,t)\rangle|1\rangle_c + |\Psi_R(n,t)\rangle|1\rangle_c \\ - |\Psi_L(n-2,t)\rangle|1\rangle_c + |\Psi_R(n-2,t)\rangle|1\rangle_c \\ + |\Psi_L(n+2,t)\rangle|0\rangle_c + |\Psi_R(n+2,t)\rangle|0\rangle_c \\ + |\mathbf{\Psi_L(n-1,t)}\rangle|\mathbf{0}\rangle_\mathbf{c} + |\mathbf{\Psi_R(n-1,t)}\rangle|\mathbf{0}\rangle_\mathbf{c} \\ - |\mathbf{\Psi_L(n+1,t)}\rangle|\mathbf{1}\rangle_\mathbf{c} + |\mathbf{\Psi_R(n+1,t)}\rangle|\mathbf{1}\rangle_\mathbf{c}\big).\end{aligned}$$

The four summands marked in bold make up the vector $|\Psi(n,t+1)\rangle$. This can be rewritten as a matrix multiplication

$$\Psi(n,t+1) = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \Psi(n+1,t) + \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \Psi(n-1,t).$$

If we denote

$$M_- = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \text{ and } M_+ = \begin{pmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix},$$

then

$$\Psi(n,t+1) = M_-\Psi(n+1,t) + M_+\Psi(n-1,t), \tag{4.1}$$

which is a difference equation with initial conditions $\Psi(0,0) = (1,0)^t$ and $\Psi(n,0) = (0,0)^t$ for all other $n \in \mathbb{Z}$. Given this difference equation, our goal

is to find an analytical expression for $\Psi_L(n,t)$ and $\Psi_R(n,t)$ since these contain the information of what the position of the particle might be. To achieve this, one usually performs a discrete-time Fourier transform. Let us briefly define the transform.

Definition 4.1 (Discrete-time Fourier Transform, DTFT)**.** Let $f : \mathbb{Z} \to \mathbb{C}$ be a complex function over the integers, then the discrete-time Fourier transform $\tilde{f} : [-\pi, \pi] \to \mathbb{C}$ is given by

$$\tilde{f}(k) = \sum_{n=-\infty}^{\infty} f(n)e^{ikn},$$

with the inverse given by

$$f(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \tilde{f}(k)e^{-ikn}\, dk. \qquad \triangle$$

Now, we can apply the DTFT to our coefficient function and get

$$\tilde{\Psi}(k,t) = \sum_n \Psi(n,t)e^{ikn}.$$

Using Equation 4.1 we arrive at

$$\tilde{\Psi}(k,t+1) = \sum_n (M_-\Psi(n+1,t) + M_+\Psi(n-1,t))e^{ikn}$$

and after rearranging some terms we get

$$\tilde{\Psi}(k,t+1) = M_k\tilde{\Psi}(k,t),$$

where $M_k = e^{-ik}M_- + e^{ik}M_+$, i.e.

$$M_k = \frac{1}{\sqrt{2}} \begin{pmatrix} -e^{-ik} & e^{-ik} \\ e^{ik} & e^{ik} \end{pmatrix}.$$

The evolution of the system can thus be described by the matrix M_k and therefore $\tilde{\Psi}(k,t) = M_k^t\tilde{\Psi}(k,0)$ with $\tilde{\Psi}(k,0) = (1,0)^t$. Our goal is now to diagonalise the matrix M_k in order to easily calculate M_k^t. Clearly, if M_k has eigenvalues $\{\lambda_k^1, \lambda_k^2\}$ with respective eigenvectors $|\Phi_k^1\rangle$, $|\Phi_k^2\rangle$, then

$$M_k^t = (\lambda_k^1)^t|\Phi_k^1\rangle\langle\Phi_k^1| + (\lambda_k^2)^t|\Phi_k^2\rangle\langle\Phi_k^2|.$$

