Discrete-time quantum walk with two-step memory

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Abstract

We examine a discrete-time quantum walk with two-step memory for a particle on a one-dimensional infinite space. The walk is defined with a four-state memory space analogous to the two-state coin space commonly used in discrete time quantum walks, and a method is presented for calculating the time evolution by using the Fourier transform. An integral expression for the probability is calculated, and this is used to produce numerical solutions for the probability distribution as a function of the time step and position. The results show two peaks in the probability distribution. One peak propagates ballistically with time, which is a common feature of quantum walks. The other peak is stationary with time and located at the initial site of the particle. This feature is not common in quantum walks and suggests that tracing the immediate history of the particle using two-step memory may represent the beginning of a transition to a classical system.

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1   Introduction

When introducing the idea of quantum random walks, it is usually helpful to begin with a brief description of what a "Walk" is. Quantum walks were motivated by applying aspects of classical walks to quantum systems [1]. In the classical walk, the particle is located at only one position and at each step in time it moves in one of several possible directions. The particle is free to take discrete steps, or "walk," around the set of connected positions. Classical walks can be studied on many different position spaces, however the simplest to consider is the one-dimensional walk. This will be especially relevant because the quantum walk discussed in this paper is also a one dimensional walk.

Consider a classical particle that is free to move on an infinite one-dimensional space of discrete positions. At each step in time the particle can move in one of two directions, say left or right. The probability that the particle moves one way or another depends on the dynamics of the system, but the most common example is the symmetric walk in which steps to the left and right are equally probable. One can think of this as flipping a coin at each time step and moving the particle to the left or right depending on whether the coin comes up heads or tails. Since there is equal probability for steps to the left and right, after a large amount of time one would expect there to be roughly equal numbers of steps in each direction. Overall, these steps will cancel out and the particle would be expected to stay in the area around where it started. The result is an approximately Gaussian probability distribution centered on the initial position of the particle [2]. This example is one of the simplest possible walks that can be considered, but it is a good illustration of the basic principles. More sophisticated statistical analysis is required to solve more complicated walks, but the goal is usually the same: find the spatial probability distribution for the particle at some later time.

Classical walks can provide good models to represent physical systems, for example, diffusion of particles [2]. In addition, the study of walks is also very important in computer science, leading to the development of various computer algorithms [3]. Due to the success of classical random walks, much of the recent interest in quantum walks is based on the belief that they will lead to deeper understanding in other fields. The most promising of these is the hope that quantum walks can be used to develop new algorithms in quantum computing. Currently, the two main techniques for analyzing quantum algorithms are *Fourier sampling* and *amplitude amplification* [4]. The former is represented in the work of Daniel Simon [5] and Peter Shor [6], and the latter is described in the work of Lov K. Grover [7]. Shor's factoring algorithm is able to factor large numbers in a time that only grows polynomially (as opposed to exponentially) with the length of the number [6], and Grover's search algorithm is able to search databases at a rate much faster than any classical algorithm [7]. However, quantum walks have recently been established as an alternative method for developing algorithms, and there have been several impressive results. For example, quantum walks have been shown to provide exponential speedup over classical computing [8], and algorithms have been developed that are able to solve problems such as searching on graphs and checking matrix multiplication [1]. With some of the possible benefits to studying quantum walks now outlined, the next step is to better describe what a quantum walk is and how it differs from the classical random walks.

1.1   Quantum Walks

Although the development of quantum walks was based on classical random walks, there are some key differences between the two. The first is that a classical particle can exist at only one position at a given time, but the quantum particle can exist in a superposition of states until a measurement takes place. This means that the state of the quantum particle can interfere at different sites leading to probability distributions that are much different than the classical distributions. A second difference between quantum and classical walks is that all time evolution in the quantum walk must be unitary, meaning that the processes are reversible. This unitary behavior becomes very important when considering the two different types of quantum walks.

The study of quantum walks can be divided into discrete-time quantum walks (DTQW) and continuous-time quantum walks (CTQW), and the two types are fundamentally different [1]. Discrete-time walks refer to evolution that occurs between small quantized steps in time; at each time step the particle changes its position. Continuous-time means that the particle can move at any of a continuous range of times and not just in discrete steps. This paper is focused on solving a DTQW so there is little need to go into CTQWs in depth. However, there are some important distinctions that should be noted. First, to produce nontrivial behavior in the DTQW, one is required to introduce a new degree of freedom to the state of the particle [1]. This degree of freedom is sometimes referred to as the "coin space" or "directionality" of the particle. CTQWs, on the other hand, do not need this extra degree of freedom. This fundamental difference between DTQWs and CTQWs means that there is not yet a known way to connect the two categories. In classical walks, continuous-time random walks can be considered a limiting case of the discrete-time walks as the time steps become very small. However, no such connection can be made for quantum walks. For more on the relationship between DTQWs and CTQWs, refer the article by A. M. Childs [1].

This paper focuses on solving a one dimensional DTWQ, so it will help to first expand on the idea of the coin space and how it works. For a one-dimensional walk, there will be two coin eigenstates corresponding to the two directions that the particle can move. For simplicity we can just refer to them as left (L) or right (R) corresponding to the direction a particle with that state will move. The position of the particle is a separate space and the full state of the particle is the tensor product of the coin state and the position state n.

$$|\psi\rangle = |coin\rangle \otimes |n\rangle \tag{1.1}$$

Note that two states with different positions could be in the same pure R state. For example, a state at position 0 and one at position 5 could both be in the same (R) coin state.

$$|\psi_1\rangle = |R\rangle \otimes |0\rangle \quad , \quad |\psi_2\rangle = |R\rangle \otimes |5\rangle$$

Also, one particle at some position could be in superposition of R and L states. For example, a state at position 0 could be in an equal superposition of (R) and (L).

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle) \otimes |0\rangle = \frac{1}{\sqrt{2}}(|R\rangle \otimes |0\rangle + |L\rangle \otimes |0\rangle)$$

Remember that the state must be normalized, as is required by quantum mechanics.

The way that the particle moves is described by the unitary evolution operator, which includes the coin operator and the shift operator. The "coin operator" acts on the particle changing its coin

state. The name coin operator is in reference to the analogy from classical walks in which a coin flip determines the direction of each step. The direction in which the particle will move depends on whether the particle is in the R or L state. This process is carried out by a separate shift operator, and the action of both operators is unitary. This process of mixing the coin state and shifting the particle is repeated many times to evolve the overall state, and the goal of quantum walks is to solve for the probability distribution of the particle at that later time. The most common example of this type of walk is the Hadamard walk. In this case the coin operator, C, acts on the coin states in the following way.

$$C|R\rangle = \frac{1}{\sqrt{2}}(|R\rangle + |L\rangle)$$

$$C|L\rangle = \frac{1}{\sqrt{2}}(|R\rangle - |L\rangle) \tag{1.2}$$

So the coin operator takes the pure coin states into equal superpositions of each coin state. The minus sign in the second equation is required to make the operator unitary. If a step to the right is considered moving in the positive direction and a step to the left is in the negative direction, the shift operator, S, acts in the following way.

$$S(|R\rangle \otimes |n\rangle) = |R\rangle \otimes |n+1\rangle$$

$$S(|L\rangle \otimes |n\rangle) = |L\rangle \otimes |n-1\rangle \tag{1.3}$$

The shift moves an R state to the right, increasing the position from n to $n+1$, and an L state to the left, decreasing the position from n to $n-1$. The total evolution operator is the combination of the coin and the shift operator

$$U = S(C \otimes I) \tag{1.4}$$

where I is the identity operator. The coin operator must be applied first because it assigns the probabilities for the particle to travel in any given direction. The evolution of the state between time steps is given by

$$|\psi_{t+1}\rangle = U|\psi_t\rangle = S(C \otimes I)|\psi_t\rangle. \tag{1.5}$$

As an example, if a particle starts in the pure (R) state at position 0, applying the operator twice gives the next two evolved states.

$$|\psi_0\rangle = |R\rangle \otimes |0\rangle$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}|L\rangle \otimes |-1\rangle + \frac{1}{\sqrt{2}}|R\rangle \otimes |1\rangle$$

$$|\psi_2\rangle = -\frac{1}{2}|L\rangle \otimes |-2\rangle + \frac{1}{2}(|R\rangle + |L\rangle) \otimes |0\rangle + \frac{1}{2}|R\rangle \otimes |2\rangle \tag{1.6}$$

Finally, the probability to find the particle at a position n is calculated using

$$P(n) = |\langle n|\psi\rangle|^2. \tag{1.7}$$

For example, the probability that the particle is found at $n = 0$ in $|\psi_2\rangle$ from Eq. (1.6) is

$$P(0) = \left| \langle 0| \left[-\frac{1}{2}|L\rangle \otimes |-2\rangle + \frac{1}{2}(|R\rangle + |L\rangle) \otimes |0\rangle + \frac{1}{2}|R\rangle \otimes |2\rangle \right] \right|^2 \tag{1.8}$$

$$P(0) = \left| \frac{1}{2}(|R\rangle + |L\rangle) \right|^2 = \frac{1}{4}\langle R|R\rangle + \frac{1}{4}\langle L|L\rangle = \frac{1}{2}. \tag{1.9}$$

Clearly, the state of the particle will expand rapidly as it evolves and at times larger than $t = 2$, the probability distributions will be much harder to calculate. A more in-depth description of this walk is given in each of the references [1,2,3,9], including how to express the state and the spatial probability distributions after many time steps.

