Two Particle Quantum Walks

Komal Sah

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1 Abstract

Classical random walks and Markov Chain methods have proved to be a powerful tool in developing stochastic algorithms. They have also provided valuable insights in Physics, Biology, Economics and Finance. Quantum analogs of the classical random walk, also known as the quantum walk, are an important tool in developing quantum search algorithms such as the Grover's algorithm. Unlike their classical counterparts, particles performing Quantum walks can be in a superposition of states. Other quantum effects such as entanglement and quantum statistics of the particles become relevant when there are multiple quantum walkers which are of particular interest in studying many body physics. In this project we study and compare classical random walk and quantum walk of one particle and two particles. We evaluate the asymptotic probability distributions, evaluate the Shannon Entropy for each of them and examine the role of the "coin" on these entropies. In addition, we look at the correlations for non-interacting two particle quantum walks to examine the role of entanglement in the case of Bosons and Fermions. Finally, we review hitting times for the two to see how quantum walks provide speed ups to the existing search algorithms.

2 Introduction

Random walks as the name suggest is a sequence of random steps taken in some discrete or contnious time. Here, we look at discrete time Random walks. Random walks are Markov Processes as the next state only depends the previous state. Randomized algorithms based on random walks and Markov chain methods have numerous applications in computer science, physics, biology and economics. Particular uses of random walk in computer science include network embedding, recommender system, link prediction, collaborative filtering, semi-supervised learning among others[7]. In physics they are used model random motions of molecules in liquids and gases(Brownian motion) to study diffusion, absorption and polymer formations. Self interacting Random walks also have found applications in Quantum Field Theory[2].

Quantum walks are the non-trivial generalization of classical random walks. Due to the superposition principle, a quantum walker follows all the possible paths simultaneously and displays Quantum coherence which is where they differ from their classical counterparts. Propagation of a single excitation in a crystal, energy transport during photosynthesis in plants and spreading of quantum information on quantum networks can are modeled using quantum walks[4]. Quantum Walks are also used in quantum search algorithms which promise speed ups to their classical counterparts.

We begin by looking at classical random walk on a grid graph before looking at Markov Chains which helps us a framework that helps us extend Random walks to any arbitrary graph. We then proceed to discuss postulates of Quantum Mechanics which necessitate the modifications to the classical random walk so that they are satisfied. We then proceed to look at Quantum walks of a single particle on a 1D lattice graph and compare it to its classical counterpart. We also point out some new features that we do not see in the classical random walk. After this we look at two non-interacting particles quantum walk on a 1D lattice graph and study correlations for the fermionic and bosonic case. Finally, we look at a simple search algorithm which shows us speedups provided by a quantum walk search algorithm.

3 Classical Random Walk

Random walk is a stochastic process, that describes a path that consists of a succession of random steps on some mathematical space. The steps of the random walk are independent and identically distributed random variables represented by $\{X_i\}$. The position of the particle, represented by χ_n , after n-steps if the walk started in the initial state x_0 is given as,

$$\chi_n = (x_0 + X_1 + X_2 + ...) + X_n \tag{1}$$
$$\chi_n = \chi_{n-1} + X_n \tag{2}$$

We observe that even though $\{X_i\}$ are independent random variables the positions χ_n are not. The simplest random walk is random walk on a discrete 1D lattice such that the particle starts at the position $x_0 = 0$ and $X_1 = +1, -1$. This random walk is also sometimes referred to as simple random walk. For an unbiased random walk we have,

$$\mathbb{P}(X_1 = 1) = \frac{1}{2} \tag{3}$$
$$\mathbb{P}(X_1 = -1) = \frac{1}{2} \tag{4}$$

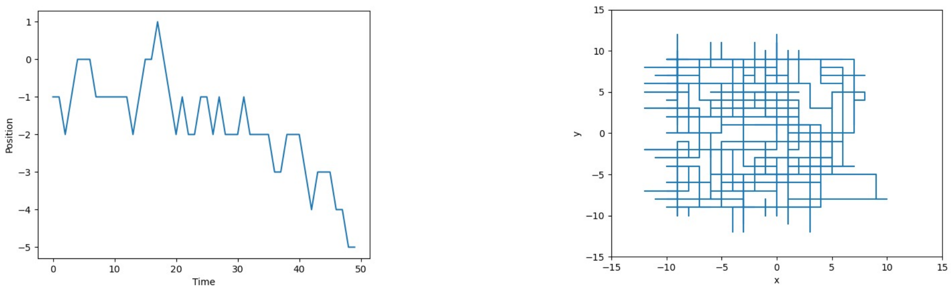
while for a biased walk we have ,

$$\mathbb{P}(X_1 = 1) = p \tag{5}$$
$$\mathbb{P}(X_1 = -1) = 1 - p \tag{6}$$

The walk is said to be biased to the right if $p > 1/2$ and it is said to be biased to the left if $p < 1/2$. This construction can be extended to higher dimensions. In case of a simple random walk of dimension - D we have,

$$X_1 = \{\pm\hat{e}_1, \pm\hat{e}_2, ..., \pm\hat{e}_D\} \tag{7}$$
$$\mathbb{P}(X_1 = \hat{e}_d) = \frac{1}{2} \tag{8}$$
$$\mathbb{P}(X_1 = -\hat{e}_d) = \frac{1}{2} \tag{9}$$

Here, $\hat{e}_d$ is a unit vector in the $\mathbb{R}^D$. Figure below shows simple random walk sequence in 1D and 2D.



