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Nature of Quantum Ultra Walks: Localization and Delocalization

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M.Sc., Emory University, GA, 2021

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Abstract

Nature of Quantum Ultra Walks: Localization and Delocalization

By Richa Sharma

Classical Random walks have proven to be a useful tool for various computational problems. Similarly, its quantum mechanical counterpart quantum walks have applications in the development of quantum algorithms specifically quantum search and element distinctness algorithm[8]. Classical random walk spreads diffusively across the geometric structure which scales proportionally to the square root of time. Homogeneous Quantum Walks, however, is ‘ballistic’, i.e., its spread scales linearly with time. This property contributes to its algorithmic applications, as it enhances quantum energy transfer on certain graphs. However, the static disorder can make quantum walks suffer Anderson-like localization which can confine the walker within a finite region for an indefinite time[11, 12, 13], taking away the quantum advantage. Therefore, the exploration of the heterogeneity in disordered systems is important for the successful realization of quantum computers. To this end, we study for a discrete-time quantum walk the effect of a quantum coin that varies randomly in space but only on a hierarchy of lattice points. Such a hierarchical system, but with a regular sequence of coins representing reflective barriers, was introduced by Boettcher et al.[3, 4, 5] who found sub-ballistic spread but no localization of the quantum particle, irrespective of barrier strength. We find that any strength of randomness on the hierarchy of lattice points by itself, without barriers, also does not localize the walk. However, applying non-trivial combinations of randomness and barrier strength on that hierarchy appears to induce transition into a localized state. This behavior of the system is determined numerically using the walk dimension d_w we extract from the mean-square displacement, averaged over repeated realizations of the randomness.

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Chapter 1

Introduction

1.1 Motivation

Quantum Walks are the quantum mechanical generalizations of the random walk. Their spread is ballistic on a regular lattice, hence making them valuable in the specific application of quantum search algorithms[8] or quantum computing in general[10]. Several interesting experimental proposals ranging from trapped ions to optical lattices for cold atoms have emerged[17, 20, 21, 22, 23, 24, 25]. However, this advantage or ballistic spreading is lost when static(position and time-independent) disorder affects the system. The quantum walks can undergo Anderson localization, which means the standard deviation or mean-squared distance of the walker from the origin stays bounded even as the time goes to infinity[26, 27, 28, 29, 30, 31]. There are theoretical [37, 38] and numerical [39] studies conducted on it as well as there is experimental evidence [17]. However, in certain cases, the quantum walks evade Anderson localization and spread sub-ballistically even in the presence of static disorder. The topology of quantum walks is also an emergent field with interesting results[34, 35, 37, 38, 39, 40].

Inspired by the ultrametric arrangement of classical barriers in diffusion problems Boettcher et al[3, 4, 5] proposed a spatially dependent hierarchical coin that analogously creates ultrametric barriers of increasing reflectivity in the quantum walks. The hierarchy, in turn, is defined by the binary decomposition of the index of the lattice sites. “Quantum Ultra Walks” at its best generates a model of sub-ballistic Quantum Walker which is not localized even if the time evolves indefinitely. In principle, these walks obtain a Quantum System whose asymptotic behavior can be modeled. However, the characteristic nature of this spreading behavior is drastically altered with the introduction of phase disorders. This thesis aims to study the Numerical results for the introduction of novel phase disorders in the model of “Quantum Ultra Walks”.

1.2 Background

This section is intended to summarize the relevant concepts and mathematical machinery required to understand the research problem and further discussions.

1.2.1 Fundamental Postulates of Quantum Mechanics

The following postulates govern the states and dynamics of a quantum systems whether its isolated or open quantum systems. Then we’ll shift our focus to the discrete quantum walks, and translate these concepts to our definition of the problems related to such systems. The kind of problem we are focusing on isn’t concerned with continuous quantum walk, however these definitions help in their understanding as well.

Postulate 1: State

State of the isolated quantum system is described by a unit-vector that exists in a d -dimensional Hilbert Space \mathcal{H}^d . The Hilbert space is an abstract vector space com-

prising complex numbers \mathbb{C} as coefficients, in which a vector is denoted by a *ket* $|\psi_i\rangle$. The properties for such vectors in the Hilbert space include, linearity, inner product (which is essentially the projection of one vector on the other represented by $\langle\psi|\phi\rangle$), norm the quantity is represented by $(|\langle\psi|\psi\rangle|^2)$. The Hilbert space dimension is described by the maximum number of linearly independent vectors that can be defined within the vector space. Linearity and dimension of the Hilbert space enables us to define the state as a linear combination of d linearly independent vectors,

$$|\psi\rangle = \sum_{i=1}^d c_i |i\rangle \quad (1.1)$$

where coefficients $c_i \in \mathbb{C}$ are the components and the set of vectors $|i\rangle$ constitute a basis for the Hilbert space \mathcal{H}^d . The summation of outer products of basis vectors is called the completion relation $\sum_{i=1}^d |i\rangle\langle i| = \mathbb{I}$.

Postulate 2: Observable

The measurable quantities of a Hermitian operators are called observable. An operator X is a linear map from vectors to vectors: $|\psi\rangle \rightarrow X|\psi\rangle$ and applicable to linear combinations due to linearity. For a given orthonormal basis, an operator can be specified by its components $\langle i|X|j\rangle = X_{ij}$. A Hermitian operator A satisfies the property $\langle i|A|j\rangle = \langle j|A|i\rangle^*$ denoted by $A = A^\dagger$ where A^\dagger is the transpose conjugate of A . The eigenvalues of A are real, and the eigenvectors corresponding to them are orthogonal. Hence, we can write a state in the Hilbert space \mathcal{H}^d as the linear combination of d eigenstates of an observable.

Postulate 3: Dynamics

A unitary operator $U(t, t')$ maps the evolution of the state at time t to time t' . Since the operator is unitary, its reversible and satisfies $U^\dagger = U^{-1}$. Operator U rotates the vectors in Hilbert space, hence their inner products and norms are preserved. However the infinitesimal time evolution for the state $|\psi\rangle$, is given by the Schrodinger

equation given as,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (1.2)$$

where H is a Hermitian operator known as the Hamiltonian of the quantum system.

For a time-independent Hamiltonian, we can write $U(t', t)$ as

$$U(t', t) = \exp \left[-\frac{i}{\hbar} H(t - t') \right]. \quad (1.3)$$

Postulate 4: Measurement

A measurement is the process to obtain information about a quantum state, which in essence collapses the quantum state. The state before measurement is assumed to be a linear combination of the eigenstates, $|\psi\rangle = \sum_i c_i |a_i\rangle$ of an observable A with eigenvalues a_i . A measurement takes the projection of the state $|\psi\rangle$ into one of the eigenstates of the observable A with eigenvalues a_i , hence giving the probability(information) to the observer about a_i as $P(a_i) = |\langle a_i | \psi \rangle|^2 = |c_i|^2$.

Postulate 5: Composite Systems

We can take tensor product of the Hilbert spaces of two individual systems which represents the Hilbert space of the composite system. For example, in the discrete quantum walk for the state of walker in position, and the internal degree of freedom(coin) of the walker constitutes the composite system for the quantum walk. Hence denoted by Hilbert space for positions and coin in tensor product given by $\mathcal{H}_p \otimes \mathcal{H}_s$. [1]

1.2.2 Geometrical Representation of Qubits

Classically we represent the data in terms of the smallest unit ‘bit’. It exists either in the states of 0 or 1. Its quantum counterpart “Qubit” is required for quantum information processing [2]. It exists in the superposition of states 0 and 1. Hence, physically it’s a two-level quantum system e.g, up and down spins of an electron or

two polarization states of a photon. Mathematically, it is defined by a unit vector in two-dimensional Hilbert space spanned by the natural orthonormal basis $|0\rangle \leftrightarrow (1, 0)^T$ and $|1\rangle \leftrightarrow (0, 1)^T$. This representation is also known as the computational basis of the qubit. One way of representing the state of a qubit is

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle,$$

where α and β are complex numbers satisfying the completeness relation $|\alpha|^2 + |\beta|^2 = 1$. Measurement on the qubit state results in the probabilities $|\alpha|^2$ and $|\beta|^2$, for the states $|0\rangle$ and $|1\rangle$ respectively. The quantum coherence is destroyed by the measurement. All qubit states can be represented on a 3-dimensional Bloch sphere, where the polar representation is,

$$|\psi\rangle = r_1 |0\rangle + r_2 e^{i\phi} |1\rangle$$

and the cartesian representation is,

$$|\psi\rangle = z |0\rangle + (x + iy) |1\rangle$$

. Using the normalization condition for a unit sphere $x^2 + y^2 + z^2 = 1$, and $r_1 = \cos \theta$ and $r_2 = \sin \theta$, where $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$. Since, we can represent all qubit states within the interval $\theta \in [0, \pi/2]$. Hence, the final form of a qubit state in Bloch sphere representation becomes

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi} |1\rangle$$

Any 2×2 matrix can be written in the basis of matrices $I, \sigma_x, \sigma_y, \sigma_z$, where σ_k are the *Pauli matrices*

$$\sigma_k = \begin{pmatrix} \delta_{k3} & \delta_{k1} - i\delta_{k2} \\ \delta_{k1} + i\delta_{k2} & -\delta_{k3} \end{pmatrix}, \quad (1.4)$$

where $k = 1, 2$, and 3 . The density matrix of the Bloch sphere can be written as,

$$\rho = \frac{1}{2}(I + \hat{n} \cdot \vec{\sigma})$$

where $\hat{n} = (n_1, n_2, n_3)$ is a 3-dimensional unit vector in spherical co-ordinates and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$. This geometrical representation is a tool to understand up and down states of the quantum walker, which are taken along $+z$ and $-z$ axis.

