Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

Trapping in Quantum Walks

Uvěznění v kvantových procházkách

Bachelor Thesis

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- Zadání práce -

Prohlášení

Prohlašuji, že jsem svou bakalářskou práci vypracovala samostatně a použila jsem pouze podklady (literaturu, projekty, SW atd.) uvedené v přiloženém seznamu.

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V Praze dne 8. 7. 2016 Tereza Štefková

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Abstrakt: Tato práce poskytuje úvod do kvantových procházek na přímce a v rovině. Na úvod podáme shrnutí základních poznatků o klasických náhodných procházkách. Poté zavedeme pojem kvantové procházky a na příkladu Hadamardovy procházky na přímce ilustrujeme základní vlastnosti této procházky. Následující část práce se zabývá efektem uvěznění, který zavedeme nejdříve pro třístavovou procházku na přímce. Dále rozšíříme pojem kvantové procházky do dimenze dva, kde studujeme uvěznění pro případ Groverovy procházky v rovině.
V poslední kapitole zavedeme pojem silného uvěznění a uvedeme třídu čtyřstavových mincí, které uvěznění vykazují.

Klíčová slova: klasická náhodná procházka, kvantová procházka, silné uvěznění, uvěznění

Title:
Trapping in Quantum Walks

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Abstract: In this thesis we provide an introduction to quantum walks on a line and on a two-dimensional lattice. We start with a brief summary of basic facts about classical random walks. Then we introduce the concept of quantum walks and illustrate its basic characteristics on the example of the Hadamard walk on a line.
The next part of the thesis deals with the effect of trapping which we firstly demonstrate on the three-state quantum walk on a line. Subsequently, we extend the model of the quantum walk to two dimensions and illustrate the existence of trapping in the case of the Grover walk on a lattice.
In the last chapter we introduce the term strong trapping and present a class of trapping four-state coins.

Key words: classical random walk, quantum walk, strong trapping, trapping

Contents

Introduction

Classical random walk is a stochastic process in probability theory with a wide range of applications. This term was introduced by Pearson in 1905 in the context of the mathematical formulation of random transport phenomena. The concept of classical random walks was used to describe for example Brownian motion as a model for microscopic diffusion. Recently, classical random walks has also been successfully utilized in theoretical computer science for algorithm development such as graph connectivity or solving 2-SAT and 3-SAT problem (for a short introduction see [1]).

Quantum walks, which are quantum mechanical analogues of classical random walks, were first introduced by Aharanov *et al* [2] in 1993 and also studied by Meyer [3] in the context of quantum cellular automata. Research in this field was initially motivated by development of quantum algorithms based on quantum walks that are considerably better than their classical counterparts in terms of computational complexity (i.e. they require less number of steps to solve the given problem). Among them, the most famous is the Grover search algorithm [4] that exhibits quadratic speed-up in comparison with the classical algorithms.

There have also been various experimental proposals and physical implementations of both quantum walks on a line and on a two-dimensional lattice using cold atoms in lattices, ion traps or polarization and orbital angular momentum of a photon (for a comprehensive review we recommend [5]).

The aim of this thesis is to review the basic facts known about discrete-time quantum walks on a line and on a two-dimensional lattice. Throughout the text we especially focus on one of the most striking behaviour of the quantum walks, namely on the effect of trapping.

The structure of this thesis is as follows. In the first chapter we briefly introduce the concept of classical random walks, touch upon its most significant properties so that we would be able to compare the classical model with its quantum analogue in the next chapter.

In chapter two we define two-state quantum walk and illustrate this concept with the help of the Hadamard walk on a line. We derive analytic expressions for the probability distribution and its limit distribution. We also summarize the most significant differences between classical random walks and quantum random walks.

In the third chapter we expand the two-state model to that of the tree-state quantum walk on a line, which exhibits phenomenon that cannot be observed in the two-state quantum walk - trapping.

In the fourth chapter the concept of the two-dimensional quantum walk on a lattice is introduced.

The last chapter focuses on a novel type of trapping observed in quantum walks in two dimensions - strong trapping and ends with a general comment on the various types of random walks introduced in the thesis.

Chapter 1

Classical random walk

Let us provide a brief introduction to classical random walks and derive its most significant properties using the simplest example of a random walk on a line and its subsequent generalization to higher dimensions.
It is important to note that there exist two types of random walks: discrete-time and continuous-time random walk. In this text we restrict ourselves only to models of discrete-time random walks.

1.1 One-dimensional random walk

A classical random walk on a line can be described as a system consisting of a particle which moves along equidistantly distributed points on a line making steps of the same length. At each step, the direction of its motion is determined by a random process, for example by a toss of a coin, which gives two possible mutually exclusive outcomes.
The crucial characteristic of this stochastic process is its probability distribution. Deriving it, we will consider a particle with the initial position at the origin ($S_0 = 0$) performing a random walk with steps of one unit. Suppose that the particle is assigned a probability p of shifting to the right and a probability $q = 1 - p$ of going to the left which can be associated with the two outcomes of the coin-flip.
The probability of finding the particle at the position x after n steps equals the probability of taking k steps to the right and l steps to the left, where k, l obviously satisfy the following relations: $x = k - l$ and $n = k + l$. This can be equivalently viewed as the probability of obtaining k times outcome p (*success*) in n flips (*trials*) of the coin. Since the next step of the random walk is independent of the previous one, the above probability is governed by the binomial distribution

$$P(S_n = x) = \binom{n}{k} p^k q^l = \binom{n}{k} p^k (1-p)^{n-k}. \tag{1.1}$$

According to the central limit theorem [6] as number of steps n tends to infinity the binomial distribution (1.1) approaches the Gaussian distribution (see Figure 1.1) with the mean value $\mu = 0$ and the variance $\sigma^2 = 1$

$$\lim_{n\to\infty} P\left(a \leq \frac{S_n - (q-p)n}{\sqrt{(4pqn)}} \leq b\right) = \int_a^b \frac{1}{\sqrt{(2\pi)}} e^{-\frac{x^2}{2}}\,\mathrm{d}x, \tag{1.2}$$

where $-\infty < a < b < +\infty$.

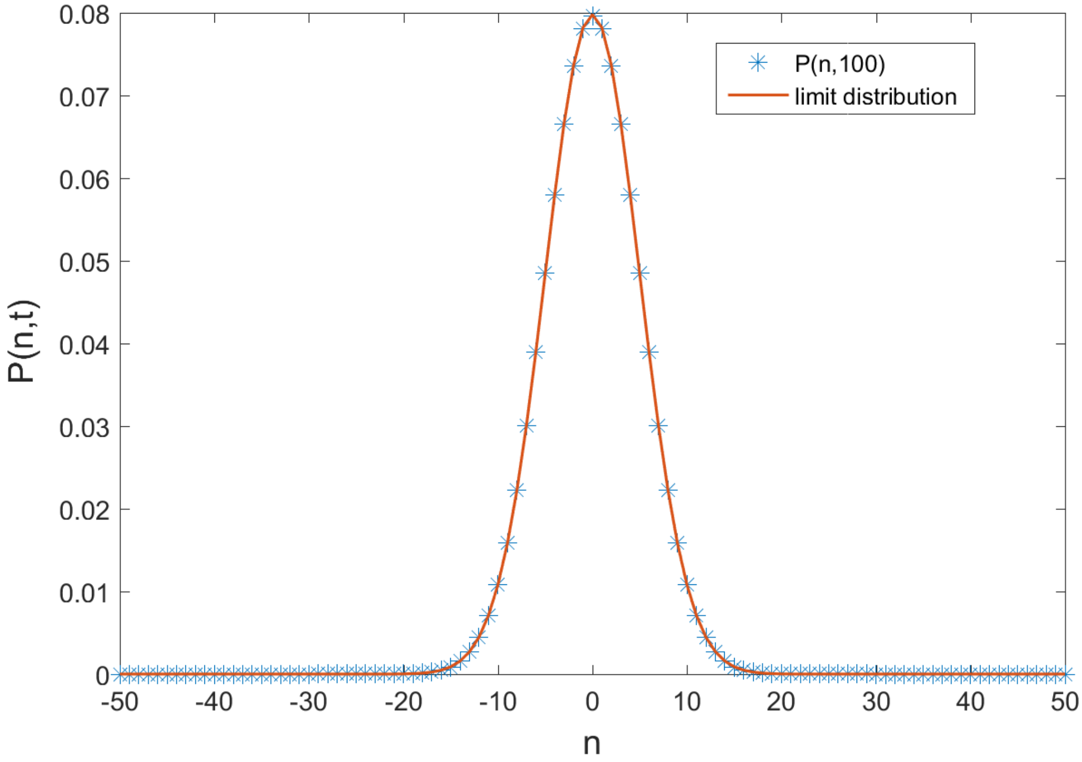

Figure 1.1: The probability distribution of the unbiased classical random walk after $t = 100$ step and its limit distribution.

1.2 Generalization to $\mathbb{Z}^d$

In this section we introduce the most straightforward generalization of the one-dimensional random walk described above. In this case the motion of the particle is restricted to d-dimensional integer lattice $\mathbb{Z}^d$ and its direction depends on a result of a coin-flip with $2d$ possible outcomes. Moreover, the coin is supposed to be 'fair', in other words, probability of the particle to jump to any of the $2d$ adjacent points is $\frac{1}{2d}$. Random walks that satisfy this condition are also referred to as simple random walks [7].
Now, using the same argument as in the previous section, we derive its probability distribution. Let us denote by $x = (x_1, \cdots, x_d)$ the position of the particle. Again we assume that the random walk starts at the origin $(0, \cdots, 0)$. Arbitrary component x_i can be rewritten as $x_i = x_{i+} - x_{i-}$, where $x_{i\pm}$ correspond to number of steps taken to the right and to the left, respectively along the i-th axis. The probability $P(S_n^d = x)$ of being at point x after n steps is given by the multinomial distribution as

$$P(S_n^d = x) = \frac{n!}{\prod_{i=1}^{d} x_{i+}!x_{i-}!} \frac{1}{(2d)^n}. \tag{1.3}$$

1.3 Returns to the origin

In the following we will be interested in one significant characteristic of classical random walks, namely in the probability of its eventual return to the origin called the Pólya number. According to this property,

random walks are classified as *recurrent*, if the Pólya number equals 1 and *transient* otherwise [8].
In the following we take advantage of the trivial fact that the probability of return is 0 for odd number of steps. Therefore, we compute the corresponding probabilities after $2n$ steps instead which leads to physically equivalent results.
Let Q be the Pólya number and p_k, q_k two sequences representing the probability that the particle is at the origin after k steps and the probability that the particle returns to the origin after k steps for the first time (for more details see [9]). The relation between these sequences is following

$$\begin{aligned} p_0 &= 1 \\ p_2 &= q_2 \\ p_4 &= q_4 + p_2 q_2 \\ &\vdots \\ p_{2k} &= q_{2k} + q_{2k-2}p_2 + \cdots + q_2 p_{2k-2} \\ &\vdots \end{aligned} \tag{1.4}$$

if we add those equation to infinity we obtain

$$\sum_{k=0}^{\infty} p_k = \sum_{k=0}^{\infty} p_k \sum_{k=1}^{\infty} q_k + 1. \tag{1.5}$$

Since also $Q = \sum_{k=1}^{\infty} q_k$ the Pólya number can be expressed as

$$Q = 1 - \frac{1}{\sum\limits_{k=0}^{\infty} p_k}. \tag{1.6}$$

This leads us to a simple criterion: The point 0 is recurrent if and only if $\sum_{k=0}^{+\infty} P(S_k = 0) = +\infty$.