1.2 Quantum Walks With Memory

Zlatko Dimcovic and Yevgeniy Kovchegov developed a framework for solving DTQW that is based on the idea of a walk with memory [9]. This means that the state of the particle includes not only its current position, but also a memory of its previous position. Keeping track of the particle's previous position can be thought of as analogous to the coin space introduced in other quantum walks. The state of the particle is then given by the tensor product of the previous and current position.

$$|\psi\rangle = |previous\rangle \otimes |current\rangle$$

If the position at a time t is $|n_t\rangle$, then the previous position is $|n_{t-1}\rangle$. So the state of the particle at the time t would be

$$|\psi_t\rangle = |n_{t-1}\rangle \otimes |n_t\rangle. \tag{1.10}$$

For a quantum walk on a one-dimensional line, a particle at a given location could have come from one of two adjacent positions. Therefore, there will be two possible memory states just like there were two coin states. For example, a particle at position n could have arrived there from $n-1$ and would be described by the state ket $|n-1\rangle \otimes |n\rangle$. Similarly, a particle that arrived from $n+1$ would be described by $|n+1\rangle \otimes |n\rangle$. The evolution operator then acts differently on the state depending on where the particle came from.

These memory states are still analogous to the coin states for the walk on a line. Consider the state $|n-1\rangle \otimes |n\rangle$. Its most recent step was to the right, so this state could also be described using the ket $|R\rangle \otimes |n\rangle$, and a direct relation can be made between the memory states and the coin states described in the previous section.

$$
\begin{aligned}
|R\rangle \otimes |n\rangle &\longleftrightarrow |n-1\rangle \otimes |n\rangle \\
|L\rangle \otimes |n\rangle &\longleftrightarrow |n+1\rangle \otimes |n\rangle
\end{aligned}
\tag{1.11}
$$

In this way, the framework for quantum walks with memory is able to exactly recreate the standard coined walk on the one dimensional line. However, this framework has proven to be more flexible than the standard coin approach when solving certain problems. For example, in their paper Dimcovic and Kovchegov were able to solve a DTQW on a binary tree, a problem that, despite much interest, had not yet been solved using standard coin methods [9]. In addition, this approach does not require one to introduce some new degree of freedom like the coin space. Instead, one just needs to extend the position space to keep track of the previous step.

The goal of this thesis is to continue to explore the idea of quantum walks with memory by expanding the memory of the particle to keep track of the previous two positions. Using two-step memory means that there are now four different possible histories that the particle can have, and the operator can act differently for each of these. We investigate the case of two-step memory quantum walks and how their behavior differs from the one-step memory and coin quantum walks. Section 2 further develops this idea and shows the process required to solve for the probability distribution of the particle at some later time.

2   Methods

The goal of this section is to describe a method for solving the time evolution of a quantum walk with two-step memory in a one-dimensional system. First we consider the case of a walk on an infinite position space and define the evolution operator that will be used in this work. This section also describes the main steps in the process of calculating how the state evolves, including the use of the spatial Fourier transform, diagonalization of the operator in the Fourier space, and finally the use of the inverse Fourier transform. Solving the one-dimensional walk results in complicated expressions that cannot be solved analytically. These expressions are solved numerically using Mathematica and the results are presented in Section 3.

2.1   Quantum Walk on an Infinite Position Space

Consider a particle that is free to move in one-dimension along an infinite space of discrete positions, $\mathbb{Z}_n$. Between any consecutive time steps the particle can move either to the left or the right. Moving to the left is considered moving in the negative direction and moving to the right is considered moving in the positive direction. Since this is a quantum system, as long as no measurements of the particle's position are taken, the state of the particle will spread out in both possible directions. This section describes how to calculate the probability distribution for the position of the particle at a later time.

The major difference between the quantum walk described in this paper and conventional quantum walks is that it uses a two-step memory. Two-step memory means that the quantum state includes the previous two positions of the particle in addition to the current position. The quantum operator then acts differently on the state depending on the previous positions. Before we can introduce this operator and how it acts on a state, we must distinguish between the four possible memory states. These states are more easily visualized by describing them each as a "tail" that points from the two previous positions to the current position.

2.2   Types of Tails

The term "tail" refers to the part of the particles state that keeps track of its previous two positions. Since there are two possible directions for the particle to move at any time, there are four possible paths it can take over two time steps. For example, consider a particle that is currently at a position n. The particle could have moved two steps in the positive direction, arriving at n from $n-2$. It could also have begun by moving in the negative direction from n, changed direction, and then moved back to n from $n-1$. Similarly, the walk could arrive at n from the positive direction in two different ways. All four of these types of tails are defined in the diagram below.

(right-right)	•——▸•——▸•	$(n-2) \to (n-1) \to n$	state $|RR\rangle$
(left-right)	•⇐——▸•	$n \to (n-1) \to n$	state $|LR\rangle$
(right-left)	•◂——⇒•	$n \to (n+1) \to n$	state $|RL\rangle$
(left-left)	•◂——•◂——	$(n+2) \to (n+1) \to n$	state $|LL\rangle$

Thus we may now refer to the memory state, or tail, in terms of the four basis kets given above. In developing the evolution operator for this system, we also be refer to the "arrows" of the tail.

These arrows are exactly those seen in the diagram above and will be described as either left or right pointing arrows. The "first arrow" in a tail is the older step that the particle took and is listed as the first entry in the tail ket. The "second arrow" in a tail is the most recent step that the particle took to arrive at its current position and is given by the second entry in the tail ket.

The full state of the particle is now given by the tensor product of the tail and position states of the particle.

$$|\psi\rangle = |tail\rangle \otimes |n\rangle \tag{2.1}$$

For example, consider a particle in the pure state $|RR\rangle \otimes |0\rangle$. The particle is currently at position $n = 0$ and it arrived there by taking two steps to the right. So this particle arrived to $n = 0$ from $n = -2$. Since this is a quantum system, the particle can also be in a superposition of states. This can be a superposition of the tail states such as

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|RR\rangle + |LL\rangle \right) \otimes |n\rangle.$$

However, superpositions of tail states and the position of the particle such as

$$|\psi\rangle = \frac{1}{\sqrt{2}} |LL\rangle \otimes |n-1\rangle + \frac{1}{\sqrt{2}} |RR\rangle \otimes |n+1\rangle$$

are also possible. The goal now is to define the quantum evolution operator and how it will act on the states.

2.3   Evolution Operator

Given that the particle is in some state at time t, the evolution of the state is described by

$$|\psi_{t+1}\rangle = U|\psi_t\rangle \tag{2.2}$$

where U is a unitary operator. Unitary means that the evolution of the system is reversible, and all time evolution operators in quantum mechanics must behave this way. The full evolution operator consists of two separate operators: the coin operator Q which operates in the tail space, and the shift operator S which operates in the position space. The coin operator assigns probabilities to move from one tail to the next based on the previous two steps. The shift operator then changes the particle's position to match the step that was implied by the change in the tail. First, we describe the coin operator in more detail.

The behavior of the operator is most easily described by referring to the separate arrows in the tail. First, notice that given some tail at time t, there are only two possible tails that the particle can have at time $t + 1$. This is because the second arrow at time t will become the first arrow at time $t + 1$. For example, a particle with tail $|LR\rangle$ at t can have only tails $|RR\rangle$ or $|RL\rangle$ at $t + 1$. So the second arrow in a particle's tail determines the first arrow in its tail after one time step.