1.2.3 Classical Random Walks

In 1905, Karl Pearson introduced the so-called 'drunkard's walk' in 2D, which led to the term random walk being coined.

“A man starts from a point O and walks l yards in a straight line; he then turns through any angle whatever and walks another l yards in a second straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + dr$ from his starting point, O.”

Lord Rayleigh provided a Gaussian large- n solution solution to the above problem as,

$$p_n(r < x < r + dr) = 2/ne^{(-r^2/n)}rdr. \quad (1.5)$$

The simplest example of a random walk is the motion of a particle on a 1-dimensional line with its outcome being determined by a coin toss. The particle shifts right or left depending on whether the outcome of the coin is head or tails. One step of the

walk is defined by application of this process a single time, and the time evolution is determined by successive steps. The exact position of the particle is not deterministic hence the time evolution is probabilistic. Instead, the probability P , which is usually given by binomial distributions,

$$P_n(t) = \frac{1}{2^t} \frac{t!}{\left(\frac{t+n}{2}\right)! \left(\frac{t-n}{2}\right)!} \quad (1.6)$$

$P_n(t)$ gives the probability of finding the particle at position $n \in \mathbb{Z}$, after some steps t . The spreading of this distribution is wider for the larger number of steps. The variance is given by,

$$\sigma^2(t) = \sum_{i=1}^R P_i(t) (n_i - \bar{n})^2 = \langle n^2 \rangle - \langle n \rangle^2 \quad (1.7)$$

where the summation is taken over the ensemble $\{n_1, \dots, n_R\}$ that contains the final positions after the R iterations of the t -step walk. The standard deviation $\sigma = \sqrt{\sigma^2}$ can also measure the spread of the walk. The variance of walker's position is linear in n for the solution given by Lord Rayleigh in eq.(4). Such spreading dynamics, which are linearly proportional to the variance, are called diffusive. [2]

1.2.4 Discrete Time Quantum Walks

The quantum model published under "Quantum Random walks" by Aharonov et.al Outperformed its classical counterpart in terms of spreading rates [7]. However, the randomness is not what constitutes an analogy between the two, rather the scheme in which we apply procedure at each step. However, the quantum model of isolated systems evolves unitarily, hence its reversible and deterministic, not random, unlike classical model. We would use the term Quantum Walks in the rest of the document in context to such models.

The model and conventional Protocol

The position of the particle in discrete-time quantum walk is associated with a state vector in the Hilbert space \mathcal{H}_p of infinite dimension which is spanned by the computational basis $\{|x\rangle : x \in \mathbb{Z}\}$. The probabilistic nature of the classical coin flip can be modeled by measuring the state of a qubit in some computational basis $c \in \{0, 1\}$. The result of the measurement determines the direction of the state evolution. This provides an internal degree of freedom to the walker, and is termed as “quantum coin”. For a one-dimensional walk on a line, the quantum coin can be selected as a two-level quantum system, with states in two-dimensional Hilbert space \mathcal{H}_c^2 . The quantum walker is a composite system which has its quantum state $|c, n\rangle$ in the Hilbert space $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$. The translation of the walker is associated with a unitary *shift/translation operator* (represented by S or T, we’re using S)

$$S = \sum_{n=-\infty}^{+\infty} (|0\rangle\langle 0| \otimes |n+1\rangle\langle n| + |1\rangle\langle 1| \otimes |n-1\rangle\langle n|)$$

which conditionally shifts the position of the walker to left or right depending on the orientation of the spin, or coin state as follows:

$$S_+ |0, n\rangle = |0, n-1\rangle$$

$$S_- |1, n\rangle = |0, n+1\rangle$$

here we split the components of S into S_+ and S_- . If we have to describe this operation as a protocol it would be summarized as follows:

We have a localized quantum walker in a two-state quantum system ($|0\rangle$ and $|1\rangle$) at its initial position, usually at $x = 0$.

- 1.) **Coin Toss:** Coin operator applied to this state, rotates it around the y-direction (by convention of Bloch sphere), most commonly used are Hadamard H , and spin rotation

R :

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad R(\theta) = e^{-i\sigma_y\theta/2} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \quad (1.8)$$

where σ_y is a Pauli Operator. This step results in the superposition of the two up and down basis states, from our initial state likely to be in just one of these states.

2.) **Shift:** Shift operator is applied to this rotated states, and based on its orientation the walker is shifted to right or left positions. Usually we shift $|0\rangle$, up states to the right and $|1\rangle$, down states to the left. This is a one step shift operator.

3.) **Evolution:** thus we can summarize the steps 1 and 2 by the application of unitary operator,

$$U = S(I_p \otimes C)$$

here, Kronecker product represents the composite system of position space, represented by I_p , and walker degrees of freedom C the coin operator. The evolution for t times of the state at t is given by $|\psi(t)\rangle$ as,

$$|\psi(t)\rangle = U^t |\psi(0)\rangle \quad (1.9)$$

4.) **Measurement:** the last step of this protocol involves projection of the $|\psi(t)\rangle$ to a specific state $|x_0\rangle$. Hence, we can measure the probability of the quantum walker in state $|x_0\rangle$.

$$|\langle x_0 | \psi(t) \rangle|^2$$

Quantum Ultra Walks

A coined quantum walk on a 1-D lattice with $P = 2^N + 1$ sites has a Hilbert space $\mathcal{H}_c \otimes \mathcal{H}_p$, here \mathcal{H}_c is a 2-dimensional coin subspace, and \mathcal{H}_p is the P -dimensional position subspace. Basis of \mathcal{H}_c is the set $|a\rangle$ for $0 \leq a \leq 1$ and \mathcal{H}_p is spanned by $|k\rangle$ with $0 \leq k \leq P - 1$. If we want to construct our hierarchy in a way that odd indexed

x share the same coin, and so do the sites that are once-, twice-, thrice-,... i -times divisible by 2. The binary decomposition of all sites except $x = 0$ can be given by

$$x(i, j) = 2^i(2j + 1) \quad (1.10)$$

where $i \geq 0$, is the hierarchy index and j is the running index, $-\infty < j < \infty$. Hence, we have one-to-one relation between $x(\neq 0)$ and pair (i, j) . In this hierarchy all the sites sharing the same value of i have an identical coin for all i i.e. $C_x(i, j) = C_i$. Thus we can transform our rotational coin to make it same for each hierarchy(i) by multiplying the argument of our coin with something that only changes value with i ,

$$R(i, \eta_i) = e^{-i(\sigma_y + \sigma_z)\left(\frac{\pi}{2} - \overbrace{\eta_0 \epsilon^i}^{\eta_i}\right)} = \begin{pmatrix} \sin(\eta_0 \epsilon^i) & \cos(\eta_0 \epsilon^i) \\ \cos(\eta_0 \epsilon^i) & -\sin(\eta_0 \epsilon^i) \end{pmatrix} \quad (1.11)$$

where $\eta_i = \eta_0 \epsilon^i$ ($0 < \epsilon \leq 1$). For the case of $\epsilon = 1$ it reproduces a spatially independent coin, hence the results for homogeneous quantum walks are reproduced. However, for the cases of $\epsilon < 1$ the transition between adjacent sites, of this hierarchy becomes increasingly difficult as $\eta_i \rightarrow 0$ for $i \rightarrow \infty$, regardless of the direction of approach.

Thus, a hierarchy of barriers emerges, in which the coin becomes ever more reflective for a walker trying to transition through respective sites. Then, the walker progressively gets confined in a tree-like ultrametric set of domains with vastly different timescales for exit. A larger domain for $i + 1$ is sandwiched between the two smaller adjacent domains at level i of the hierarchy, which gives rise to the ultrametric hierarchy. Fig.1.1 represents the barriers of this hierarchy[3, 4, 5, 6, 36].

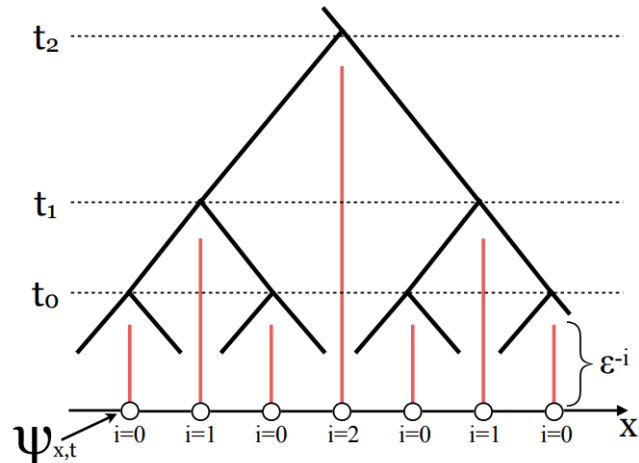


Figure 1.1: The Hierarchy of reflective barriers (ε^{-i}) is dependent on the tuning parameter (ε) and site index i . For higher indices the barriers are higher and harder to transit between sites.