Now, we use this criterion to prove recurrence or transience for simple random walks in dimensions 1, 2 and 3.
For a one-dimensional simple random walk the probability of finding the particle at the origin can be written according to equation (1.1) as

$$P(S_{2n}^{1D} = 0) = \binom{2n}{n}\frac{1}{2^{2n}}, \tag{1.7}$$

which can be rewritten, using Stirlig's formula, [1] as

$$P(S_{2n}^{1D} = 0) \approx \frac{1}{\sqrt{\pi n}}. \tag{1.8}$$

Since the series $\sum_{n=1}^{\infty} \frac{1}{\sqrt{n}}$ is divergent, one-dimensional random walk is recurrent according to the above criterion.
For a two-dimensional walk the corresponding probability is given as

$$P(S_{2n}^{2D} = 0) = \frac{1}{4^{2n}} \sum_{k=0}^{n} \frac{(2n)!}{(k!)^2((n-k)!)^2} = \frac{1}{4^{2n}}\binom{2n}{n}^2. \tag{1.9}$$

[1] Stirling's formula: $n! \approx \sqrt{2\pi n}\, n^n\, e^{-n}$

Similarly, this can be approximated as

$$P(S_{2n}^{2D} = 0) \approx \frac{1}{\pi n}. \tag{1.10}$$

Again, the corresponding series is divergent, hence random walk in dimension two is reccurent.
In the three dimensions the probability of finding the particle at the origin after $2n$ steps is given as

$$P(S_{2n}^{3D} = 0) = \frac{1}{6^{2n}} \sum_{j,k=0}^{j+k\leq n} \frac{(2n)!}{(k!)^2 (j!)^2 ((n-k-j)!)^2}. \tag{1.11}$$

After some algebra (for detailed computation see [10]) we get

$$P(S_{2n}^{3D} = 0) \approx \frac{const}{\sqrt{n^3}}. \tag{1.12}$$

In this case the series converges. As a result, three-dimensional random walk is transient.
It can be shown that simple random walks in dimension $d > 3$ are transient [8].

1.4 Markov chains

A classical random walk can also be viewed as a Markov chain (for a detailed introduction to Markov chains see [11]), which is a random process where the next step is independent of the previous evolution. In the following we give a notion of Markov chains with the example of classical random walk on a d-regular graph [2].
Let G be d-regular graph and I set of its vertices. We denote as p_n the probability distribution over vertices I after n steps, i.e. its components satisfy $0 \leq p_{n_i} \leq 1$, $i \in I$ and $\sum_{i\in I} p_{n_i} = 1$.
The evolution is generated by the transition matrix P, where $0 \leq P_{ij} \leq 1$ and $\sum_{j\in I} P_{ij} = 1$. At the same time, the element P_{ij} equals the probability of going from vertex i to vertex j. The probability distribution over I after the n-th step of random walk is then given as $p_n = P\, p_{n-1}$.
We illustrate the idea of a Markov chain with the example of a simple classical random walk on a circle of N vertices. In this case the transition matrix is given as

$$P = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & & 0 \\ 0 & 1 & 0 & 1 & & & \vdots \\ 0 & 0 & 1 & 0 & \ddots & & \\ \vdots & \vdots & & \ddots & & 1 & 0 \\ 0 & & & & 1 & 0 & 1 \\ 1 & 0 & \cdots & & 0 & 1 & 0 \end{pmatrix} \tag{1.13}$$

and the probability distribution after n steps is given by $p_n = P^n\, p_0$. The probability distribution of this random walk approaches the stationary distribution $p_\infty = (\frac{1}{N}, \cdots, \frac{1}{N})$ [12].

There exist several other characteristics that describe important aspects of the behaviour of random walks. The most important of them for the application of random walks in computer science are the so-called *hitting time* and *mixing time* [12].

[2] D-regular graphs are graphs with vertex-degree d, in other words each vertex has d outgoing edges.

Hitting time H_{ij} is the expected number of steps before the vertex j is visited for the first time during the evolution of the random walk starting from vertex i.
On the other hand, *mixing time* represents the number of steps before the probability distribution of the classical random walk is close enough to its limit distribution.

In this chapter we summarized several basic facts about classical random walks so that we could compare this model with that of a quantum walk which we introduce in the next chapter.

Chapter 2

One-dimensional quantum walk

Quantum walk is the quantum-mechanical counterpart of the classical random walk. The simplest example of the quantum walk is a one-dimensional walk on a line, which consists of a quantum particle that makes steps of the same length of one unit either to the left or to the right.
At this point we note that in the following we restrict ourselves to the so-called discrete-time quantum walks. Similarly to classical random walks, there also exist continuous-time quantum walks. Unlike the discrete-time quantum walks, the continuous-time quantum walks do not use a coin and their time evolution is given by the unitary operator $U(t) = \exp(-iHt)$, where H represents the Hamiltonian of the system [13].

2.1 Definition of the one-dimensional two-state quantum walk on a line

Let us now describe the model of a two-state quantum walk on a line.
The position of the particle at each time can be described by a vector from Hilbert space $\mathcal{H}_p$ spanned by the basis states $\{\,|n\rangle\,; n \in \mathbb{Z}\,\}$.
To obtain non-trivial correctly defined quantum walk we use an additional degree of freedom called a coin. In case of the two-state quantum walk, the coin is assigned a coin space $\mathcal{H}_c$ spanned by two basis states we denote $|L\rangle$ and $|R\rangle$ corresponding to the direction of motion to the left and to the right. In the following, we associate $|L\rangle$ and $|R\rangle$ with $\binom{1}{0}$ and $\binom{0}{1}$, respectively.
The state of the whole system is thus represented by a vector from Hilbert space $\mathcal{H}$, where $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$ is the tensor product of Hilbert spaces $\mathcal{H}_c$ and $\mathcal{H}_p$.
The evolution of a quantum walk is a unitary process on the Hilbert space $\mathcal{H}$, which comprises of two subsequent transformations of the state vector. First, the coin state is rendered in a superposition by the application of the coin operator C, which acts on the coin space $\mathcal{H}_c$ and resembles a coin-flip in the classical random walk. Subsequently, we realize the translation of the particle using conditional step operator S on the state vector that moves the particle to the adjacent integer point on a line according to the outcome of the previous coin-flip. The unitary step operator S can be described as follows

$$S = |L\rangle\langle L| \otimes \sum_{n\in\mathbb{Z}} |n-1\rangle\langle n| + |R\rangle\langle R| \otimes \sum_{n\in\mathbb{Z}} |n+1\rangle\langle n|\,. \tag{2.1}$$

Each step of the quantum walk is then realized by the unitary operator U

$$U = S\,(C \otimes I) \tag{2.2}$$

which gives the following expression for the state of the quantum walk after t steps with the initial state $|\psi(0)\rangle$

$$|\psi(t)\rangle = U^t |\psi(0)\rangle . \tag{2.3}$$

Before we proceed, let us denote by $\psi_R(n,t)$, $\psi_L(n,t)$ the probability amplitude of finding the particle at point n after t steps with the coin-state value R and L, respectively. We also define vector of these amplitudes as

$$\psi(n,t) = \begin{pmatrix} \psi_L(n,t) \\ \psi_R(n,t) \end{pmatrix} = \psi_L(n,t)|L\rangle + \psi_R(n,t)|R\rangle . \tag{2.4}$$

The corresponding probability is then given by

$$P(n,t) = |\psi_L(n,t)|^2 + |\psi_R(n,t)|^2. \tag{2.5}$$

In this notation, the time evolution (2.3) attains the following form

$$|\psi(t)\rangle = \sum_{n\in\mathbb{Z}} \Big(\psi_L(n,t)|L\rangle + \psi(n,t)|R\rangle \Big) \otimes |n\rangle . \tag{2.6}$$

2.2 The Hadamard walk on a line

In the previous section we described the time evolution of a quantum walk as a successive application of a unitary operator. Now, we will try to obtain general expressions for amplitudes of the particle being at the position n at given time t in the case of the so-called Hadamard walk which is a typical example of a quantum walk on a line. The unitary operation on the coin space is represented by the Hadamard operator

$$\hat{H} = \frac{1}{\sqrt{2}}\Big(|L\rangle\langle L| + |L\rangle\langle R| + |R\rangle\langle L| - |R\rangle\langle R| \Big) \tag{2.7}$$

which has this form in the basis $|L\rangle = \binom{1}{0}$, $|R\rangle = \binom{0}{1}$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{2.8}$$

It is worth to note that the Hadamard walk is a balanced quantum walk which means that in one step the probability of going to the left equals probability of shifting to the right.

There exist two major methods of quantum walk analysis. One of them, the combinatorial approach, is based on the same principle as the method used in the section concerning classical random walk: the desired probability is given as a sum of amplitudes of all the paths ending at point n after t steps.
However, in our case we will follow the so-called Schrödinger approach which was first employed by Nayak and Vishwanath [14]. The basic principle of this method is to transform the time evolution of the probability amplitude using the Discrete-Time Fourier Transform (see Appendix) analyse it in the Fourier domain and then transform it back to the spatial domain with the help of the Inverse Fourier Transform. This method represent the major method for analysis of quantum walks with homogeneous coin (e. i. the coin operator does not change during the time evolution and also stays the same for every position n) since this homogeneous quantum walks take a simple form in the Fourier domain.

In the following we demonstrate the Schrödinger approach on the example of the Hadamard walk. Obviously, in the $(t+1)$-th step of the walk only the amplitudes at the adjacent points $\psi(n-1,t)$ and $\psi(n+1,t)$

contribute to the amplitude $\psi(n,t+1)$. After the application of the Hadamard operator on $\psi(n-1,t)$ and $\psi(n+1,t)$, respectively, we obtain

$$\hat{H}\psi(n\pm 1,t) = \frac{1}{\sqrt{2}}\begin{pmatrix}\psi_L(n\pm 1,t)+\psi_R(n\pm 1,t)\\ \psi_L(n\pm 1,t)-\psi_R(n\pm 1,t)\end{pmatrix} \tag{2.9}$$

$$= \frac{1}{\sqrt{2}}\Big(\psi_L(n\pm 1,t)+\psi_R(n\pm 1)\Big)|L\rangle + \frac{1}{\sqrt{2}}\Big(\psi_L(n\pm 1,t)-\psi_R(n\pm 1,t)\Big)|R\rangle\,. \tag{2.10}$$

Taking into consideration only the contributions to the probability amplitude $\psi(n,t+1)$ we derive the following recurrent relation

$$\psi(n,t+1) = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ 0 & 0\end{pmatrix}\psi(n+1,t) + \begin{pmatrix}0 & 0\\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}\psi(n-1,t) \tag{2.11}$$

where we denote

$$H_L = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ 0 & 0\end{pmatrix},\quad H_R = \begin{pmatrix}0 & 0\\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}. \tag{2.12}$$

The evolution of the Hadamard walk starting from the initial state $(\,\alpha\,|L\rangle+\beta\,|R\rangle\,)\otimes|0\rangle$, $|\alpha|^2+|\beta|^2 = 1$, is then given as the solution of the above recurrence with the initial condition $\psi(0,0) = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ and $\psi(n,0) = \begin{pmatrix}0\\ 0\end{pmatrix}$ for $n \neq 0$.