In [4] it is shown that the eigenvalues of the matrix M_k are $\lambda_k^1 = e^{i\omega_k}$ and $\lambda_k^2 = e^{i(\pi-\omega_k)}$ where $\omega_k \in [-\pi/2, \pi/2]$ satisfies $\sin(\omega_k) = \frac{\sin k}{\sqrt{2}}$. The corresponding eigenvectors are

$$\Phi_k^1 = \frac{1}{\sqrt{2N(k)}} \begin{pmatrix} e^{-ik} \\ \sqrt{2}e^{i\omega_k} + e^{-ik} \end{pmatrix},$$
$$\Phi_k^2 = \frac{1}{\sqrt{2N(\pi-k)}} \begin{pmatrix} e^{-ik} \\ -\sqrt{2}e^{-i\omega_k} + e^{-ik} \end{pmatrix},$$

where the normalisation factor $N(k)$ is given by

$$N(k) = (1 + \cos^2 k) + \cos k\sqrt{1 + \cos^2 k}.$$

In the Fourier basis the initial state is given by $\tilde{\Psi}(k, 0) = (1, 0)^t$ for all k. Therefore, we get that the wave function at time t may be written as

$$\begin{aligned}\tilde{\Psi}_L(k,t) &= \frac{1}{2}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right) e^{i\omega_k t} \\ &\quad + \frac{(-1)^t}{2}\left(1 - \frac{\cos k}{\sqrt{1+\cos^2 k}}\right) e^{-i\omega_k t}, \\ \tilde{\Psi}_R(k,t) &= \frac{e^{-ik}}{2\sqrt{1+\cos^2 k}}\left(e^{i\omega_k t} - (-1)^t e^{-i\omega_k t}\right).\end{aligned}$$

By using the inverse Fourier transform the authors of [4] proved the following Lemma.

Lemma 4.2. *Let $|\psi_0\rangle = |0\rangle_c \otimes |0\rangle_p$ be the initial state of a discrete quantum random walk on a line with the Hadamard coin. Then*

$$\Psi_L(n,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{-ie^{ik}}{2\sqrt{1+\cos^2 k}}\left(e^{-i(\omega_k t - kn)}\right)\, dk$$

and

$$\Psi_R(n,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right)\left(e^{-i(\omega_k t - kn)}\right)\, dk,$$

where $\omega_k = \sin^{-1}\left(\frac{\sin k}{\sqrt{2}}\right)$ and $\omega_k \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$.

As in the simulation, we see that the amplitudes for even n at odd t or odd n at even t respectively are zero. Ideally, we can describe the behaviour of $\Psi(n,t)$ as $t \to \infty$ or equivalently find an asymptotic expression for

$$P(n,t) = |\Psi_L(n,t)|^2 + |\Psi_R(n,t)|^2 \quad \text{as } t \to \infty.$$

The integrals in the lemma above are of the form

$$I(\alpha, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(k) e^{i\phi(k,\alpha)t}\, dk,$$

where $\alpha = n/t$. There exist methods in complex analysis to study their asymptotic behaviour, so-called stationary phase approximation. With their use, the authors of [4] proved the following theorems.

Theorem 4.3. *Let $\epsilon > 0$ be any constant and α be in the interval $(-\frac{1}{\sqrt{2}}+\epsilon, \frac{1}{\sqrt{2}}-\epsilon)$. Then, as $t \to \infty$, we have*

$$|\Psi_L(n,t)|^2 \sim \frac{2}{\pi t\sqrt{1-2\alpha^2}} \cos^2\left(-\omega t + \frac{\pi}{4} - \rho\right),$$
$$|\Psi_R(n,t)|^2 \sim \frac{2(1+\alpha)}{\pi(1-\alpha)t\sqrt{1-2\alpha^2}} \cos^2\left(-\omega t + \frac{\pi}{4}\right),$$

where $\omega = \alpha\rho + \theta$, $\rho = \arg(-B + \sqrt{\Delta})$, $\theta = \arg(B + 2 + \sqrt{\Delta})$, $B = \frac{2\alpha}{1-\alpha}$ and $\Delta = B^2 - 4(B+1)$.