(a) Simple Random Walk Sequence in 1D

(b) Simple Random Walk Sequence in 2D

Figure 1: Simple Random walk sequences in different dimensions

3.1 Random Walk as a Markov Chain

Markov chains help us study random walks on a more general non-geometric setting. Random walks on a d-regular graph $G = (V, E)$ instead of the physical space can be studied using the Markov chain formalism. Here $V = \{i\}$ are the vertices and $E = \{(i, j)\}$ are the edges of the graph G. The simple random walk in 1D is random walk on a line and simple random walk in 2D is a random walk on a square grid graph. The state space for a random walk is then simply the vertices $\mathcal{S} = V = \{i\}$ of the graph. The random walk is then given by the transition matrix T of dimension

$n(\mathcal{S}) \times n(\mathcal{S})$ where, T_{ij} or the elements of the matrix gives the probability of transition from vertex i to vertex j such that $\sum_{j \in V} T_{ij} = 1$. The transition matrix T preserves normalization and is stochastic. The initial state is then represented by a vector- μ of length $\mathbb{R}^{n(\mathcal{S})}$. The state after one step is then given as, $\mu(t=1) = \mu T$. The asymptotic probability distribution $\mu(t \to \infty)\pi$ is then simply the eigenvector of T corresponding to eigenvalue 1. Using Markov chains we can also calculate the hitting time, which is an upperbound on the time taken to reach a marked vertex, for an arbitrary graph. Hitting time is one of the quantities which helps us compare generic search alogorithms based on classical and quantum walks.

3.1.1 1D Random walk

We give the Markov chain representation of a simple 1D random walk with periodic boundary conditions as shown below.

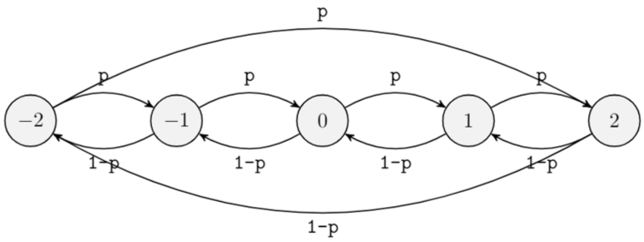


Figure 2: Simple Random Walk Markov Chain

The state space for this chain is $\mathcal{S} = \{0, \pm 1, \pm 2\}$. The transition matrix for this graph is given as,

$$T = \begin{bmatrix} 0 & p & 0 & 0 & 1-p \\ 1-p & 0 & p & 0 & 0 \\ 0 & 1-p & 0 & p & 0 \\ 0 & 0 & 1-p & 0 & p \\ p & 0 & 0 & 1-p & 0 \end{bmatrix} = T^{(L)} + T^{(R)} \tag{10}$$

$$T^{(R)} = p \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} T^{(L)} = (1-p) \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{11}$$

The asymptotic probability distribution for the Markov chain when $p = 1/2$ is given by $\pi = \left\{\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\right\}$. This simple representation provides us a framework for extending the Random Walk to the quantum systems. The probabilities are replaced with "coin operators" and the transition matrix is replaced by a unitary operator.

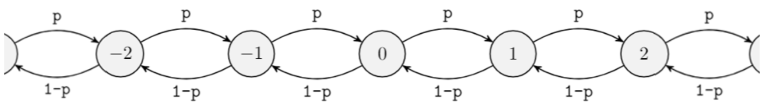


Figure 3: Random Walk of infinite 1D Chain

We also use the construction above to study Random Walk on an infinite 1D lattice graph. The state space is an open set $\mathcal{S} = \{0, \pm 1, \pm 2 ...\}$ in this case. The asymptotic probability distribution for this system is a Gaussian distribution. The most probable state (or lattice point) is dependent upon p or the bias of the "coin". If $p > 1/2$ then we see the walk is biased to the right while we say it is biased to the left for $p/2$. The figure [4] shows the asymptotic distribution for infinite Random walks with varying bias.

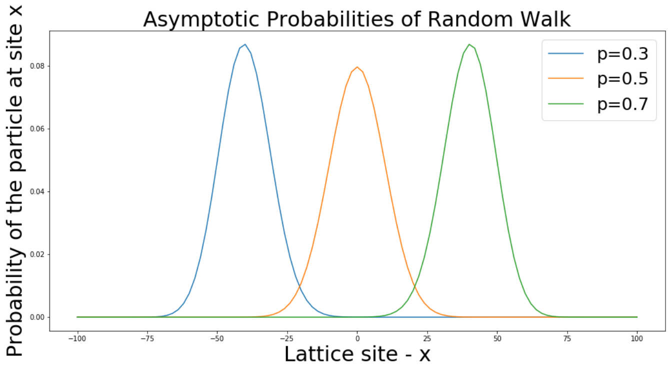


Figure 4: Asymptotic distribution for infinite Random walks with varying bias.

