- Final report -
A model of confined quantum random walk

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Abstract

This report summarizes our research process on the behaviour of quantum random walks within the specific model of the Creutz ladder. We begin by introducing fundamental concepts related to classical random walks, quantum random walks and some key differences between them. We then focus on our specific case study, examining the property of localization. By utilizing combinatorial methods and providing some visualization, we obtained interesting results regarding the confinement of the particle on the quantum lattice.

1 Introduction

1.1 Classical random walks (CRW)

1.1.1 Discrete CRW in 1D

Random walk (RW) is a mathematical process that describes a path consisting of a series of random steps. It can be applied in various fields, particularly in physics, it could be used to model the diffusion of particles in a medium.

In our project, we focused on the simplest classical RW, which is in 1D. Basically, assuming that there is a particle at the origin of the integer line, each turn the particle can move to the left (right) by 1 unit with the probability p_L (p_R) with $p_L + p_R = 1$. Since the probability of finding the particle d units away from the origin equals to the probability of finding it $d-1$ ($d+1$) units away from the origin then moving right (left) to reach the distance d, we could write down the master equation

$$P(d, t+1) = p_R P(d-1, t) + p_L P(d+1, t), \tag{1}$$

where $P(d,t)$ is the probability of finding the particle $d \in \mathbb{Z}$ units away from the origin after $t \in \mathbb{N}$ turns. This equation describes how the probability $P(d,t)$ evolves in time with initial condition $P(0,0) = 1, P(d \neq 0, 0) = 0$.

We derived the expression of $P(d,t)$ by examining the polynomial

$$(p_L \chi_L + p_R \chi_R)^T, \tag{2}$$

where χ_L, χ_R are dummy variances representing the particle moves left or right accordingly. We denote $n_L(n_R)$ the number of steps the particle takes to left (right) after T turns then if the particle is found at d after T turns, $n_R + n_L = T, n_R - n_L = d$. That means $n_R = (T+d)/2, n_L = (T-d)/2$, which is why d must have the same parity as T and the probability $P(d,T)$ equals to the coefficient of the term $\chi_R^{n_R}\chi_L^{n_L}$ in Eq. (2)

$$P(d,T) = \binom{T}{n_R} p_R^{n_R} p_L^{n_L} = \binom{T}{\frac{T+d}{2}} p_R^{\frac{T+d}{2}} p_L^{\frac{T-d}{2}}. \tag{3}$$

We can see that the mean distance of the particle from the origin after T turns is

$$\langle d \rangle = \sum_{d=-T,-T+2,\cdots}^{T} dP(d,T) \tag{4}$$

and the variance $\langle d^2 \rangle$, which tells us about the dispersion of the particle is

$$\langle d^2 \rangle = \sum_{d=-T,-T+2,\cdots}^{T} d^2 P(d,T). \tag{5}$$

Considering the simple case of symmetric walk ($p_L = p_R = 1/2$), we can see that the mean distance in this case $\langle d \rangle = 0$ since the particle has equal chance to move left or right each turn and notably, the variance $\langle d^2 \rangle = T$, proved by denoting $j = (T+d)/2$ and we have

$$\begin{aligned}
\langle d^2 \rangle &= \frac{1}{2^T} \sum_{j=0}^{T} (T-2j)^2 \binom{T}{j} = \frac{1}{2^T} \left(T^2 \sum_{j=0}^{T} \binom{T}{j} - 4T \sum_{j=0}^{T} j \binom{T}{j} + 4 \sum_{j=0}^{T} j^2 \binom{T}{j} \right) \\
&= \frac{1}{2^T} \left(T^2 2^T - 4T^2 \sum_{j=0}^{T-1} \binom{T-1}{j} + 4T \sum_{j=0}^{T-1} j \binom{T-1}{j} + 4T \sum_{j=0}^{T-1} \binom{T-1}{j} \right) \\
&= \frac{1}{2^T} \left(T^2 2^T - 4T^2 2^{T-1} + 4T(T-1) 2^{T-2} + 4T 2^{T-1} \right) = T.
\end{aligned} \tag{6}$$

That means the particle will mostly be $\sqrt{\langle d^2 \rangle} = \sqrt{T}$ unit distance away after T turns. That is, to cover the same distance as a normal particle moving in one direction, a random walk particle needs T^2 time instead of T.