The coin operator assigns the probability that the particle will move either left or right during a time step. For this quantum walk, we define the coin so that there is a positive probability $p < 1$ that between t and $t + 1$ the particle moves in the same direction as the first arrow in the tail at t. Then the probability that the particle moves the opposite direction as the first arrow in its tail is $1 - p$. For example, if the particle has a tail $|RL\rangle$, then the first arrow is to the right. This means

there is a probability p that its next step is to the right and a probability $p - 1$ that its next step is to the left. The operator can also be thought of as the probability that the tail state maintains its recent behavior. If it continued moving in the same direction at the previous time step, then the probability that it keeps moving in that direction is p. If the particle changed direction at the previous time step, then there is a probability p that it will change direction again in the current step. We can now write how the coin operator acts on each of the four tail kets.

$$
\begin{aligned}
Q|RR\rangle &= \sqrt{p}\,|RR\rangle + \sqrt{1-p}\,|RL\rangle \\
Q|LR\rangle &= \sqrt{1-p}\,|RR\rangle + -\sqrt{p}\,|RL\rangle \\
Q|RL\rangle &= -\sqrt{p}\,|LR\rangle + \sqrt{1-p}\,|LL\rangle \\
Q|LL\rangle &= \sqrt{1-p}\,|LR\rangle + \sqrt{p}\,|LL\rangle.
\end{aligned}
\tag{2.3}
$$

These four relations can also be written in matrix notation.

$$
\begin{pmatrix} |RR\rangle_{t+1} \\ |LR\rangle_{t+1} \\ |RL\rangle_{t+1} \\ |LL\rangle_{t+1} \end{pmatrix} = Q \begin{pmatrix} |RR\rangle_t \\ |LR\rangle_t \\ |RL\rangle_t \\ |LL\rangle_t \end{pmatrix}, \quad Q = \begin{bmatrix} \sqrt{p} & \sqrt{1-p} & 0 & 0 \\ 0 & 0 & -\sqrt{p} & \sqrt{1-p} \\ \sqrt{1-p} & -\sqrt{p} & 0 & 0 \\ 0 & 0 & \sqrt{1-p} & \sqrt{p} \end{bmatrix}.
\tag{2.4}
$$

There are a few comments to be made on the operator Q. First, the terms $\sqrt{p}$ and $\sqrt{1-p}$ are used instead of p and $1 - p$ because the operator must be expressed in terms of the probability amplitudes. The actual probabilities to measure the associated tails are the squares of the probability amplitudes, which would give p and $1 - p$ as required. Also, negative signs have been used on two of the entries. This was necessary to make the operator unitary, but it does not affect the probabilities. Finally, notice there are only two nonzero entries in each column of the operator Q. This reflects the fact that any tail has only two possible changes it can make between time steps. Now that the coin operator has been defined, we move on to the shift operator S.

The behavior of the shift operator is closely related to the coin operator because the way in which the tail state changes implies the direction that the particle moved. For example, if the tail changes from $|RR\rangle$ to $|RL\rangle$ during some time step, then the particle must have moved to the left during that step. This means that the shift operator must decrease the position by one during that step. Similarly, if the tail implies that the particle moved to the right, the shift operator must increase the position by one. The shift operator can now be defined as

$$
\begin{aligned}
S =&\Pi_{RR} \otimes \sum_n |n+1\rangle\langle n| + \Pi_{LR} \otimes \sum_n |n+1\rangle\langle n| \\
&+ \Pi_{RL} \otimes \sum_n |n-1\rangle\langle n| + \Pi_{LL} \otimes \sum_n |n-1\rangle\langle n|,
\end{aligned}
\tag{2.5}
$$

where Π_{ij} are the projection operators corresponding to the tail states. The role of the projectors is to select one of the tail states, and then the sums shift all positions with that tail state in the appropriate direction. Consider the first of the four terms in the shift operator. The projector Π_{RR} selects all the parts of the state that have the tail $|RR\rangle$. Then, since that tail implies that the most recent step was to the right, the sum shifts all the positions from $|n\rangle$ to $|n+1\rangle$.

Finally, the coin and shift operators must be combined to give the total evolution operator U.

$$
U = S(Q \otimes I)
\tag{2.6}
$$

The term in parentheses operates first, mixing the tail states and assigning probabilities for the particle to move either left or right. This term includes the identity operator because the action of the coin does not yet change the position states. Rather, the coin operator Q changes the tail states and determines which direction the positions will be shifted. The shift operator S then acts on the position of the particle to move it in the correct direction. So the overall evolution of the state of the particle is a series of mixing the tail states and then shifting the positions. An example help to will illustrate how the total evolution operator works. Consider a particle that starts in the state

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|RR\rangle \otimes (|1\rangle + |4\rangle). \tag{2.7}$$

This particle is in an equal superposition of the positions $n = 1$ and $n = 4$, and both parts are in the tail state $|RR\rangle$. To evolve the state, we first act with the coin and the identity.

$$(Q \otimes I)|\psi_0\rangle = (Q \otimes I)\left[\frac{1}{\sqrt{2}}|RR\rangle \otimes (|1\rangle + |4\rangle)\right] = \frac{1}{\sqrt{2}}Q|RR\rangle \otimes I(|1\rangle + |4\rangle)$$

$$= \frac{1}{\sqrt{2}}\left(\sqrt{p}|RR\rangle + \sqrt{1-p}|RL\rangle\right) \otimes (|1\rangle + |4\rangle)$$

$$= \sqrt{\frac{p}{2}}|RR\rangle \otimes (|1\rangle + |4\rangle) + \sqrt{\frac{1-p}{2}}|RL\rangle \otimes (|1\rangle + |4\rangle) \tag{2.8}$$

Now to complete the evolution, we apply the shift operator to this state. Notice that only the terms from the shift operator that have the Π_{RR} and Π_{RL} projectors will be able to operate.

$$|\psi_1\rangle = S(Q \otimes I)|\psi_0\rangle$$

$$= \left[\Pi_{RR} \otimes \sum_n |n+1\rangle\langle n| + \Pi_{RL} \otimes \sum_n |n-1\rangle\langle n|\right]$$

$$\times \left[\sqrt{\frac{p}{2}}|RR\rangle \otimes (|1\rangle + |4\rangle) + \sqrt{\frac{1-p}{2}}|RL\rangle \otimes (|1\rangle + |4\rangle)\right]$$

$$= \sqrt{\frac{p}{2}}|RR\rangle \otimes \left[\sum_n |n+1\rangle\langle n|(|1\rangle + |4\rangle)\right] + \sqrt{\frac{1-p}{2}}|RL\rangle \otimes \left[\sum_n |n-1\rangle\langle n|(|1\rangle + |4\rangle)\right]$$

$$= \sqrt{\frac{p}{2}}|RR\rangle \otimes (|2\rangle + |5\rangle) + \sqrt{\frac{1-p}{2}}|RL\rangle \otimes (|0\rangle + |3\rangle)$$

$$= \sqrt{\frac{1-p}{2}}|RL\rangle \otimes |0\rangle + \sqrt{\frac{p}{2}}|RR\rangle \otimes |2\rangle + \sqrt{\frac{1-p}{2}}|RL\rangle \otimes |3\rangle + \sqrt{\frac{p}{2}}|RR\rangle \otimes |5\rangle \tag{2.9}$$

There are now four different terms in the state. The parts of the particle's state that were at $n = 1$ and $n = 4$ each split, moving in both the left and right directions. The probability that the state would move in either direction was assigned by the coin operator. From this simple example, it is already clear that the state of the particle expands rapidly and the expressions become very complicated. Evolutions after a large numbers of time steps would be extremely difficult to calculate by simply applying the operator U many times. Another method utilizing the Fourier transform is necessary to calculate the state at much later times.

Now we define the notation that will be used to express any possible state of the particle. Consider a general state at time t given by

$$|\psi_t\rangle = \sum_{n\in\mathbb{Z}} \Big(a_t(n)|RR\rangle + b_t(n)|LR\rangle + c_t(n)|RL\rangle + d_t(n)|LL\rangle \Big) \otimes |n\rangle. \tag{2.10}$$

The state of the particle is in a superposition of all the possible positions. In addition, at each position the particle is in a superposition of each of the four tail states. We have defined $a_t(n)...d_t(n)$ as the amplitudes of each tail state at the position n. Applying the operator U gives the probability amplitudes at t in terms of the amplitudes at the previous time $t-1$.

$$\begin{aligned}
a_t(n) &= \quad\;\; \sqrt{p}\, a_{t-1}(n-1) + \sqrt{1-p}\, b_{t-1}(n-1) \\
b_t(n) &= \quad -\sqrt{p}\, c_{t-1}(n-1) + \sqrt{1-p}\, d_{t-1}(n-1) \\
c_t(n) &= \sqrt{1-p}\, a_{t-1}(n+1) - \quad\;\; \sqrt{p}\, b_{t-1}(n+1) \\
d_t(n) &= \sqrt{1-p}\, c_{t-1}(n+1) + \quad\;\; \sqrt{p}\, d_{t-1}(n+1).
\end{aligned} \tag{2.11}$$

The goal is to solve these recurrence relations so that they can be applied to some initial state to predict the amplitudes at a later time. Once all four of the tail amplitudes are known as a function of the position n, then the probability distibution for finding the particle at n is given by

$$\begin{aligned}
P_t(n) &= |\langle n|\psi_t\rangle|^2 \\
&= \left| \langle n| \sum_{n\in\mathbb{Z}} \Big(a_t(n)|RR\rangle + b_t(n)|LR\rangle + c_t(n)|RL\rangle + d_t(n)|LL\rangle \Big) \otimes |n\rangle \right|^2 \\
&= \left| \Big(a_t(n)|RR\rangle + b_t(n)|LR\rangle + c_t(n)|RL\rangle + d_t(n)|LL\rangle \Big) \otimes \sum_{n\in\mathbb{Z}} \langle n|n\rangle \right|^2
\end{aligned}$$

$$P_t(n) = |a_t(n)|^2 + |b_t(n)|^2 + |c_t(n)|^2 + |d_t(n)|^2. \tag{2.12}$$

Therefore, the probability distribution for the position of the particle is given by the sum of the squares of each of the four tail state probability amplitudes. The four recursion relations above can be solved to find the amplitudes at any time, but the solution requires the use of the Fourier transform. This transforms the amplitudes from functions of position, n, to functions of spatial frequency, k. In the Fourier space the evolution operator can be diagonalized, and this allows us to analytically solve for the amplitudes after any number of time steps.

