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QUANTUM WALK ON INTEGERS AND MAXIMUM LIKELIHOOD PARAMETRIC ESTIMATION

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Dedicated to my family

Abstract

Classical statistics and quantum mechanics are two important research fields of mathematics and natural sciences. We make a blend of these by creating a novel algorithm for the determination of an unknown matrix, by estimating the values of a single parameter from which the matrix elements are assumed to be determined. Basics of statistical parametric estimation theory and theory of quantum walks (QWs) are the main ingredients of the method. Among the various methodologies employed in parametric estimation theory e.g. the methods of moments, the Bayesian methodology and maximum likelihood estimation, we choose the latter one to combine with the formalism of QW on integers in order to accomplish the task of estimation. The QW enters in the estimation algorithm via its so called reshuffling matrix which operates in the "quantum coin" Hilbert space. Using elements from representation theory of the ISO(2) Lie algebra (a.k.a. Euclidean algebra), from the formalism of completely positive trace preserving maps, and from basic theory of Chebyshev polynomials, the dynamics of finite steps of QW is completely derived analytically. Constructing and evaluating the analogue of quantum statistical moments for the walker's position operator, and by introducing simplifying assumptions in the form of closed paths for QWer, we end up with the likelihood function. Imposing the maximum likelihood condition, finally leads to validation of value intervals for the solicited parametric estimation.

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In memory of my grandfather George.

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1 Introduction

The aim of my thesis is to describe a very simple procedure of finding the elements of a matrix. Firstly, we set a matrix with the elements that we search. We insert this matrix on the QW as the so called reshuffling matrix. The unknown elements of the initial matrix are now elements of the QW. After that, we calculate the occupation probability distribution of the position of the walker. The occupation probability distribution contains the elements of the matrix that we search. Thus, we consider the occupation probability distribution as a probability density function with parameters the unknown elements. The final and most important step is the estimation procedure. The starting point is the probability density function with the parameters that we set. We create the stochastic likelihood function using the probability density function. The objective is to maximize the stochastic likelihood function for the parameters with methods of calculus. The critical points of the stochastic likelihood function are the candidates for the title of the maximum likelihood estimator. We choose the critical point that satisfies the criterion of the second derivative for each one of the parameters and this critical point is the maximum likelihood estimator for each one of the parameters. The maximum likelihood estimators are the values for the elements of the initial unknown matrix. Thus, we find the unknown elements with the maximization of a stochastical function.

My thesis has two areas of study, QW and statistics. The problem that I tackle is estimation via QW. I will describe my method briefly. I made maximum likelihood estimation with the help of the QW. I did it in order to check if the maximum likelihood estimation method works with the QW. My target was to understand if I can use maximum likelihood estimation in order to search the parameter of a matrix, which is involved as a reshuffling matrix of a QW. I applied maximum likelihood estimation with the probability density function extracted from a QW. I used Chebyshev polynomials in order to solve the problem of applying maximum likelihood estimation with a QW. I provide an outline of my thesis.

Chapter 2. Mathematical Preliminaries. We expand all these concepts and mathematical background that is required for the understanding of the thesis. If the reader feels confident, may omit the study of this chapter.

Chapter 3. Quantum Walk on Integers. We talk about the fundamentals of the QW on the line of the integers.

Chapter 4. Estimation Theory. This chapter refers to the maximum likelihood estimation method.

Chapter 5. Parametric Estimation via QW. We apply a special method of maximum likelihood estimation, using a probability density function extracted from a QW.

2 Mathematical Preliminaries

2.1 Postulates of Quantum Mechanics

We now provide the postulates of quantum mechanics [18] upon which we build up our work on QWs. In quantum mechanics there are two mathematical formalisms to describe a physical quantum system. The state vectors and the density operators. Both approaches are mathematically equivalent and consequently choosing one or the other is a matter of convenient description of the properties of the system to be studied. We formulate Postulates $1, 2, 3$ and 4 in the parlance of state vectors and additionally define density operators in the context of Postulate 1.

State Space

The postulate provides the mathematical framework with which we describe closed (that is isolated) physical systems. **Postulate 1**: Each isolated physical system is associated with a Hilbert space $\mathcal{H}$, herein after known as the state space of the system. The physical system is completely described by its state vector, which is a unit vector $|\psi\rangle \in \mathcal{H}$. The dimension of $\mathcal{H}$ depends on the specific degrees of freedom of the physical property under consideration. Postulate 1 implies that a linear combination of state vectors is a state vector. This is known as the superposition principle and it is a quantum mechanical description of physical systems. In particular any vector state $|\psi\rangle$ may be desrcibed as a superposition of basis states

$$\{|e_i\rangle \in \mathcal{H}\} = e_i, i = 1, 2, ..., n, \tag{1}$$

i.e

$$|\psi\rangle = \sum_i c_i |e_i\rangle, \tag{2}$$

where $c_i \in \mathbb{C}, i = 1, 2, ..., n$.

An alternative description of quantum states is given by the density operator (also called density matrix). The density operator is positive Hermitian and has trace equal to 1. A quantum system whose state $|\psi\rangle$ is known exactly is said to be in a pure state. The density operator in a pure state is given by

$$\rho = |\psi\rangle \langle\psi|. \tag{3}$$

A density operator also describes mixed quantum states. A mixed state may be obtained from a source randomly producing pure states. For example, suppose that a quantum system has a quantum state picked from a set of posssible quantum states $\{|\psi\rangle_i\}$ according to a probability distribution $\{p_i\}$. Then, its density operator is given by

$$\rho = \sum_i p_i |\psi\rangle_{ii} \langle\psi|. \tag{4}$$

Density operators do not uniquely represent a probability distribution over pure states as it is possible to have two different quantum state ensembles giving rise to the same density operator.

The qubit

In mathematical computation, information is stored and manipulated in the form of bits. The mathematical structure of a classical bit is rather simple. It suffices to define two logical values, traditionally labelled as $\{0, 1\}$, and to relate these values to two different outcomes of a classical measurement. So, classical bit lives in a scalar space.

In quantum computation, information is stored, manipulated and measured in the form of qubits. A qubit is a physically entity described by the laws of quantum mechanics. Simple examples of qubits include two orthogonal polarizations of a photon (e.g. horizontal and vertical), the alignment of a $\left(spin - \frac{1}{2}\right)$ nuclear spin in a magnetic field or two states of an electron orbiting atom. A qubit may be mathematically represented as a unit vector in a two dimensional Hilbert $|\psi\rangle \in \mathcal{H}^2$. A qubit $|\psi\rangle$ may be written in general form as

$$|\psi\rangle = a\,|p\rangle + \beta\,|q\rangle\,, \tag{5}$$

where $\alpha, \beta \in \mathbb{C}$, and

$$|\alpha|^2 + |\beta|^2 = 1, \tag{6}$$

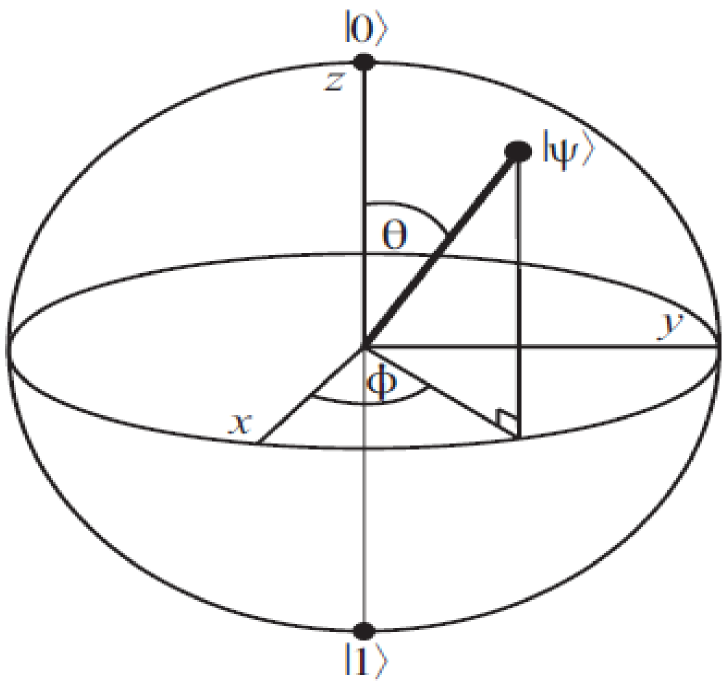
and $\{|p\rangle\,, |q\rangle\}$ is an arbitrary basis spanning $\mathcal{H}^2$. The choice of $\{|p\rangle\,, |q\rangle\}$ is often $\{|0\rangle\,, |1\rangle\}$, the so called computational basis states which form an orthonormal basis for $\mathcal{H}^2$. In general $|\psi\rangle$ is a coherent superposition of the basis states $|p\rangle$ and $|q\rangle$ and can be prepared in an infinite number of ways simply by varying the values of the complex coefficients α and β subject to the normalization constraint. We can rewrite $|\psi\rangle$ as