1.1.2 Continuous CRW in 1D

We had solved the discrete version using combinatorics, we then studied how to transform discrete RW to continuous version by using Taylor's approximation. Because we advance time in dt and distance in dx unit, where the limit dt, dx will be taken to 0, working with probability density function (pdf) $\rho(x,t)$ instead of probability $P(x,t)$ is appropriate. They are related by the relation that the probability $P(x,t)$ to find the particle near the position x is $\rho(x,t)dx$. From Eq. (1) we get the evolution equation for the pdf

$$\rho(x, t+dt) = p_R \rho(x - dx, t) + p_L \rho(x + dx, t). \tag{7}$$

We again simply consider the symmetric random walk, then perform a first-order Taylor expansion on the left-hand side of Eq. (7) wrt x and a second-order Taylor expansion on the right-hand side wrt t and obtain the diffusion equation

$$\frac{\partial \rho(x,t)}{\partial t} = D \frac{\partial^2 \rho(x,t)}{\partial x^2}, \tag{8}$$

where the diffusion constant $D = dx^2/2dt$. Solving this second order PDE with the initial condition $\rho(x,0) = \delta(x)$, where $\delta(x)$ is the dirac-delta function, we obtain the pdf $\rho(x,t)$ given by Gaussian distribution

$$\rho(x,t) = \frac{1}{\sqrt{4\pi Dt}} exp\left(-\frac{x^2}{4Dt}\right). \tag{9}$$

So that the mean wrt time $\langle d(t)\rangle = 0$ and the variance wrt time $\langle d^2(t)\rangle = 2Dt$. Hence, the scaling of the variance $\langle d^2\rangle = O(T)$ (diffusive regime) similar to that in the discrete version. Nevertheless, the probabilities in the two version are not the same. As the probability of finding the particle at the specific point in continuous RW is indeed 0, we consider the probability $P(I,t)$ of finding the particle located within a certain interval I. We simulated a particular case and obtained the plot in figure 1. The probability $P(I,t)$ in term

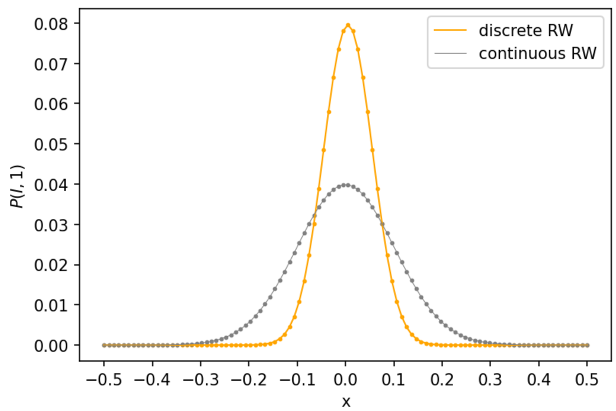


Figure 1: The probability of finding the particle at a distance d from the origin, where $d \in I = [x, x+dx)$, after time $t = 1$, with the units of distance and time for the discrete RW (dx and dt) both being 0.01.

of discrete RW means the probability of finding the particle after time t in half-open interval $I = [x, x+dx)$, which is simply the probability of finding it at the position x. As demonstrated, the probability of finding the particle near the origin is higher in discrete version, which intuitively could be seen as the result of the position and time step in continuous RW approaching 0 making it a continuous range of possible positions rather than being confined to discrete steps. This results in the smoother, broader curve for the continuous random walk compared to the sharper peak seen in the discrete case.

1.1.3 The 2-SAT problem and CRW algorithm

[...]
- Introduce k-SAT problem, 2-SAT problem solved by CRW algorithm.
- Proof.
- Scaling of algorithms –> motivation for quantum algorithms which could solve the problem faster.

1.2 Quantum random walk (QRW)

We started this section by a simple example of phase interference showing why quantum algorithms could be faster and saw that due to constructive wave interference, quantum random walk could achieve the ballistic regime ($\langle d^2\rangle = O(T^2)$). Furthermore, if the phase information is lost, the quantum random walk and classical random walk coincide. It is also a way to make a quantum random walk into a classical walk, namely phase decoherence in the coin space.

We defined the quantum random walk analogously by using coin to control movement of the particle. However, the coin is no longer classical but a quantum coin and we work with system wave function $|\psi\rangle$ instead of probability P.