Theorem 4.4. *Let $n = \alpha t \to \infty$ with α fixed. In case $-1 < \alpha < -1/\sqrt{2}$ or $1/\sqrt{2} < \alpha < 1$, there exists a constant $c > 1$ for which*

$$|\Psi_L(n,t)|^2 = \mathcal{O}(c^{-n}) \text{ and } |\Psi_R(n,t)|^2 = \mathcal{O}(c^{-n}).$$

Theorem 4.5. *Let π_t denote the uniform distribution on $\mathbb{Z} \cap [-t/\sqrt{2}, t/\sqrt{2}]$. There exists a constant $\delta < 1$ such that for all t sufficiently large, $\|P(\cdot, t) - \pi_t\| \leq \delta$.*

4.1.1 Comparison of the Random Walks on the Line

The conclusions we can draw from these theorems are the following. First, Theorem 4.3 tell us that the wave function is almost uniformly spread in a region for which α is in the interval $[-1/\sqrt{2}, 1/\sqrt{2}]$ and Theorem 4.4 gives us the fact that the wave function decays very quickly outside that region. Second, by integrating the functions in Theorem 4.3 it is possible to see that almost all the probability is concentrated in $[(-1/\sqrt{2}+\epsilon)t, (1/\sqrt{2}-\epsilon)t]$, namely a probability of $1 - \frac{2\epsilon}{\pi} - \frac{\mathcal{O}(1)}{t}$.

Furthermore, we see that the probability "spreads" in linear time, i.e. is in $[-t/\sqrt{2}, t/\sqrt{2}]$. In [5] as well as in [6] it is again proven that the standard deviation of the discrete quantum random walk on the line is $\mathcal{O}(t)$ instead of $\sqrt{t}$, as we have seen for the classical random walk on the integers in the beginning of Chapter 2.

For the time being, let us continue with analysing the theorems above. We have defined what the *mixing time* is for classical random walks and we will use the same definition here. According to Theorem 4.5, we get that the quantum random walk is mixing in *linear time*. This is again in contrast to the classical case where we have shown that the random walk on the line mixes in quadratic time.

4.2 Limit theorems for Quantum Random Walks

In this section we will look into results about limit theorems that describe the state of the system after a certain number of steps. Notably, the contributions by Norio Konno in his publications [5], [7], [8] and [9] are discussed.

As before, at each position we have a vector in $\mathbb{C}^2$ such that the square of the absolute value is the probability of the particle being at that position, i.e.

$$\Psi(k,n) = \begin{pmatrix} \Psi_L(k,n) \\ \Psi_R(k,n) \end{pmatrix}.$$

From now on, time will be denoted by $n \in \{1,2,\ldots\}$ and the location by $k \in \mathbb{Z}$. To this end, let

$$\Phi = \{(\alpha,\beta)^t \in \mathbb{C}^2 : |\alpha|^2 + |\beta|^2 = 1\}$$

denote the set of initial coin states of a one-dimensional quantum random walk. Furthermore, let X_n^φ denote a walk at time n that started at position $|0\rangle$ with the initial coin state $\varphi \in \Phi$. The evolution operator of $\Psi(k,n)$ is given by a *unitary matrix*

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

where $a, b, c, d \in \mathbb{C}$. Similarly as before, the evolution can be written as

$$\Psi(k,n) = P\Psi(k+1,n) + Q\Psi(k-1,n),$$

where

$$P = \begin{pmatrix} a & b \\ 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 0 \\ c & d \end{pmatrix}$$

and k denotes the location and n the time. The unitarity of $U = P + Q$ ensures that this always defines a probability distribution for the location. In order to study $\mathbb{P}\left[X_n^\varphi = k\right]$ for $n + k$ even, one can analyse the number of steps to the left and the number of steps to the right using the matrices P and Q. For l (steps to the left) and m (steps to the right) with $l + m = n$ and $m - l = k$ we look at