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}\,|0\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|1\rangle\right), \tag{7}$$

where γ, θ and $\phi \in \mathbb{R}$. Since, $e^{i\gamma}$ has no observable effects, we can ignore it. Thus,

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|1\rangle\,. \tag{8}$$

The numbers θ and ϕ define a point on the unit 3-dimensional sphere known as Bloch Sphere [8].



Bloch Sphere representation of a qubit $|\psi\rangle$

(Bloch Sphere)

When we know with certainty the initial state of the qubit, we have to use a vector representation. An example of this statement is to prepare a qubit in the state

$$|\psi\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \tag{9}$$

that is an equally weighted superposition of the canonical basis $\{|0\rangle, |1\rangle\}$. However, let us consider a different scenario in which a qubit $|\Psi\rangle$ is initially prepared in one of the quantum states $\{|\psi\rangle_1, |\psi\rangle_2, |\psi\rangle_3, ..., |\psi\rangle_n\}$ where each one of the states is selected with probability $\frac{1}{n}$. We do not know what state was chosen to prepare $|\Psi\rangle$ but we do know that only preparations $|\psi\rangle_i \in \{1, 2, ..., n\}$ are allowed. In this case, a convenient representation for $|\Psi\rangle$ is the associated density operator

$$\rho_\Psi = \frac{1}{n}\sum_{k=1}^{n} |\psi\rangle_{kk} \langle\psi|. \tag{10}$$

Evolution of a closed quantum system

Postulate 2 (Unitary Operator Version)

The evolution of a closed quantum system with state vector $|\Psi\rangle$ is described by a unitary transformation $\widetilde{U}$. The state of a system at time t_2 according to its state at time t_1 is given by

$$|\Psi(t_2)\rangle = \tilde{U}\,|\Psi(t_1)\rangle\,. \tag{11}$$

Postulate 2 only describes the mathematical properties that an evolution operator must have. The specific evolution operator required to describe the behaviour of a particular quantum system depends on the system itself. In the case of single qubits, any unitary operator can be realised in physical systems. Postulate 2 can also be stated with the famous Schrödinger equation.

Postulate 2 (Hermitian Operator Version)

The evolution of a closed quantum system is described by Schrödinger equation

$$i\hbar\frac{d\,|\psi\rangle}{dt} = \tilde{\mathbf{H}}\,|\psi\rangle\,, \tag{12}$$

where $\hbar$ is Planck's constant and $\tilde{\mathbf{H}}$ is a fixed Hermitian operator known as the Hamiltonian of the closed system. We have to note that $\tilde{\mathbf{H}}$ is the Hamiltonian of Postulate 2 and H is the Hadamard operator. The Hamiltonian of particular physical systems must be determined and calculated for each case. The search of the Hamiltonian of a particular physical system is a difficult task. The effect of the Hadamard operator is represented in the following two equations

$$H\,|0\rangle = \frac{1}{\sqrt{2}}\left\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right\}|0\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right), \tag{13}$$

and

$$H\,|1\rangle = \frac{1}{\sqrt{2}}\left\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right\}|1\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{14}$$

Quantum Measurements

In quantum mechanics, measurement is a non trivial and highly counter intuitive process. Firstly, because measurement outcomes are inherently probabilistic, i.e. regardless the carefulness in the preparation of a measurement procedure, the possible outcomes of such a measurement will be distributed according to a certain probability distribution. Secondly, once a measurement has been performed, a quantum system is unavoidably altered due to the interaction with measurement apparatus. Consequently, for an arbitrary quantum system, pre measurement and post measurement quantum states are different in general.

Postulate 3

Quantum measurements are described by a set of measurements operators $\left\{\tilde{M}_m\right\}$, index m labels the different measurement outcomes which act on the state space of the system being measured. Measurement outcomes correspond to values of observables, such as position, energy and momentum, which are Hamiltonian operators corresponding to physically measurable quantities. Let

$|\psi\rangle$ be the state of the quantum system immediately before the measurment. Then, the probability that result m occurs is given by

$$p(m) = \langle\psi| \tilde{M}_m^\dagger \tilde{M}_m |\psi\rangle, \tag{15}$$

and the post measurement state is

$$|\psi\rangle_{pm} = \frac{\tilde{M}_m |\psi\rangle}{\sqrt{\langle\psi| \tilde{M}_m^\dagger \tilde{M}_m |\psi\rangle}}. \tag{16}$$

Operators $\tilde{M}_m$ must satisfy the completeness relation, i.e.

$$\sum_m \tilde{M}_m^\dagger \tilde{M}_m = \mathbf{1}, \tag{17}$$

because that guarantees that probabilities $p(m)$ will sum to one

$$\sum_m \langle\psi| \tilde{M}_m^\dagger \tilde{M}_m |\psi\rangle = \sum_m p(m) = 1. \tag{18}$$

Let us work out a simple example. Assume we have a polarized photon with associated polarization orientations horizontal and vertical. The horizontal polarization direction is denoted by $|0\rangle$ and the vertical polarization direction is denoted by $|1\rangle$. Thus, an arbitrary initial state for our photon can be desrcibed by the quantum state

$$|\psi\rangle = a|0\rangle + \beta|1\rangle, \tag{19}$$

where α and β are complex numbers constrained by the normalization condition

$$|\alpha|^2 + |\beta|^2 = 1, \tag{20}$$

and $\{|0\rangle, |1\rangle\}$ is the computational basis spanning $\mathcal{H}^2$. Now, we construct two measurement operators

$$\tilde{M}_0 = |0\rangle\langle 0|, \tag{21}$$

and

$$\tilde{M}_1 = |1\rangle\langle 1|, \tag{22}$$

and two measurement outcomes α_0, α_1. Then, the full observable used for measurement in this experiment is

$$\tilde{M} = \alpha_0 |0\rangle\langle 0| + \alpha_1 |1\rangle\langle 1|. \tag{23}$$

According to Postulate 3, the probabilities of obtaining outcome α_0 or outcome α_1 are given by

$$p(\alpha_0) = |\alpha|^2, \tag{24}$$

and

$$p(\alpha_1) = |\beta|^2. \tag{25}$$

Corresponding to post measurement quantum states are as follows. If

$$outcome = \alpha_0, \tag{26}$$

then

$$|\psi\rangle_{pm} = |0\rangle\,, \tag{27}$$

and if

$$outcome = \alpha_1, \tag{28}$$

then

$$|\psi\rangle_{pm} = |1\rangle\,. \tag{29}$$

Composite Quantum systems

We now focus on the mathematical description of a composite quantum system, i.e. a system made up of several different physical systems.

Postulate 4 The state space of a composite quantum system as the tensor product of the component system state spaces.