1.2.5 Localization: Absence of diffusion

The models discussed in the previous sections described perfect Quantum Walks, which are only existent theoretically. If we implement these models anywhere in the nature imperfections are inevitable. We would encounter noise in these models in the form of decoherence and disorder, which effects these quantum walks in interesting ways. Decoherence involves unwanted couplings to the environment (since it is an open quantum system), that causes loss of information and renders the walk non-unitary with non-hermitian \mathcal{H}_{eff} . Kendon reviewed these systems in detail in her paper in 2007 [41]. This research proposal would be focused on noise in the form of disorder. When we characterize decoherence we refer to distortion of the walk's evolution in terms of action of imperfect operators or random measurements in which the information is lost, whereas disorder is characterized by the variations in the structure of the Hamiltonian away from the ideal.

Hamiltonian

Static disorders in experimental setups might be introduced because of the errors that limit us from having the perfect Hamiltonian, usually due to uneven site energies or bond lengths. Mathematically, static disorders are represented by small perturbations to the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_s + \mathcal{H}_b = \mathcal{H}_0 + \sum_i \epsilon_i |i\rangle \langle i| + \sum_{\substack{i,j \\ i \neq j}} \epsilon_{i,j} \mathcal{H}_{i,j} |i\rangle \langle j|, \quad (1.12)$$

where $\mathcal{H}_0, \mathcal{H}_s, \mathcal{H}_b$ represents the ideal, site disorder, and bond disorder Hamiltonians, respectively. This equation results in the perturbation of the eigenstates of the system, with corresponding energy shifts and additional couplings. If the system's evolution remains unitary, we can predict the disruptions in the system's evolution.

Dynamical Localization

Anderson[11] in 1958 discovered that disorder leads to the localization of the quantum states. This discovery countered the “naive” physical intuition related to the transport in a metal with a strong concentration of impurities don't proceed by tunneling from impurity to another, rather completely stops above a threshold concentration. Hence if the particle is initially concentrated at the origin, there would be a finite probability of finding the particle at the origin even when we measure the state after a long time. Hence, the wave function of the particle is exponentially localized inside a region characterized by a localization length l . In the Hamiltonian discussed in equation 13, if we have take ϵ as the representation of the random site energies, and we can take a uniform distribution for $\epsilon = \mathcal{U}(-W/2, W/2)$, with a band width W . We can replicate the model proposed by Anderson which exhibit complete localization for any disordered strength(measured by W) in one or two dimensions. The

wavefunction can be expressed as,

$$\text{Lim}_{x \rightarrow \infty} \sim e^{\pm x/l}, \quad l \sim 1/\lambda$$

Where λ is the maximum Lyapunov exponent. The characteristic length scale is the function energy for the wavefunctions. For the eigenvalues of our Hamiltonian, these solutions would be decaying in both directions. Hence we can summarize, the spectrum of the Anderson Hamiltonian is a discrete spectrum of exponentially localized wave functions, whose characteristic localization length is given by the inverse of the Lyapunov exponent of the transfer matrix product.

1.3 Methods

The simulation of the Quantum Walks for a spatially variant coin is reproduced using the Python libraries. The testing of our system is done via the reproduction of the results of the Boettcher[3] and Flach et al.[35]. The following sections elaborate on the methodologies and practices incorporated for the testing and tuning of our system. The next chapter showcases these results as well as the simulations for the hypothetical “critical transitioning point” for our quantum walks systems.

The simplest way to introduce the phase disorders is through the shift matrix corresponding to the left or right shift of the Quantum Walker. Since Anderson localization is a well-established property in Quantum Tunnelling and similar transport processes we would first verify our system of quantum walks by simulating phase disorders at each site of the lattice.

After the general tests of our system and verification of Flach et al.[35] results we then move on to our novel disorders which are correlated by hierarchy and describe their methodology. The next sections mention the tuning of our system and the numerical analysis concepts we are utilizing.

1.3.1 Simulation of Heterogeneous Quantum Walks

Following the conventional Quantum Walks protocol, the homogeneous quantum walks were generated. The simulation of Hadamard walks with a superposition of spin-up and spin-down at the origin of the walker produced well established results of the ballistic spread of the walk. Now, in order to simulate Boettcher et al.[3, 4, 5], hierarchical quantum walks where the reflectivity of the walker increases with a tunable parameter (i.e, ε) are created using spatially variant coin matrix shown in eq.1.13. This matrix changes the phase of rotation/reflection θ in correspondence to this equation $\theta \equiv \eta_0 \epsilon^i$, where i is the hierarchical index as explained in 1.2.4 under Hierarchical Quantum Walks. The simulations are realized using Python’s library numpy functionality for sin and cosine which helped in the reduction of computational costs of otherwise tensor multiplication. The details of the same are given in Appendix B. The results of this system of “Quantum Ultra Walks” are uploaded in the GitHub repository as the open-source software, details of the same are given in Appendix B. The software written supports the creation of snapshot at any evolved state along with the ability to calculate standard deviation of the Quantum Walker. The reproduction of the results of Boettcher et al. are given in the next chapter under section 2.1. The tunability of the entire system with the parameter ε showcases the increasing reflectivity of the 1-D lattice which works against the quantum walker to escape ballistically. However, the system is never localized for the walker, which is still able to evade and collide with the absorbing wall placed at infinity.

1.3.2 Uncorrelated phase disorders in the lattice

In Flach et.al [35] they've introduced 4 types of disorders in the general coin operator given in terms of 4 angles $\phi, \phi_1, \phi_2,$ and θ

$$U = e^{i\phi} \begin{pmatrix} e^{i\phi_1} \cos \theta & e^{i\phi_2} \sin \theta \\ -e^{-i\phi_2} \sin \theta & e^{-i\phi_1} \cos \theta \end{pmatrix} \quad (1.13)$$

The disorder in phase ϕ_1 does not lead to the localization since it only modifies the phase difference between neighboring sites, while keeping the amplitude ratio unchanged. However, the uncorrelated disorder in all other quantum coin angles θ, ϕ and ϕ_2 leads to Anderson Localization. The use of static disorder has been implemented with its probability distribution function given by,

$$\mathcal{P}(x) = 1/(2W), x_0 - W \leq x \leq x_0 + W$$

and $\mathcal{P}(x) = 0$ elsewhere, with x_0 as average with disorder strength in $0 \leq W \leq \pi$. The results published in Flach et. al [35] are shown in the Fig.1.2, where Localization length within the allowed bands of ω , indicated by vertical red lines, is differentiated on the basis of W . The Localization length peaks at $\omega = \pi/2$ and is shown to be maximum for $W = \pi/20$. Since, the relationship of localization length at $\omega = \pi/2$ is inversely proportional to W , and there is a considerable gap in blue band and red band, its fair to assume there is a critical point where the transition of sub-ballistic Quantum Walker to completely localized Quantum Walker takes place. This investigation has been made and the results are confirmed and presented in Chapter 2.2.

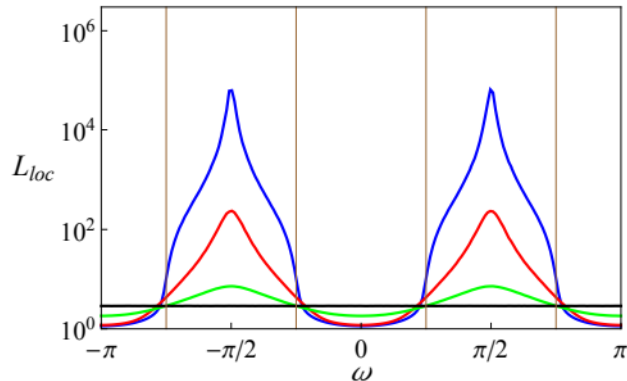


Figure 1.2: This figure is sourced from Flach et al. [35], and it illustrates the dependence of the localization length on the frequency ω (the eigenfrequencies of the solution for transfer matrix) for phase disorder-induced with ϕ . From top to bottom at $\omega = \pi/2$: $W = \pi/20, \pi/5, \pi/2, \pi$. Here at $\theta = \pi/4$ the red vertical lines indicate the boundaries of the allowed bands.

1.3.3 Disorders correlated by hierarchy

The introduction of novel disorders are done to conduct simulations to find out the behaviour of the walker in constrained randomness. The selection of phase disorders are completely random but would only be done a maximal of 21 times in a system which evolves a million times. We are interested in correlating our disorders with our hierarchical barriers that decided upon by the index of each lattice site which is a power of 2. These phase disorders will induce randomness at each of hierarchically indexed lattice points for the evolution of the quantum walker in this system. We've utilized the hash map functionality given by dictionaries in python to simulate these phase disorders at exact spatial points on the 1-D lattice.

Even if we don't increase the reflectivity of our system these induced disorders will sure to effect the ballistic behaviour. This ansatz is confirmed with the results for such system, where the homogeneous walks with hierarchical disorders produce sub-ballistic behaviour. The results are elaborated in section 2.3.