$$\Xi(l,m) = \sum P^{l_1} Q^{m_1} P^{l_2} Q^{m_2} \cdots P^{l_n} Q^{m_n},$$

	P	Q	R	S
P	aP	bR	aR	bP
Q	cS	dQ	cQ	dS
R	cP	dR	cR	dP
S	aS	bQ	aQ	bS

Table 4.1: Multiplication by row times column

summed over all $l_j, m_j \geq 0$ satisfying $m_1 + \ldots + m_n = m$ and $l_1 + \ldots + l_n = l$. Then, we have that

$$\mathbb{P}\big[X_n^\varphi = k\big] = (\Xi(l,m)\varphi)^*(\Xi(l,m)\varphi).$$

For example, determining $\mathbb{P}\big[X_4^\varphi = -2\big]$ leads to the expression

$$\Xi(3,1) = P^3Q + P^2QP + PQP^2 + QP^3.$$

Using the relations in Table 4.1 where

$$R = \begin{pmatrix} c & d \\ 0 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & 0 \\ a & b \end{pmatrix}$$

we can simplify any expression of Ξ down to the form

$$\Xi(l,m) = p_n(l,m)P + q_n(l,m)Q + r_n(l,m)R + s_n(l,m)S.$$

In our example we would end up with

$$\Xi(3,1) = 2abcP + a^2bR + a^2cS.$$

The idea of the paper was to use combinatorial methods in order to determine the coefficients in this expression. This is the content of the next lemma.

Lemma 4.6. *Consider a quantum random walk X_n^φ in one dimension with $abcd \neq 0$. Suppose that $l, m \geq 0$ with $l + m = n$, then we have*

(i) for $\min\{l,m\} \geq 1$,

$$\Xi(l,m) = a^l\overline{a}^m(\det U)^m \sum_{\gamma=1}^{\min\{l,m\}} \left(-\frac{|b|^2}{|a|^2}\right)^\gamma \binom{l-1}{\gamma-1}\binom{m-1}{\gamma-1} \times \\ \times \left[\frac{l-\gamma}{a\gamma}P + \frac{m-\gamma}{\overline{a}\gamma\det U}Q - \frac{1}{\overline{b}\det U}R + \frac{1}{b}S\right],$$

(ii) for $l \geq 1$, $m = 0$,

$$\Xi(l, 0) = a^{l-1} P,$$

(iii) for $l = 0$, $m \geq 1$,

$$\Xi(0, m) = (\det U)^{m-1} \overline{a}^{m-1} Q.$$

From this lemma the characteristic function of X_n^φ is obtained and in turn from this the mth moment can be derived in a standard fashion.

Definition 4.7 (Characteristic function and mth moment)**.** For a scalar random variable X the characteristic function φ_X is defined as the expected value of e^{itX} where $t \in \mathbb{R}$, i.e.

$$\varphi_X(t) = \mathrm{E}[e^{itX}] = \int_R e^{itx} f_X(t)\, dx.$$

If the characteristic function is m times differentiable at zero, then the mth moment can be calculated by

$$\mathrm{E}[X^m] = i^{-m} \frac{d^m \varphi_X(t)}{dt^m}\Big|_{t=0}.$$

△

Using this fact, the author derives the following theorem for the mth moment of the quantum random walk's amplitude distribution.

Theorem 4.8. *Consider again a quantum random walk* X_n^φ *with* $abcd \neq 0$ *and* $\varphi = (\alpha, \beta)^t$.