- If we have n quantum systems expressed as state vectors labeled $|\psi\rangle_1\,, |\psi\rangle_2\,, ..., |\psi\rangle_n$ then the joint state of the total system is given by

$$|\psi\rangle_T = |\psi\rangle_1 \otimes |\psi\rangle_2 \otimes ... \otimes |\psi\rangle_n\,. \tag{30}$$

- Similarly, if we have n quantum systems expressed as density operators $\rho_1, \rho_2, ..., \rho_n$ then the joint state of the local system is given by

$$\rho_T = \rho_1 \otimes \rho_2 \otimes ... \otimes \rho_n \tag{31}$$

  (in the absence of any knowledge of correlations).

Reduced Density operator

Let us suppose we have a density operator describing a composite quantum system C and we are interested in studying the properties of one subsystem of C (such a situation would happen for example if after creating a bipartitte quantum system we had access to only one particle). The description of such a subsystem as provided by the reduced density operator.

Definition 1 *Let A,B be two physical systems whose state is described by a density operator ρ^{AB}. The reduced density operator for a system A is defined as*

$$\rho^A = Tr_B\left\{\rho^{AB}\right\}, \tag{32}$$

where Tr_B is the partial trace over system B. The partial trace is given by

$$Tr_B\left\{|a_1\rangle\langle a_2| \otimes |\beta_1\rangle\langle\beta_2|\right\} \equiv |a_1\rangle\langle a_2|\, Tr\left\{|\beta_1\rangle\langle\beta_2|\right\} \equiv |a_1\rangle\langle a_2|\,\langle\beta_1\,|\beta_2\rangle\,. \tag{33}$$

2.2 Various Definitions

Definition 2 *Inner product vector space. An inner product vector space V is a complex vector space, equiped with an inner product $\langle \cdot\, |\cdot\rangle : V \times V \longrightarrow \mathbb{C}$,satisfying the following axioms. $\forall a, b, c, d \in V, \gamma, \delta \in \mathbb{C}$*

1)

$$\langle a\, |b\rangle = \langle b\, |a\rangle^{*}, \tag{34}$$

2)

$$\langle a\, |a\rangle \geq 0, \tag{35}$$

and

$$\langle a\, |a\rangle = 0 \Longleftrightarrow a = 0, \tag{36}$$

3)

$$\langle a\, |\gamma b + \delta c\rangle = \gamma \langle a\, |b\rangle + \delta \langle a\, |c\rangle\, . \tag{37}$$

The inner product introduces the norm on

$$V: \;\; \|a\| = \sqrt{\langle a\, |a\rangle}. \tag{38}$$

Definition 3 *Functional. Let V be a vector space over a field F. A linear functional is a linear function $f : V \longrightarrow F$.*

Definition 4 *Dirac notation. Let $\mathcal{H}$ be a Hilbert space. A vector $\psi \in \mathcal{H}$ is denoted $|\psi\rangle$ and is referred as a ket. The corresponding linear functional is denoted $\langle\psi|$ and is referred as bra. Thus, $\langle\cdot|$ can be seen as an operator that maps each state ϕ into a functional $\langle\phi|$ such that*

$$\langle\phi|\,(|\psi\rangle) = \langle\phi\, |\psi\rangle\, . \tag{39}$$

We define

$$|\psi\rangle^{\dagger} \equiv \langle\psi|\, . \tag{40}$$

Column and row representation of kets and bras. Let $\mathcal{H}$ be an n-dimensional Hilbert space. Then, $|\psi\rangle \in \mathcal{H}$ can be represented as an n dimensional column vector, and its corresponding functional $\langle\psi| \in \mathcal{H}^{*}$ can be seen as an n dimensional row vector. Therefore, $\langle\phi\, |\psi\rangle$ is the usual row column matrix operator that computes the inner product in finite dimensional vector spaces. $|\psi\rangle \leftrightarrow \langle\psi|$ corresonds to transposition and conjuction

We now discuss linear operator in Hilbert spaces and their outer product representation.

Definition 5 *Linear Operator. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. Then, a linear operator A is a linear function between $\mathcal{H}_1$ and $\mathcal{H}_2$ i.e. A:$\mathcal{H}_1 \longrightarrow \mathcal{H}_2$ such that*

$$\forall \;\; |\psi_i\rangle \in \mathcal{H}_1, a_j \in \mathbb{C} \Longrightarrow A\left(\sum_m a_m\, |\psi\rangle_m\right) = \sum_m A\,(|\psi\rangle_m) = \sum_m a_m\, |\phi\rangle_m\, , \tag{41}$$

with $|\phi\rangle_m \in \mathcal{H}_2$.

Definition 6 *Outer product representation. Let* $|\psi\rangle, |a\rangle \in \mathcal{H}_1$ *and* $|\phi\rangle \in \mathcal{H}_2$*. Then, the outer product* $|\phi\rangle\langle\psi|$ *is the linear operator from* $\mathcal{H}_1$ *to* $\mathcal{H}_2$ *defined by*

$$(|\phi\rangle\langle\psi|)(|a\rangle) \equiv |\phi\rangle\langle\psi|a\rangle \equiv \langle\psi|a\rangle|\phi\rangle. \tag{42}$$

Definition 7 *Hermitian operator. Let* $\mathcal{H}$ *be a finite Hilbert space and* $A{:}\mathcal{H} \longrightarrow \mathcal{H}$ *a linear operator. If*

$$A = A^\dagger, \tag{43}$$

then A *is a Hermitian operator.*

Definition 8 *Positive operator. Let* $\mathcal{H}$ *be a Hilbert space and* $A{:}\mathcal{H} \longrightarrow \mathcal{H}$ *a linear operator.* A *is a positive operator if and only if*

$$\forall\ |\psi\rangle \in \mathcal{H} \Longrightarrow \langle\psi|A|\psi\rangle \geq 0. \tag{44}$$

Definition 9 *Unitary operator. Let* $\mathcal{H}$ *be a Hilbert space and* $U{:}\ \mathcal{H} \longrightarrow \mathcal{H}$ *a linear operator.* U *is a unitary operator if* $UU^\dagger = \mathbf{1} = U^\dagger U$ *where* $\mathbf{1}$ *is the identity operator. Unitary operators are the key elements in the formulation of quantum mechanics because they preserve the inner product between vectors.*

$$\text{If } |\beta\rangle = U|b\rangle \text{ and } |\delta\rangle = U|d\rangle \Longrightarrow \langle\beta|\delta\rangle = \langle b|U^\dagger U|d\rangle = \langle b|\mathbf{1}|d\rangle = \langle b|d\rangle. \tag{45}$$

Definition 10 *Normal Operator. Let* $\mathcal{H}$ *Hilbert space and* $A{:}\mathcal{H} \longrightarrow \mathcal{H}$ *a linear operator.* A *is normal if*

$$AA^\dagger = A^\dagger A. \tag{46}$$

Unitary and Hermitian operators are both normal matrices.

Theorem 11 (Spectral Theorem) *For every normal operator* A *acting on a finite dimensional Hilbert space* $\mathcal{H}$*, there is an orthonormal basis of* $\mathcal{H}$ *consisting of the eigenvectors* $|a_i\rangle$ *of* A*. Thus, the spectral decomposition of the operator* A *is*

$$A = \sum_i \lambda_i |a_i\rangle\langle a_i|, \tag{47}$$

where λ_i *are the eigenvalues of the operator* A*.*

Definition 12 *Operator functions. Let* $f : \mathbb{C} \longrightarrow \mathbb{C}$ *be a function and*

$$A = \sum_i \lambda_i |i\rangle\langle i|, \tag{48}$$

be a spectral decomposition for a normal operator A*. Then, the operator function* $f(A)$ *is defined by*

$$f(A) = \sum_i f(\lambda_i)|i\rangle\langle i|. \tag{49}$$

2.3 Pauli Matrices

The Pauli matrices are a set of three $2x2$ complex matrices which are Hermitian and Unitary. They are indicated by the greek letter σ and are defined as follows