3.1.2 Shannon Entropy of the Random walk

We calculate the entropy of the 1D random walk after a large number of steps as a function of the bias of the walk. Shannon entropy is defined as, $H(X) = -\sum_{x\in X} p(x)\log p(x)$. In our case the entropy is given as, $p(x)$ is the probability of each state after t steps given by $\mu(t \to infty)$. The sum is over all states in $\mathcal{S}$. We compare this entropy with the Shannon entropy of the quantum walk that we look at later. We do this to see if it can be used as a single parameter to distinguish the two without having to consider the entire probability distribution. The figure below shows the values obtained. We see that the entropy decreases as the walk becomes more biased in one direction compared to the other which is expected as it reduces uncertainty in the motion of the random walker.

p	Entropy
0.1	3.62
0.2	4.04
0.3	4.24
0.4	4.39
0.5	4.37

Figure 5: Entropy of 1D Random Walk for varying bias in the walk

3.1.3 Two non-interacting Random Walkers on a 1D Graph

We now proceed to extend our formalism to study two non-interacting random walkers on a 1D Graph. The state space for a two particle Random walk is $\mathcal{S} = \mathcal{S}_1 \otimes \mathcal{S}_2$ where $\mathcal{S}_i = V = \{i\}$ represents the state of one of the random walkers. The transition matrix is then $T = T_1 \otimes T_2$, where T_i is the transition matrix for a single random walker on a graph. The elements of the transition matrix T gives us the probability of the system from state $\{\{i_1\},\{i_2\}\}$ to state $\{\{j_1\},\{j_2\}\}$. The matrix T can be now used to obtain the asymptotic joint probability distribution $\Pi \in \mathbb{R}^{n(\mathcal{S})} \times \mathbb{R}^{n(\mathcal{S})}$. Since, the particles are non-interacting this is simply direct product of the asymptotic probability distribution of the single random walkers that we had obtained before i.e, $\Pi = \pi \otimes \pi$. The correlation is also 0 for the two classical non-interacting random walkers.

We will now move onto extending the ideas developed earlier to study Quantum walks involving one and two particles.

4 Quantum Walk

Quantum Walk differs from classical Random walk because the quantum walker must obey postulates of Quantum Mechanics that are stated below. We explore the variations in the probability distributions of a random walker as a result of these postulates.

1. The set of all quantum states is contained in the Hilbert space which is complete. Quantum states are represented by vectors of complex number often represented by kets-$\{|\psi\rangle\}$ that lie in the Hilbert space. These states in some ways are analogous to the Markov states that we defined earlier.

2. The basis quantum states of the Hilbert space, given by $\{|i\rangle\}$ are orthonormal to each other.

$$\langle i|j\rangle = \delta_{ij} \tag{12}$$

   Any superpositions of these orthonormal basis states also lies in the Hilbert space. This distinguishes the Hilbert space from the $\mathcal{S}$ that we had defined earlier for the classical system.

3. Physical observables in quantum mechanics are represented by operators. Any measurement of an observable gives us an eigenvalue which is the classical physical quantity corresponding to the operator.

4. Any measurement of the quantum system alters the system. The state right after measurement is the normalized eigenstate of the eigenvalue that was observed. Thus, if we make a measurement of the quantum walker at every step, we would end up with the classical random walk.

5. The time evolution of a quantum system is given by a unitary operator. A unitary operator preserves that normalization of a quantum state.

$$|\psi(t)\rangle = U(t,t_0)\,|\psi(t_0)\rangle \tag{13}$$

$$\sum_i |\langle i|\psi(t_0)\rangle|^2 = 1 = \sum_i |\langle i|\psi(t)\rangle|^2 \tag{14}$$

   Thus, to observe the "quantum" nature of a random walk the transition matrix T must be replaced by a Unitary operator that gives the Quantum walk.

4.1 Single Particle Quantum Walk on 1D Graph

4.1.1 "Quantizing" the Random Walk - Unitary Operator construction

We first construct the unitary operator for quantum walk on discrete 1D lattice graph. The construction used here is the specific Quantum Markov Chain construction for a simple 1D quantum walk. The unitary operator for the simple unbiased 1D quantum walk is given as,

$$U = (I \otimes H)\cdot S \tag{15}$$

$$H = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \tag{16}$$

$$S = |R\rangle\langle R| \otimes \sum_j |j+1\rangle\langle j| + |R\rangle\langle R| \otimes \sum_j |j\rangle\langle j-1| \tag{17}$$

The probability of transition is given by H also called as the coin operator. The unbiased coin operator is the Hadamard operator shown above. The coin operator is different from its classical analog as it allows for the superposition of states. The S operator serves to shift the operator. We observe that the unitary operator has dimensions $\mathbb{C}^{2n} \times \mathbb{C}^{2n}$, where n is the number of lattice points or vertices in our 1D graph. This is differs from 1D random walk on a graph with n sites where the transition matrix has dimensions $\mathbb{R}^n \times \mathbb{R}^n$.