The QRW works in the Hilbert space which is the tensor product $\mathcal{H}_d \otimes \mathcal{H}_c$, where $\mathcal{H}_d$ is the position space with the shifting operator $\hat{S}$ and $\mathcal{H}_c$ is the coin space with the tossing operator $\hat{C}$. Therefore, the discrete time Schodinger evolution equation of the particle can be described by

$$|\psi_{t+1}\rangle = \hat{S}\hat{C}\,|\psi_t\rangle = (\hat{S}\hat{C})^{t+1}\,|\psi_0\rangle\,. \tag{10}$$

We particularly worked with an example of discrete state $\{|n\rangle\}$ ($n \in \mathbb{Z}$) and a common coin operator, the Hadamard coin operator which is given by

$$\hat{C} = \hat{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{11}$$

By updating the rule of QRW similar to the Eq. (1) then using Fourier transform to solve the wave function, we finally obtained that the scaling of variance in QRW is $O(T^2)$.

2 Quantum random walk on a lattice

We have seen above the dispersion rate of QRW in 1D with a quadratic speed up over a classical random walk, the scaling of variance $\langle d^2\rangle = O(T)$ or $O(T^2)$ means that the particle can move to the infinity with a finite probability. So in the next phase of the project we mainly focused on another interesting case of QRW, which is called localization and has $\langle d^2\rangle = O(1)$. We introduce a model and study the randomness on it.

2.1 Creutz ladder model

The Creutz ladder is a quantum toy lattice in which the electrons are localized. The Hamiltonian of the

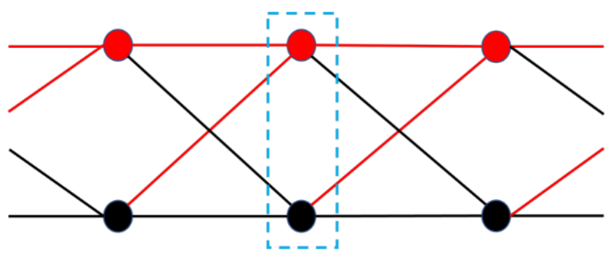


Figure 2: Creutz ladder with threading magnetic field. The red edge has hopping amplitude 1 and the black edge has hopping amplitude -1. The blue-dashed square is a unit cell of the ladder. Each cell has two sites/orbitals (red site and black site)

system with the creation and annihilation operators is given by

$$\begin{aligned}\hat{H}_{\text{Creutz}} = &\sum_j \Big[\Big(\hat{c}^\dagger_{j+1,r}\hat{c}_{j,r} - \hat{c}^\dagger_{j+1,b}\hat{c}_{j,b}\Big) + \Big(\hat{c}^\dagger_{j+1,r}\hat{c}_{j,b} - \hat{c}^\dagger_{j+1,b}\hat{c}_{j,r}\Big) \\ &+ \Big(\hat{c}^\dagger_{j,r}\hat{c}_{j+1,r} - \hat{c}^\dagger_{j,b}\hat{c}_{j+1,b}\Big) + \Big(\hat{c}^\dagger_{j,b}\hat{c}_{j+1,r} - \hat{c}^\dagger_{j,r}\hat{c}_{j+1,b}\Big)\Big]\,. \end{aligned} \tag{12}$$

Our task is Fourier transforming $\hat{H}$ into the momentum space k, obtaining

$$\hat{H} = \int_{-\pi}^{\pi} \mathrm{dk}\, \begin{bmatrix} \hat{c}^\dagger_{r,j} & \hat{c}^\dagger_{b,j} \end{bmatrix} H(k) \begin{bmatrix} \hat{c}_{r,j} \\ \hat{c}_{b,j} \end{bmatrix}, \quad H(k) = \begin{bmatrix} 2\cos k & 2i\sin k \\ -2i\sin k & -2\cos k \end{bmatrix}, \tag{13}$$

the Bloch-Hamiltonian matrix $H(k)$ has the eigenvalues independent of k. Deducing its corresponding eigenvector $|g_n(k)\rangle$, one can imply that the particle is localized by constructing the Wannier functions

$$|w_n(k)\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \mathrm{dk}\; e^{ijk}\,|g_n(k)\rangle\,. \tag{14}$$

The Wannier functions are localized at the $0-th$ and $1-st$ unit cell. Since the energy bands $\lambda_n(k)$ are flat (independent of k), the Wannier functions are also eigenstates of the Hamiltonian. The localization property is proved for this model.

2.2 Introduce randomness into the model

Now we consider if the localization still holds when we simulate a quantum random walk on it by introducing the coin operator $\hat{C}$ and the shifting operator $\hat{S}$. The new system studied can be described in this figure.