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{50}$$

They have also the following properties

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = -i\sigma_x\sigma_y\sigma_z = \mathbf{1}, \tag{51}$$

$$\det(\sigma_i) = -1, i = x, y, z, \tag{52}$$

$$Tr\{\sigma_i\} = 0, i = x, y, z. \tag{53}$$

2.4 Superoperator - CPTP maps

We have a random density matrix ρ. The operator that acts on the density matrix ρ is called superoperator, is represented as $\mathcal{E}$ and the action is described as

$$\rho \xrightarrow{\mathcal{E}} \mathcal{E}(\rho). \tag{54}$$

The superoperator $\mathcal{E}$ must satisfy the following conditions.
Linearity

$$\mathcal{E}(\sum_i a_i\rho_i) = \sum_i a_i\mathcal{E}(\rho_i), \tag{55}$$

and

$$0 \leq Tr[\mathcal{E}(\rho)] \leq 1. \tag{56}$$

A superoperator is CPTP if the following extra conditions are satisfied

$$\forall\ \rho > 0 \implies \mathcal{E}(\rho) > 0, \tag{57}$$

and

$$Tr\{\mathcal{E}(\rho)\} = Tr\{\rho\}. \tag{58}$$

The most known representation of a superoperator $\mathcal{E}(\rho)$ is the representation

$$\mathcal{E}(\rho) = \sum_i A_i\rho A_i^\dagger, \tag{59}$$

where the operators A_i are linear and

$$\sum_i A_i^\dagger A_i \leq \mathbf{1}. \tag{60}$$

We call the operators A_i generators of the superoperator $\mathcal{E}(\rho)$. The set of the generators A_i of the superoperator $\mathcal{E}$ is not unique. A superoperator can be given by many different sets of generators. If the superoperator has

$$Tr\{\mathcal{E}(\rho)\} = Tr\rho = 1, \tag{61}$$

is linear

$$\mathcal{E}\left(\sum_i p_i \rho_i\right) = \sum_i p_i \mathcal{E}\left(\rho_i\ \right) \tag{62}$$

and $(\mathbf{1} \otimes \mathcal{E})\,\rho$ is a positive operator then there is a Kraus analysis or operator sum representation as follows

$$\mathcal{E}\left(\rho\right) = \sum_k A_k \rho A_k^{\dagger}, \tag{63}$$

where

$$A_i A_i^{\dagger} = \mathbf{1} \ \ \text{(trace precerving condition)} \tag{64}$$

Matrices A_i and $A_i^{\dagger}$ are called Kraus operators. Furthermore, If

$$\mathcal{E}\left(\mathbf{1}\right) = \mathbf{1}, \tag{65}$$

then $\mathcal{E}$ is called unital map.

2.5 Tensor Product

Now we focus on the tensor product, a method to build vector spaces from other vector spaces. The tensor product is crucial to representing mutliparticle quantum systems.

Definition 13 *Let V and W be vector spaces (over a field F) of dimension m and n respectively. Let X be the tensor of V and W, i.e. $X = V \otimes W$. The elements of X are linear combinations of vectors $|a\rangle \otimes |b\rangle$ where $|a\rangle \in V$ and $|b\rangle \in W$. In particular, if $\{|i\rangle\}$ and $\{|j\rangle\}$ are orthonormal bases for V and W then $\{|i\rangle \otimes |j\rangle\}$ is a basis for X. Let A and B be linear operators on V and W respectively. Then $\forall\ |a\rangle_1, |a\rangle_2 \in V\ , |b\rangle_1, |b_2\rangle \in W$ and $\gamma \in F \Longrightarrow$*

1)

$$\gamma\left(|a\rangle_1 \otimes |b\rangle_1\right) = \left(\gamma\,|a\rangle_1\right) \otimes |b\rangle_1 = |a\rangle_1 \otimes \left(\gamma\,|b\rangle_1\right), \tag{66}$$

2)

$$\left(|a\rangle_1 + |a\rangle_2\right) \otimes |b\rangle_1 = |a\rangle_1 \otimes |b\rangle_1 + |a\rangle_2 \otimes |b\rangle_1\,, \tag{67}$$

3)

$$|a\rangle_1 \otimes \left(|b\rangle_1 + |b\rangle_2\right) = |a\rangle_1 \otimes |b\rangle_1 + |a\rangle_1 \otimes |b\rangle_2\,, \tag{68}$$

4)

$$A \otimes B\left(|a\rangle_1 \otimes |b\rangle_1\right) = A\,|a\rangle_1 \otimes B\,|b\rangle_1\,, \tag{69}$$

5) A generalization of the previous step is straighforward. Let $|a\rangle_i \in V, |b\rangle_i \in W$ and $t_i \in F \Longrightarrow$

$$A \otimes B\left(\sum_i t_i\,|a\rangle_i \otimes |b\rangle_i\right) = \sum_i t_i A\,|a\rangle_i \otimes B\,|b\rangle_i\,. \tag{70}$$

A short hand notation for $|a\rangle \otimes |b\rangle$ is simply $|ab\rangle$ or $|a,b\rangle$. Furthermore, the tensor product of $|a\rangle$ with n times $|a\rangle \otimes |a\rangle \otimes ... \otimes |a\rangle$ can also be conveniently written as $|a\rangle^{\otimes n}$. The kronecker product is a convenient and simple matrix representation of the tensor product. Let $A = (a_{ij})\,, B = (b_{ij})$ be two matrices of order $m \times n$ and $p \times q$ respectively.

$$A = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix}, \tag{71}$$

and

$$B = \begin{bmatrix} b_{11} & \cdot & \cdot & \cdot & b_{1q} \\ \cdot & & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot \\ b_{p1} & \cdot & \cdot & \cdot & b_{pq} \end{bmatrix}, \tag{72}$$

Then $A \otimes B$ is given by

$$A \otimes B = \begin{bmatrix} a_{11} & \cdot & \cdot & \cdot & a_{1n} \\ \cdot & & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot \\ a_{m1} & \cdot & \cdot & \cdot & a_{mn} \end{bmatrix} \otimes \begin{bmatrix} b_{11} & \cdot & \cdot & \cdot & b_{1q} \\ \cdot & & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot \\ b_{p1} & \cdot & \cdot & \cdot & b_{pq} \end{bmatrix}. \tag{73}$$

Thus,

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdot & \cdot & \cdot & a_{1n}B \\ \cdot & & & & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & & & & \cdot \\ a_{m1}B & \cdot & \cdot & \cdot & a_{mn}B \end{bmatrix}, \tag{74}$$

where the matrix $A \otimes B$ is of order $mp \times nq$.

2.6 Trace and Partial Trace

Let $A \in M_n(F)$ be a matrix of order n with entries (a_{ij}) from a field F. The trace of the matrix A is defined as

$$Tr\,\{A\} = \sum_i a_{ii}. \tag{75}$$

The trace of a matrix A is the sum of all diagonal elements of the matrix. We consider V, W two finite dimensional vector spaces with dimensions m and n, respectively. For the space V we denote as $L(V)$ the space of linear operators on V. The partial trace over the space V, Tr_V, is a mapping

$$T \in L(V \otimes W) \longrightarrow Tr_W(T) \in L(V), \tag{76}$$

and

$$Tr_V : L(V \otimes W) \longrightarrow L(V), \tag{77}$$

such that

$$Tr_V(R \otimes S) = [TrR]S, \forall R \in L(V), \forall S \in L(W). \tag{78}$$

Example 14 *We consider the matrix*

$$A = \begin{bmatrix} 1 & 2 \\ 4 & 5 \end{bmatrix}. \tag{79}$$

The trace of the matrix A is

$$TrA = a_{1,1} + a_{2,2} = 1 + 5 = 6. \tag{80}$$

Example 15 *We consider the matrix*

$$Z = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \tag{81}$$

where A, B, C, D are matrices. The Z matrix can be expressed as

$$Z = |0\rangle \langle 0| \otimes A + |0\rangle \langle 1| \otimes B + |1\rangle \langle 0| \otimes C + |1\rangle \langle 1| \otimes D. \tag{82}$$

The partial trace of the matrix Z is

$$Tr_V \{Z\} = \underbrace{[Tr\,|0\rangle \langle 0|]}_{1} A + \underbrace{[Tr\,|0\rangle \langle 1|]}_{0} B + \underbrace{[Tr\,|1\rangle \langle 0|]}_{0} C + \underbrace{[Tr\,|1\rangle \langle 1|]}_{1} D. \tag{83}$$