2.4   Fourier Transform

Due to the translational invariance of the position space, the evolution of the quantum walk has a much simpler representation in the Fourier space. Therefore, the general strategy for solving the recurrence relations is to first use the Fourier transform on each of the four equations. These equations are then combined into a matrix form for the evolution operator in the Fourier space. We then diagonalize the operator so that it can easily be raised to the power of t. This greatly simplifies the algebra because when a diagonal matrix is raised to some power, each diagonal element is just

raised to that power. The diagonalized operator is applied to some initial state to get the amplitudes at a later time. Finally, we carry out the inverse Fourier transform to return the amplitudes the position space.

The Fourier transform is defined as

$$\widehat{f}(k) = \sum_{n \in \mathbb{Z}} f(n)e^{i k n}, \tag{2.13}$$

We start by applying the transform to the equation for the amplitude $a(n)$.

$$\widehat{a}_t(k) = \sum_{n \in \mathbb{Z}} a_t(n)e^{i k n}$$
$$= \sum_{n \in \mathbb{Z}} [\sqrt{p}a_{t-1}(n-1) + \sqrt{1-p}b_{t-1}(n-1)]e^{i k n} \tag{2.14}$$

Distributing the exponent and rearranging we can rewrite Eq. (2.14) as

$$\widehat{a}_t(k) = \sqrt{p}e^{i k} \sum_{n \in \mathbb{Z}} a_{t-1}(n-1)e^{i k (n-1)} + \sqrt{1-p}e^{i k} \sum_{n \in \mathbb{Z}} b_{t-1}(n-1)e^{i k (n-1)}. \tag{2.15}$$

Changing the index from n to $n-1$ has no effect on the sum since the sum runs from negative to positive infinity. So the terms in the sums are themselves Fourier transforms. The $\widehat{a}_t(k)$ coefficient can finally be expressed as

$$\widehat{a}_t(k) = \sqrt{p}e^{i k}\widehat{a}_{t-1}(k) + \sqrt{1-p}e^{i k}\widehat{b}_{t-1}(k) \tag{2.16}$$

Transforming the other three coefficients from (2.11) in a similar way we get

$$\begin{aligned}
\widehat{b}_t(k) &= -\sqrt{p}e^{i k} \ \widehat{c}_t(k) + \sqrt{1-p}e^{i k} \ \widehat{d}_t(k) \\
\widehat{c}_t(k) &= \sqrt{1-p}e^{-i k} \ \widehat{a}_t(k) - \sqrt{p}e^{-i k} \ \widehat{b}_t(k) \\
\widehat{d}_t(k) &= \sqrt{1-p}e^{-i k} \ \widehat{c}_t(k) + \sqrt{p}e^{-i k} \ \widehat{d}_t(k).
\end{aligned} \tag{2.17}$$

We can now see why the Fourier transform helps with the calculation. The four recursion relations in the Fourier space are only functions of k. However, the recursion relations from (2.11) are in terms of $n-1$, n, and $n+1$. Combining (2.16) and (2.17) we get the matrix M, the evolution operator in the Fourier space.

$$|v_t\rangle = \begin{pmatrix} \widehat{a}_t \\ \widehat{b}_t \\ \widehat{c}_t \\ \widehat{d}_t \end{pmatrix} = M \begin{pmatrix} \widehat{a}_{t-1} \\ \widehat{b}_{t-1} \\ \widehat{c}_{t-1} \\ \widehat{d}_{t-1} \end{pmatrix} = M^t \begin{pmatrix} \widehat{a}_0 \\ \widehat{b}_0 \\ \widehat{c}_0 \\ \widehat{d}_0 \end{pmatrix} \tag{2.18}$$

$$M = \begin{bmatrix} \sqrt{p}\,e^{i k} & \sqrt{1-p}\,e^{i k} & 0 & 0 \\ 0 & 0 & -\sqrt{p}\,e^{i k} & \sqrt{1-p}\,e^{i k} \\ \sqrt{1-p}\,e^{-i k} & -\sqrt{p}\,e^{-i k} & 0 & 0 \\ 0 & 0 & \sqrt{1-p}\,e^{-i k} & \sqrt{p}\,e^{-i k} \end{bmatrix}. \tag{2.19}$$

The state vector $|v_t\rangle$ has been defined as the vector whose components are the four probability amplitudes $\widehat{a}_t...\widehat{d}_t$. The matrix M is now diagonalized to make it easier to solve for $|v_t\rangle$ which will give the probability amplitudes at some later time. In the next subsection 2.5 we solve for the four eigenvalues and eigenvectors which are then used to form the diagonal operator.

2.5   Diagonalizing the Operator M

The first step in diagonalizing the matrix M is to solve for the eigenvalues. The four eigenvalues are obtained by solving the equation

$$det(M - I\lambda) = 0 \tag{2.20}$$

for λ. Taking the determinant of

$$M = \begin{bmatrix} \sqrt{p}\,e^{ik} - \lambda & \sqrt{1-p}\,e^{ik} & 0 & 0 \\ 0 & -\lambda & -\sqrt{p}\,e^{ik} & \sqrt{1-p}\,e^{ik} \\ \sqrt{1-p}\,e^{-ik} & -\sqrt{p}\,e^{-ik} & -\lambda & 0 \\ 0 & 0 & \sqrt{1-p}\,e^{-ik} & \sqrt{p}\,e^{-ik} - \lambda \end{bmatrix}, \tag{2.21}$$

gives the characteristic equation

$$\lambda^4 - \left(\sqrt{p}\,e^{ik} + \sqrt{p}\,e^{-ik}\right)\lambda^3 + \left(\sqrt{p}\,e^{-ik} + \sqrt{p}\,e^{ik}\right)\lambda - 1 = 0. \tag{2.22}$$

Using the exponential form of the cosine function we can rewrite Eq. (2.22).

$$\lambda^4 - (2\sqrt{p}\cos k)\lambda^3 + (2\sqrt{p}\cos k)\lambda - 1 = 0. \tag{2.23}$$

Finally, solving this equation for the eigenvalues we get

$$\lambda_1 = 1 \quad , \quad \lambda_2 = -1$$
$$\lambda_3 = \sqrt{p}\cos k + i\sqrt{1 - p\cos^2 k} \quad , \quad \lambda_4 = \sqrt{p}\cos k - i\sqrt{1 - p\cos^2 k}. \tag{2.24}$$

At this point it is helpful to note that the eigenvalues of a unitary operator must always have a norm of one, so $|\lambda_i| = 1$. This means that the two complex eigenvalues must be points on the unit circle and the four eigenvalues can then be expressed as

$$\lambda_1 = 1, \quad \lambda_2 = -1, \quad \lambda_3 = e^{i\omega_k}, \quad \lambda_4 = e^{-i\omega_k}, \quad \text{where} \quad \omega_k = \cos^{-1}(\sqrt{p}\cos k). \tag{2.25}$$

Now that the eigenvalues are known, the eigenvectors $|V_i\rangle$ of the matrix M can be found by solving

$$(M - I\lambda_i)|V_i\rangle = 0$$

$$\begin{bmatrix} \sqrt{p}\,e^{ik} - \lambda & \sqrt{1-p}\,e^{ik} & 0 & 0 \\ 0 & -\lambda & -\sqrt{q}\,e^{ik} & \sqrt{1-q}\,e^{ik} \\ \sqrt{1-p}\,e^{-ik} & -\sqrt{p}\,e^{-ik} & -\lambda & 0 \\ 0 & 0 & \sqrt{1-q}\,e^{-ik} & \sqrt{q}\,e^{-ik} - \lambda \end{bmatrix} \begin{pmatrix} 1 \\ \alpha_i \\ \beta_i \\ \gamma_i \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.26}$$