As we have already mentioned, the task of computing analytic expression for the probability amplitude $\psi_(n,t)$ is considerably simplified in the Fourier domain. We therefore transform the recurrence (2.11) using the Discrete-Time Fourier Transform (Appendix (5.10))

$$\tilde{\psi}(k,t+1) = \sum_{n\in\mathbb{Z}}\left(H_L\,\psi(n+1,t) + H_R\,\psi(n-1,t)\right)e^{ikn} \tag{2.13}$$

which can be rewritten as

$$\begin{aligned}\tilde{\psi}(k,t+1) &= e^{-ik}H_L\sum_{n\in\mathbb{Z}}\psi(n+1,t)e^{ik(n+1)} + e^{ik}H_R\sum_{n\in\mathbb{Z}}\psi(n-1,t)e^{ik(n-1)}\\ &= (e^{-ik}H_L + e^{ik}H_R)\,\tilde{\psi}(k,t)\\ &= \tilde{U}(k)\,\tilde{\psi}(k,t)\end{aligned} \tag{2.14}$$

where

$$\tilde{U}(k) = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-ik} & e^{-ik}\\ e^{ik} & -e^{ik}\end{pmatrix} = \begin{pmatrix}e^{-ik} & 0\\ 0 & e^{ik}\end{pmatrix}H. \tag{2.15}$$

The recurrence (2.14) is thus easily rewritten as

$$\tilde{\psi}(k,t) = \tilde{U}^t(k)\,\tilde{\psi}(k,0). \tag{2.16}$$

As a result, our problem is reduced to the task of computing $\tilde{U}^t(k)$ which is easy in case of a diagonal matrix. We therefore compute eigenvalues $\lambda_1(k) = e^{-i\omega_k}, \lambda_2(k) = e^{i(\pi+\omega_k)}$ and the corresponding eigenvectors v_1, v_2 of the matrix $\tilde{U}(k)$

$$v_1(k) = \frac{1}{\sqrt{2}}\left(\left(1+\cos^2 k\right) - \cos k\sqrt{1+\cos^2 k}\right)^{-\frac{1}{2}}\begin{pmatrix}e^{-ik}\\ \sqrt{2}e^{-i\omega_k} - e^{-ik}\end{pmatrix} \tag{2.17}$$

$$v_2(k) = \frac{1}{\sqrt{2}}\left(\left(1+\cos^2 k\right) + cosk\sqrt{1+\cos^2 k}\right)^{-\frac{1}{2}}\begin{pmatrix}e^{-ik}\\ -\sqrt{2}e^{i\omega_k} - e^{-ik}\end{pmatrix} \tag{2.18}$$

where $\omega_k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ satisfies the relation $\sin\omega_k = \frac{\sin k}{\sqrt{2}}$.
The matrix $\tilde{U}^t(k)$ then can be written in the form of a diagonal matrix as

$$\tilde{U}^t(k) = \lambda_1^t(k)\ |v_1(k)\rangle \langle v_1(k)| + \lambda_2^t(k)\ |v_2(k)\rangle \langle v_2(k)| \tag{2.19}$$

which yields the following formula

$$\tilde{\psi}(k,t) = e^{-i\omega_k t}\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle |v_1(k)\rangle + e^{i(\pi+\omega_k)t}\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle |v_2(k)\rangle \tag{2.20}$$

where $\tilde{\psi}(k,0) = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ is the Fourier transform of the initial state.
If we now return to the spatial domain using Inverse Fourier Transform (see Appendix (5.11)), we obtain the general expressions for probability amplitude $\psi(n,t)$ as

$$\psi(n,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{\psi}(k,t)e^{-ink}\mathrm{d}k \tag{2.21}$$

2.3 Asymptotic behaviour of the Hadamard walk

To obtain the asymptotic form of the probability distribution for the Hadamard walk, we now follow the approach used in [15] which is based on the weak limit theorem obtained by Grimmett *et al* [16] who introduced the method of moments to derive it. The r-th moment [1] of the position operator n is given as

$$\langle n^r\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{\psi}^*(k,t)\left(i\frac{\mathrm{d}}{\mathrm{d}k}\right)^r \tilde{\psi}(k,t)\mathrm{d}k, \tag{2.22}$$

where $\left(i\frac{\mathrm{d}}{\mathrm{d}k}\right)$ is the Fourier transform of the position operator n. In the next step we express $\tilde{\psi}(k,t)$ in terms of (2.20)

$$\langle n^r\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} \tilde{\psi}^*(k,t)\left(i\frac{\mathrm{d}}{\mathrm{d}k}\right)^r \left(e^{-i\omega_k t}\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle v_1(k) + e^{i(\pi+\omega_k)t}\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle v_2(k)\right)\mathrm{d}k$$

and apply the position operator $\left(i\frac{\mathrm{d}}{\mathrm{d}k}\right)$. We consider only the contributions to the integrand in which the variable t is of order at least r

$$\begin{aligned}\langle n^r\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi}\Bigg(& t^r\left(\frac{\mathrm{d}\omega_k}{\mathrm{d}k}\right)^r e^{-i\omega_k t}\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\left\langle\tilde{\psi}(k,t)\middle|v_1(k)\right\rangle\\ &+(-1)^r t^r\left(\frac{\mathrm{d}\omega_k}{\mathrm{d}k}\right)^r e^{i(\pi+\omega_k)t}\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\left\langle\tilde{\psi}(k,t)\middle|v_2(k)\right\rangle\Bigg)\mathrm{d}k + O(t^{r-1}).\end{aligned}$$

Using again the formula (2.20) the r-th moment of the position operator n reads

$$\langle n^r\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} t^r\left(\frac{\mathrm{d}\omega_k}{\mathrm{d}k}\right)^r\left(\left|\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 + (-1)^r\left|\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2\right)\mathrm{d}k + O(t^{r-1}).$$

[1] R-th moment the operator X in quantum mechanics is given as $\langle X^r\rangle = \langle\psi|X^r|\psi\rangle$

If we subsequently rescale the position operator by number of steps t we obtain

$$\left\langle\left(\frac{n}{t}\right)^r\right\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{\mathrm{d}\omega_k}{\mathrm{d}k}\right)^r\left(\left|\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 + (-1)^r\left|\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2\right)\mathrm{d}k + O(t^{-1}) \tag{2.23}$$

which converges to the r-th moment of a variable [16]

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{\mathrm{d}\omega_k}{\mathrm{d}k}\right)^r\left(\left|\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 + (-1)^r\left|\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2\right)\mathrm{d}k = \lim_{t\to+\infty}\left\langle\left(\frac{n}{t}\right)^r\right\rangle = \langle v^r\rangle = \int v^r w(v)\mathrm{d}v. \tag{2.24}$$

We can express the following terms in the above relation as

$$\left|\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 + \left|\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 = 1 \tag{2.25}$$

$$\left|\left\langle v_1(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 - \left|\left\langle v_2(k)\middle|\tilde{\psi}(k,0)\right\rangle\right|^2 = -\frac{\cos k}{\sqrt{(1+\cos^2 k)}}\left(|\alpha|^2 - |\beta|^2 + \bar{\alpha}\beta + \alpha\bar{\beta}\right) \tag{2.26}$$

Using the substitution

$$v = -\frac{\mathrm{d}\omega_k}{\mathrm{d}k} = -\frac{\cos k}{\sqrt{1+\cos^2 k}},\ \mathrm{d}v = \frac{\sin k}{\sqrt{(1+\cos^2 k)^3}}\mathrm{d}k \tag{2.27}$$

and its inverse

$$\cos k = -\frac{v}{\sqrt{1-v^2}},\ \sin k = \pm\sqrt{\frac{1-2v^2}{1-v^2}} \tag{2.28}$$

we obtain the $\langle v^r\rangle$ in the following form due to the symmetries of the integrand

$$\langle v^r\rangle = \int_{-\frac{1}{\sqrt{2}}}^{-\frac{1}{\sqrt{2}}} v^r\,\frac{1-\left(|\alpha|^2 - |\beta|^2 + \bar{\alpha}\beta + \alpha\bar{\beta}\right)v}{\pi(1-v^2)\sqrt{1-2v^2}}\mathrm{d}v \tag{2.29}$$

which yields the probability density of the variable v as

$$w(v) = \frac{1-\left(|\alpha|^2 - |\beta|^2 + \bar{\alpha}\beta + \alpha\bar{\beta}\right)v}{\pi(1-v^2)\sqrt{1-2v^2}}. \tag{2.30}$$

Let us comment on the most general two-state quantum walk on a line. The general unitary two-dimensional matrix can be written in the following form

$$C = \begin{pmatrix} \sqrt{\rho} & \sqrt{1-\rho}e^{i\theta} \\ \sqrt{1-\rho}e^{i\varphi} & -\sqrt{\rho}e^{i(\theta+\varphi)} \end{pmatrix}, \tag{2.31}$$

where $\rho \in (0,1)$, $0 \leq \theta$ and $\varphi \leq \pi$. The global phase of the coin operator was removed since it is irrelevant for quantum walks with homogeneous coin.

In [17] Tregenna *et al* analysed quantum walk with the coin (2.31) and found the eigenvalues of this operator in the Fourier domain as $\lambda_{1,2} = \pm e^{i\delta}e^{\pm\omega_k}$, where $\delta = \frac{\theta+\varphi}{2}$ and ω_k satisfy relation $\sin\omega_k = \sqrt{\rho}\sin(k-\delta)$. Notice that the eigenvalues are dependent of variable k for all two-state quantum walks on a line.