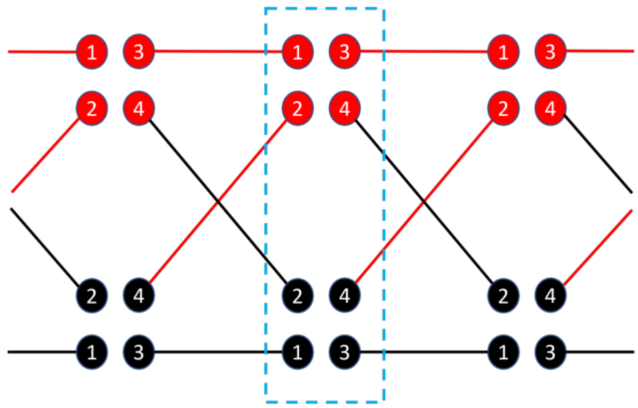


Figure 3: We incorporate the coin space into the lattice space by introducing additional sites/orbitals per unit cell. Since each red/black site in the original Creutz-ladder has 4 edges, the dimension of the coin space for each red/black site is 4.

To be specific, we model the coin flip operator using Grover G_4 coin because it is symmetric wrt all coin states

$$G_4 = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}, \quad C = Id \otimes G_4, \tag{15}$$

and the shifting operator is given by

$$\begin{aligned} S = \sum_i \big(& -|i-1,3R\rangle\langle i,1R| - |i+1,1R\rangle\langle i,3R| - |i-1,4B\rangle\langle i,2R| \\ & + |i+1,2B\rangle\langle i,4R| + |i-1,3B\rangle\langle i,1B| + |i+1,1B\rangle\langle i,3B| \\ & + |i-1,4R\rangle\langle i,2B| - |i+1,2R\rangle\langle i,4B| \big), \end{aligned} \tag{16}$$

where, for instance, the state $|i,3R\rangle$ describing that the drunkard walker is located at the red orbital of the $i-th$ unit cell, and the coin state is 3.
Following the previous problem, we investigated the "Bloch energy" and saw it is flat. However, the existence of flat bands does not guarantee the localization so we continued working more using combinatorial approach. Denoting $|\psi_n, t\rangle$ the amplitude vector of finding the particle in $n-th$ unit cell at time t, we can write a master equation for the time evolution of the particle

$$|\psi_n, t+1\rangle = F|\psi_{n-1}, t\rangle + B|\psi_{n+1}, t\rangle, \tag{17}$$

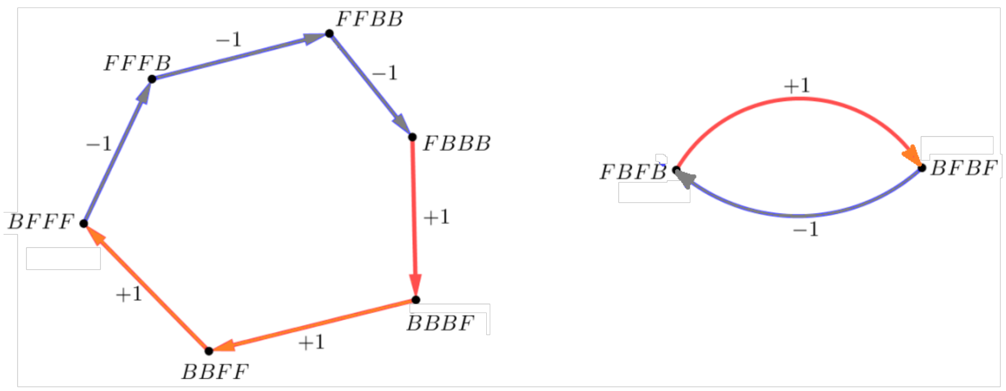
where F, B are respectively the *forward* and *backward* operators. We found the expression of F and B based on the shifting operator and tensor product with $\hat{C}$. Applying the Jordan decomposition to F and B, we proved that

$$F^4 = 0 = B^4 \tag{18}$$

which hints that the particle cannot move beyond $|d| = 3$. We then proved the foresight utilizing combinatorial method. The master equation can be expressed as the sequence of F, B, we made a table of product between these operators $\{FF, FB, BF, BB\}$.