Solving Eq. (2.26) for each of the coefficients $\alpha_i, \beta_i, \gamma_i$ gives the equation for the eigenvectors in terms of the eigenvalues λ_i.

$$\alpha_i = \frac{\lambda_i e^{-ik} - \sqrt{p}}{\sqrt{1-p}}, \quad \beta_i = \frac{\lambda_i^{-1} e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}}, \quad \text{and} \quad \gamma_i = \frac{\sqrt{p}e^{-3ik} - \lambda_i^{-1}e^{-2ik}}{\sqrt{p}e^{-ik} - \lambda_i}. \tag{2.27}$$

The expressions for $\alpha_i, \beta_i, \gamma_i$ given by Eq. (2.27) are elements of the eigenvectors and become important when calculating each of the tail amplitudes. The general expression for the eigenvectors is

$$|v_i\rangle = \begin{pmatrix} 1 \\ \alpha_i \\ \beta_i \\ \gamma_i \end{pmatrix} = \begin{pmatrix} 1 \\ \left(\frac{\lambda_i e^{-ik} - \sqrt{p}}{\sqrt{1-p}}\right) \\ \left(\frac{\lambda_i^{-1} e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}}\right) \\ \left(\frac{\sqrt{p}e^{-3ik} - \lambda_i^{-1}e^{-2ik}}{\sqrt{p}e^{-ik} - \lambda_i}\right) \end{pmatrix}. \tag{2.28}$$

We now write the four eigenvalues and the corresponding eigenvectors.

$$\lambda_1 = 1, \quad \lambda_2 = -1, \quad \lambda_3 = e^{i\omega_k}, \quad \lambda_4 = e^{-i\omega_k}, \quad \text{where} \quad \omega_k = \cos^{-1}(\sqrt{p}\cos k) \tag{2.29}$$

$$|v_1\rangle = \begin{pmatrix} 1 \\ \frac{e^{-ik} - \sqrt{p}}{\sqrt{1-p}} \\ \frac{e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}} \\ e^{-2ik} \end{pmatrix}, \quad |v_2\rangle = \begin{pmatrix} 1 \\ \frac{-e^{-ik} - \sqrt{p}}{\sqrt{1-p}} \\ \frac{-e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}} \\ e^{-2ik} \end{pmatrix}$$

$$|v_3\rangle = \begin{pmatrix} 1 \\ \frac{e^{i\omega_k}e^{-ik} - \sqrt{p}}{\sqrt{1-p}} \\ \frac{e^{-i\omega_k}e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}} \\ \frac{\sqrt{p}e^{-3ik} - e^{-i\omega_k}e^{-2ik}}{\sqrt{p}e^{-ik} - e^{i\omega_k}} \end{pmatrix}, \quad |v_4\rangle = \begin{pmatrix} 1 \\ \frac{e^{-i\omega_k}e^{-ik} - \sqrt{p}}{\sqrt{1-p}} \\ \frac{e^{i\omega_k}e^{-ik} - \sqrt{p}e^{-2ik}}{\sqrt{1-p}} \\ \frac{\sqrt{p}e^{-3ik} - e^{i\omega_k}e^{-2ik}}{\sqrt{p}e^{-ik} - e^{-i\omega_k}} \end{pmatrix}. \tag{2.30}$$

Using the eigenvalues and eigenvectors, we construct the diagonalized operator. The best way to do this without having to change from the $|v_i\rangle$ basis is to use the spectral decomposition of M. This is given by

$$M = \sum_{i=1}^{4} \lambda_i \frac{|v_i\rangle\langle v_i|}{\langle v_i|v_i\rangle}. \tag{2.31}$$

The spectral decomposition is a sum of the projection operators for each of the eigenvectors weighted by the eigenvalues. The inner products in the denominator are required because the four eigenvectors obtained above were not normalized. The real benefit of this form is that raising it to the power t simply raises the eigenvalues to that power.

$$M^t = \sum_{i=1}^{4} (\lambda_i)^t \frac{|v_i\rangle\langle v_i|}{\langle v_i|v_i\rangle}. \tag{2.32}$$

We finally have everything we need to calculate how the state of the particle will change after any number of time steps. If $|v_0\rangle$ is the vector that gives the initial tail amplitudes in the Fourier space, then after t time steps the state will be

$$|v_t\rangle = M^t|v_0\rangle = \left(\sum_{i=1}^{4} (\lambda_i)^t \frac{|v_i\rangle\langle v_i|}{\langle v_i|v_i\rangle}\right) |v_0\rangle. \tag{2.33}$$

For simplicity, we assume that the particle starts out in the pure state $|RR\rangle$. So the initial vector will be the unit vector $|v_0\rangle = |e_1\rangle$. Since each of the vectors $|v_i\rangle$ were chosen so that their first entry was one, this means that $\langle v_i|v_0\rangle = \langle v_i|e_1\rangle = 1$. Given the initial state $|RR\rangle$, the final state of the particle in the Fourier space will be

$$|v_t\rangle = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle}|v_i\rangle \quad \longrightarrow \quad \begin{pmatrix} \widehat{a}_t \\ \widehat{b}_t \\ \widehat{c}_t \\ \widehat{d}_t \end{pmatrix} = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle} \begin{pmatrix} 1 \\ \alpha_i \\ \beta_i \\ \gamma_i \end{pmatrix}. \tag{2.34}$$

Finally, this gives the four equations for the tail amplitudes after the particle has evolved for a time t.

$$\widehat{a}_t = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle} \quad , \quad \widehat{b}_t = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle}\alpha_i$$

$$\widehat{c}_t = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle}\beta_i \quad , \quad \widehat{d}_t = \sum_{i=1}^{4} \frac{(\lambda_i)^t}{\langle v_i|v_i\rangle}\gamma_i \tag{2.35}$$

Each amplitude has four terms that contain eigenvalues and eigenvectors. We have already solved for all of the elements contained in these terms. However, these amplitudes are still in the Fourier space. Before we can calculate the probability distribution for the particle, we must use the inverse Fourier transform to return each of the terms above to the position space.

2.6 Inverse Fourier Transform

The inverse Fourier transform is defined as

$$f(n) = \frac{1}{2\pi} \int_0^{2\pi} f(k)e^{-ikn}dk \tag{2.36}$$

This inverse transform must be applied to each of the expressions in (2.35) to find the tail amplitudes as functions of position. Finally, these amplitudes will be used to calculate the probability distribution for the position of the particle using Eq. (2.12)

$$P_t(n) = |a_t(n)|^2 + |b_t(n)|^2 + |c_t(n)|^2 + |d_t(n)|^2.$$

The probability distributions is calculated numerically and presented in the Section 3.

3   Results

This section presents the plots for the tail amplitudes and the total probability distribution of the particle. Each result is evaluated at time steps 99, 100, 199, and 200. These times were chosen to show evolution over a single step and over larger time intervals. When calculating the evolution of the particle, one must first find the four probability amplitudes $a_t(n)$ through $d_t(n)$, so the plots for these are presented first. The amplitude plots share similar features that also appear in the probability distribution.

3.1   Tail Probability Amplitudes

In Section 2.5 we solved for each of the tail amplitudes in terms of t and k. To return to the original position space, we apply the inverse Fourier transform defined by Eq. (2.36) to each expression from (2.35). The integral for the $a_t(n)$ is

$$
\begin{aligned}
a_t(n) &= \frac{1}{2\pi} \int_0^{2\pi} \left[\sum_{i=1}^4 \frac{(\lambda_i)^t}{\langle v_i | v_i \rangle} \right] dk \\
&= \frac{1}{2\pi} \int_0^{2\pi} \left[\frac{1-p}{4(1-\sqrt{p}\cos k)} + (-1)^t \frac{1-p}{4(1+\sqrt{p}\cos k)} \right. \\
&\qquad\qquad + e^{+t(i\omega_k)} \frac{1 + p - 2p\cos^2 k + 2(\sqrt{p}\sin k)\sqrt{1 - p\cos^2 k}}{4\left(1 - p\cos^2 k\right)} \\
&\qquad\qquad \left. + e^{-t(i\omega_k)} \frac{1 + p - 2p\cos^2 k - 2(\sqrt{p}\sin k)\sqrt{1 - p\cos^2 k}}{4\left(1 - p\cos^2 k\right)} \right] e^{-ikn} dk
\end{aligned}
\tag{3.1}
$$

where ω_k and the eigenvalues λ_i are given by Eq. (2.25). The full integral from Eq. (3.1) is not solved analytically, but it is still an exact solution for the tail amplitude. Instead of solving analytically, the expression is integrated numerically and Fig. 1 shows the result for the integral.