Thus,

$$Tr_V \{Z\} = A + D. \tag{84}$$

2.7 Density Matrix - Operator

A matrix ρ is called density matrix if and only if $\rho > 0$ [positive eigenvalues], $\rho = \rho^\dagger$ [2 real eigenvalues] and $Tr\{\rho\} = 1$ [sum of the eigenvalues=1]. If $Tr\{\rho^2\} = 1$ then the densiy matrix ρ describes a pure quantum state and if $Tr\rho^2 < 1$ then the density matrix ρ describes a mixed state. The set of all density matrices on the Hilbert space $\mathcal{H}$ is defined as

$$\Delta(\mathcal{H}) = \left\{\rho \in Lin(\mathcal{H}) \;\; s.t. \; \rho^\dagger = \rho, \rho > 0, Tr\{\rho\} = 1\right\}. \tag{85}$$

$$\text{If } \rho^2 = \rho \text{ then } \rho = |\psi\rangle \langle\psi| \;\; [\text{projector operator}]. \tag{86}$$

2.8 Hilbert Space and its Dual

We consider a Hilbert space $\mathcal{H} = \mathbb{C}^{n\times 1}$ which contains vectors, polynomials and matrices. Each vector is defined as $|\rangle \in \mathcal{H}$ and it is called ket. Its dual space is $\mathcal{H}^* = \mathbb{C}^{1\times n}$ and each vector is defined as $\langle| \in \mathcal{H}^*$.

Example 16 *Discrete and Continuous Hilbert Spaces*

We consider the continuous Hilbert space $\mathcal{H}^\phi = \left\{|\phi\rangle, \frac{d\phi}{2\pi}\right\}_{\phi\in[0,2\pi)}$ and its dual $\mathcal{H}^{\phi*} = \left\{\langle\phi|, \frac{d\phi}{2\pi}\right\}_{\phi\in[0,2\pi)}$. The completeness is described as

$$\int_0^{2\pi} |\phi\rangle\langle\phi| \frac{d\phi}{2\pi} = \mathbf{1}. \tag{87}$$

We consider the discrete Hilbert space $\mathcal{H}^m = \{|m\rangle\}_{m\in\mathbb{Z}}$ and its dual $\mathcal{H}^{m*} = \{\langle m|\}_{m\in\mathbb{Z}}$. The completeness is described as

$$\sum_{m\in\mathbb{Z}} |m\rangle\langle m| = \mathbf{1}. \tag{88}$$

2.9 Dirac Delta Function

Dirac function with centre 0

$$\delta(x) = \begin{cases} 0, x \in \mathbb{R} \\ \infty, x = 0 \end{cases}. \tag{89}$$

Dirac function with centre $a \in \mathbb{R}$

$$\delta(x-a) = \begin{cases} 0, x \neq a \\ \infty, x = a \end{cases}. \tag{90}$$

For a function $f(x)$, its Dirac transformation with center α is

$$f(a) = \int_{-\infty}^{+\infty} \delta(x-a) f(x)\, dx, \tag{91}$$

where

$$\int_{-\infty}^{\infty} \delta(x-a)dx = 1, a > 0. \tag{92}$$

2.10 Classical Statistics

The branch of Mathematics that deals with random phenomena is the probability theory [24]. An example of a random phenomenon is the throwing of a coin. The base for the mathematical study of random phenomena is a typical mathematical structure called probability space.

The uncertainty of a stochastical experiment $(\Omega, \mathcal{A})$ is determined on the structure of the space with probability $(\Omega, \mathcal{A}, P)$ of the experiment as follows.

1) The sample space Ω consists of all the possible results ϖ of the stochastical experiment and it reflects the kind of the information that we have or request from the experiment

2) Th $\sigma-$algebra $\mathcal{A}$ of the possibilities of the experiment

a) contains the Ω space

b)

$$\forall A \in \mathcal{A} \Longrightarrow A^c \in \mathcal{A}, \tag{93}$$

c)

$$\forall \left(A_i\right)_{i=1}^{\infty} \in \mathcal{A} \Longrightarrow \bigcap_{i=1}^{\infty} A_i \in \mathcal{A}. \tag{94}$$

The delicacy of $\mathcal{A} \subseteq \mathcal{P}_0 = \{A : A \subseteq \Omega\}$, reflects the detail of the information that we have or request from our experiment.

3) The likely function P of the experiment (Ω, A) is a function $P : A \in \mathcal{A} \longrightarrow P(A) \in [0,1]$ such that $P(\Omega) = 1$,

$$P\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} P\left(A_i\right), \tag{95}$$

and

$$\forall \ \left(A_i\right)_{i=1}^{\infty} \in \mathcal{A}, \tag{96}$$

where A_i is a sequence of independent and disjoint possibilities.

The likely function P on $\mathcal{A}$ defines the distribution of the total "probability mass" on the space Ω and it reflects the frequency whereby are happening or could be happen the various possibilities $A \in \mathcal{A}$ of the experiment $(\Omega, \mathcal{A})$.

Definition 17 (possibilities independecy) *A group of possibilities $A_1, A_2, .., A_n, ..$ is called a group of independent possibilities if and only if the possibilities of each finite subgroup are independent.*

2.10.1 Statistical Random Variable

Definition 18 (random variable) *An experiment is a situation with a set of possible outcomes. Let $(\Omega, \mathcal{A})$ an experiment, then a function $X : \varpi \in \Omega \mapsto X(\varpi) \in \mathbb{R}$ is called random variable (r.v.) if and only if $(X \leq x) = \{\varpi \in \Omega : X \leq x\} \in \mathcal{A}, \forall x \in \mathbb{R}$. The random variable X is the function that depicts the set Ω of all the possible results ϖ of an experiment.*

Definition 19 (discrete random variable) *The random variables $x_1, .., x_n$ that their carrier is a discrete finite or countable set of distinct values of the form $S_x = \{x_1 < x_2 < ... < x_n < ...\}$ and their distribution is determined from a probability density function (p.d.f) $p_X : \mathbb{R} \longmapsto [0, +\infty)$ where*

$$p_X(x) = P(X = x), \tag{97}$$

such that $p_X(x) \geq 0$,$\forall x \in S_x$ and

$$\sum_{x \in S_X} p_X(x) = 1, \tag{98}$$

are called discrete random variables.

Definition 20 (continuous random variable) *The random variables $x_1, ..., x_n$ that their carrier is a set of the form (a, β) ,where $-\infty \leq a < \beta \leq \infty$ and their distribution is determined from a probability density function (p.d.f.) $f_X : \mathbb{R} \longmapsto [0, +\infty)$ such that $f_X(x) \geq 0,\ \forall x > 0,$ where*

$$\int_{\mathbb{R}} f_X(x)\, dx = 1, \tag{99}$$

and

$$P(x \in B) = \int_B f_X(x)\, dx, \tag{100}$$

$\forall B \in \mathcal{B}$, are called continuous random variables. Furthermore, a random variable is called continuous if $P(X = x) = 0, -\infty < x < +\infty$.