The initial state is defined on a $\mathbb{C}^{2n}$ space. It is given as $|j\rangle\,|d\rangle$. The first ket $|j\rangle$ is defined on $\mathbb{C}^n$ space which is similar to μ which is defined on $\mathbb{R}^n$. This ket indicates the lattice point of the graph. The second ket $|d\rangle$ is defined on $\mathbb{C}^2$ space. It lies in the Hilbert space of the coin operator. Physically, it corresponds to the initial direction of quantum walker. The kets $|L\rangle$ and

$|R\rangle$ indicate the direction left and right respectively. Since, quantum objects propagate as waves we have to contend with the direction of the initial state of the walker as well. This nature results in interference upon propagation. In figure below we compare the first few steps of classical and quantum walks.

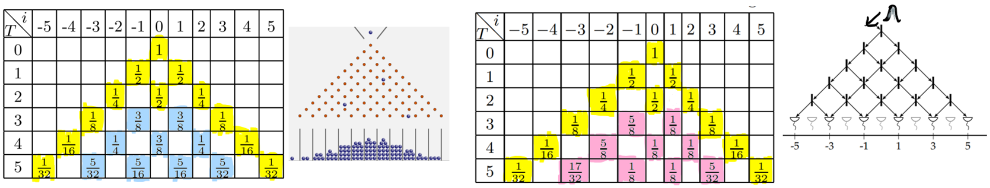


Figure 6: Steps of Classical Random walk (left) and Quantum Walk (right). The most probable position of a classical walk is in the center while it is towards the left for quantum walk in this case. The walks can be visualized using a galton board for classical random walks and optical Galton board for a quantum walk.[3]

4.1.2 Asymptotic Probability Distribution - Spectrum of Single Particle Quantum Walk

The asymptotic probability distribution of a quantum walk is determined by finding the eigenvalues of the unitary operator with absolute value 1. All the eigenvalues of the unitary operator are of the form,

$$U|\lambda\rangle = e^{i\lambda}|\lambda\rangle \tag{18}$$

The above expression implies that there would be multiple eigenstates (asymptotic probability distributions) as there are multiple eigenvalues with absolute value 1. The number of degenerate eigenstates is $2n$ with n being the number of sites in the system. The shift operator S has n eigenstates with eigenvalues that have absolute value 1 while the coin operator has 2 such eigenstates. In order to find these eigenstates we change to the momentum basis to diagonalize S. We then solve the block diagonalized matrix for the eigenstates. Since, the coin operator has 2 eigenstates, each value of k in the momenum space has two possible eigenstates. Physically, the two bands of eigenvalues correspond to a eigenstate that moves to the left and right. For a general coin operator as indicated below, we calculate the eigenvalues as outlined in [5].

$$H = \begin{bmatrix} \sqrt{R}e^{i\alpha} & \sqrt{1-R}e^{-i\beta} \\ -\sqrt{1-R}e^{i\beta} & \sqrt{R}e^{-i\alpha} \end{bmatrix} \tag{19}$$

$$R \in [0,1] \tag{20}$$

$$\alpha, \beta \in [0,1] \tag{21}$$

The eigenvalues of the unitary operator are given below. The figure shows the two bands of eigenvalues for different coin parameters R.

$$e^{i\lambda} = e^{i\beta}[\sqrt{R}\cos(\alpha - 2\pi k/N) \pm i\sqrt{1 - R\cos^2(\alpha - 2\pi k/N)}] \tag{22}$$

The corresponding eigenstates are given as,

$$|\lambda\rangle = s|k\rangle [|L\rangle - \frac{h_{00}(\lambda,k)}{h_{01}(k)}|R\rangle] + e^{(}i\omega)s'|k'\rangle [|0\rangle - \frac{h_{00}(\lambda,k')}{h_{01}(k')}|R\rangle] \tag{23}$$

$$k' = -k + \frac{\alpha n}{\pi} \tag{24}$$

$$h_{00} = \sqrt{R}e^{i(\alpha+\beta-\frac{2\pi k}{n})} - e^{i\lambda} \tag{25}$$

$$h_{10} = -\sqrt{1-R}e^{i(2\beta+\frac{2\pi k}{n})} \tag{26}$$

$$h_{01} = \sqrt{1-R}e^{-i\frac{2\pi k}{n}} \tag{27}$$

$$h_{11} = \sqrt{R}e^{-i(-\alpha-\beta-\frac{2\pi k}{n})} - e^{i\lambda} \tag{28}$$