   The other three probability amplitudes are calculated in the same way as $a_t(n)$ by applying the inverse Fourier transform. The integral expressions are extremely similar to Eq. (3.1), except that each term is multiplied by α_i for $b_t(n)$, β_i for $c_t(n)$, and γ_i for $d_t(n)$.

$$
b_t(n) = \frac{1}{2\pi} \int_0^{2\pi} \left[\sum_{i=1}^4 \frac{(\lambda_i)^t}{\langle v_i | v_i \rangle} \alpha_i \right] dk \quad , \quad c_t(n) = \frac{1}{2\pi} \int_0^{2\pi} \left[\sum_{i=1}^4 \frac{(\lambda_i)^t}{\langle v_i | v_i \rangle} \beta_i \right] dk
$$
$$
d_t(n) = \frac{1}{2\pi} \int_0^{2\pi} \left[\sum_{i=1}^4 \frac{(\lambda_i)^t}{\langle v_i | v_i \rangle} \gamma_i \right] dk
\tag{3.2}
$$

The factors α_i, β_i, and γ_i are given by Eq. (2.27). These coefficients are also calculated by numerical integration, and the results are presented in Figs. 2, 3, and 4.
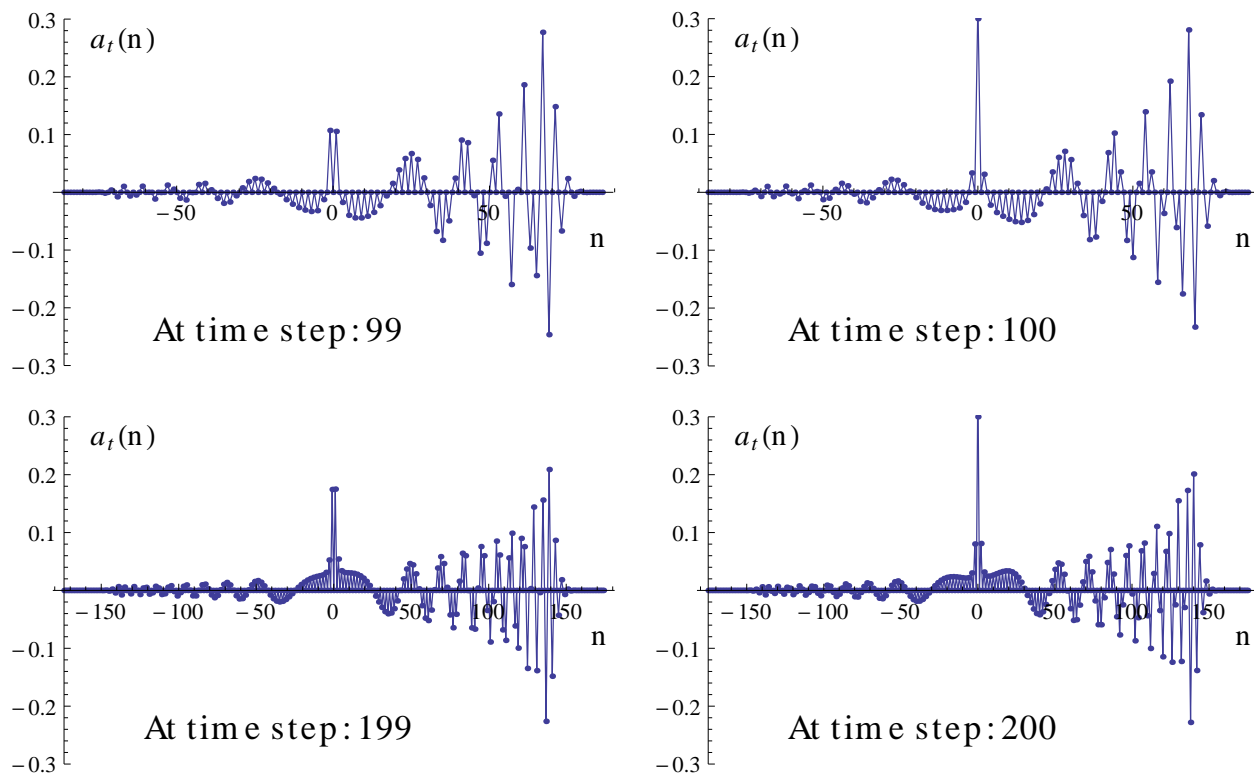
Figure 1: Probability amplitude $a_t(n)$ as a function of position for time steps 99, 100, 199, 200.
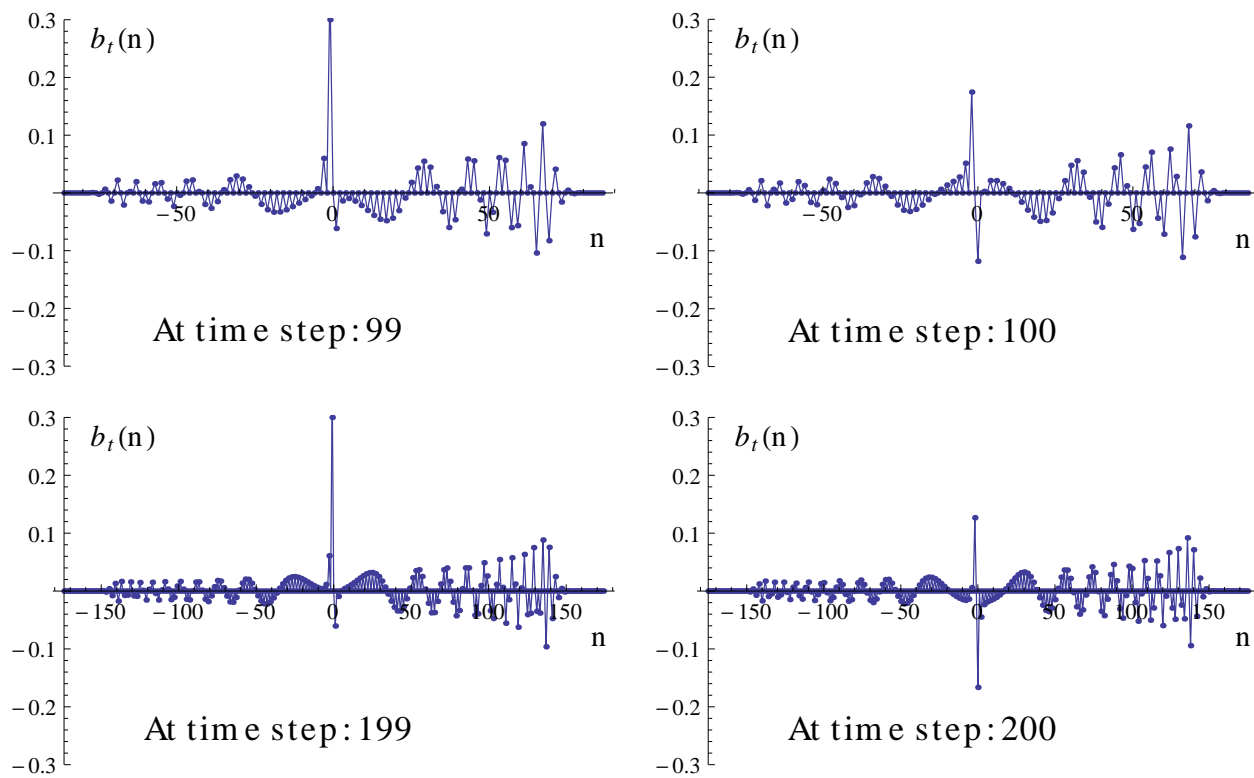
Figure 2: Probability amplitude $b_t(n)$ as a function of position for time steps 99, 100, 199, 200.
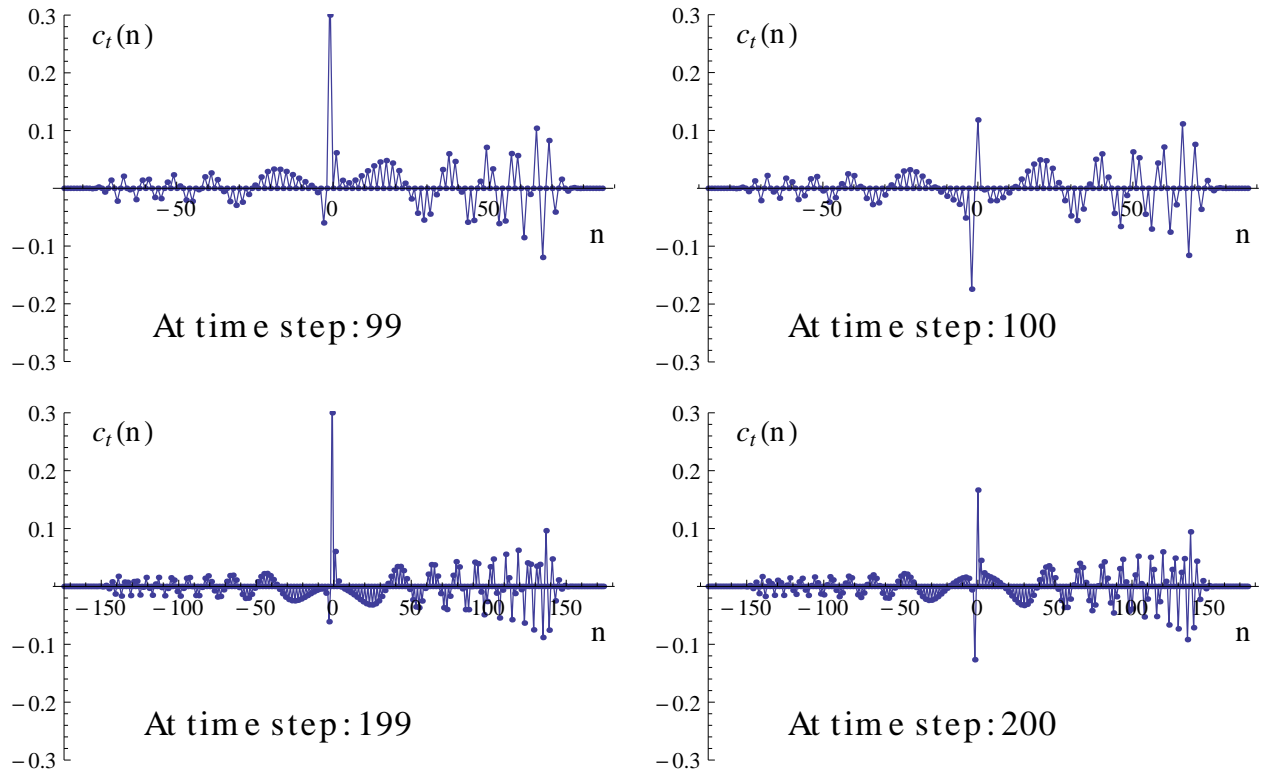
Figure 3:   Probability amplitude $c_t(n)$ as a function of position for time steps 99, 100, 199, 200.
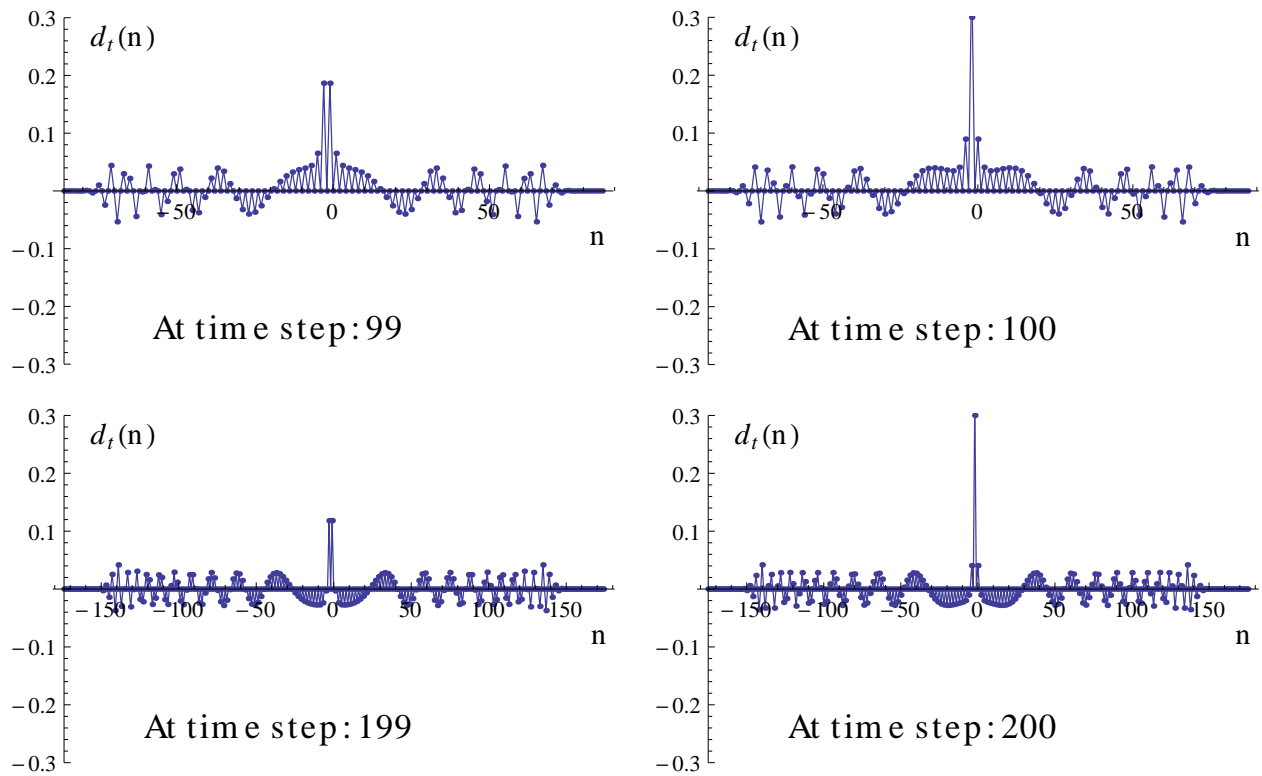
Figure 4:   Probability amplitude $d_t(n)$ as a function of position for time steps 99, 100, 199, 200.