Diffusion Constants and Intercepts

The analysis of the results are done by observing the intercepts of the logarithmic scale of standard-deviation per logarithmic time-scale vs per logarithmic time scale. The reason for using this scales and our interest in the intercept is explained by the following equation. If our mean-square displacement equation for the quantum walker can be written as,

$$\sigma(t) \sim t^{1/d_w}, \quad (1.14)$$

where d_w is the walk dimension which characterizes the nature of the walk e.g. walk is purely diffusive at $d_w = 2$ and so on. If we take logarithmic scale on both sides we get,

$$\log \sigma(t) = \log C + \frac{1}{d_w} \log t \quad (1.15)$$

where C is some constant of proportionality. After taking out a factor of $\log t$, and renormalizing $\log C$ to be 1 we get the following equation.

$$\frac{\log \sigma(t)}{\log t} = \frac{1}{\log t} + \frac{1}{d_w} \quad (1.16)$$

So if our graphs we analyze $1/d_w$ we can find the behaviour of the quantum walk. Since, d_w is the inherent characteristic of the walk, if our value of the intercept are closer to 0 for millionth numerical evolution of the system it clearly implies that it takes infinite time for the quantum walker to evade localized state. Hence, we can have general idea of the nature of our system by observing the intercepts in the graphs for the above mentioned scaling.

Increasing the reflectivity of the hierarchy

Since in our system the reflectivity can be tuned by using the parameter ϵ as we have $\theta \equiv \eta_0 \epsilon^i$ for the hierarchical coin, we can involve some tuning of this parameters

to extrapolate whether the walker experiences transitions between its spreading behaviour. The interest in studying this kind of system is to establish the differences between homogeneous quantum walks from the heterogeneous quantum walks. The results related to these extrapolations are presented in section 2.4.

Chapter 2

Results

2.1 Behaviours of homogeneous and heterogeneous Quantum Walks

The proposed walk by Boettcher et.al[3] in Quantum Ultra Walk is 1D walk which is strongly spatially variant but with the hierarchical repetition of coins. Boettcher termed it as "Quantum Ultra Walks", which is inspired by the ultra-metric arrangement of barriers in Classical diffusion problems[3, 4]. The introduction of inhomogeneity in the lattice for the quantum walks changes its asymptotic behaviour. The walk dimension d_w^{QW} ranges from 1 to infinity which basically represents the spreading behavior of the walker where $d_w = 2$ implying diffusive behaviour and $d_w = \infty$ implying localization. Since the ordinary diffusion problems shows quite robust diffusion in the hierarchy below a threshold, for the walk to become sub-diffusive the threshold of the hierarchy was required to be increased. The hierarchy produces reflective barriers at the indexed sites of the 1-D lattice and as the index increases the time barriers increases for the particle to escape the particular site as the reflection due to hierarchical coins increases [3]. This heterogeneous model of the walk produces sub-ballistic plots as shown below in Figure 2.1. This sub-ballistic behaviour charac-

terizes the slowing down of the ballistic spread inversely proportional to the tuning parameter ε . The tuning parameter increases the reflectivity with its decreasing value which in the limiting case of $\varepsilon \rightarrow 0$ gives the case of pauli X matrix which reflects the quantum state on the z-basis. The Standard deviation plots are represented in the following figures for the homogeneous and heterogeneous walks to make the reader realize the differences between them.

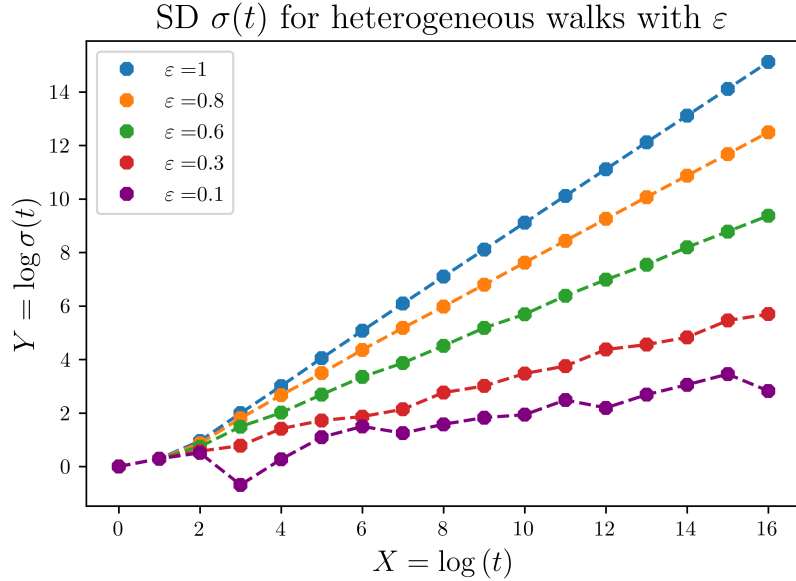


Figure 2.1: This figure illustrates the Standard Deviation on Log-Log scale for the various $\varepsilon(s)$ in order to represent how the increasing reflectivity in the 1D lattice of the Quantum Walks affects the ballistic behaviour. Different $\varepsilon(s)$, tuning parameters, are given which are inversely proportional to the reflectivity of the heterogeneous walks.

2.2 Localization for regular phase disorders

The results for the case when phase disorders affect each lattice site verifies the Figure 1.2 hence the results of Flach et.al [35]. The intercepts are close to 0 in the limit of infinite time evaluations, which we have taken as 2^{17} . The extrapolated intercept using linear regression for the last 5 data points have shown to come out in the limit of 0 in the 3 standard cases of disorder strength W 's yet in the case of $W = 0.05\pi$,

it comes out as around the value $1/d_w = 0.3$. This result verifies the non-localized sub-ballistic behaviour of quantum walks for weak disorder strength, $W = 0.05\pi$. The interesting observation from the plot one can make is the gap in the intercept values for the rest of $W(s)$ and $W = 0.05\pi$ which further solidifies our assumption that a critical point(i.e in parameter W) exists which makes the sub-ballistic walk localized.

2.2.1 Homogeneity affected by phase disorders

The regular disorder shows standard localization plots confirming the analysis given in Flach et.al [35], and we see the occurrence of sub-ballistic walks. We know in the Homogeneous i.e spatially invariant coin walks we can't tune the reflectivity of the system but with spatially variant coin such tuning is possible. The following Fig.2.2 shows how increasing the reflectivity of the system converges the intercept.

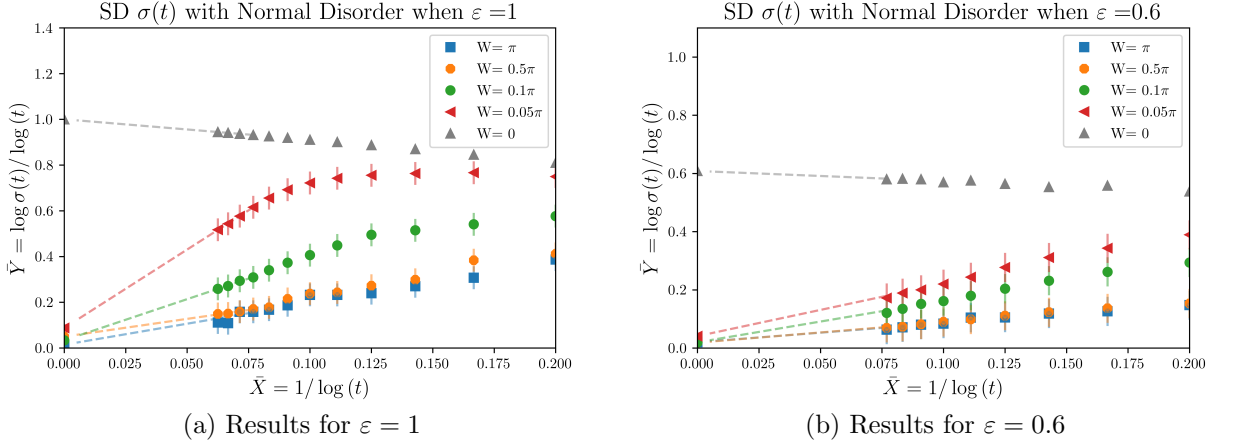


Figure 2.2: Figure (a) and (b) illustrates spreading behaviour for systems with $\varepsilon = 1, 0.6$ affected by normal disorder, which affects each lattice point. Intercept corresponds to the inverse walk-dimension $1/d_w$, and is plotted for different values of disorder strength W . Figure 3.1 shows that $1/d_w$ scales linearly with ε hence at $W = 0$, $1/d_w = \varepsilon$ which serves as the confirmation for accuracy of figures above. As the reflectivity of the system increases which is inversely correlated to the ε the system is indicative of more localized behaviour of the walker. Length of Vertical Error bars in (a) are 0.04 (averaged over 25 runs) while (b) has 0.05 (averaged over 20 runs).

2.2.2 Phase disorders in Heterogeneous systems

The heterogeneous system of quantum walks which is controlled by a tuning parameter ε gives us the possibility to extrapolate the systems for such critical points where the transitions occur. The data collected from probing the system for turning sub-ballistic to localized walk showcases the transition point of this system given in the Figure 2.2 b).

2.3 System affected by phase disorders correlated with Hierarchical indices

We introduced novel phase disorders in our system of Quantum Walks to analyze the differences in the spreading behaviour from the spatial disorders. The problem of disorders helps us to realize the breaking point of our quantum systems. One of the primary reasons for introducing disorders such that they are hierarchically correlated is because of the ease of mathematical modeling of them using re-normalization groups.