Definition 21 (Borel Algebra) *The smallest $\sigma-$algebra that contains all the semi straight lines $(-\infty, x]$ is called the Borel set and is defined as*

$$\mathcal{B} = \sigma\{(-\infty, x], x \in \mathbb{R}\}. \tag{101}$$

2.10.2 Probability Density Function

Definition 22 (discrete density function) *Let $X : \Omega \longrightarrow A$ be a discrete random variable. Since the outcomes of an experiment are uncertain in general, we associate with each outcome $x \in A$ a probability $p_X(x)$ where $p_X(x) = P(X = x)$ .The real function p_x that is defined on $\mathbb{R}$ as $p_X(x) = P(X = x)$ is called discrete probability density function of x. A number x is called possible value of the function p if $p_X(x) > 0$.Furthermore, a real function $p(x)$ defined on $\mathbb{R}$ is called discrete probability density function if the following properties are satisfied 1) The density function is positive*

$$p_X(x) \geq 0, \forall x \in \mathbb{R}. \tag{102}$$

2) The possibility

$$\{x : p_X(x) \neq 0\}, \tag{103}$$

is finite or infinity countable subset of $\mathbb{R}$. *Suppose that* $\{x_1, x_2, ...\}$ *is that set. Then*

$$\sum_i p_X(x_i) = 1. \tag{104}$$

Definition 23 ***(continuous density function)*** *Continuous probability density function is a non negative function* $f_x(x)$ *such that*

$$\int_{-\infty}^{+\infty} f_X(x)\, dx = 1. \tag{105}$$

2.10.3 Indicator Function

The indicator function is defined as

$$1_A(x) = \begin{cases} 1, \text{if } x \in A \\ 0, \text{if x} \notin A \end{cases}. \tag{106}$$

2.10.4 Probability Distribution

Probability distribution assigns a probability to each measurable subset of the possible outcomes of a random experiment survey, or procedure of statistical inference. A probability distribution can either be univariate or multivariate. A univariate distribution gives the probabilities of a single random variable taking on various alternative values. A multivariate distribution gives the probabilities of a random vector taking on various combinations of values. We describe below some common univariate discrete and continuous probability distributions.

Discrete Probability Distributions Binominal $B(n, r)$ with parameters $(n, r) \in \Theta = \mathbb{N} \times [0, 1]$. The probability density function is defined as

$$p_X(x|n, r) = \binom{n}{r} r^x (1-r)^{n-x} 1_{S_X^B}(x), \tag{107}$$

and the carrier is $S_X^B = \{0, 1, ..., n\}$.

The Binomial distribution describes experiments that consist of a number of idependent identical trials with two possible outcomes. Sucess with probability r and failure with probability $q = 1 - r$. Thus, the random variable $X =$ number of sucesses can take any value from $\{0, 1, ..., n\}$ and its distribution is described by the Binomial distribution. The probability $p_X(x)$ of obtaining x sucesses from n trials is given by

$$p_X(x|n, r) = \binom{n}{r} r^x (1-r)^{n-x} 1_{S_X^B}(x). \tag{108}$$

Poisson $P(\lambda)$ with parameter $\lambda \in \Theta = (0, +\infty)$. The probability density function is defined as

$$p_X\left(x|\lambda\right)=e^{-\lambda}\frac{\lambda^x}{x!}1_{S_X^P}\left(x\right) \tag{109}$$

and the carrier is $S_X^P=\{0,1,...\}$.

Continuous Probability Distributions Normal Distribution $N\left(\mu,\sigma^2\right)$ with parameters $\left(\mu,\sigma^2\right)\in\mathbb{R}\times\mathbb{R}_+$. The probability density function is defined as

$$f\left(x|\mu,\sigma^2\right)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left\{-\frac{\left(x-\mu\right)^2}{2\sigma^2}\right\}1_{S_X^N}\left(x\right), \tag{110}$$

and the carrier is $S_X^N=\{-\infty,+\infty\}$.

Gamma Distribution $\Gamma\left(\alpha,\lambda\right)$ with parameters $\left(a,\lambda\right)\in\mathbb{R}_+^2$. The probability density function is defined as

$$f\left(x|a,\lambda\right)=\frac{\lambda^a}{\Gamma\left(a\right)}x^{a-1}e^{-\lambda x}1_{S_X^\Gamma}\left(x\right), \tag{111}$$

where

$$\Gamma\left(a\right)=\int_0^{+\infty}\left\{x^{a-1}e^{-x}\right\}dx, a>0, \Gamma\left(a+1\right)=a\Gamma\left(a\right), a>0, \Gamma\left(\frac{1}{2}\right)=\sqrt{\pi}, \Gamma\left(n\right)=\left(n-1\right), \tag{112}$$

and the carrier is $S_X^\Gamma=\{1,2,...\}$.

Geometrical Distribution $Geom\left(p\right)$ with parameter p. The probability density function is defined as

$$P\left(X=x\right)=p\left(1-p\right)^{x-1}1_{S_X^G}\left(x\right), \tag{113}$$

and the carrier is $S_X^G=\{1,2,...\}$.

2.10.5 Multivariate Random Variables

Definition 24 ***(multivariate random variable)*** *A vector* $\underset{\sim}{x}=\left(x_1,...,x_n\right)^T$ *of real random variables defined on the same space with probability* $\left(\Omega,\mathcal{A},P\right)$ *is called* $n-$*dimensional or multivariate random variable.*

We denote a r dimensional vector of the $\mathbb{R}^r$ space as $\underset{\sim}{X}=\left(X_1,...,X_r\right)$. For each $\varpi\in\Omega$ we obtain the functional vector $X\left(\varpi\right)=\left(X_1\left(\varpi\right),...,X_r\left(\varpi\right)\right)$.

Example 25 *The probability density function of the n-dimensional normal distribution* $N_n\left(\bar{\mu},\pm\right)$ *where* $\bar{\mu}\in\mathbb{R}^n, \pm\in\mathbb{R}^n\times\mathbb{R}^n$ *(is a symmetrical and positive definite matrix) is defined as*

$$f_n\left(\underset{\sim}{x}|\bar{\mu},\pm\right)=\frac{1}{\left(2\pi\right)^{\frac{n}{2}}\left|\Sigma\right|^{\frac{1}{2}}}\exp\left\{-\frac{1}{2}\left(\underset{\sim}{x}-\bar{\mu}\right)^T\Sigma^{-1}\left(\underset{\sim}{x}-\bar{\mu}\right)\right\}1\left(\underset{\sim}{x}\in\mathbb{R}^n\right). \tag{114}$$

For $n = 2$, $\underline{\mathrm{x}} \sim N_2(\bar{\mu}, \Sigma) \equiv N_2(\mu_1, \mu_2 | \sigma_1^2, \sigma_2^2 | \rho)$ the probability density function is defined as

$$\begin{aligned} f_2(x_1, x_2) &= \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \\ &\quad \times \exp\{-\frac{1}{2(1-\rho^2)}\left[\left(\frac{x_1-\mu_1}{\sigma_1}\right)^2 + \left(\frac{x_2-\mu_2}{\sigma_2}\right)^2 - 2\rho\left(\frac{x_1-\mu_1}{\sigma_1}\right)\left(\frac{x_2-\mu_2}{\sigma_2}\right)\right]\}, \end{aligned} \tag{115}$$

where $x_1, x_2 \in \mathbb{R}$ with parameters $\mu_1, \mu_2 \in \mathbb{R}$ and $\sigma_1^2, \sigma_2^2 > 0$, $\rho \in [-1, 1]$.

Definition 26 *The random variables $x_1, ..., x_n$ defined on the same $(\Omega, \mathcal{A}, P)$ are called independent if and only if for each $B_1, ..., B_n \in \mathcal{B}$, the possibilities $(x_1 \in B_1), ..., (x_n \in B_n)$ are independent, i.e.*