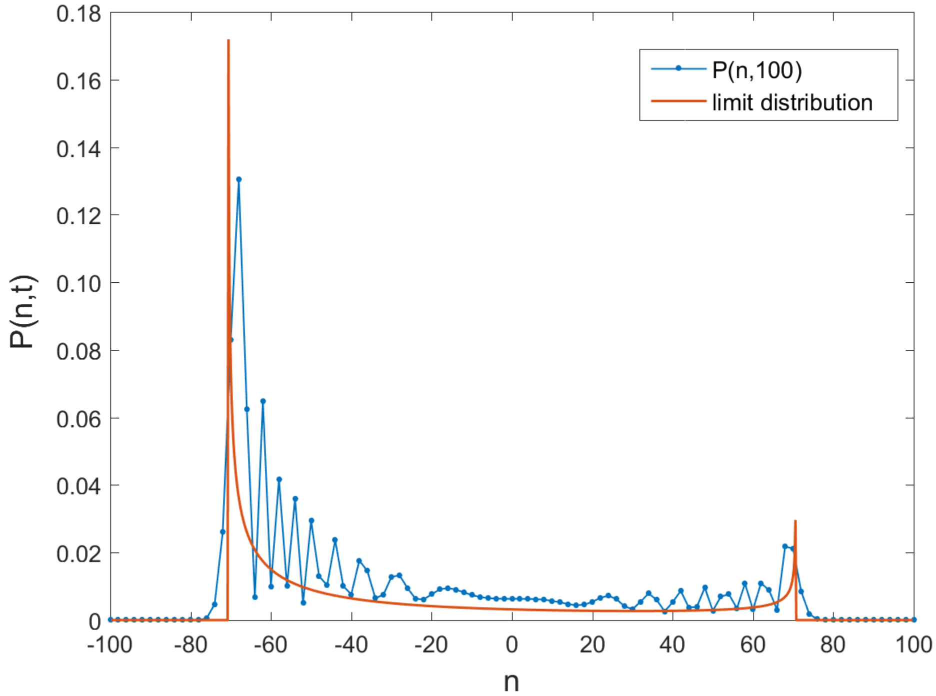

Figure 2.1: The probability distribution of the Hadamard walk after $t = 100$ step with the limit distribution (2.30) of the variable $\frac{n}{t}$ normalized by $\frac{1}{t}$.

2.4 Quantum walk vs. classical random walk

We have seen that the classical random walk is a stochastic process which satisfies the Markov property. In contrast, the model of a homogeneous quantum walk described above is a deterministic process since every step of this walk is governed by one unitary transformation. Moreover, the requirement of "memorylessness" of the random walk cannot be satisfied in the case of its quantum counterpart since every unitary process is reversible. The probabilistic nature of the quantum walk stems solely from the quantumness of the particle.
The limit distributions of those two types of walks exhibit significant differences. The limit distribution of the quantum walk does not have one peak centered around the origin since, due to the quantum-mechanical properties of the particle, the amplitudes interfere (compare Figure 1.1 and Figure 2.1).
As can be seen from the comparison of the limit distributions, more precisely from the scaling factor of the probability distribution (1.2) and (2.30), the quantum walk propagates quadratically faster. This feature of quantum walks is utilized in quantum algorithm development.

Chapter 3

Three-state quantum walk on a line

In this chapter we extend the model of the two-state quantum walk on a line to that of the three-state quantum walk to demonstrate one remarkable property of quantum walks called trapping, previously referred to as localization. We note that similar effect can be observed in case of four-state quantum walks on a lattice.

3.1 Definition of the one-dimensional three-state quantum walk on a line

In the case of the three-state quantum walk there are three possible states of the coin (the internal degree of freedom): in one step of the walk the particle can move to the left, to the right or stay at its current position. The coin space thus has to be augmented by a basis vector which we denote by $|S\rangle$ representing the option with no motion. We choose the following basis of the coin space

$$\mathcal{H}_c = \text{span}\left\{|L\rangle, |S\rangle, |R\rangle\right\} = \text{span}\left\{\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}\right\}. \tag{3.1}$$

The corresponding shift operator S is given by

$$S = |L\rangle\langle L| \otimes \sum_{n\in\mathbb{Z}} |n-1\rangle\langle n| + |S\rangle\langle S| \otimes \sum_{n\in\mathbb{Z}} |n\rangle\langle n| + |R\rangle\langle R| \otimes \sum_{n\in\mathbb{Z}} |n+1\rangle\langle n| \tag{3.2}$$

and every step of the walk is a unitary process represented by the evolution operator U (2.2). Again, we denote by

$$\psi(n,t) = \begin{pmatrix}\psi_L(n,t)\\ \psi_S(n,t)\\ \psi_R(n,t)\end{pmatrix} \tag{3.3}$$

the vector of the probability amplitudes of the particle being after t steps of the walk at point n corresponding to the coin states $|L\rangle$, $|S\rangle$ and $|R\rangle$.

3.2 The Grover walk on a line

The most typical example of a three-state quantum walk on a line is that with the Grover operator as the coin which was extensively studied by Konno *et al* [18]. In the above basis (3.1), the Grover operator is given by

$$G = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}. \tag{3.4}$$

Again, we assume that the particle starts the walk with the initial state

$$\psi(0,0) = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}, \ \psi(n,0) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \text{for } n \neq 0, \tag{3.5}$$

where $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$.
Using the same idea as in the case of the Hadamard walk, we obtain the time evolution of the Grover walk in the following form

$$\psi(n,t+1) = G_L\,\psi(n+1,t) + G_S\,\psi(n,t) + G_R\,\psi(n-1,t), \tag{3.6}$$

where we have denoted

$$G_L = \frac{1}{3}\begin{pmatrix} -1 & 2 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ G_S = \frac{1}{3}\begin{pmatrix} 0 & 0 & 0 \\ 2 & -1 & 2 \\ 0 & 0 & 0 \end{pmatrix}, \ G_R = \frac{1}{3}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 2 & 2 & -1 \end{pmatrix}. \tag{3.7}$$

Subsequent application of the Discrete-Time Fourier Transform (5.10) gives the time evolution in the Fourier domain as

$$\tilde{\psi}(k,t+1) = \frac{1}{3}\begin{pmatrix} e^{-ik} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{ik} \end{pmatrix}\begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}\tilde{\psi}(k,t) = \tilde{U}(k)\,\tilde{\psi}(k,t) \tag{3.8}$$

where $\tilde{U}(k)$ represents the Fourier transform of the evolution operator U.
The solution of the recurrence (3.8) in the Fourier space is again reduced to a successive application of the evolution operator $\tilde{U}(k)$ on the initial state $\tilde{\psi}(k,0) = \psi(0,0)$, i. e.

$$\tilde{\psi}(k,t) = \tilde{U}^t(k)\,\tilde{\psi}(k,0). \tag{3.9}$$

Again, we diagonalize the unitary matrix $\tilde{U}(k)$ so that we can compute its t-th power as

$$\tilde{U}^t(k) = \sum_{j=1}^{3} \lambda_j^t(k) \left|v_j(k)\right\rangle \left\langle v_j(k)\right|. \tag{3.10}$$

The eigenvalues of the evolution operator $\tilde{U}(k)$ are given by

$$\begin{aligned} \lambda_1 &= e^{-i\omega_k} \\ \lambda_2 &= 1 \\ \lambda_3 &= e^{i\omega_k} \end{aligned} \tag{3.11}$$

where ω_k satisfies for $k \in [-\pi, \pi)$ conditions

$$\cos\omega_k = -\frac{1}{3}(2 + \cos k) \tag{3.12}$$

$$\sin\omega_k = \frac{1}{3}\sqrt{(5 + \cos k)(1 - \cos k)}. \tag{3.13}$$

The corresponding eigenvectors are obtained as

$$v_{1,3}(k) = \sqrt{2\left(\frac{1}{1+\cos(\omega_k \mp k)} + \frac{1}{1+\cos\omega_k} + \frac{1}{1+\cos(\omega_k \pm k)}\right)^{-1}} \begin{pmatrix} \frac{1}{1+e^{i(\mp\omega_k + k)}} \\ \frac{1}{1+e^{i\mp\omega_k}} \\ \frac{1}{1+e^{i(\mp\omega_k - k)}} \end{pmatrix} \tag{3.14}$$

$$v_2(k) = \sqrt{\frac{1+\cos k}{5+\cos k}} \begin{pmatrix} \frac{1}{1+e^{ik}} \\ \frac{1}{2} \\ \frac{1}{1+e^{-ik}} \end{pmatrix}. \tag{3.15}$$

The recurrence (3.9) has the following expression in the orthonormal basis formed by the eigenvectors (3.14) and (3.15)

$$\tilde{\psi}(k,t) = \sum_{j=1}^{3} \lambda_j^t(k) \left\langle v_j(k) \middle| \tilde{\psi}(k,0) \right\rangle \left| v_j(k) \right\rangle \tag{3.16}$$

and the desired probability $\psi(n,t)$ is then obtained by the Inverse Fourier Transform (Appendix (5.11)) as

$$\psi(n,t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{j=1}^{3} \lambda_j^t(k) \left\langle v_j(k) \middle| \tilde{\psi}(k,0) \right\rangle \left| v_j(k) \right\rangle e^{-ikn} \mathrm{d}k \tag{3.17}$$

which can be equivalently written as

$$\psi(n,t) = \begin{pmatrix} \psi_L(n,t) \\ \psi_S(n,t) \\ \psi_R(n,t) \end{pmatrix} = \sum_{j=1}^{3} \begin{pmatrix} \psi_L^j(n,t) \\ \psi_S^j(n,t) \\ \psi_R^j(n,t) \end{pmatrix} \tag{3.18}$$

where

$$\psi_l^j(n,t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \lambda_j^t \left\langle v_j(k) \middle| \tilde{\psi}(k,0) \right\rangle \left| v_j(k) \right\rangle e^{-ikn} \mathrm{d}k \tag{3.19}$$

for the coin-state values $l = L, S, R$.

The major difference between the Hadamard walk and the discussed Grover walk is the existence of the eigenvalue λ_2 independent of k. This feature is responsible for the phenomenon which cannot be observed in the two-state quantum walk - trapping. We have seen from the limit distribution (2.30) that the probability of finding the particle at the fixed position in the limit as number of steps t tends to infinity converges to zero in case of the two-state quantum walk. The particle is trapped at the initial position if the probability of finding it there does not vanish after infinitely many steps. We will verify in the next section that the Grover walk exhibits trapping.