The introduction of the Novel Phase disorders in our system of Quantum Walks is made to study the characteristic behaviour of the spreading of the Quantum Walks. The Quantum ultra walk model introduced by Boettcher et al. concluded this system has finite d_w^{QW} for all the $\varepsilon(s)$ except for the trivial case of $\varepsilon = 0$, which makes the spatially variant coin matrix to be Pauli-X matrix which is essentially reflective, hence the quantum walker would be trivially localized. The trivial case doesn't provide us with much information about realizing the walks in the physical world. We would discuss the significance of the problem and analysis of the simulation results in detail in chapter 3. The novel disorders introduced are as the name suggests hierarchically correlated which means there can only be maximal $N+1$ random and unique disorders

if the Quantum Walker evolves 2^N times. And at each hierarchical index, they added the same phase randomness to the coin matrix. So if we evolve our system for a million time-steps maximally it can only have 21 random phase disorders introduced within this system. The coin matrix which is spatially variant and is correlated to the hierarchical index gives us an interesting system to evolve and tune. The equation 1.16 gave us new $\bar{Y} = \frac{\log \sigma(t)}{\log t}$ and $\bar{X} = \frac{1}{\log t}$ scales for us to plot our standard deviation data on. The data for standard deviation is smoothed by iterating over 100 times with the disorders and averaging. The last five points are used in extrapolating d_w intercept using linear regression.

2.3.1 Novel Disorder introduced with $\varepsilon = 1$

The case for $\varepsilon = 1$ produces a homogeneous quantum walks system. We performed the analysis of the spreading dynamics over four different $W = (s)$. The figure 2.3 a) illustrates the results. Results for $W = 0$, although not part of the experiment, were included in the Figure 2.3 as a visual aid to understand the difference between disordered affected and unaffected behavior. None of these walks shows localized behavior. It is understandable as a fact that this system doesn't have the threshold of randomness required to stop the transport of the walker. The correlated disorders still add interesting mechanisms in the mathematical solvable hierarchical model of quantum walks representing the further halt in their spread.

2.4 Increasing Reflectivity(ε^{-1}) of the system

The tuning of the system is done by decreasing the reflectivity parameter. For the sufficiently large time limit, the approximations for d_w obtained through the intercepts are taken into account to categorize the spreading behavior. The changing of ε helps us differentiates between the Homogeneous $\varepsilon = 1$ and the Heterogeneous walks

$0 \leq \varepsilon < 1$ when they are unaffected by disorders. The results for various $\varepsilon(s)$ are presented over the selected disorder strengths. We want to illustrate how this tuning of the parameter changes the $1/d_w$ making it smaller and smaller until it approaches the limiting behavior at $1/d_w \sim 0$. These values are presented in Table 2.1 for a comprehensive understanding of the variables of this Quantum Walks system and their corresponding behavior.

2.4.1 Heterogeneity and hierarchical phase disorders effects

The presence of critical points for transition is indicated in this system by the results presented in the following Figure 2.3. The results show transitioning of Nearly Ballistic behavior into sub-diffusive and sub-ballistic behavior indicative of plausible localization when the ε crosses a certain threshold.

2.4.2 Indicators of Localized, sub-ballistic and ballistic behaviour

On the basis of the extrapolated intercept in the limit of large time-steps (2^{17}), we are able to assemble the results in a tabular format that categorizes different spreading behaviour of the Quantum Walks. As the results for the correlation of disorder strengths with localization are already established with more the strength, smaller the localization length. The tabulated results in Table 2.1 indicates various plausible transitions between spreading behaviour, an accompanying polar plot in Fig.2.4 provides a more visual representation of such transitions.

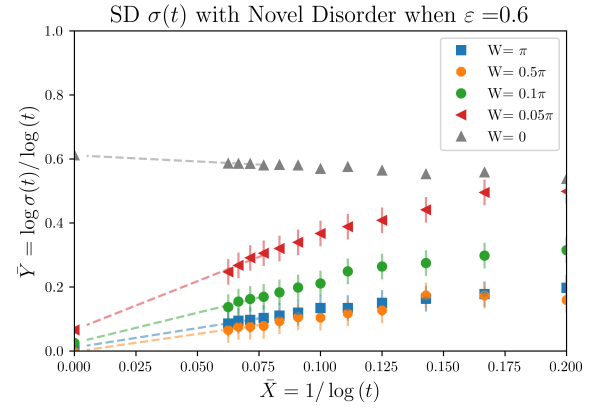
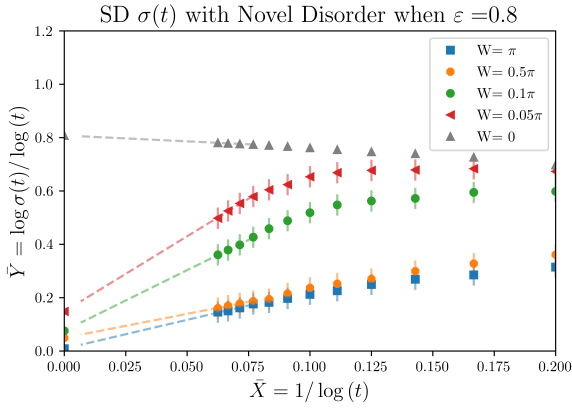
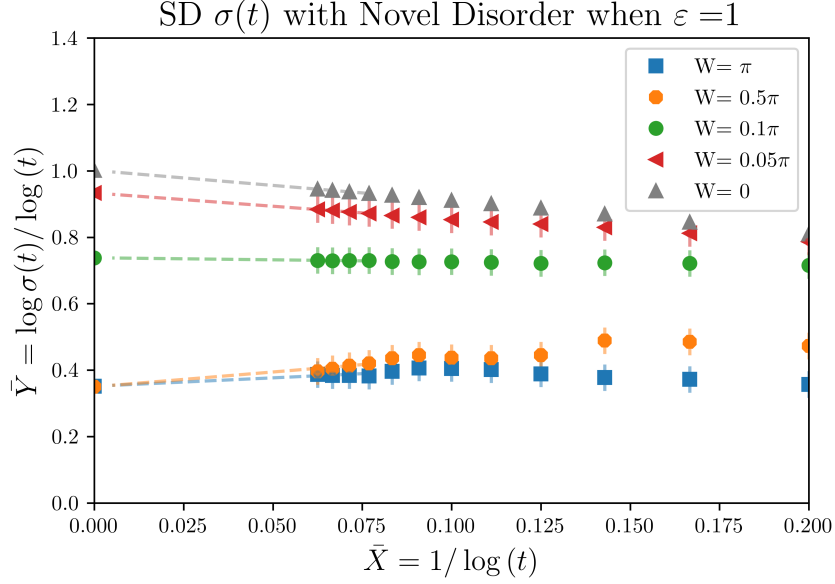


Figure 2.3: Figure (a),(b), and (c) illustrates the spreading behavior for systems with respective $\varepsilon(s) = 1, 0.8, 0.6$ affected by the novel disorder, which affects only 21 lattice points for a million time-steps. These results indicate that system seemingly localizes a particle as reflectivity increases (ε decreases) for sufficiently high disorder strength, W . These results are tabulated in Table 2.1. Length of Vertical Error bars in (a) & (c) are 0.02 (averaged over 50 runs) while (b) has 0.04 (averaged over 25 runs)

Table 2.1: Values of Intercept($1/d_w$) and corresponding disorder strengths, ε and categorical spreading behaviour

Disorder Strength(W)	Epsilon(ε)	Intercept($1/d_w^{QW}$)	Behaviour
Nearly Ballistic and Sub-Ballistic ($1 > 1/d_w > 0.5$)			
0.05π	1	0.9	Nearly Ballistic
0.01π	1	0.7	Sub-Ballistic
0.05π	0.9	0.6	Sub-Ballistic
Diffusive and Sub-Diffusive ($0.5 \geq 1/d_w \geq 0.1$)			
0.33π	1	0.5	Diffusive
0.05π	0.8	0.5	Diffusive
0.01π	0.9	0.4	Sub-Diffusive
π	1	0.3	Sub-Diffusive
0.01π	0.8	0.25	Sub-Diffusive
Localized ($1/d_w \ll 0.1 \sim 0$)			
π	0.8	~ 0	Localized
0.5π	0.6	~ 0	Localized

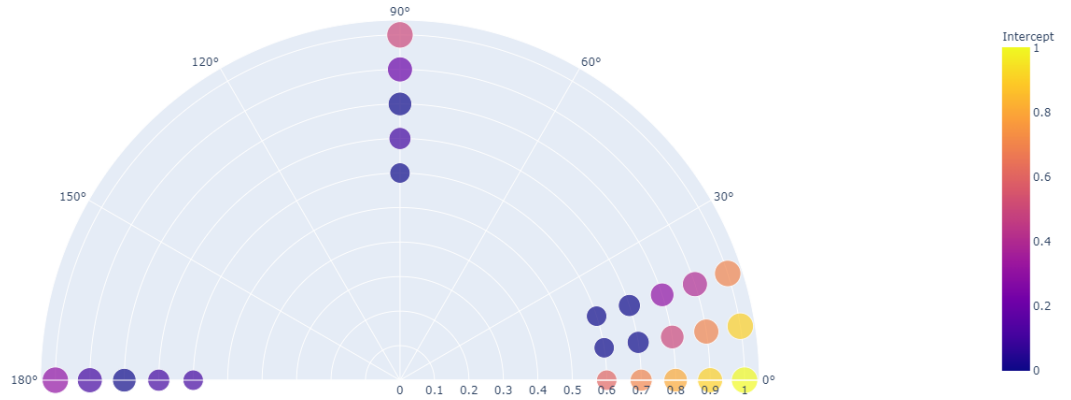


Figure 2.4: Polar plot with radius r given by ε and θ given by W in range of 0 and π and differentiated based on the Intercept as shown in the color gradient bar to the right.