3.2   Probability Distribution

The four tail amplitudes have been calculated, so we can finally use Eq. (2.12) to calculate the probability distribution of the particle as a function of time and position. Fig. 5 shows the results for the probability.

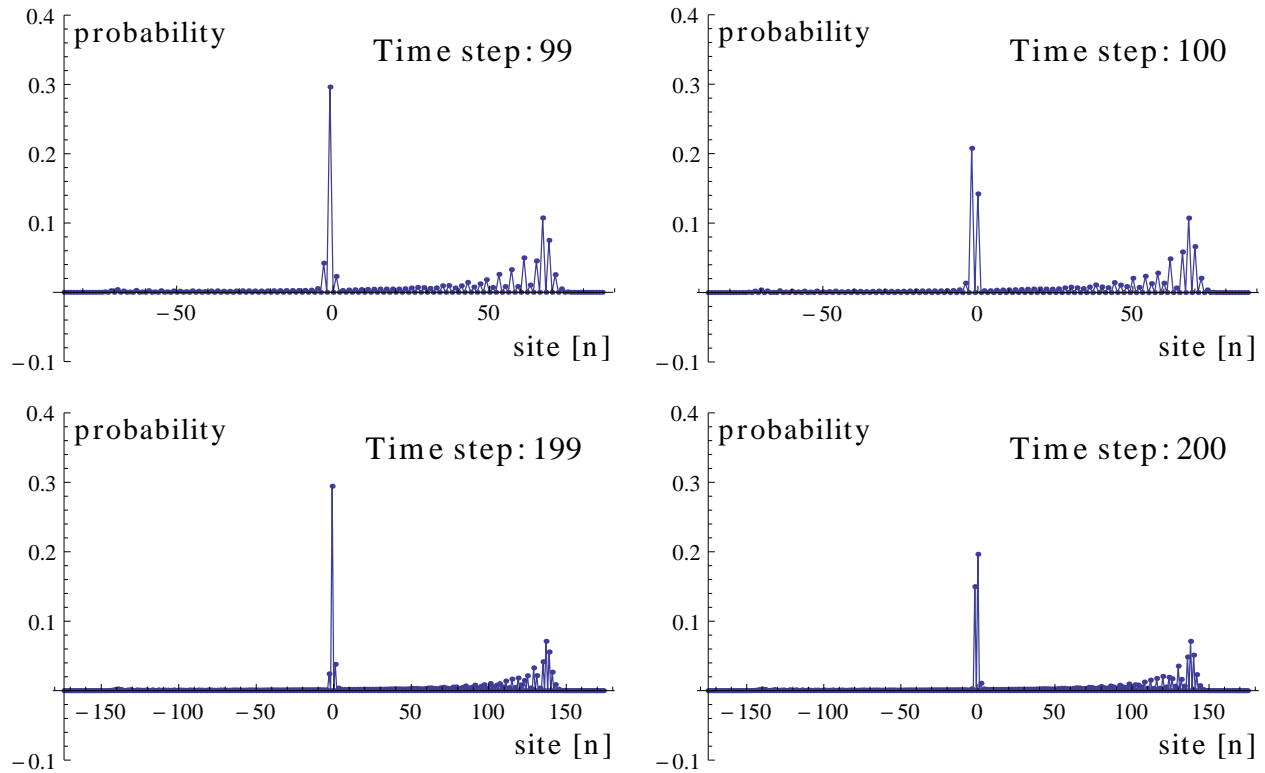$$P_t(n) = |a_t(n)|^2 + |b_t(n)|^2 + |c_t(n)|^2 + |d_t(n)|^2 \, .$$

Figure 5:   Probability distribution $P_t(n)$ for the particle as a function of position for time steps 99, 100, 199, 200.