3.3 Probability of being at the origin in the limit

Let us now compute the analytic expression for the probability $P(0,\infty)$ of being at the origin as number of steps t tends to infinity which is a limit of the expression

$$P(0,t)=\sum_{j=1}^{3}|\psi_L^j(0,t)|^2+\sum_{j=1}^{3}|\psi_S^j(0,t)|^2+\sum_{j=1}^{3}|\psi_R^j(0,t)|^2. \tag{3.20}$$

The probability amplitudes $\psi_j^1(0,t)$ and $\psi_j^3(0,t)$ take the form of integrals of oscillating functions $e^{\mp i\omega_k t}$ which converge to 0 as t tends to infinity (follows from the Riemann-Lebesgue lemma). Hence the only contribution to the probability $P(0,\infty)$ would be that of $\psi_j^2(0,t)$. However, since the eigenvalue λ_2 equals unity the $\psi_j^2(0,t)=\psi_j^2(0)$ is independent of t. After some algebra, we can rewrite integrals $\psi_j^2(0)$ (3.19) as

$$\begin{aligned}
\psi_L^2(0) &= \frac{\alpha+\beta+\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\cos k+1}{\cos k+5}\mathrm{d}k+\frac{\alpha-\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\sin^2 k}{(\cos k+5)(\cos k+1)}\mathrm{d}k+i\frac{\beta+2\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\sin k}{\cos k+5}\mathrm{d}k\\
\psi_S^2(0) &= \frac{\alpha+\beta+\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\cos k+1}{\cos k+5}\mathrm{d}k+i\frac{\gamma-\alpha}{2\pi}\int_{-\pi}^{\pi}\frac{\sin k}{\cos k+5}\mathrm{d}k \qquad (3.21)\\
\psi_R^2(0) &= \frac{\alpha+\beta+\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\cos k+1}{\cos k+5}\mathrm{d}k+\frac{-\alpha+\gamma}{2\pi}\int_{-\pi}^{\pi}\frac{\sin^2 k}{(\cos k+5)(\cos k+1)}\mathrm{d}k+i\frac{-2\alpha-\beta}{2\pi}\int_{-\pi}^{\pi}\frac{\sin k}{\cos k+5}\mathrm{d}k
\end{aligned}$$

The solution of the above equations is

$$\psi_L^2(0)=\frac{\sqrt{6}}{6}\alpha+\left(-\frac{\sqrt{6}}{3}+1\right)\beta+\left(-\frac{5\sqrt{6}}{6}+2\right)\gamma \tag{3.22}$$

$$\psi_S^2(0)=\left(-\frac{\sqrt{6}}{3}+1\right)(\alpha+\beta+\gamma) \tag{3.23}$$

$$\psi_R^2(0)=\left(-\frac{5\sqrt{6}}{6}+2\right)\alpha+\left(-\frac{\sqrt{6}}{3}+1\right)\beta+\frac{\sqrt{6}}{6}\gamma \tag{3.24}$$

which yields the trapping probability at the origin as

$$\begin{aligned}
P(0,\infty) &= |\psi_L^2(0)|^2+|\psi_S^2(0)|^2+|\psi_R^2(0)|^2 && (3.25)\\
&= (5-2\sqrt{6})\left(1+|\alpha+\beta|^2+|\beta+\gamma|^2-2|\beta|^2\right). && (3.26)
\end{aligned}$$

Note that the probability $P(0,\infty)$ depends only on the initial state of the quantum walk and is greater than 0 except for one special choice of the localized initial state

$$\psi_G=\begin{pmatrix}\alpha\\ \beta\\ \gamma\end{pmatrix}=\frac{1}{\sqrt{6}}\begin{pmatrix}1\\ -2\\ 1\end{pmatrix}, \tag{3.27}$$

which is a solution of

$$|\psi_L^2(0)|^2=|\psi_S^2(0)|^2=|\psi_R^2(0)|^2=0. \tag{3.28}$$

It can be readily verified that this solution is orthogonal to the eigenvector $v_2(k)$. Indeed, if we start the Grover walk with the state ψ_G the component responsible for trapping ψ_j^2 vanishes. Since the coin is three-dimensional we are able to find orthogonal basis spanned by vectors $v_2(k)$, ψ_G and v. However, the vector v is not independent of k and thus cannot represent localized initial state. In other words, we have shown that the Grover walk exhibits trapping except for one particular initial state ψ_G (see Figure 3.1).

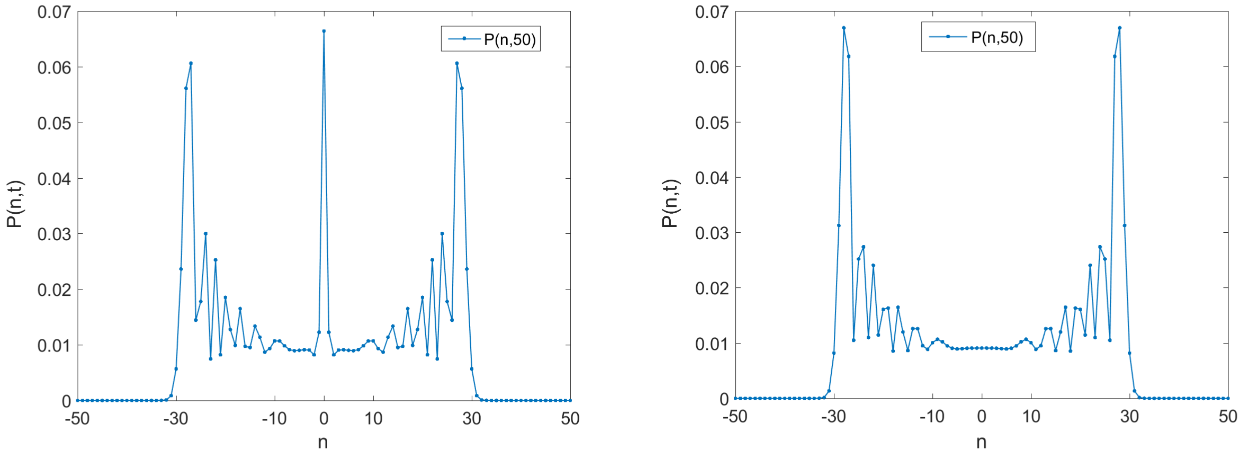

Figure 3.1: The probability distribution of the Grover walk on a line after $t = 50$ steps with the initial states $\psi = \frac{1}{\sqrt{3}}(1, -1, 1)^T$ (on the left) and $\psi_G = \frac{1}{\sqrt{6}}(1, -2, 1)^T$ (on the right).

3.4 General three-dimensional coin exhibiting trapping

Štefaňák *et al* [19] found two classes of three-dimensional unitary operators C exhibiting trapping. As we have already mentioned, this effect is conditioned by the existence of an eigenvalue in the point spectrum. We now outline their method and show that in the case of the three-state quantum walk on a line the trapping can be avoided by a suitable choice of the initial state.
Any three-dimensional coin operator has the following form in the Fourier domain

$$\tilde{U}(k) = \begin{pmatrix} e^{-ik} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{ik} \end{pmatrix} C. \tag{3.29}$$

It is easily shown that to obtain non-trivial, correctly defined quantum walk, $\tilde{U}(k)$ has to have exactly one eigenvalue independent of k.
The eigenvalues of the general three-dimensional, trapping coin thus can be written in the form

$$\lambda_2 = e^{i\varphi}, \ \lambda_{1,3}(k) = e^{\pm i\omega_k}. \tag{3.30}$$

Obviously, these eigenvalues must satisfy the characteristic equation

$$\det\left(\tilde{U}(k) - \lambda\right) = (\lambda_1 - \lambda)(\lambda_2 - \lambda)(\lambda_3 - \lambda) = 0. \tag{3.31}$$

Subsequent comparison of the terms with the same power of λ leads to conditions for elements of the coin operator C.
In [19] the authors parametrized the general three-dimensional matrix, applied these conditions together with conditions on a U(3) group and obtained two classes of coin operators which exhibit non-trivial time evolution.
In the first case, the coin operator C_1 depends on five parameters γ_2, γ_4, γ_5, θ_{13} and θ_{23} which satisfy

following conditions: $\theta_{13}, \theta_{23} \neq \pm\frac{\pi}{2},\ \theta_{23} \neq 0,\ \gamma_1 = \gamma_2 + \gamma_4$ with angles in the interval $(-\pi, \pi)$.

$$C_1 = \begin{pmatrix} e^{i(\gamma_2+\gamma_4)} \cos\theta_{13} \cos\theta_{23} & e^{i\gamma_2} \cos\theta_{13} \sin\theta_{23} & e^{-i\gamma_5} \sin\theta_{13} \\ -e^{i\gamma_4} \cos\theta_{23}(1 + \sin\theta_{13}) \sin\theta_{23} & \cos^2\theta_{23} - \sin\theta_{13} \sin^2\theta_{23} & e^{-i(\gamma_2+\gamma_5)} \cos\theta_{13} \sin\theta_{23} \\ e^{i\gamma_5}(-\cos^2\theta_{23} \sin\theta_{13} + \sin^2\theta_{23}) & -e^{-i(\gamma_4-\gamma_5)} \cos\theta_{23}(1 + \sin\theta_{13}) \sin\theta_{23} & e^{-i(\gamma_2+\gamma_4)} \cos\theta_{13} \cos\theta_{23} \end{pmatrix} \tag{3.32}$$

The second class C_2 depends on six parameters $\gamma_1,\ \gamma_2,\ \gamma_4,\ \gamma_5,\ \delta$ and θ_{23}. The evolution of the quantum walk driven by this operator is non-trivial if following holds: $\theta_{13}, \theta_{23} \neq \pm\frac{\pi}{2},\ \delta \neq \gamma_1 - \gamma_2 - \gamma_4,\ \sin\theta_{13} = -\frac{\sin\kappa}{\sin(\delta+\kappa)}$.

$$C_2 = \begin{pmatrix} e^{i\gamma_1} \cos\theta_{23} B & e^{i\gamma_2} B \sin\theta_{23} & -e^{-i(\delta+\gamma_5)} A \sin\kappa \\ -e^{i(\gamma_1-\gamma_2)} A \sin\theta_{23} \cos\theta_{23} \delta & e^{i\kappa}(\cos^2\theta_{23} + e^{i\delta} A \sin^2\theta_{23} \sin\kappa) & e^{-i(\gamma_1-\gamma_4+\gamma_5)} B \sin\theta_{23} \\ e^{i\gamma_5}(\sin^2\theta_{23} + e^{i\delta} \cos^2\theta_{23} A \sin\kappa) & -e^{-i(\gamma_4-\gamma_5)} A \sin\theta_{23} \cos\theta_{23} \sin\delta & e^{-i\gamma_1} \cos\theta_{23} B \end{pmatrix} \tag{3.33}$$

where $\kappa = \gamma_2 + \gamma_4 - \gamma_1$, $A = \frac{1}{\sin(\delta+\kappa)}$, $B = \sqrt{A^2 \sin\delta \sin(\delta + 2\kappa)}$.
In [19] they also derived the eigenvectors corresponding to the eigenvalue λ_2 for both of the classes C_1 and C_2 as

$$v_1(k) = \begin{pmatrix} -e^{-i\gamma_5}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \sin\theta_{23} \\ e^{i(k-\gamma_2-\gamma_5)}\left(\sin\frac{\theta_{13}}{2} - \cos\frac{\theta_{13}}{2}\right) + e^{i(\gamma_4-\gamma_5)}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \cos\theta_{23} \\ -e^{ik}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \sin\theta_{23} \end{pmatrix} \tag{3.34}$$

$$v_2(k) = \begin{pmatrix} e^{i(\gamma_2+\gamma_4)} \sin\delta \sin\theta_{23} \\ -e^{i(\gamma_1+\gamma_4)} \sin\delta \cos\theta_{23} + e^{i(k+\gamma_4)} \sqrt{\sin\delta \sin(\delta + 2\kappa)} \\ e^{i(k+\gamma_1+\gamma_5)} \sin\delta \sin\theta_{13} \end{pmatrix}. \tag{3.35}$$