$$P(x_1 \in B_1, ..., x_n \in B_n) = \prod_{i=1}^{n} P(x_i \in B_i). \tag{116}$$

3 Theory of Quantum Walk

3.1 Introduction

A stochastic process is a system which involves in time undergoing chance fluctuations. We can describe such a system with a family of random variables $\{X_t\}$ where X_t measures, at time t the property of the system which is of interest. Random walks are a particular type of stochastic processes, and are relevant as mathematical entities as well as in many fields like physics and computer science. A particular kind of stochastic process is a classical random walk (CRW) on a line. The simplest classical walk on a line consists of a particle (the walker) jumping to either left or right depending on the outcomes of a probability system (the coin) with (at least) two mutually exclusive results, i.e. the particle moves according to a probability distribution. The generalization to random walks on spaces of higher dimensions (graphs) is straightforward. An example of a random walk on a graph is a particle moving on a lattice where each node has six vertices and the particle moves according to the outcomes produced by tossing a dice. CRWs, a subset of stochastic process (that is, processes whose evolution involves chance) have proved to be a very powerful tool for the development of stochastic algorithms. The main idea behind the mechanics of CRWs is the following. Assume we have a particle (walker) that is allowed to move on a lattice. The actual movements of the particle on the lattice, i.e. the evolution of the system, are performed according to a probability distribution. This process is clearly stochastic and it is known as a CRW on a line. The quantum mechanical counterparts of random walks are the QWs. There are two models of QWs. The first model is called discrete QW and it consists of two quantum mechanical systems (a walker and a coin) as well as an evolution operator which is applied to both systems only in discrete time steps. In the second model named continuous QWs the evolution operator of the system can be applied at any time. In both cases the QW is performed on discrete graph. The key idea behind QWs is to apply the corresponding evolution operator to the initial quantum state several times, without performing intermediate measurements. By doing so, quantum interference will cause a behaviour radically different from that of a CRW. Discrete QWs on a line is the most studied model of discrete QWs [2], [8]. In order to perform a discrete QW with non trivial evolution it was proposed to use an additional quantum system, a coin. Thus, a discrete QW comprises two quantum systems, coin and walker along with a coin unitary operator (to toss a coin) and a conditional shift operator (to displace the walker either left or right depending on the accompanying coin state component). The walker is a quantum system living in a Hilbert space of an infinite but countable dimension $\mathcal{H}_w$. It is customary to use vectors from the canonical (computational) basis of $\mathcal{H}_w$ as position states for the walker. Thus, we denote the walker as $|position\rangle \in \mathcal{H}_w$, and affirm that the canonical basis states $|i\rangle_w$ that span $\mathcal{H}_w$ as well as any superposition of the form $\sum_i a_i |i\rangle_w$ subject to

$$\sum_i |a_i|^2 = 1, \tag{117}$$

are valid states for $|position\rangle$. The walker is usually initialised at the origin, i.e.

$$|position\rangle_{initial} = |0\rangle_w \,. \tag{118}$$

The coin is a quantum system living in a two dimensional Hilbert space $\mathcal{H}_c$. The coin may take the canonical basis states $|0\rangle$ and $|1\rangle$ as well as any superposition of these basis states. Therefore, $|coin\rangle \in \mathcal{H}_c$ and a general normalised state of the coin may be as

$$|coin\rangle = a\,|0\rangle_c + b\,|1\rangle_c \,, \tag{119}$$

where

$$|a|^2 + |b|^2 = 1. \tag{120}$$

An initial state of a QW can be defined as

$$|\psi\rangle_{initial} = |position\rangle_{initial} \otimes |coin\rangle_{initial} \,. \tag{121}$$

The evolution of a QW is divided into two parts that closely resemble the behaviour of a CRW. In the classical case, chance plays a key role in the evolution of the system. This is evident in the following example. We first toss a coin (either biased or unbiased) and then, depending on the coin outcome, the walker moves one step either to the right or to the left. In quantum case the equivalent of the previous process is to apply an evolution operator to the coin state followed by a conditional shift operator to the total quantum system. The purpose of the coin operator is to render the coin state in superposition, and the randomness is introduced by perfoming a measurement on the system after both evolution operators have been applied to the total quantum system several times.

3.2 Quantum Walk on Integers

Preliminaries. Let a random walker hopping on the line of the integers $\mathbb{Z}$. The position of the walker is described as $|m\rangle\,, m \in \mathbb{Z}$ and the number of the step is enumerated as $n \in \{1, 2, ...\}$. The move of the walker is decided from the toss of a coin. The coin tossing "drives" the walk. If the coin heads, then the walker goes left with a direction to the negative side. If the coin tails, then the walker goes right with a direction to the positive side. We have two systems. The coin and the walker system. The two systems interact each other. Each system is described by a Hilbert space. The coin Hilbert space

$$\mathcal{H}_c = span\,\{|+\rangle = heads, |-\rangle = tails\}\,, \tag{122}$$

admits as basis the vectors $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$. On $\mathcal{H}_c$ operate the step operators, i.e. $\{P_+, P_-\} \in End(\mathcal{H}_c)$. The walker Hilbert space is $\mathcal{H}_w = span\,\{|m\rangle\}_{m\in\mathbb{Z}}$ .On $\mathcal{H}_w$ operate the step operators $E_\pm$ and the position operator L i.e. $\{E_\pm, L\} \in End(\mathcal{H}_w)$.

The quantum system of the coin is described by the density matrix ρ_c and the quantum system of the walker is described by the density matrix ρ_w. We use the tensor product $\otimes$ to create the total space $\mathcal{H}_c \otimes \mathcal{H}_w$. The system in the total space $\mathcal{H}_c \otimes \mathcal{H}_w$ is described by the density matrix $\rho_c \otimes \rho_w$ if there is no coupling between the two systems. The $\rho_c \otimes \rho_w$ is a separable density matrix of the composition of coin and walker systems. We define a CRW step via the action of the unitary operator

$$V_{cl} = P_+ \otimes E_+ + P_- \otimes E_-, \tag{123}$$

in the total space $\mathcal{H}_c \otimes \mathcal{H}_w$, with the following unitary transformation

$$\rho_c \otimes \rho_w \rightarrow V_{cl} \left(\rho_c \otimes \rho_w\right) V_{cl}^{\dagger}. \tag{124}$$

If the total system $\rho_c \otimes \rho_w$ is decoupled initially, i.e. $\rho_c \otimes \rho_w$, then action of V_{cl} creates a coupling of the two systems. Subsequently after the action of the classical, we eliminate the coin quantum system by tracing out its operators, as follows

$$\begin{aligned} \rho_c \otimes \rho_w & \overset{\text{unitary transformation}}{\rightarrow} V_{cl}(\rho_c \otimes \rho_w)V_{cl}^{\dagger} \\ & \overset{\text{decoupling}}{\rightarrow} Tr_c(V_{cl}(\rho_c \otimes \rho_w)V_{cl}^{\dagger}). \end{aligned} \tag{125}$$

The partial trace for the coin space is a dynamic realization of the coin tossing process. The CRWer density matrix will now be expressed by means of the CPTP map $\mathcal{E}_{V_{cl}}(\rho_w)$ operating on the walker degree of freedom as follows

$$\mathcal{E}_{V_{cl}}(\rho_w) = Tr_c \left\{ V_{cl}(\rho_c \otimes \rho_w)V_{cl}^{\dagger} \right\}. \tag{126}$$

This map is identified with a single step and subsequent steps are identified with successive actions of $\mathcal{E}_{V_{cl}}$. For n steps the action of $\mathcal{E}_{V_{cl}}$ is described as

$$\mathcal{E}_{V_{cl}}^{n}(\rho_w) = \mathcal{E}_{V_{cl}}(\rho_w^{n-1}) = Tr_c \left\{ V_{cl}(\rho_c \otimes \rho_w^{n-1})V_{cl}^{\dagger} \right\}, \tag{127}$$

while for the $(n+1)$ th step it reads

$$\mathcal{E}_{V_{cl}}^{n+1}(\rho_w) = \mathcal{E}_{V_{cl}}(\rho_w^{n}) = Tr_c \left\{ V_{cl}(\rho_c \otimes \rho_w^{n})V_{cl}^{\dagger} \right\}. \tag{128}$$

We quantize the above CRW using a quantization rule (see below for details). We examine two quantization rules, the U rule and the ε rule. This time we use the U rule. The transformation

$$V_{cl} \rightarrow V_q = (V_{cl} U \otimes \mathbf{1}) \tag{129}$$

will occur, where the matrix U is the coin evolution operator and $\mathbf{1}$ is the shift operator. The QW density matrix is now

$$\mathcal{E}_{V_q}\left(\rho_w\right) = Tr_c \left\{ V_q \left(\rho_c \otimes \rho_w\right) V_q^{\dagger} \right\}. \tag{130}$$

The occupation probability distribution of the position states of the walker system after one evolution step occurs if we calculate the diagonal elements of $\mathcal{E}_{V_{cl}}(\rho_w)$ using the eigenbasis $|m\rangle$ of the position operator L, is

$$p_m = \langle m| \, \mathcal{E}_{V_{cl}}(\rho_w) \, |m\rangle \, . \tag{131}$$

After n evolution steps the occupation probability distribution will be

$$p_m^{(n)} = \langle m| \, \mathcal{E}_{V_{cl}}(\rho_w^{(n)}) \, |m\rangle \, , m = 0, \pm 1, \pm 2, ... \tag{132}$$

The QW deals in a quantum way the coin and walker systems. The target of our master thesis is a general and systematic framework of quantization of classical walks. The CRW is a transformation into a QW via a quantization rule. The essential feature for this transformation is the dynamic interactions among the two physical systems. The coin system has two sides (head, tails). Each side represents a movement to the left or to the right. We denote the density matrix of the coin as $\rho_c \in \Delta_c(\mathcal{H})$. The walker states vectors are labelled by integers and in this way we denote the direction of the motion of the walker and the density matrix of the walker is denoted as $\rho_w \in \Delta_w(\mathcal{H})$.