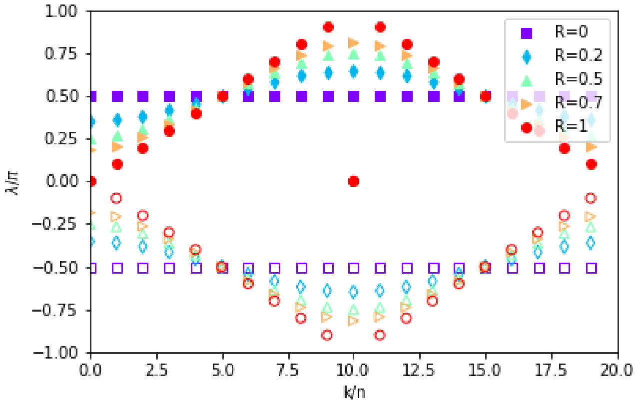
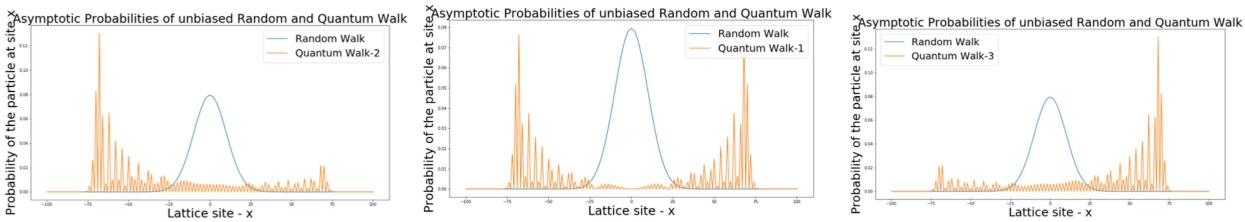


Figure 7: Eigenvalue λ of the unitary operator as a function of k/n where k is a value in the momentum lattice of 1D lattice graph with n sites.The different bands correspond to different values of R.



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

Figure 8: Asymptotic states for the unbiased classical and quantum walk starting at site $|0\rangle$. Direction of the initial state determines asymptotic state attained for quantum walk.

s, s', ω are free parameters that are chosen such to give us the two orthonormal eigenstates corresponding to a single value of k. The figure below shows numerically calculated eigenstates for the Hadamard coin operator.

Comparing with the classical Random walk case we make two obervations.

1. The asymptotic state is dependent on the direction of the initial state even if the initial positions states are the same.
2. The quantum walker drifts away from the center while the classical random walker is continues to remain around the center. This property is the reason why search algorithms based on quantum walk are faster than their classical counterparts.

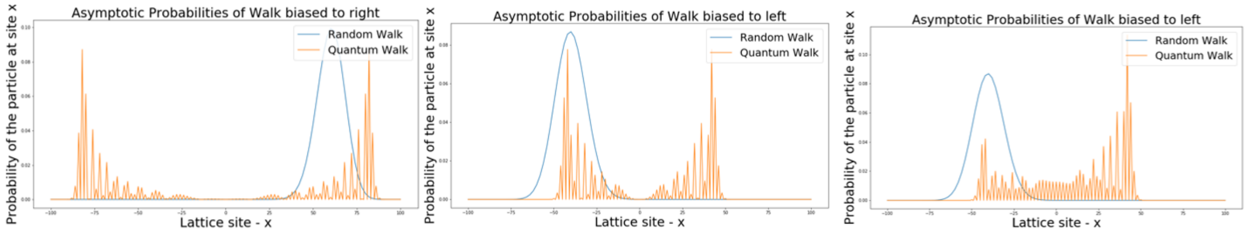
4.1.3 Role of the coin operator

The figure below shows numerically calculated eigenstates for a biased coin operator and compares it to its classical counterparts. Comparing with the classical Random walk case we make two obervations.

1. The asymptotic state is dependent on the direction of the initial state even if the initial positions states are the same.
2. The quantum walker and classical random walker drift away from the center.
3. If the initial direction of the quantum walker is towards right it will drift to the right even if the bias is in the opposite direction

4.1.4 Shannon Entropy of the Quantum walk

We study entropy of the quantum walk as a function of the bias of the coin operator and as a function of initial direction. We observe that just like the classical random walk increasing the bias



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

Figure 9: Asymptotic states for the biased classical and quantum walk starting at site $|0\rangle$.The bias $p = 0.7, R = \sqrt{0.7}$ for the first plot and $p = 0.2, R = \sqrt{0.2}$ for the other two plots

of the coin-$p = R^2$ decreases the entropy. The entropy of the quantum walk is larger than that of the classical random walk for the same bias. That could be an indicator of that the Quantum walk spreading more than the classical walk resulting in greater uncertainty and hence entropy.

The entropy as a function of initial function of the directions is a little more harder to analyse clearly. We observe that the entropy is larger when the initial direction is more biased towards one direction compared to the other. The entropy is least when the direction of the initial walk is not biased. I am unsure how to explain this in terms of uncertainty in the motion of the quantum walker. Perhaps using a quantum information measure such as Von-neumann entropy would make sense here?

p	Entropy
0.1	4.79
0.2	5.16
0.3	5.34
0.4	5.41
0.5	5.43

Initial State	Entropy
$\lvert\psi(0)\rangle = \lvert 0R\rangle$	5.43
$\lvert\psi(0)\rangle = \sqrt{0.9}\lvert 0R\rangle + i\sqrt{0.1}\lvert 0L\rangle$	5.12
$\lvert\psi(0)\rangle = \sqrt{0.7}\lvert 0R\rangle + i\sqrt{0.3}\lvert 0L\rangle$	4.54
$\lvert\psi(0)\rangle = \frac{1}{\sqrt{2}}(\lvert 0R\rangle + i\lvert 0L\rangle)$	4.23
$\lvert\psi(0)\rangle = \sqrt{0.3}\lvert 0R\rangle + i\sqrt{0.7}\lvert 0L\rangle$	4.54
$\lvert\psi(0)\rangle = \sqrt{0.1}\lvert 0R\rangle + i\sqrt{0.9}\lvert 0L\rangle$	5.12
$\lvert\psi(0)\rangle = \lvert 0L\rangle$	5.43