Now we show that for general three-dimensional trapping coin there exists localized initial state that is orthogonal to eigenvector corresponding to the constant eigenvalue and thus results in propagating walk. Let us denote such states by ψ_1, ψ_2 corresponding to the class C_1 and C_2, respectively. These states must satisfy the following relation for every k

$$\langle v_i(k)|\psi_i\rangle = 0,\ \psi_i = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix},\ i = 1, 2 \tag{3.36}$$

In the case of the first class C_1 we obtain the following relations (in k^i, i represents the power of k):

$$k^0 :\ \alpha e^{i\gamma_5}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \sin\theta_{23} = \beta e^{-i(\gamma_4-\gamma_5)}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \cos\theta_{23} \tag{3.37}$$

$$k^1 :\ \beta e^{-i(k-\gamma_2-\gamma_5)}\left(\sin\frac{\theta_{13}}{2} - \cos\frac{\theta_{13}}{2}\right) = \gamma e^{-ik}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \sin\theta_{23} \tag{3.38}$$

with the solution

$$\psi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\gamma_4} \cos\theta_{23}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \\ \sin\theta_{23}\left(\sin\frac{\theta_{13}}{2} + \cos\frac{\theta_{13}}{2}\right) \\ e^{i(\gamma_2+\gamma_5)}\left(\sin\frac{\theta_{13}}{2} - \cos\frac{\theta_{13}}{2}\right) \end{pmatrix} \tag{3.39}$$

For the class C_2 the equation (3.36) gives:

$$k^0 :\ \alpha e^{-i(\gamma_1+\gamma_2)} \sin\delta \sin\theta_{23} = \beta e^{-i(\gamma_1+\gamma_4)} \sin\delta \cos\theta_{23} \tag{3.40}$$

$$k^1 :\ -\beta e^{-i(k+\gamma_4)} \sqrt{\sin\delta \sin(\delta + 2\kappa)} = \gamma e^{-i(k+\gamma_1+\gamma_5)} \sin\delta \sin\theta_{13}. \tag{3.41}$$

with the corresponding solution

$$\psi_2 = \frac{\sin(\delta+\kappa)}{\sqrt{\sin\delta\left(\sin^2\kappa\sin\delta+\sin^3(\delta+\kappa)\sin^2\theta_{23}\right)}}\begin{pmatrix} e^{-i(\gamma_1-\gamma_2)}\cos\theta_{23}\sin\theta_{13}\sin\delta \\ \sin\theta_{23}\sin\ \theta_{13}\sin\delta \\ -e^{-i(\gamma_4-\gamma_1-\gamma_5)}\sqrt{\sin\delta\sin(\delta+\kappa)}\sin\theta_{23} \end{pmatrix}. \tag{3.42}$$

In this chapter we presented a striking property of quantum walks - trapping. We note that the effect of trapping does not have a classical analogue. Indeed, if the probability of leaving the current position is non-zero the classical random walk diffuses. Hence, trapping is purely quantum phenomenon.

Chapter 4

Two-dimensional quantum walk

Let us now focus on a quantum walk on a two-dimensional lattice. We will see that in certain aspects this type of quantum walk differs considerably from the one-dimensional case. The major difference is that the two-dimensional quantum walk allows for the trapping effect even in the case of a leaving walk.

4.1 Definition of the two-dimensional quantum walk on a lattice

The basic concept is similar to that of the quantum walk on a line. The particle is assigned a Hilbert space $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p$, where the coin space $\mathcal{H}_c$ is spanned by vectors

$$\{ |L\rangle , |D\rangle , |U\rangle , |R\rangle\} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\} \tag{4.1}$$

corresponding to all four possible directions of movement: to the left, down, up and to the right. The position on the lattice is given by a vector from the Hilbert space $\mathcal{H}_p = \text{span}\{ |p\rangle = |n, m\rangle \mid n, m \in \mathbb{Z}\}$, where n, m represent the coordinates of the particle on the lattice. The conditional shift operator takes the form

$$\begin{aligned} S = \sum_{n,m \in \mathbb{Z}} \Big(& |L\rangle \langle L| \otimes |n-1, m\rangle \langle n, m| + |D\rangle \langle D| \otimes |n, m-1\rangle |n, m\rangle \\ & + |U\rangle \langle U| \otimes |n, m+1\rangle \langle n, m| + |R\rangle \langle R| \otimes |n+1, m\rangle \langle n, m| \Big). \end{aligned} \tag{4.2}$$

One step of this quantum walk is again given by (2.2) and its state after t steps with the normalized initial state $|\psi(0)\rangle = (\alpha |L\rangle + \beta |D\rangle + \gamma |U\rangle + \delta |R\rangle) \otimes |0, 0\rangle$ localized at the origin corresponds to

$$|\psi(t)\rangle = \sum_{n,m \in \mathbb{Z}} \Big(\psi_L(n, m, t) |L\rangle + \psi_D(n, m, t) |D\rangle + \psi_U(n, m, t) |U\rangle + \psi_R(n, m, t) |R\rangle \Big) \otimes |n, m\rangle , \tag{4.3}$$

where $\psi_j(n, m, t)$, $j = L, D, U, R$ are again components of the vector of the probability amplitudes $\psi(n, m, t)$ analogous to (2.4).

4.2 Two-dimensional Grover walk

In this section we give a typical example of a quantum walk on a two-dimensional lattice with the help of the Grover walk represented by the four-dimensional Grover coin

$$G = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}. \tag{4.4}$$

The time evolution, obtained by similar reasoning as that of the Hadamard walk (2.11), attains the following form

$$\psi(n, m, t+1) = G_L\,\psi(n+1, m, t) + G_D\,\psi(n, m+1, t) + G_U\,\psi(n, m-1, t) + G_R\,\psi(n-1, m, t) \tag{4.5}$$

where $G_j,\ j = L, D, U, R$ represent

$$G_L = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},\ G_D = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},\ G_U = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix},\ G_R = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & -1 \end{pmatrix}. \tag{4.6}$$

Using the two-dimensional Discrete-Time Fourier Transform (see Appendix 5.12) we derive the time evolution of the Grover walk in the Fourier domain as

$$\begin{aligned}
\tilde{\psi}(k, l, t+1) &= \sum_{n,m\in\mathbb{Z}} \psi(n, m, t)\, e^{ikn} e^{ilm} \\
&= e^{-ik} G_L \sum_{n,m\in\mathbb{Z}} \psi(n+1, m, t)\, e^{ik(n+1)} e^{ilm} + e^{-il} G_D \sum_{n,m\in\mathbb{Z}} \psi(n, m+1, t)\, e^{ikn} e^{il(m+1)} \\
&\quad + e^{il} G_U \sum_{n,m\in\mathbb{Z}} \psi(n, m-1, t)\, e^{ikn} e^{il(m-1)} + e^{ik} G_R \sum_{n,m\in\mathbb{Z}} \psi(n-1, m, t)\, e^{ik(n-1)} e^{ilm} \\
&= \left(e^{-ik} G_L + e^{-il} G_D + e^{il} G_U + e^{ik} G_R\right) \tilde{\psi}(k, l, t) \\
&= \tilde{U}(k, l)\, \tilde{\psi}(k, l, t) \\
&= \tilde{U}^t(k, l)\, \tilde{\psi}(k, l, 0).
\end{aligned} \tag{4.7}$$

The recurrence (4.7) represents the time evolution of the Grover walk with the initial state $\tilde{\psi}(k, l, 0) = \psi(0, 0, 0) = (\alpha, \beta, \gamma, \delta)^T$ in the Fourier domain with the transformed step operator

$$\tilde{U}(k, l) = \begin{pmatrix} e^{-ik} & 0 & 0 & 0 \\ 0 & e^{-il} & 0 & 0 \\ 0 & 0 & e^{il} & 0 \\ 0 & 0 & 0 & e^{ik} \end{pmatrix} G. \tag{4.8}$$

The solution of the recurrence (4.7) has the following form

$$\tilde{\psi}(k, l, t) = \sum_{j=1}^{4} \lambda_j^t(k, l) \left\langle v_j(k, l) \middle| \tilde{\psi}(k, l, 0) \right\rangle \left| v_j(k, l) \right\rangle \tag{4.9}$$

where

$$\lambda_1 = 1,\ \lambda_2 = -1,\ \lambda_3 = e^{i\omega(k,l)},\ \lambda_4 = e^{-i\omega(k,l)} \tag{4.10}$$

represent the eigenvalues of the operator (4.8) where $\omega(k,l)$ is given as

$$\cos\omega(k,l) = -\frac{1}{2}(\cos k + \cos l)\,,\ k,l \in [-\pi,\pi) \tag{4.11}$$

with the corresponding eigenvectors

$$v_j(k,l) = \begin{pmatrix} \left(\lambda_j\, e^{il}+1\right)\left(\lambda_j\, e^{-ik}+1\right)\left(\lambda_j\, e^{-il}+1\right) \\ \left(\lambda_j\, e^{ik}+1\right)\left(\lambda_j\, e^{-ik}+1\right)\left(\lambda_j\, e^{-il}+1\right) \\ \left(\lambda_j\, e^{il}+1\right)\left(\lambda_j\, e^{ik}\ +1\right)\left(\lambda_j\, e^{-ik}+1\right) \\ \left(\lambda_j\, e^{il}+1\right)\left(\lambda_j\, e^{ik}\ +1\right)\left(\lambda_j\, e^{-il}+1\right) \end{pmatrix}. \tag{4.12}$$

Notice that again we obtained eigenvalues independent of k and l. This implies that the two-dimensional quantum walk driven by the Grover coin is trapped at the origin, which was verified by Konno in [20]. Again, the trapping can be avoided by a suitable choice of the initial state, namely by choosing an initially localized state without an overlap with eigenvectors v_1 and v_2 that are responsible for trapping. Similarly to the three-state quantum walk on a line, these initial states must be orthogonal to the eigenvectors v_1 and v_2. Solving the equation

$$\left\langle v_j(k,l) \middle| \psi_G \right\rangle = 0, j = 1,2 \tag{4.13}$$

for every k, l yields exactly one initially localized state $\psi_G = \frac{1}{2}(1,-1,-1,1)^T$ which results in a propagating quantum walk (compare Figure 4.1 and Figure 4.2).

There is a significant difference between the trapping effect in the case of the four-state quantum walk on a lattice and in the case of the three-state quantum walk on a line. The four-state quantum walk introduced above belongs to the so-called leaving walks, which means that at each step the particle is forced to leave its current position. Unlike in the case of the quantum walk on a line, the four-state quantum walk can exhibit trapping even if it has zero probability of staying at the same point in one step of the walk. This is one of many examples of counter-intuitive nature of quantum mechanics.