Chapter 3

Discussion

3.1 Heterogeneity in Quantum Walks

The "Quantum Ultra Walk" model, which was proposed by Boettcher [3, 4, 5, 6], utilized a coin that depends on the hierarchical index. This model was loosely inspired by the ultra-metric arrangement of barriers in the classical diffusion problem. The same model was applied for the Classical Random walks as well as for the Quantum Random walks. The ability to mathematically model the asymptotic spreading behavior made it a relevant problem to pursue. Boettcher concluded that using this model no localization is achieved, unless it is for the trivial case of $\varepsilon = 0$. This model makes the Quantum Walks more reflective and therefore slowing down the ballistic spread of the walks to the category of sub-ballistic behavior. When we compare this to the results of Anderson Localization proposed in Anderson's seminal work in 1958, he attributed the decay of the wave functions to the Quantum Reflections in the lattice. The disordered case however is a completely uncorrelated form of Quantum Reflections, whereas the introduction of ultra-metric walks is done by using cleverly correlated indices. These indices produce the spatially variant coins which have the same 'reflectivity' at each index. Hence the complete decay of the wave function is

never realized and no localization occurs in this model.

3.2 Disorder Strength and localization length

The reasoning to incorporate the phase disorders, proposed in the Flach et al.[35] is to explore this system for critical change in the spreading behavior. Even though no exact critical point is determined but we can identify it exists in the range $W = 0.05\pi$ and $W = 0.3\pi$ for the change in ballistic to sub-diffusive behavior, and similarly for other transitions. The critical point we talk about in the thesis is in the context of a change of the categorical spreading behavior instead of the localization to delocalization transitions which is the usual context for such studies of the criticality of the system. Our, motive was to observe the differences from the regular disorders that affect the interaction of the wavefunction at each lattice point from the novel disorders which only differ at hierarchical indices.

From Flach et.al[35] and Anderson's investigation of the quantum transport, we already are familiar with the fact that higher the disorder strength lower the localization length hence a more localized Quantum System. Anderson proposed in his seminal paper given a strong disorder the system will be localized no matter the dimension d [11]. To understand Anderson localization in a more intuitive sense it is the result of the Quantum reflections in the lattice that makes the wave function halt. However, Anderson didn't study the delocalization and critical behavior of this system. In higher dimensions(d) ($d > 3$) the phenomenon of delocalization exists, and the critical disorder state is dependent on the energy of the eigenstate. In the case of phase disorders, the maximum you can choose is π , after which the repetition of the disorders starts as it completes the circular phase at π . The choice of our novel disorder only allows a maximum of 21 points given that the system is able to evolve a million times which is our computational limit at the moment. In Flach et

al.[35] we see when the phase disorder is $\ll \pi$, we end up with a greater localization length. The simulations we produced verified this result with the finite value of d_w for the disorder strength($W = 0.05\pi$). However, as we increase the reflectivity of the system it crosses the threshold towards lower localization length or in a higher d_w . While making such analysis we need to ensure the limits of the number of time-steps and what constitutes as infinite d_w are clearly established. We have to understand the results produced from these simulations can only stipulate at best the behavioral changes of the system and predict how the system evolves in these experimental novel disorders, but we still can't fully prove the localization through these methods. To accomplish that one has to incorporate the mathematical methods that we would briefly discuss in the next section.

3.3 Re-normalization and Mathematical modeling of the Quantum System

The existent mathematical methods to ensure the complete halt to the propagation of the wave function localization of eigenstates are Dynamical Transport also known as locator expansion originally by Anderson, localization of eigenstates (characterized by Inverse Participation ratio), spectral analysis and continuity of the spectrum.[11, 12] Asymptotically tracing the behaviour of such quantum walks require the careful study of the system utilizing the mathematical tools at hand. Renormalization groups are a mathematical technique that essentially is coarse-graining of any physical systems to observe its characteristics in a larger space. This technique is applied in the 1-D lattice of quantum ultra walks. The equation of the propagator(time-evolution operator) for our quantum system is,

$$\mathcal{U} = \sum_x A_x |x + 1\rangle \langle x| + B_x |x - 1\rangle \langle x| + M_x |x\rangle \langle x| \quad (3.1)$$

here A_x, B_x and M_x describes the hopping operators for transitions to left, right or the same lattice sites respectively. These operators can be mapped out to corresponding projectors S^A, S^B and S^M . The equations expressing this $A_x = S^A C_x, B_x = S^B C_x$ and $M_x = S^M C_x$ with $S^A + S^B + S^M = \mathcal{I}_r$, with lowest dimension $r=2$ for the unitary coins C_x [3, 5]. These hopping matrices are renormalizable for the given quantum system, where hierarchically correlated indices reproduce the spatially variant coin. This forms mathematically solvable system utilizing which we can conclusively model the spreading behaviour of these walks. The results produced by Boettcher [3] have been presented in Figure 3.1 which are worth the mention to understand the complete motivation to solve problems.

One of the motivations to propose a system like Quantum Ultra Walks was to analyze its asymptotic behaviour by using Renormalization group. The Figure 3.1 shows the results for the scaling of $1/d_w$ with respect to ε and it's clear to see the non-zero finite value of inverse walk dimension exists for the $\varepsilon \neq 0$. The solution of the quantum walk model with novel disorders haven't been worked upon yet. The work presented in this thesis shows a glimpse of the possible categorical spreading behaviour of the quantum walk.

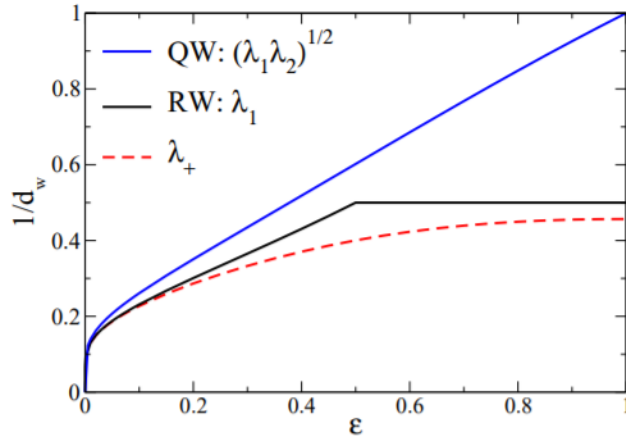


Figure 3.1: This plot is sourced from Boettcher et.al[3] which illustrates the scaling of inverse walk dimension $1/d_w$ for the classical and quantum walks with ultrametric barriers. The dashed line represents the unphysical solution (eigenvalue λ_+) of the system.

Chapter 4

Further Studies

4.1 Novel Phase Disorders

The investigation of the effects of novel correlated disorders on the quantum system was inspired from the paper of Flach et.al [35]. In this work they have concluded for a general coin operator the disorder in ϕ, ϕ_2, θ results in the Anderson Localization of the eigenstates. The investigation of the phase disorder in this thesis was limited to the ϕ phase. Due to the disorder being hierarchically correlated we were able to have a Quantum system that's solvable with the re-normalization groups. We can design other such novel systems that are mathematically solvable using RG techniques. However the careful selection of combination of the disorders at each indices are required. We have to ensure that they uphold the hierarchy of the system. One such potential candidate would be having disorders for any index k , $k + 1$ -indexed lattice points for θ , and at regular indices k -indexed lattice points for ϕ . These lattice points will have more pronounced Quantum reflections and more prominent decay of the transient solution of the wavefunction .

4.2 Quantum Advantage of Quantum Walks modeling

The Quantum Walks are at the forefront of the developing Quantum Technologies. They have drastically different behaviour on certain graphs compared to their classical analog of random walks. This behaviour of the quantum walks on G_N graphs leads to the faster information transfer and many are helpful in developing quantum algorithms. The studies are done whether Quantum Walks provide the same advantages in the arbitrary graphs without the underlying symmetries. Work of Melkinov et.al[42] provided with the insights of predicting the quantum advantage of such walks on these arbitrary graphs just by looking at the graph. They've accomplished this by using convolutional neural networks. These neural networks learn from the graph such that it eliminates the need to conduct real simulations of the classical and quantum walks on these graphs to conclude for the same. More importantly this method proposed helps in design of automated novel large scale quantum circuits. This level of interconnected applications of exploring the systems with Quantum Walks exist in this field. Although, the work we had done in this thesis has no direct correlation to establishing the Quantum Advantage but it paves the way to know where the clear disadvantage of the system exist. The realization of any structure or quantum circuits would end up creating disorders due to various factors mentioned earlier in this thesis, our job is to create more resources towards the understanding of the behaviour in such situations.