(i) When m *is odd, we have*

$$\begin{aligned}
&\mathrm{E}[(X_n^\varphi)^m] \\
&= |a|^{2(n-1)} \Big[-n^m \left(\left(|a|^2 - |b|^2\right) \left(|\alpha|^2 - |\beta|^2\right) + 2(a\alpha\overline{b\beta} + \overline{a\alpha} b\beta) \right) \Big] \\
&+ \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2} \right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \\
&\times \binom{n-k-1}{\delta-1} \frac{(n-2k)^{m+1}}{\gamma\delta} \Bigg[- \left(n(|a|^2 - |b|^2) + \gamma + \delta \right) \\
&\times \left(|\alpha|^2 - |\beta|^2\right) + \left(\frac{\gamma+\delta}{|b|^2} - 2n \right) (a\alpha\overline{b\beta} + \overline{a\alpha} b\beta) \Bigg].
\end{aligned}$$

(ii) When m is even, we have

$$\begin{aligned}\mathrm{E}[(X_n^{\varphi})^m] = |a|^{2(n-1)} \Bigg[& n^m \\ & + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \sum_{\gamma=1}^{k} \sum_{\delta=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{\gamma+\delta} \binom{k-1}{\gamma-1} \binom{k-1}{\delta-1} \binom{n-k-1}{\gamma-1} \\ & \times \binom{n-k-1}{\delta-1} \frac{(n-2k)^m}{\gamma\delta} \left((n-k)^2 + k^2 - n(\gamma+\delta) + \frac{2\gamma\delta}{|b|^2}\right) \Bigg].\end{aligned}$$

So, in the case where m is even the mth moment is independent of the initial state φ.

Furthermore, Konno proves a weak limit theorem for the quantum random walk.

Theorem 4.9. *We assume $abcd \neq 0$. If $n \to \infty$, then*

$$\frac{X_n^{\varphi}}{n} \Rightarrow Z^{\varphi},$$

where Z^{φ} has a density

$$f(x) = \frac{\sqrt{1-|a|^2}}{\pi(1-x^2)\sqrt{|a|^2-x^2}} \left[1 - \left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2}\right) x\right]$$

for $x \in (-|a|, |a|)$ with

$$\begin{aligned}&\mathrm{E}[Z^{\varphi}] = -\left(|\alpha|^2 - |\beta|^2 + \frac{a\alpha\overline{b\beta} + \overline{a\alpha}b\beta}{|a|^2}\right) \times \left(1 - \sqrt{1-|a|^2}\right), \\ &\mathrm{E}[(Z^{\varphi})^2] = 1 - \sqrt{1-|a|^2}.\end{aligned}$$

Here, "$\Rightarrow$" means convergence in distribution.

The density function allows for some observations regarding the initial state of the system. Define

$$\begin{aligned}\Phi_s &= \left\{\varphi \in \Phi \mid \forall n \in \mathbb{Z}_{\geq 0} \forall k \in \mathbb{Z} : \mathbb{P}\left[X_n^{\varphi} = k\right] = \mathbb{P}\left[X_n^{\varphi} = -k\right]\right\}, \\ \Phi_0 &= \left\{\varphi \in \Phi \mid \forall n \in \mathbb{Z}_{\geq 0} : \mathrm{E}[X_n^{\varphi}] = 0\right\}, \\ \Phi_{\perp} &= \left\{(\alpha, \beta)^t \in \Phi \mid |\alpha| = |\beta|, a\alpha\overline{b\beta} + \overline{a\alpha}b\beta = 0\right\}.\end{aligned}$$

Konno uses Theorem 4.8 to prove that these sets are indeed equal.

Theorem 4.10. *Assume that $abcd \neq 0$. Then we have*

$$\Phi_s = \Phi_0 = \Phi_\perp.$$

To finish this section, we want to see what these theorems mean for the quantum random walk with the Hadamard coin, i.e.

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

We have seen that the distribution of the quantum random walk on the line with the Hadamard coin operator is quite different from the distribution of the classical random walk on the line whose distribution is a binomial one. By Theorem 4.9 we can state that for $-1/\sqrt{2} < a < b < 1/\sqrt{2}$ as $n \to \infty$,

$$\mathbb{P}\big[a \leq X_n^\varphi/n \leq b\big] \to \int_a^b \frac{1 - (|\alpha|^2 - |\beta|^2 + \alpha\overline{\beta} + \overline{\alpha}\beta)x}{\pi(1-x^2)\sqrt{1-2x^2}}\, dx,$$

for any initial state $\varphi = (\alpha, \beta)^t$.