4   Discussion

We now discuss the important features of the results presented in Section 3. We start by discussing the probability amplitudes for the tail states, and then consider the overall probability. The probability distribution for the DTQW with two-step memory shows behavior typical of quantum walks, but we also see the emergence of classical behavior.

4.1   Tail Probability Amplitudes

Calculating the tail probability amplitudes was the focus of most of the work in the Section 2 because we must know each of them before calculating the probability. However, they are not as physically meaningful as the probability distribution because they do not actually represent the probability to find the particle at a given position and time. Instead, they give only that probability that a given *tail state* is measured. For example, if we had some way of measuring the current position of the particle as well as the previous two positions, then $a_t(n)$ would allow us to calculate the probability that we measure the $|RR\rangle$ tail state. In addition, the plots in Figs. 1, 2, 3, and 4 are *probability amplitudes*, not probabilities. This is why the amplitude values are able to take on both positive and negative values.

The tail amplitudes do show the same features that are seen in the probability distribution. First, Figs. 1, 2, 3, and 4 all show a sharp central peak located around the original location of the particle. This implies that there is a strong probability that the particle would be found at the same position it started at. The central peak does oscillate between time steps, but it does not after large amounts of time. Mathematically, the stationary peak is caused by the first two terms in each of the integrals. For example, the $a_t(n)$ coefficient is given by Eq. (3.1) where we see that the first two terms are only time dependent due to the $(-1)^t$. The integral of these two terms will be different for positive or negative t, but it does not depend on how much time has passed. The 1 and -1 eigenvalues lead to similar stationary central peaks in each of the other three tail amplitudes as well.

The results for the tails also show peaks in the amplitude that move away from the original location of the particle. Fig. 1 illustrates this clearly with a peak propagating to the right with time. We can also see that the peak propagates ballistically, or linearly with t. At time step $t = 100$ the peak appears around $n = 70$, while at time step $t = 200$ the peak is around $n = 140$. Also, the amplitude of the propagating peaks is different for each of the four plots. For example, the propagating peak in $a_t(n)$ is always larger than in $b_t(n)$ or $c_t(n)$ (Figs. 2 and 3), and $d_t(n)$ (Fig. 4) has such small peaks that we do not even the directionality that we did in the other plots. This behavior is seen because of the initial state of the particle and shows that the initial state has a strong effect on the evolution of the particle.

Finally, notice that for each of the figures, half of the points are always zero. This must be the case because the particle can only change its position by one at any time step. For example, if the particle starts at an even position, then it must move one step to the left or right at the next time step and must end on an odd position. No matter how many steps are taken, the particle can only be found at an even *or* an odd numbered position. This still applies to our quantum particle, even though it spreads out over many positions as it evolves.

4.2   Probability Distribution

The probability distribution Fig. 5 is the final result for the quantum walk with two-step memory, and gives the actual probability that the particle will be measured at a given time and position. It is calculated from the tail amplitudes according to Eq. (2.12) and shows the same major features that were seen in the probability amplitudes: ballistic propagation and a stationary central peak.

The peak that propagates to the right spreads ballistically, and this is a very common feature of other quantum walks. However, the propagation of a DTQW with two-step memory is much more directional than most other walks. Fig. 5 shows that there is an extremely small probability that the particle is found to the left of its original position, and the direction in which the particle is likely to propagate depends on the initial tail state of the particle. For example, if we had chosen the initial state to be $|LL\rangle$, then the propagation of the particle would be predominately to the left. The ability to direct the propagation could be very useful when considering the algorithmic uses of the quantum walk with two-step memory.

The other major feature in the probability distribution is the stationary peak around the original position of the particle. This is not a feature that is commonly seen in quantum walks and represents the emergence of classical behavior. This means that keeping track of the added step of memory is likely the beginning of a transition to a classical system. One explanation is that when keeping track of one more position, we must know the exact path that the particle took over the last two time steps. This eliminates some of the possible paths in the path integral, thus decreasing the interference between paths. This is a very interesting result and should be explored further. Similar stationary peaks have been seen in the paper by Brun, Carteret, and Ambainis [2]. They also suggest that they are transitioning to classical behavior, but they do so in a much different way than presented above. They use multiple quantum coins to decrease the interference and find that only in the limit of a different coin at each time step does the quantum behavior of the particle disappear.

5   Conclusion

The framework for quantum walks with memory has proven useful for solving some problems that have not yet been solved using standard coin methods. This thesis explored the effect of extending the memory of the quantum state. The walk presented is a discrete-time quantum walk with two-step memory, meaning that the state of the particle keeps track of its current position as well as its previous two positions. The walk defined propagates on a one-dimensional discrete position space, so the effect of this extended memory is that there are four possible paths by which a particle can reach a given position. We define these as the four possible "tail" states and they are analogous to the two coin states commonly used when solving quantum walks. The evolution operator for the walk describes how the particle propagates in one direction or the other depending on the tail state. This walk is then solved to give the probability distribution for the particle as a function of time step and position.

The walk presented above is defined on an infinite position space with a specific initial state and a general method is presented for solving such a walk. The method for calculating the probability distribution of the particle focuses mainly on solving for the probability amplitudes of each possible tail state. First one must use the evolution operator to generate four recursion relations for the tail amplitudes. These relations express each amplitude in terms of the tail amplitudes at the previous time step. To solve the recursion relations, one needs to use the Fourier transform to express the equations in the Fourier space and then express the four equations in matrix form. It is then possible to diagonalize the matrix and calculate the probability amplitudes after any number of time steps. Finally, the inverse Fourier transform is applied to express each of the amplitudes in the original position space and the probability amplitudes can be combined to yield the probability distribution for the particle.

The four tail amplitudes are very complicated integrals that we do not solve analytically. Instead, the integrals were evaluated numerically at different time steps to generate the plots for the amplitudes as a function of position. These plots are then combined to calculate the probability distribution for the particle. Although most of the work goes into solving for the four tail amplitudes, these plots are less physically meaningful than the probability distribution which actually gives the likelihood that the particle is found at a given time and position.

The probability distribution for the particle shows two main features. First we have ballistically propagating peaks which are a common feature of quantum walks. These peaks spread at a rate directly proportional to the time, unlike the diffusive propagation typical of classical walks in which the rate is proportional to $\sqrt{t}$. However, the propagation in the case of the two-step memory walk appears to be much more directional than seen in other quantum walks. This directionality obviously depends on the initial state of the particle, so one could change the directionality by choosing an initial state with a tail that points in a given direction. This behavior could prove to be useful when considering the algorithmic uses of quantum walks with memory.

The other main feature of the probability distribution is a stationary peak located at the initial position of the particle, and this is not a common feature seen in quantum walks. Mathematically, the central peak is caused by the eigenvalues 1 and -1 that were found when diagonalizing the evolution operator. The stationary states associated with these eigenvalues do not decreases in amplitude as the time step increases. Instead, they create a sharp narrow peak that oscillates between successive steps but does not diminish with time. Physically, the central peak represents

the emergence of a classical feature in this quantum walk and suggests that keeping track of two steps of memory may be the start of a transition to a classical system. One explanation for this is that keeping track of the previous positions reduces some of the interference in the path integral for the particle because the path it took over the previous two steps is known.

Similar stationary peaks in the probability distribution have been seen in the work of Brun, Carteret, and Ambainis, and they also claim that this is a transition to classical behavior [2]. However, their approach is much different than the one presented above. Instead they use multiple different coin operators and coin operators of higher dimension to diminish the interference in the path integral.

Future work will continue to explore the properties of quantum walks with memory. First, it would be interesting to consider how the particle would evolve if allowed to propagate on a finite one dimensional space, such as a ring. In the case of periodic boundary conditions, the propagating peaks in the probability distribution will move around the ring instead of spreading out infinitely. This would allow the peaks to interfere with one another, and it is not clear what features to expect in the final probability distribution. We would also like to explore the effects of extending the memory of the particle to a larger number of steps. The quantum walk with two-step memory showed classical behavior, and it is important to investigate whether this transition to a classical random walk will continue as we increase the memory to keep track of a large number of steps.

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