Figure 10: Entropy of 1D Quantum Walk for varying bias of the coin operator and as initial direction of the walker

4.2 Two non-interacting Particle Quantum Walk

We look at quantum walk of two non-interacting particles using the formalism discussed in [6]. We explore two particle Quantum walks because it allows us to explore the effect of entanglement and quantum statistics. The Hilbert space for a two particle Quantum walk is $\mathbb{C}_n \otimes \mathbb{C}_n$. The unitary matrix is then $U = U_1 \otimes U_2$, where $U_i = (I \otimes H_i) \cdot S$ where $i \in 1, 2$ is the unitary matrix for a single quantum walker on a graph. The dimensions of the unitary matrix U is $\mathbb{C}_{2n^2} \otimes \mathbb{C}_{2n^2}$. The operators H_1 and H_2 are the coin operators for the first and second quantum walker respectively.The operators S_1 and S_2 are the shift operators for the first and second quantum walker respectively.

The initial state of the quantum walkers is described in the space $\mathbb{C}_{2n^2}$. The initial state can be a pure state given as,

$$|\Psi(0)\rangle = |j_1\rangle |d_1\rangle |j_2\rangle |d_2\rangle \tag{29}$$

Here, $|j_1\rangle |d_1\rangle$ and $|j_2\rangle |d_2\rangle$ indicates the initial position and direction of the first and second quantum walkers respectively. The initial state of each of the walkers can also be a superposed state.

Unlike the classical system, the initial state can also be in an entangled state

$$|\Psi(0)\rangle = \alpha_1 |\psi(0)\rangle_1 |\psi(0)\rangle_2 + \alpha_2 |\psi(0)\rangle_2 |\psi(0)\rangle_1 \tag{30}$$

$$\alpha_1^2 + \alpha_2^2 = 1 \tag{31}$$

The degree of entanglement of the initial state is given by P_E defined as,

$$P_E = \alpha_1 \alpha_2 \tag{32}$$

The initial state as a fermionic entangled state is given below. The fermionic state satisfies the fermion statistics and is the most negatively entangled state with degree of entanglement given as $P_E = -1/2$.

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}} |\psi(0)\rangle_1 |\psi(0)\rangle_2 - \frac{1}{\sqrt{2}} |\psi(0)\rangle_2 |\psi(0)\rangle_1 \tag{33}$$

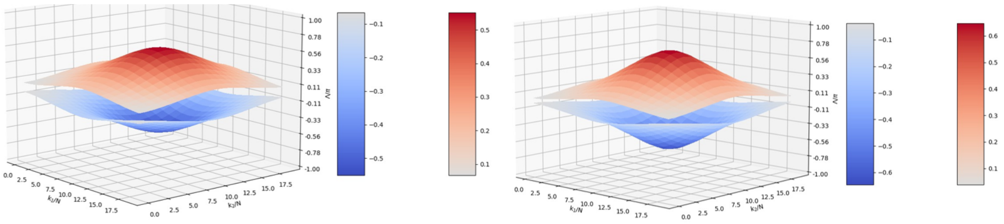
It can also be an Bosonic entangled state given below. The bosonic state satisfies the boson statistics and is the most positively entangled state with degree of entanglement given as $P_E = 1/2$.

$$|\Psi(0)\rangle = \frac{1}{\sqrt{2}} |\psi(0)\rangle_1 |\psi(0)\rangle_2 + \frac{1}{\sqrt{2}} |\psi(0)\rangle_2 |\psi(0)\rangle_1 \tag{34}$$

The correlation as we will see later is non-zero for these entangled states even though they are not interacting [6]. We look at Quantum walk of two particles starting in a pure state, fermionic and bosonic entangled states.

4.2.1 Asymptotic Probability Distribution - Spectrum of Two Particle Quantum Walk

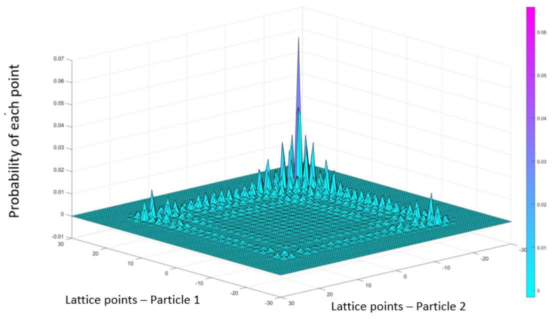
The spectrum or the asymptotic states of a two particle Quantum walk is given by a direct product of one particle eigenstates $|\lambda\rangle$ that is given in equation-23 i.e, $|\Lambda\rangle = |\lambda_1\rangle |\lambda_2\rangle$. The figure shows the four bands of eigenvalues for different coin parameters R_1 and R_2. Two of the bands overlap and as $\Lambda = \lambda_1\lambda_2 = \lambda_2\lambda_1$. The bands below are for different biases $R_1 = R_2$.