It is a well-known fact that for $n \to \infty$ a binomially distributed random variable $Y \sim \mathrm{Bin}(n, p)$ converges to a normally distributed random variable. Therefore, for the classical simple random walk starting at 0 if $-\infty < a < b < \infty$ as $n \to \infty$,

$$\mathbb{P}\big[a \leq Y_n^0/\sqrt{n} \leq b\big] \to \int_a^b \frac{e^{-x^2/2}}{\sqrt{2\pi}}\, dx.$$

This result is often called *De Moivre*[2]*-Laplace*[3] *theorem*. In case the initial state is chosen from Φ_s and thus the quantum random walk is symmetric the formula simplifies. For example, using $\varphi = (1/\sqrt{2}, i/\sqrt{2})^t$, we arrive at the following quantum version of the De Moivre-Laplace theorem

$$\mathbb{P}\big[a \leq X_n^\varphi/n \leq b\big] \to \int_a^b \frac{1}{\pi(1-x^2)\sqrt{1-2x^2}}\, dx \quad \text{as } n \to \infty.$$

In conclusion, it is shown that the quantum random walk also admits a weak limit theorem just as the classical one. However, the behaviour differs greatly. For example, the distribution has two peaks at the end points of the support. We will now go on with a continuous-time version and state similar limit theorems.

[2] Abraham de Moivre (* 26 May 1667, Vitry-le-François; † 27 November 1754, London) French mathematician

[3] Pierre-Simon Laplace (* 23 March 1749, Beaumont-en-Auge; † 5 March 1827, Paris) French mathematician

4.3 The Continuous-time Quantum Random Walk

In [10] the authors design a quantum random walk that traverses a decision tree starting at the root. Their approach is a process that runs continuously in time but on a discrete space – a tree. First, we will introduce the model for a continuous-time quantum random walk as Fahri and Gutmann did in their paper and also briefly talk about the limit theorems that Konno produced in [9]. For ease of notation we will also define the continuous-time quantum random walk on the line.

First, we introduce an adjacency matrix A as follows:

$$A = \begin{array}{c} \\ \vdots \\ -3 \\ -2 \\ -1 \\ 0 \\ 1 \\ 2 \\ 3 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccccc} \cdots & -3 & -2 & -1 & 0 & 1 & 2 & 3 & \cdots \end{array} \\ \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 1 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 1 & 0 & 1 & 0 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 1 & 0 & 1 & 0 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 1 & 0 & 1 & \cdots \\ \cdots & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array}$$

The *amplitude wave function* of the walk at time t, Ψ_t, is defined by

$$\Psi_t = U_t \Psi_0,$$

where

$$U_t = e^{itA/2}.$$

Clearly, A is a unitary matrix. As the initial state, we take

$$\Psi_0 = (\ldots, 0, 0, 0, 1, 0, 0, 0, \ldots)^t.$$

Let $\Psi_t(x)$ be the amplitude wave function at location x and time t. The probability of a particle being at location x at time t is given, as usual, by the square of the absolute value, i.e.

$$P_t(x) = |\Psi_t(x)|^2.$$

In [9] the operator U_t is calculated explicitly by use of the *Bessel*[4] *function*. We omit the proof as it is rather technical, but the result is as follows.