Chapter 5

Summary

5.1 Results

We have studied the Nature of Quantum Walks which are characterized by hierarchically repeating spatially variant coins. This creates a hierarchical set of barriers of relative reflectivity(ε^{-i}) where ε is the tuning parameter in the range of $0 < \varepsilon < 1$ and i is the corresponding hierarchical index on a 1D line. The results of Standard Deviation for such heterogeneous walks have been illustrated in the Figure 2.1 and it reestablishes the fact that heterogeneity in the lattice for such Quantum Walks slow down the spread ultimately to be sub-ballistic but do not localize the walker even if the system evolves indefinitely. This can be briefly summarized using the inverse walk parameter $1/d_w$ which would be a finite number for these Quantum Ultra Walks for any ε other than the trivial case of 0. Further, the results proved the works of Flach et.al where they introduce phase disorders in the ϕ of general coin matrix at every lattice point and it completely localizes the walker for strong disorders. However for the weak disorders where $W \ll \pi$, the underlying heterogeneity of this Quantum System which makes it more reflective at hierarchical indexed points, shows results of localization when the parameter ϵ of the system is reduced. The results for $\varepsilon = 0.6$

shows results which are indicative of plausible complete localization of the Quantum Walker in this system. This just proves the intuition one would have for this physical system which is more reflective barriers there are harder it is for the Walker to evade the localization. At last the results were presented for the simulations for our Novel Disorders, which were spatially correlated by the hierarchical index which also decides the reflectivity of the barriers in this Quantum System. Figures 2.4 and 2.5 illustrates the results of the simulations for such disorders for the $\varepsilon = 1$ and $\varepsilon = 0.8, 0.6$ respectively. For the case of $\varepsilon = 1$, the simulations are not indicative of any plausible localization in the system as the lowest value of the inverse walk dimension is $1/d_w \sim 0.4$, which can be characterized as the sub-diffusive at best. And the highest value of $1/d_w = 0.9$ is indicative of sub-ballistic behaviour which is again the same as the results of Standard Deviation for heterogeneous systems. But as the parameter is tuned down to the values of $\varepsilon = 0.8, 0.6$, the spreading behaviour is indicative of a localized walker for strong disorders at $W = \pi, 0.5\pi$. The weaker disordered lattices still made walker sub-diffusive and the weakest case at $W = 0.05\pi$ showed the results of $1/d_w < 0.1$, which is outstanding comparing its almost ballistic behaviour for $\varepsilon = 1$. This is an interesting outcome which verifies the physical intuition for the applicability of phase disorders in the lattice that has hierarchically reflective barriers. Since, fundamentally Anderson localization is the outcome of the interaction of Quantum Waves at these disorders which halts its transport by making lattice ultimately more reflective.

5.2 Discussion

The relevance of the model for “Quantum Ultra Walks” is due to its ability for its asymptotic behaviour to be modeled mathematically. The already established fact for this system is that other than the trivial case of $\varepsilon = 0$ this model is never lo-

calized. The slowest spreading behaviour for these walks are sub-ballistic. These results have been conclusively proved in the Chapter 2 and their physical meaning has been elaborated in Chapter 3. The inverse correlation of the Disorder Strength and the localization length is also shown to be true and is discussed in the Chapter 3.2. Essentially for the regular phase disorders present at each lattice point we obtain a completely localized system for strong disorders but for weak disorders the system is sub-diffusive at best. The results for such weak disorders are tuned by the parameter ε which increases the reflectivity of the hierarchical barriers in this system. And intrinsically, the more the system is reflective the easier it is to halt the spread of the walker and localize it. This proves to be very much the case for our experimental novel disorders that were hierarchically correlated. The interesting thing about these phase disorders were at each index i they would produce the same random value, which in a system that evolves 2^N times can maximally be $N + 1$. This only creates N unique random phase disorders in the system which were ultimately not sufficient for the complete localization of the quantum walker. However when the system is made to be more reflective (tuning of ε) we obtain results that are indicative of the increasing difficulty for the walker to evade the localization. Hence, it differentiates between the spreading behaviours caused by two fundamentally different phase disorders. However, this work at its best can only serve as the indicator for the localized or delocalized behaviour of the quantum walks. The renormalization group techniques discussed in Chapter 3.3 discusses how the asymptotic scaling of d_w differ from the projected values from its simulations. Numerical results for such problems always have constraints of computational resources which puts an upper limit on the time evolution for such walks. We can not effectively calculate the exact value for d_w through such Numerical results as the detailed analytical work would be required for the same.

5.3 Conclusion

This thesis studies the indicators of localization for the system of hierarchical quantum walks. These walks are termed as Quantum Ultra Walks characterized by its unique arrangement of barriers of reflectivity. The thesis delved into the proven cases of Anderson localization in such systems and explored the nature of such localizations for weak disorders (disorder strength $W \ll \pi$). Then, the introduction of the Novel Disorder helped in exploring the Nature of these localized systems further. The indicated characteristic behaviour was tabulated and categorized. The categorical results were tabulated using the extrapolated values using linear regression for the inverse dimension of Quantum walks. The constraints created by the Novel disorder seemed to have slowed down the spread of the quantum walks but not essentially localize the homogeneous quantum walks that are fully ballistic. However, these results still have to rely on the solution from Asymptotic Analysis from Re-normalization groups to verify the stipulated behaviour.

Appendix A

Open-Source QWalks Software

Qwalks software implements the discrete time quantum walks models which are spatially variant and dependent of the tuning parameter ε . It provides general functionalities of statistical measures and dynamics of quantum walks. This is the first of its kind project that deals with Anderson Localization in a spatially dependent disorders which were based on the the publications of Boettcher[3, 4, 5] and Flach et.al[35].

Currently the software offers the implementation of:

- 1.) **QWdisorders** which supports both spatially independent and dependent disorders and showcases the results for localization, sub-ballistic spread, and divergent walks.
- 2.) **QWevolve** supports the static snapshots at any time-step and can be used in the creation of gif(s) for the time-evolution of our Quantum Walks such as the following for hadamard walks, and spatially variant hierarchical walks which see different probability amplitudes due to hierarchy.

The codebase is available in both python and C++ at the github link :

<https://github.com/rshar95/QWalks-Software.git>

The python code base is completely Cythonized and parallelized which makes the simulations faster than the corresponding C++ code base.

Appendix B

Optimizing Quantum Simulations

We have initially written the code for our system in Python, due to the obvious debugging advantages and helpful libraries. Python is a dynamically typed high-level language, which means it's build upon C and stores variables in memory stack which would be otherwise stored as bytes. This inefficiency slows down the processing speed of the entire routine exponentially compared to its C++ counterpart.

Also, the computational power required for processing spatially variant matrices over a large time-evolution puts a lot of strain on the CPU(s) and GPU(s). We needed to optimize our code to overcome these inefficiencies. The time taken to process this program was noticeably cut when matrix multiplication was done for the lattice point $N - n$ to $N + n$ where n is the the time step and N is the number of time-steps. The initialized state in the lattice exists at $\psi_i[N]$. Since, other entries were 0 anyways this helps in reducing multiplication processing of these entries. The example of the method **QWevolve** is given in the following listing. The comments are provider for the accessibility of the code to the reader. This method uses two parameters ϵ (tuning parameter of our system) and N (time-steps).

```

1 def QWevolve(eps, N):
2     a = 1 / sqrt(2.0)    #initializing the up-state array
3     b = 1j / sqrt(2.0)  #initializing the down-state array

```

```

4     r1 = rotation(N,eps) #initializing rotation matrix
5     #array to store a particular state
6     psi = np.zeros((2, 2 * N + 1), dtype=complex)
7     #array to store all the states of evolution
8     psi_t = zeros((2, 2*N + 1, N+1), dtype = complex)
9     psi_t[:, :, 0] = psi
10    psi[0,N] = a
11    psi[1, N] = b
12
13    for n in range(1, N + 1):
14        # rotation of the quantum state at the lattice point
15        psi[:,N-n:N+n+1] = np.einsum("ijk,jk->ik", r1[:, :, N-n:N+n+1],
16            psi[:,N-n:N+n+1], optimize="optimal")
17        psi[0] = roll(psi[0], 1) # shift up
18        psi[1] = roll(psi[1], -1) # shift down
19        psi_t[:, :, n] = psi
20    return psi_t

```

Listing B.1: Python Code for optimized evolution

This optimization was quite useful in progressing this code but we still needed to make our code more statically typed for the efficient use of R.A.M. We utilized the python-C interface Cython. Python is build upon C hence it has engine for implementing all the functionalities of C and C++. These can be accessed through converting the existing python code to statically typed Cython. Here we were just required to define all the types of the variables to the corresponding C types. The exponential processing time speed up was quite rewarding after going through this process. An example of such interfacing is given in the following code listing, where you can clearly observe the only required changes to the code was of required type-casting to corresponding C variables.

```

1 #defining functions using cdef or cpdef for smart Cython
2 cdef QWevolve(float eps, long N):

```

```

3  #cython interfacing: type-casting to C
4  cdef float a;
5  cdef double complex b;
6  cdef numpy.ndarray[double complex, ndim=3] r;
7  cdef numpy.ndarray[double complex, ndim=2] psi;
8  cdef numpy.ndarray[double complex, ndim=3] psi_t;
9  #original code
10 a = 1 / sqrt(2.0) #initializing the up-state array
11 b = 1j / sqrt(2.0) #initializing the down-state array
12 r = rotation(N,eps) #initializing rotation matrix
13 psi = np.zeros((2, 2 * N + 1), dtype=complex)
14 psi_t = zeros((2, 2*N + 1, N+1), dtype = complex)
15 psi_t[:, :, 0] = psi
16 psi[0, N] = a
17 psi[1, N] = b
18 for n in range(1, N + 1):
19     psi[:, N-n:N+n+1] = np.einsum("ijk, jk->ik", r1[:, :, N-n:N+n+1],
20         psi[:, N-n:N+n+1], optimize="optimal")
21     psi[0] = roll(psi[0], 1) # shift up
22     psi[1] = roll(psi[1], -1) # shift down
23     psi_t[:, :, n] = psi
24 return psi_t