$R_1 = R_2 = 0.5$ $R_1 = R_2 = 0.7$

Figure 11: Eigenvalue Λ of the unitary operator as a function of k_1/n and k_2/n where k_i is a value in the momentum lattice of 1D lattice graph with n sites.The different bands correspond to different values of R_1, R_2.

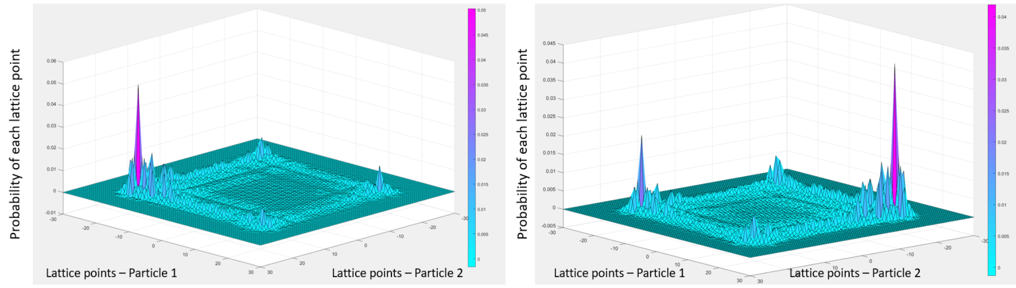
Pure state The figure [12] shows the asymptotic state of pure state obtained numerically for an unbiased coin operator.The asymptotic probability distribution is product of the single particle probability distributions. This is similar to its classical case of two non-interacting random walkers.



$\psi(0) = |0L\rangle_1 |0R\rangle_2$

Figure 12: The asymptotic probability distribution is product of the single particle probability distribution with one walker drifting to left and the other to right

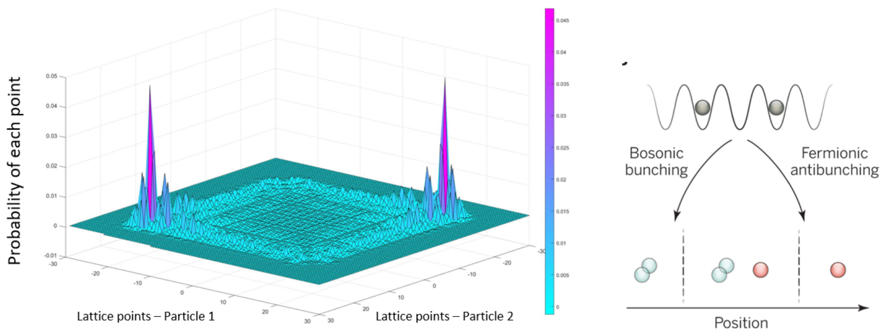
Entangled States The figure [13] shows the asymptotic state of entangled state obtained numerically for an unbiased coin operator. The asymptotic probability distribution is not a simple product of the single particle probability distributions. The asymptotic probability distribution approaches that of pure states on decreasing the degree of entanglement.



$\Psi(0) = \frac{1}{\sqrt{5}}|0L\rangle_1|0R\rangle_2 - \frac{2}{\sqrt{5}}|0R\rangle_1|0L\rangle_2$ $\Psi(0) = \frac{1}{\sqrt{3}}|0L\rangle_1|0R\rangle_2 - \frac{\sqrt{2}}{\sqrt{3}}|0R\rangle_1|0L\rangle_2$

Figure 13: The asymptotic probability distribution is not a simple product of the single particle probability distribution. The degree of entanglement is 0.4 for the figure on the left and 0.47 for the figure on the right

Fermionic Entangled State The figure [14] shows the asymptotic state of fermionic entangled state obtained numerically for an unbiased coin operator. The asymptotic probability distribution is not a simple product of the single particle probability distributions. We see that the fermions move away from each other eventhough there is no repulsive interactions.



$\psi(0) = \frac{1}{\sqrt{2}}(|0L\rangle_1|0R\rangle_2 - |0R\rangle_1|0L\rangle_2)$

Figure 14: The asymptotic probability distribution is not a simple product of the single particle probability distribution. Fermionic antibunching is observed in the figure

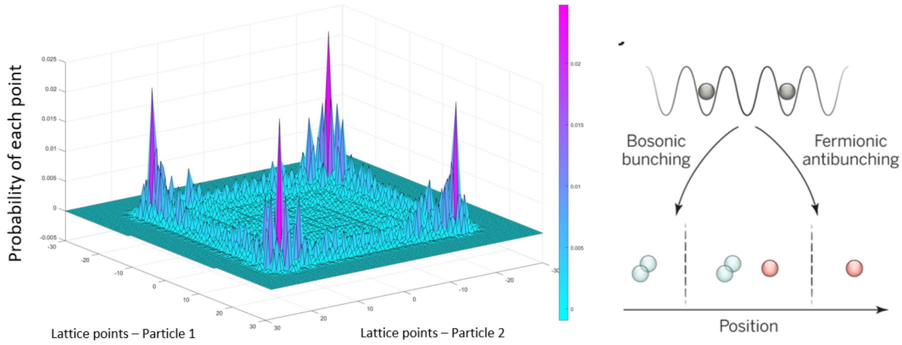
Bosonic Entangled State The figure [15] shows the asymptotic state of bosonic entangled state obtained numerically for an unbiased coin operator. The asymptotic probability distribution is not a simple product of the single particle probability distributions. We see that the bosons move towards each other eventhough there is no attractive interactions.