	FF	FB	BF	BB
FF	0	*	0	*
FB	0	*	0	*
BF	*	0	*	0
BB	*	0	*	0

For every sequence with $|n(F) - n(B)| \geq 4$, the sequence will contains at least 1 subsequence from $\{FFFF, FFBF, FBFF, FBBF, BFFB, BFBB, BBFB, BBBB\}$ that means no matter which path we departed from the origin, the particle cannot escape the $|d| = 3$ region as hinted by the Jordan decomposition. It is because there are only 2 possible types of sequence that the product does not equal zero $(\cdots FFFBBBFFFBBB\cdots)$ with $\max|n(F) - n(B)| = 3$ and $(\cdots FBFBFB\cdots)$ with $\max|n(F) - n(B)| = 1$.



3 Visualization

Along with doing the analytical tasks, we also numerically simulated the quantum walk on the lattice, and checked some cases by comparing the plot with what we expected from analytical solution. One of these is to numerically check that if the particle is at the origin at $T = 0$, the particle will never be 3 unit cells away from the origin.

As we can see in the plot, if $|d| > 3$ the probability of finding the particle equals zero, which goes hand-in-hand with the laid-out mathematical solution.

We also discovered that after a certain period of time, there is a repeating pattern of particle location probability. This will also be our further research direction to explain this recurring phenomenon.

4 Discussion

This study investigates quantum random walks (QRWs) within the Creutz ladder model, revealing significant localization. The results enhance our understanding of QRWs and their applications in quantum researchs. We demonstrated diffusive behavior in classical random walks and ballistic behavior in QRWs. Introducing randomness via a Grover coin operator in the Creutz ladder model provided a novel approach to QRWs in a confined lattice. These findings align with previous research and suggest that structured lattices with quantum coins and shifting operators can induce significant localization, beneficial for designing quantum

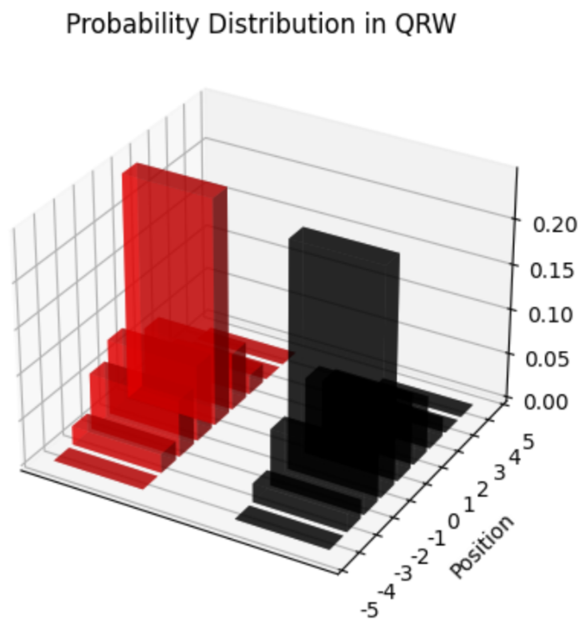


Figure 4: The average probability of particle position after a period of time T has passed

algorithms requiring controlled particle movement.
However, the project is of a preliminary research nature, applying acquired knowledge to study a specific topic under the instruction of our mentors, so there are still limitations. We wish to learn more deeply with fully grasp and broader comprehension of this field in the future.

5 Conclusion

The principal conclusions derived from our research are as follows:

1. **Validation of Classical and Quantum Walk Regimes**: We demonstrated the anticipated diffusive behavior in classical random walks and ballistic behavior in quantum random walks for some simple cases.

2. **Localization within the Creutz Ladder Model**: By incorporating randomness via the Grover coin operator and employing combinatorial methods, we established that the particle's movement is confined to $|d| \leq 3$.

3. **Numerical Confirmation**: Our numerical simulations substantiated the analytical findings, indicating a zero probability of the particle traversing beyond the specified confined range.

These findings contribute significantly to our comprehension of QRWs and their potential applications. The demonstrated confinement of quantum walks within the Creutz ladder model suggests promising avenues for future research into controlled quantum systems and their practical implementations.

6 Recommendations

Based on the insights gleaned from our study, we propose the following directions for further research:

1. **Exploration of Alternative Lattice Models**: Investigating various lattice structures and their effects on QRW behavior could provide deeper insights into the factors influencing localization.

2. **Development of Quantum Algorithms**: Exploiting the confinement properties observed in our study to design new quantum algorithms that necessitate precise control of quantum particle movements.
3. **Experimental Validation**: Conducting empirical studies to validate our theoretical and numerical findings within real-world quantum systems.

These recommendations aim to solidify the understanding of QRWs and expand their applicability across diverse quantum technologies.

7 References