4.3 General four-dimensional trapping coin

Let us now consider general trapping four-state coin governing a two-dimensional quantum walk. We have already seen that the trapping effect stems from the existence of a constant eigenvalue. Let us denote by λ an eigenvalue of the operator $\tilde{U}(k,l)$, which is the Fourier transform of the general coin C

$$\tilde{U}(k,l) = \mathrm{diag}\left(e^{-ik}, e^{-il}, e^{il}, e^{ik}\right)\, C = \begin{pmatrix} e^{-ik} & 0 & 0 & 0 \\ 0 & e^{-il} & 0 & 0 \\ 0 & 0 & e^{il} & 0 \\ 0 & 0 & 0 & e^{ik} \end{pmatrix} \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{24} & c_{34} & c_{44} \end{pmatrix} \tag{4.14}$$

The eigenvalue λ obviously satisfies the characteristic equation

$$\begin{aligned} \det\left(\tilde{U}(k,l) - \lambda\right) = \lambda^4 - \lambda^3 \left(c_{11}\, e^{-ik} + c_{22}\, e^{-il} + c_{33}\, e^{il} + c_{44}\, e^{il}\right) + \\ \lambda^2 \left(C_{14} + C_{23} + C_{12}\, e^{-ik} e^{-il} + C_{13}\, e^{-ik} e^{il} + C_{24}\, e^{ik} e^{-il} + C_{34}\, e^{ik} e^{il}\right) \\ - \lambda \left(C_{123}\, e^{-ik} + C_{124}\, e^{-il} + C_{134}\, e^{il} + C_{234}\, e^{ik}\right) \det(C) = 0, \end{aligned} \tag{4.15}$$

where we have denoted

$$C_{ij} = \det\begin{pmatrix} c_{ii} & c_{ij} \\ c_{ji} & c_{jj} \end{pmatrix} \text{ and } C_{ijk} = \det\begin{pmatrix} c_{ii} & c_{ij} & c_{ik} \\ c_{ji} & c_{jj} & c_{jk} \\ c_{ki} & c_{kj} & c_{kk} \end{pmatrix}. \tag{4.16}$$

Let us now assume that λ lies in the point spectrum of the operator (4.14), i. e. λ is a k, l-independent eigenvalue. The equation (4.15) holds for every k, l which leads to the following relations

$$\begin{aligned} \lambda^4 + \lambda^2\,(C_{14} + C_{23}) + \det(C) &= 0 \\ \lambda^3 \left(c_{11}\,e^{-ik} + c_{22}\,e^{-il} + c_{33}\,e^{il} + c_{44}\,e^{il}\right) + \lambda \left(C_{123}\,e^{-ik} + C_{124}\,e^{-il} + C_{134}\,e^{il} + C_{234}\,e^{ik}\right) &= 0 \\ \lambda^2 \left(C_{12}\,e^{-ik}e^{-il} + C_{13}\,e^{-ik}e^{il} + C_{24}\,e^{ik}e^{-il} + C_{34}\,e^{ik}e^{il}\right) &= 0. \end{aligned} \tag{4.17}$$

One can immediately see that if λ is a constant eingevalue of the operator (4.14) then $-\lambda$ is in the spectrum since it satisfies relations (4.17).
Considering a coin with three constant eigenvalues, we find out that the last one has to be k, l-independent as well. This readily follows from the relation $\det(\tilde{U}(k, l)) = \det(C)$ which stems from (4.14). However, coin operator with four constant eigenvalues results in a quantum walk with trivial time evolution. Hence, the general trapping four-state coin possesses a pair of constant eigenvalues λ, $-\lambda$.
Relations (4.17), together with the conditions on U(4) group, represent requirements on the general four-state trapping coin. However, solving these equations analytically appears to be practically impossible. In the next chapter we present an alternative approach for the construction of the trapping coins.

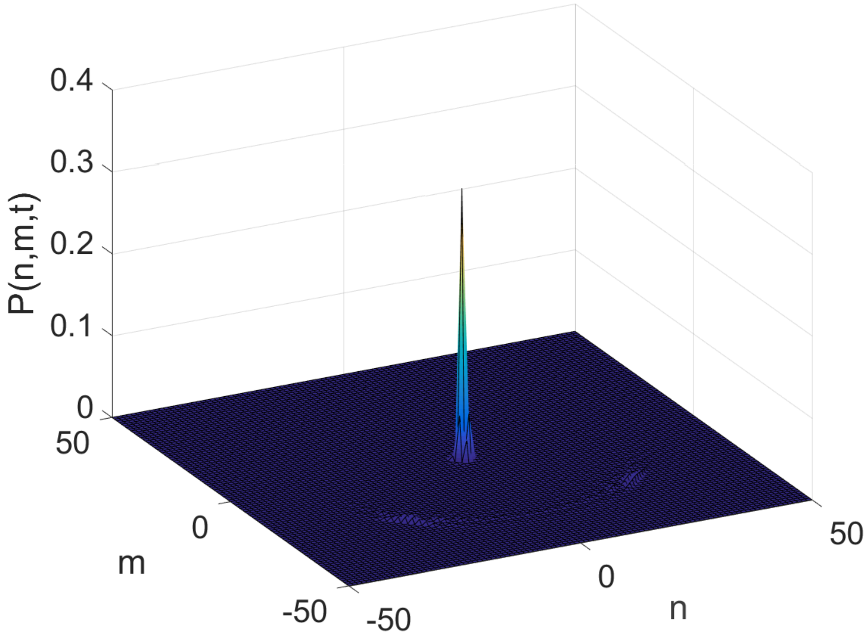

Figure 4.1: The probability distribution of the Grover walk on a two-dimensional lattice after $t = 50$ steps with the initial state $\psi = \frac{1}{2}(1, -1, 1, 1)^T$.

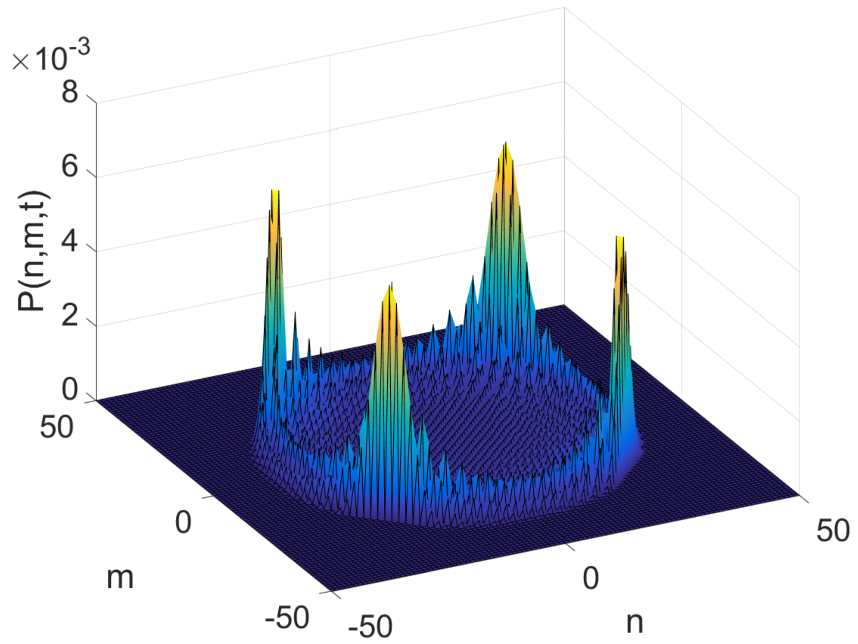

Figure 4.2: The probability distribution of the Grover walk on a two-dimensional lattice after $t = 50$ steps with the initial state $\psi_G = \frac{1}{2}(1, -1, -1, 1)^T$.

Chapter 5

Strong trapping

We now introduce stronger version of the trapping effect considered in the previous two chapters. Strongly trapped quantum walks exhibit a wide range of interesting properties such as non-trivial topological phases or possible utilization for the quantum search [21].

5.1 Definition of strong trapping effect

Let us consider a two-dimensional quantum walk on a lattice driven by the following coin operator

$$C_{STR} = \frac{1}{2\sqrt{2}}\begin{pmatrix} -\sqrt{3} & \sqrt{3} & 1 & 1 \\ 1 & -1 & \sqrt{3} & \sqrt{3} \\ \sqrt{3} & \sqrt{3} & -1 & 1 \\ 1 & 1 & \sqrt{3} & -\sqrt{3} \end{pmatrix}. \tag{5.1}$$

It is easily verified that the Fourier transform $\tilde{U}(k,l)$ of this operator given by the equation (4.14) has eigenvalues in the form (4.10) where

$$\cos\omega(k,l) = -\frac{\sqrt{3}\cos k + \cos l}{2\sqrt{2}},\ k,l \in [-\pi,\pi) \tag{5.2}$$

and eigenvectors corresponding to the pair of constant eigenvalues λ_1, λ_2 given as

$$v_{1,2}(k,l) = \begin{pmatrix} \sqrt{2} \pm e^{il} \\ \sqrt{2} \pm \sqrt{3}e^{ik} \\ \pm\sqrt{3}e^{il} + \sqrt{2}e^{ik}e^{il} \\ \pm e^{ik} + \sqrt{2}e^{ik}e^{il} \end{pmatrix}. \tag{5.3}$$

There is a striking difference between the Grover walk defined in the previous chapter and the quantum walk driven by the coin operator (5.1), namely the non-existence of the vector orthogonal to the eigenvectors $v_1(k,l)$ and $v_2(k,l)$ in the latter case. Indeed, the equation (4.13) yields only a trivial solution in this case. In other words, the quantum walk is trapped for arbitrary choice of localized initial state. This phenomenon, called strong trapping, was defined by Kollár *et al* in [21] where they introduced a class of four-dimensional trapping coins using a constructive approach.
General coin from this class depends on 7 real parameters $\alpha_1,\ \alpha_2,\ \beta_1,\ \beta_2,\ \delta_1,\ \delta_2$ and φ and has the following form

$$C_S = \begin{pmatrix} e^{-i(\alpha_1+\alpha_2)}\cos\delta_1\cos\delta_2 & -e^{-i(\alpha_2+\beta_1)}\sin\delta_1\cos\delta_2 & -e^{-i(\alpha_1+\beta_2)}\cos\delta_1\sin\delta_2 & e^{-i(\beta_1+\beta_2+\varphi)}\sin\delta_1\sin\delta_2 \\ e^{-i(\alpha_1-\beta_2)}\cos\delta_1\sin\delta_2 & -e^{-i(\beta_1-\beta_2)}\sin\delta_1\sin\delta_2 & e^{-i(\alpha_1-\alpha_2)}\cos\delta_1\cos\delta_2 & -e^{i(\alpha_2-\beta_1-\varphi)}\sin\delta_1\cos\delta_2 \\ e^{-i(\alpha_2-\beta_1)}\sin\delta_1\cos\delta_2 & e^{i(\alpha_1-\alpha_2)}\cos\delta_1\cos\delta_2 & -e^{i(\beta_1-\beta_2)}\sin\delta_1\sin\delta_2 & -e^{i(\alpha_1-\beta_2-\varphi)}\cos\delta_1\sin\delta_2 \\ e^{i(\beta_1+\beta_2+\varphi)}\sin\delta_1\sin\delta_2 & e^{i(\alpha_1+\beta_2+\varphi)}\cos\delta_1\sin\delta_2 & e^{i(\alpha_2+\beta_1+\varphi)}\sin\delta_1\cos\delta_2 & e^{i(\alpha_1+\alpha_2)}\cos\delta_1\cos\delta_2 \end{pmatrix}. \tag{5.4}$$