4.2.2 Joint Entropy of the two particle Quantum walk

We calculate the joint entropy for different degrees of entanglement for the unbiased quantum walks that shown in the previous section. The results are stated below. We observe that Joint Entropy increases with the degree of entanglement. However, the values of Joint Entropy which are in bits indicate that it may not be a good quantity for measuring a quantum system. Calculating the quantum analog might be more helpful in analysis of such a system. Another good quantity might be Entropy rate which I was unable to calculate.

4.2.3 Correlations non-interacting quantum walks

Correlation between the spatial probability distributions of the two particle Quantum walk can be calculated using the single particle quantum walk distribution which is given by $\left\langle |_i \langle\psi|\psi\rangle_i|^2 \right\rangle$ and the joint probability distribution of the two particle Quantum Walk which is given by $\left\langle | \langle\Psi|\Psi\rangle |^2 \right\rangle$.



$\psi(0) = \frac{1}{\sqrt{2}}(|0L\rangle_1|0R\rangle_2 + |0R\rangle_1|0L\rangle_2)$

Figure 15: The asymptotic probability distribution is not a simple product of the single particle probability distribution. Bosonic bunching is observed in the figure

P_F	Joint Entropy
0	7.811
-0.4	8.532
-0.4714	8.729
-0.5	8.8106
0.5	8.8106
-0.4714	8.729
0.471405	8.532

Figure 16: Joint Entropy for varying degrees of entaglement

In each of the cases here, $|\psi\rangle$ and $|\Psi\rangle$ are the state of the particle after N steps. The correlation function is given as,

$$C_{12} = \left\langle | \langle \Psi | \Psi \rangle |^2 \right\rangle - \left\langle |_1 \langle \psi | \psi \rangle_1 |^2 \right\rangle \left\langle |_2 \langle \psi | \psi \rangle_2 |^2 \right\rangle \tag{35}$$

The correlation evaluated this way was obtained in [6] and is shown below.

Nb. of steps N	10	20	30	40	60	100
Init. c. $\lvert\psi_0^-\rangle_{12}$	-16.8	-69.8	-153.5	-276.2	-619.7	-1718.3
Init. c. $\lvert\psi_0^S\rangle_{12}$	0	0	0	0	0	0
Init. c. $\lvert\psi_0^+\rangle_{12}$	4.8	7.3	13.7	15.1	23.1	39.1

Figure 17: Correlation after N steps for the fermionic state(first row), pure state(second row) and bosonic state(last row)[6]

We observe that for two particle non-interacting quantum walk:

1. There is no correlation between the quantum walkers if the initial state was a pure state
2. The two quantum walks are anticorrelated if the initial state was an entangled fermionic state.
3. The two quantum walks are correlated if the initial state was an entangled bosonic state.

4.2.4 Hitting time- Comparing quantum and Classical search algorithms

A simple search algorithm on a graph G where some vertices are marked such that $M \subset V$ can be formulated by taking a stochastic matrix T and modifying it such that the algorithm stops when a marked vertex is found[1]. The modified matrix is given below.

$$T'_{ij} = \begin{cases} 0 & \text{if } j \in M \text{ and } i = j \\ 1 & \text{if } j \in M \text{ and } i \neq j \\ T_{ij} & \text{if } j \notin M \end{cases}$$

It can be shown that the number of steps a quantum walk algorithm takes to find a marked vertex is in the order $O(1/\sqrt{1 - \|T_M\|})$ where T_M corresponds to the block of the matrix T' corresponding to the marked vertices. The classical algorithm takes steps of the order $O(1/(1 - \|T_M\|))$[1]. Comparing the two we can see that a quantum search algorithm is faster.

5 Conclusions and outlook

We studied the construction of classical and quantum random walks using Markov Chain and quantum Markov Chains respectively. We calculated the asymptotic probability distribution in each case and found the entropy of this asymptotic state for both the walks. We then compared these quantities for both the classical and quantum random walks. We also looked at the correlations for non-interacting two particle walks and learnt that entanglement and quantum statistics affect it. We also examined a simple search algorithm based on these walks and compared the performance of the two. We saw that quantum walk provided square root speed ups over the random walk algorithm.

However, several questions remain unanswered. The first being what information measures are suitable for the two walks. The classical Shannon entropy was used for both the classical and the quantum case but this may be incorrect. The second is, can the asymptotic states of the quantum walk provide us any insight into many body physics. The third question is can a second quantized formalism be developed for the discrete quantum walk as bosonisation or fermionisation of a state becomes more cumbersome on increasing the number of quantum walkers. Additionally, a Quantum Markov chain method for a non-geometric graph has not been discussed and may help address some of the questions.

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