[4] Friedrich Bessel (* 22 July 1784, Minden; † 17 March 1846, Königsberg) German astronomer, mathematician, physicist and geodesist

Theorem 4.11. *An explicit form of U_t is given by*

$$U_t = \begin{array}{c} \\ \vdots \\ -2 \\ -1 \\ 0 \\ 1 \\ 2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccccccc} \cdots & -2 & -1 & 0 & 1 & 2 & \cdots \end{array} \\ \begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & J_0(t) & iJ_1(t) & i^2J_2(t) & i^3J_3(t) & i^4J_4(t) & \cdots \\ \cdots & iJ_1(t) & J_0(t) & iJ_1(t) & i^2J_2(t) & i^3J_3(t) & \cdots \\ \cdots & i^2J_2(t) & iJ_1(t) & J_0(t) & iJ_1(t) & i^2J_2(t) & \cdots \\ \cdots & i^3J_3(t) & i^2J_2(t) & iJ_1(t) & J_0(t) & iJ_1(t) & \cdots \\ \cdots & i^4J_4(t) & i^3J_3(t) & i^2J_2(t) & iJ_1(t) & J_0(t) & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array}$$

That is, the (l, m) component of U_t is given by $i^{|l-m|}J_{|l-m|}(t)$, where $J_k(t)$ is the Bessel function of the first kind of order k given by

$$J_k(t) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\Gamma(m+k+1)} \left(\frac{t}{2}\right)^{2m+k}.$$

By looking at a column of U_t one immediately obtains the following corollary.

Corollary 4.12. *The amplitude wave function is given by*

$$\Psi_t = (\ldots, i^2J_2(t), iJ_1(t), J_0(t), iJ_1(t), i^2J_2(t), \ldots)^t.$$

Therefore, one has that $\Psi_t(x) = i^{|x|}J_{|x|}(t)$ for any location $x \in \mathbb{Z}$ and time $t \geq 0$.

Since $J_{-x}(t) = (-1)^x J_x(t)$, as can be seen by the series definition, we get another easy conclusion.

Corollary 4.13. *The probability distribution is*

$$P_t(x) = J_{|x|}^2(t) = J_x^2(t),$$

for any location $x \in \mathbb{Z}$ and time $t \geq 0$.

Finally, we want to state the weak limit theorem for the continuous-time quantum random walk as well and take a look at its moments.

Theorem 4.14. *Let X_t be a continuous-time quantum random walk on $\mathbb{Z}$. If $t \to \infty$, then*

$$\frac{X_t}{t} \Rightarrow Z,$$

where Z has the density

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}}\chi_{(-1,1)}(x).$$

Here, $\chi_{(-1,1)}$ is the indicator function on the interval $(-1,1)$.

Noting that

$$\int_{-1}^{1} \frac{x^{2m}}{\pi\sqrt{1-x^2}}\,dx = \frac{2}{\pi}\int_0^{\pi/2} \sin^{2m}\varphi\,d\varphi = \frac{(2m-1)!!}{(2m)!!},$$

where

$$n!! = \begin{cases} n(n-2)\cdots 5\cdot 3\cdot 1, & n \text{ odd}, \\ n(n-2)\cdots 6\cdot 4\cdot 2, & n \text{ even}, \end{cases}$$

we deduce the following corollary.

Corollary 4.15. *For $m = 1, 2, \ldots$,*

$$\mathrm{E}[(X_t/t)^{2m}] \to \frac{(2m-1)!!}{(2m)!!} \quad \textit{as } t \to \infty.$$

Using the moments, we may calculate the standard deviation and are able to see that

$$\sigma_{(c)}(t)/t \to 1/\sqrt{2} \quad \text{as } t \to \infty.$$

approaches a certain value for the continuous-time quantum random walk. In the same manner, we can use Theorem 4.8 to see that

$$\sigma_{(d)}(n)/n \to \sqrt{(2-\sqrt{2})/2} \quad \text{as } n \to \infty$$

for the discrete-time quantum random walk. This gives a rigorous proof that the quantum random walk's standard deviation grows like t or n respectively instead of $\sqrt{t}$ or $\sqrt{n}$ for their classical counterparts.

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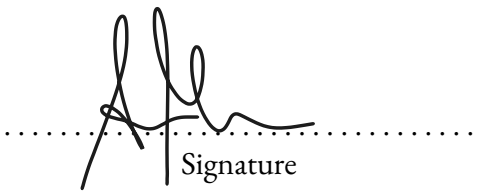

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