```

Listing B.2: Cython interfacing with existing python code

The next speed-up was achieved after invoking multiple cores of our CPU(s) to process these Quantum Simulations in parallel. We had two functions where we had to average the standard deviations calculated from particular disorders to minimize the errors. Hence, we ran this for loop in parallel using Joblib library of the python which smoothly runs these kinds of tasks. Next for a similar for-loop which ran these QWalks simulations for different disorder strengths we successfully processed them in parallel.

```
1 import joblib
2 from joblib import Parallel, delayed
3
4 def QWparallel(eps,w):
5     cdef int k
6     cdef numpy.ndarray[double, ndim=1] standard_dev1
7     with joblib.parallel_backend(backend="threading"):
8         parallel = Parallel(verbose=5)
9         standard_dev1= np.sum(parallel([delayed(qw_split_avg)(k,eps,
10 w) for k in range(1)]),axis=0)
11     return standard_dev1
```

Listing B.3: Parallel processing using Joblib

This QWalks software ultimately provided a good testing framework for these parallel libraries, one other candidate that was considered was Ray. Since, integration of Ray isn't feasible with Cython we picked Joblib for these tasks. But Ray is a very powerful library written specifically for Linux and its Ray Dashboard which is a hosted interface provides great insights in observing your processes across multiple threads.

Bibliography

- [1] J. Sakurai **Modern Quantum Mechanics**
- [2] R. Portugal, **Quantum Walks and Search Algorithms.**(Springer, Berlin, 2013).
- [3] S Boettcher. **Quantum ultra-walks: Walks on a line with hierarchical spatial heterogeneity.**
- [4] S. Boettcher, S. Li, and R. Portugal, J. Phys. A 50, 125302 (2017). Physical Review Research 2 (2), 023411
- [5] Stefan Boettcher, Shanshan Li. **Analysis of coined quantum walks with renormalization.** Physical Review A 97 (1), 012309
- [6] S. Falkner and S. Boettcher, Phys. Rev. A 90, 012307 (2014).
- [7] D. Aharonov, Y., Davidovich, L., Zagury, N.: **Quantum random walks..** Phys. Rev. A 48(2), 1687–1690 (1993)
- [8] N. Shenvi, J. Kempe, and R.B. Whaley. **A quantum random walk search algorithm..** Phys. Rev. A, 67(5):052307, 2003.
- [9] Ambainis, A., Kempe, J., Rivosh, A. **Coins make quantum walks faster..** Proceedings of the Sixteenth Annual ACM-SIAM Symposium on Discrete Algorithms, pp. 1099–1108. SIAM, Philadelphia (2005)

- [10] N. B. Lovett, S. Cooper, M. Everitt, M. Trevers, and V. Kendon **Universal quantum computation using the discrete-time quantum walk** Phys. Rev. A 81, 042330 (2010).
- [11] Anderson, P. W. **Absence of diffusion in certain random lattices**. Physical review 109, 1492 (1958).
- [12] Chandrashekar, C. **Disordered-quantum-walk-induced localization of a bose-einstein condensate**. Physical Review A 83, 022320 (2011).
- [13] Edge, J. M. Asboth, J. K. **Localization, delocalization, and topological transitions in disordered two-dimensional quantum walks**. Phys. Rev. B 91, 104202 (2015).
- [14] Zhang, R., Xue, P. Twamley, J. **One-dimensional quantum walks with single-point phase defects**. Physical Review A 89, 042317(2014).
- [15] Li, Z., Izaac, J. Wang, J. Physical **Position-defect-induced reflection, trapping, transmission, and resonance in quantum walks**. Review A 87, 012314 (2013).
- [16] Zhang, R. Xue, P **Two-dimensional quantum walk with position-dependent phase defects**. Quantum Information Processing 13,1825–1839 (2014).
- [17] Schreiber, A. et al. **Decoherence and disorder in quantum walks: from ballistic spread to localization**. Physical review letters 106,180403 (2011).
- [18] Salimi, S. Yosefani, R. **Asymptotic entanglement in 1d quantum walks with a time-dependent coined**. International Journal of Modern Physics B 26, 1250112 (2012).

- [19] Kitagawa, T. **Topological phenomena in quantum walks: elementary introduction to the physics of topological phases.** Quantum Information Processes 11, 1107 (2012)
- [20] F. Zahring, G. Kirchmair, R. Gerritsma, E. Solano, R. Blatt, and C. F. Roos, **Realization of a Quantum Walk with One and Two Trapped Ions** Phys. Rev. Lett. 104, 100503 (2010).
- [21] H. Schmitz, R. Matjeschk, Ch. Schneider, J. Glueckert, M. Enderlein, T. Huber, and T. Schaetz **Quantum Walk of a Trapped Ion in Phase Space** Phys. Rev. Lett. 103, 090504 (2009).
- [22] M. Karski, L. Forster, J.-M. Choi, A. Steffen, W. Alt, D. Meschede, and A. Widera, **Quantum Walk in Position Space with Single Optically Trapped Atoms** Science 325, 174 (2009).
- [23] M. Genske, W. Alt, A. Steffen, A. H. Werner, R. F. Werner, D. Meschede, and A. Alberti, **Electric Quantum Walks with Individual Atoms** Phys. Rev. Lett. 110, 190601 (2013).
- [24] A. Schreiber, K. N. Cassemiro, V. Potocek, A. Gabris, P. J. Mosley, E. Andersson, I. Jex, and C. Silberhorn, **Photons Walking the Line: A Quantum Walk with Adjustable Coin Operations** Phys. Rev. Lett. 104, 050502 (2010).
- [25] A. Peruzzo, M. Lobino, J. C. F. Matthews, N. Matsuda, A. Politi, K. Poulios, X.-Q. Zhou, Y. Lahini, N. Ismail, K. W. Whoff et al., **Quantum Walks of Correlated Photons** Science 329, 1500 (2010).
- [26] Kitagawa, T., Rudner, M. S., Berg, E. Demler, E. **Exploring topological phases with quantum walks.** Physical Review A 82, 033429(2010).

- [27] Kitagawa, T. et al. **Observation of topologically protected bound states in photonic quantum walks.** Nature communications 3, 882(2012).
- [28] Yutaka Shikano and Hosho Katsura, **Localization and fractality in inhomogeneous quantum walks with self-duality.** Phys. Rev. E 82, 031122 (2010).
- [29] Hideaki Obuse and Norio Kawakami, **Topological phases and delocalization of quantum walks in random environments.** Phys. Rev. B 84, 195139 (2011).
- [30] T. Chattaraj and R. V. Krems, **Effects of long-range hopping and interactions on quantum walks in ordered and disordered lattices.** Phys. Rev. A 94, 023601 (2016)
- [31] Hideaki Obuse and Norio Kawakami, **Topological phases and delocalization of quantum walks in random environments,** Physical Review B 84, 195139 (2011).
- [32] Zeng, M., Yong, E.H., **Discrete-Time Quantum Walk with Phase Disorder: Localization and Entanglement Entropy.** Sci Rep 7, 12024 (2017).
- [33] Peng Xue et.al. **A one-dimensional quantum walk with multiple-rotation on the coin** arXiv:1404.1611
- [34] CVC Mendes et.al, **Localization properties of a discrete-time 1D quantum walk with generalized exponential correlated disorder** Physics Letters A, 2021 - Elsevier
- [35] I. Vakulchyk, M. V. Fistul, P. Qin, and S. Flach, **Anderson localization in generalized discrete time quantum walks** Phys. Rev. B 96, 144204
- [36] F. L. Marquezino, R. Portugal, S. Boettcher, **Quantum Search Algorithms on Hierarchical Networks** arXiv:1205.0529

- [37] A. Joye and M. Merkli, *J. Stat. Phys.* **140**, 1025 (2010). **Dynamical Localization of Quantum Walks in Random Environments**
- [38] A. Ahlbrecht, V. B. Scholz, and A. H. Werner, *J. Math. Phys.* **52**, 102201 (2011). **Disordered quantum walks in one lattice dimension**
- [39] F. De Nicola, L. Sansoni, A. Crespi, R. Ramponi, R. Osellame, V. Giovannetti, R. Fazio, P. Mataloni, and F. Sciarrino, *Phys. Rev. A* **89**, 032322 (2014). **Quantum simulation of bosonic-fermionic noninteracting particles in disordered systems via a quantum walk**
- [40] Tibor Rakovszky and Janos K. Asboth *Phys. Rev. A* **92**, 052311 **Localization, delocalization, and topological phase transitions in the one-dimensional split-step quantum walk**
- [41] V. Kendon, **Decoherence in quantum walks – a review.** *Mathematical Structures in Comp. Sci.* **17** (2007), no. 6, 1169–12
- [42] Alexey A Melnikov, Leonid E Fedichkin, and Alexander Alodjants, **Predicting quantum advantage by quantum walk with convolutional neural networks.** *New J. Phys.* **21** (2019) 125002