In [21] they also analysed quantum walks driven by the coin operator (5.4) in the Fourier domain and obtained the eigenvectors corresponding to the constant eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$ as

$$v_{1,2}(k,l) = \frac{1}{2}\begin{pmatrix} -e^{i\beta_1}\sin\delta_1 \mp e^{-i\beta_1}e^{il}\sin\delta_2 \\ -e^{-i\alpha_1}\cos\delta_1 \pm e^{i\alpha_2}e^{ik}\cos\delta_2 \\ \mp e^{i\alpha_2}e^{il}\cos\delta_2 + e^{i\alpha_1}e^{ik}e^{il}\cos\delta_1 \\ \mp e^{i(\beta_2+\varphi)}e^{ik}\sin\delta_2 - e^{i(\beta_1+\varphi)}e^{ik}e^{il}\sin\delta_1 \end{pmatrix}. \tag{5.5}$$

In this case the relation (4.13) leads to the condition

$$\cos 2\delta_1 = \cos 2\delta_2 \tag{5.6}$$

which means that strong trapping is avoided for the coins satisfying (5.6). Indeed, in this case there exists initially localized state that results in non-trapped quantum walk given by

$$\psi(0,0,0) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\beta_1}\cos\delta_1 \\ -e^{-i\alpha_1}\sin\delta_1 \\ -e^{-i(\alpha_2+\beta_1-\beta_2)}\sin\delta_1 \\ -e^{-i(\alpha_1+\alpha_2-\beta_2-\varphi)}\cos\delta_1 \end{pmatrix},\ \psi(n,m,0) = \begin{pmatrix}0\\0\\0\\0\end{pmatrix} \text{ for } n,m \neq 0. \tag{5.7}$$

In the previous chapter we studied the Grover walk on a lattice which belongs to the weakly trapped quantum walks, i. e. walks that escape for the choice of the initial state (5.7). If we compare the spectra of weakly trapping and strongly trapping coins, we see that the spectrum is gapless in the former case, whereas in case of the strong trapping walks there appear gaps around $\omega(k,l) = 0$ (see Figure 5.1 and Figure 5.2). This implies the existence of non-trivial topological phases (for an introduction to topological phases see [22]).

5.2 General notes on the trapping in classical and quantum walks

Let us now comment on the most significant differences between various types of classical random walk and quantum walks regarding the effect of trapping.
The classical random walk is not trapped unless the probability of leaving the current position is zero. In other words, the trapping does not have a classical analogue.
As we have already discussed in the previous chapter, contrary to the four-state quantum walk on a lattice, the two-state (leaving) one-dimensional quantum walk does not exhibit trapping since it cannot possess k-independent eigenvalue.
In chapter 3 we also observed that for an arbitrary one-dimensional three-state trapping walk the trapping effect could be avoided by one special choice of the initial state. This became more complicated in the case of the two-dimensional quantum walks which are classified as weakly trapped, if the trapping can be avoided, or strongly trapped otherwise.

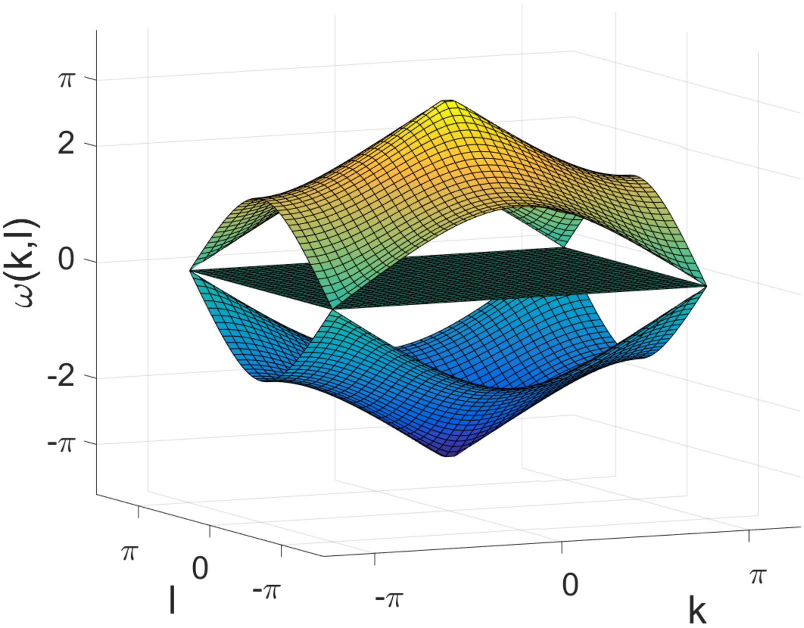

Figure 5.1: The spectrum of the Grover coin (4.4).

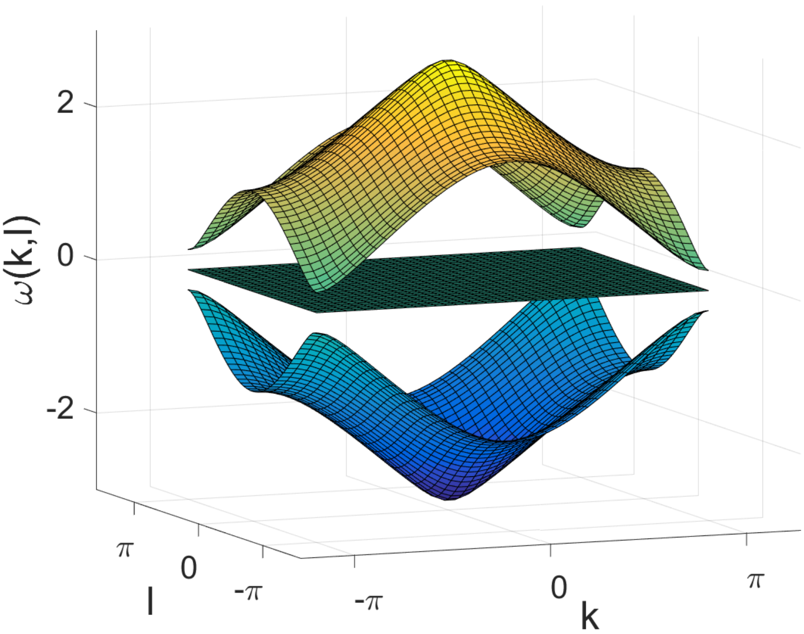

Figure 5.2: The spectrum of the strongly trapping coin operator (5.1).

Conclusion

In this thesis we have summarized the concept of quantum walks in dimensions one and two.
In the first chapter we outlined basic information about classical random walks such as the limit distribution, the recurrence properties or hitting and mixing time of random walks.
In the second chapter we introduced quantum walk on a line and illustrated methods of analysis with the example of the Hadamard walk. We also commented on the most significant differences between the models of the classical and quantum walks.
In the third chapter we described the three-state quantum walk on a line and showed that the three-state quantum walk driven by the Grover coin exhibits trapping. We also presented the general form of three-state trapping coins.
The last two chapters dealt with the effect of trapping in leaving quantum walks on a two-dimensional lattices. We saw that the trapping effect in dimension two represents a more complex phenomenon and that the four-state trapping coins can be classified as weakly or strongly trapping according to whether the trapping can be avoided or not.
However, there still remain open questions. On the contrary to the three-state quantum walk on a line, the form of the general strongly trapping coin is yet to be determined. Once we have obtained this form, there arise questions related to the stability of the trapping effect on a lattice under perturbations, such as the dependence of the coin on small changes of its parameters or the underlying lattice. These characteristics are extremely important for physical implementation of quantum walks. Strongly trapping coin could also be potentially utilized for wave-packet manipulation. The wave-packet could be trapped or released by switching form a trapping to a non-trapping coin.

Appendix

Fourier Transform

Let $f \in L^1(\mathrm{R}^n)$. The Fourier transform $\mathcal{F} : L^1(\mathrm{R}^n) \mapsto C(\mathrm{R}^n)$ of the function f defined as

$$(\mathcal{F} f)(y) = \int_{-\infty}^{\infty} e^{iy \cdot x} f(x) \, \mathrm{d}^n x \tag{5.8}$$

is a bounded function.
The Fourier transform has some interesting properties:

Linearity: $a \in \mathbb{C},\ f, g \in L^1(\mathrm{R}^n)$

$$\Big(\mathcal{F}\left(af(x) + g(x)\right)\Big)(y) = a\Big(\mathcal{F} f(x)\Big)(y) + \Big(\mathcal{F} g(x)\Big)(y).$$

Modulation: $b \in \mathrm{R}^n,\ f \in L^1(\mathrm{R}^n)$

$$\left(\mathcal{F} f(x)\right)(y + b) = \left(\mathcal{F} e^{ibx} f(x)\right)(y).$$

Translation: $b \in \mathrm{R}^n,\ f \in L^1(\mathrm{R}^n)$

$$\left(\mathcal{F} f(x - b)\right)(y) = e^{iby}\left(\mathcal{F} f(x)\right)(y).$$

Scaling: $c \in \mathrm{R},\ c \neq 0,\ f \in L^1(\mathrm{R}^n)$

$$\left(\mathcal{F} f(cx)\right)(y) = \frac{1}{|c|^n}\left(\mathcal{F} f(x)\right)\left(\frac{y}{c}\right).$$

Conjugation: $f \in L^1(\mathrm{R}^n)$

$$\left(\mathcal{F}\overline{f(x)}\right)(y) = \overline{\left(\mathcal{F} f(x)\right)\,(-y)}.$$

Fourier transform is injective. The inverse transform is given as

$$(\mathcal{F}^{-1} f)(x) = \frac{1}{(2\pi)^n}\int_{-\infty}^{\infty} e^{-iy \cdot x} f(y) \, \mathrm{d}^n y. \tag{5.9}$$

However, in this thesis we use the so-called Discrete-Time Fourier Transform to analyse discrete-time quantum walks.

Discrete-Time Fourier Transform

The Discrete-Time Fourier Transform $\tilde{f}$ of a complex valued function f over integers is defined as follows:

$$\tilde{f}(k) = \sum_{n \in \mathbb{Z}} f(n)\, e^{ikn} \tag{5.10}$$

with the corresponding inverse transform

$$f(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \tilde{f}(k)\, e^{-ikn}\, \mathrm{d}k. \tag{5.11}$$

The above relations can also be generalized to two-dimensional spaces as

$$\tilde{f}(k,l) = \sum_{n,m \in \mathbb{Z}} f(n,m)\, e^{i(kn+lm)} \tag{5.12}$$

$$f(n,m) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \tilde{f}(k,l)\, e^{-i(kn+lm)}\, \mathrm{d}k\, \mathrm{d}l. \tag{5.13}$$

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