Qws create position probability distributions which give rise to statistical moments that have a different distribution law than those of CRWs. QWs helped for the invention of newer and faster algorithms in quantum computation like the Grover algorithm.

The standard deviation of a QW is $O(t)$ and the corresponding of a classical walk is $O\left(\sqrt{t}\right)$ where t is the number of the steps. The QW diffuses quadratically faster. The classical walk lives in the subballistic regime and the QW lives in the ballistic regime.

3.3 Group Theory of QW

The coin Hilbert space $\mathcal{H}_c = l_2(\{+,-\}) = span\{|+\rangle, |-\rangle\}$, is spanned by the orthogonal vectors $\langle + |-\rangle = \langle - |+\rangle = 0$, that form a complete basis, i.e.

$$|+\rangle\langle +| + |-\rangle\langle -| = \mathbf{1}. \tag{133}$$

The projectors in the basis vectors $\{|+\rangle, |-\rangle\}$ of coin space are $P_+ = |+\rangle\langle +|$, $P_- = |-\rangle\langle -|$, and satisfy the orthogonality relation $P_+P_- = 0$, and the completeness relation

$$P_+ + P_- = \mathbf{1}_{H_c}. \tag{134}$$

The walker Hilbert space $\mathcal{H}_w = l_2(\mathbb{Z}) = span\{|m\rangle\}_{m\in\mathbb{Z}}$, is spanned by the orthogonal vectors $\langle m | m'\rangle = \delta_{mm'}$, that form a complete basis i.e.

$$\sum_{m\in\mathbb{Z}} |m\rangle\langle m| = \mathbf{1}_{H_w}. \tag{135}$$

We can use a new basis for Hilbert space for the walker which results from the application of the discrete Fourier transform $\mathcal{F}$ to the vector $span\,(|m\rangle)_{m\in\mathbb{Z}}$. The resulting space will be denoted $\mathcal{H}_w^*$, it is the dual space of $\mathcal{H}_w$, and reads

$$\mathcal{H}_w^* = L_2\left([k, k+2\pi), \frac{d\phi}{2\pi}\right) = \left\{|\phi\rangle\,; \phi \in [k, k+2\pi), \frac{d\phi}{2\pi}\right\} \approx l_2\left(\mathbb{Z}\right), \tag{136}$$

for some $0 \leq k < 2\pi$, where

$$|\phi\rangle = \sum_{m\in\mathbb{Z}} e^{i\phi m}\,|m\rangle\,. \tag{137}$$

The generalized orthonormality of the elements of the dual space is

$$\langle \phi\,|\phi'\rangle = \delta(\phi - \phi') = \sum_{n\in\mathbb{Z}} e^{in\left(\phi-\phi'\right)}, \tag{138}$$

and the completeness reads is

$$\int_k^{k+2\pi} |\phi\rangle\,\langle\phi|\,\frac{d\phi}{2\pi} = \mathbf{1}_{H_w^*}. \tag{139}$$

Vectors $|m\rangle$ and $|\phi\rangle$ are connected as follows
$|\phi\rangle \rightarrow |m\rangle$

$$|m\rangle = \int_k^{k+2\pi} e^{-im\phi}\,|\phi\rangle\,\frac{d\phi}{2\pi}, \tag{140}$$

$|m\rangle \rightarrow |\phi\rangle$

$$|\phi\rangle = \sum_{m\in\mathbb{Z}} e^{i\phi m}\,|m\rangle\,. \tag{141}$$

Similarly the completeness relations and the respective resolution of units $\mathbf{1}_{H_w^*}$ and $\mathbf{1}_{H_w}$ are connected as follows
$\mathbf{1}_{H_w^*} \rightarrow \mathbf{1}_{H_w}$

$$\begin{aligned}\mathbf{1}_{H_w^*} &= \int_k^{k+2\pi} |\phi\rangle\,\langle\phi|\,\frac{d\phi}{2\pi} = \sum_{mm'} \underbrace{\int_k^{k+2\pi} e^{i\phi m} e^{-i\phi m'}\frac{d\phi}{2\pi}}_{\delta_{mm'}}\,|m\rangle\,\langle m'| \\ &= \sum_{mm'} |m\rangle\,\langle m'|\,\delta_{mm'} = \mathbf{1}_{H_w},\end{aligned} \tag{142}$$

where $\mathcal{B} = [k, k+2\pi) \equiv S^1$ is called in the Brillouin Zone in the context of physics applications and is identified with a 1 dimensional circle S^1;
$\mathbf{1}_{H_w} \rightarrow \mathbf{1}_{H_w^*}$

$$
\begin{aligned}
\mathbf{1}_{H_w} &= \sum_m |m\rangle\langle m| = \sum_m \int_k^{k+2\pi}\int_k^{k+2\pi} e^{im\phi}\,|\phi\rangle\langle\phi'|\,e^{-im\phi'}\frac{d\phi}{2\pi}\frac{d\phi'}{2\pi} \\
&= \int_k^{k+2\pi}\int_k^{k+2\pi} \underbrace{\left(\sum_m e^{im\left(\phi-\phi'\right)}\right)}_{\delta(\phi-\phi')}|\phi\rangle\langle\phi'|\,\frac{d\phi}{2\pi}\frac{d\phi'}{2\pi} \\
&= \int_k^{k+2\pi}|\phi\rangle\langle\phi|\,\frac{d\phi}{2\pi} = \mathbf{1}_{H_w^*}.
\end{aligned}
\tag{143}
$$

3.4 The Euclidean algebra generators acting on spaces $\mathcal{H}_w$ and $\mathcal{H}_w^*$

Next, we are study the main points of the Euclidean algebra and its representations in the spaces H_w and H_w^*. More explicitly, we study the operators involved in the theory of QW, their defining commutation relations, actions on vectors spaces H_w and H_w^* and the associated matrix representation and functional representations carrying by the coressponding discrete and continuous basis vectors of these spaces.

We consider the algebra $ISO\,(2)$ with generators

$$ISO\,(2) = span\,\{L, E_+, E_-\}\,. \tag{144}$$

The position L and step operators $E_+, E_-,$ are connected by the following commutation relations

$$[L, E_\pm] = \pm E_\pm, \;\; \left[E_+, E_-\right] = 0. \tag{145}$$

The action of step operator $E_\pm$ on $|m\rangle$ is

$$E_\pm\,|m\rangle = |m\pm 1\rangle\,. \tag{146}$$

Furthermore, we can take the a power of the operator $E_\pm$ such that

$$(E_\pm)^a\,|m\rangle = E_{\pm a}\,|m\rangle = |m\pm a\rangle\,, a\in\mathbb{Z}.$$

The position operator L admits basis vectors $|m\rangle\in\mathcal{H}_w,$ as eigenvectors i.e. $L\,|m\rangle = m\,|m\rangle$. Therefore, the matrix representation of $ISO\,(2)$ generators in the discrete $m-$basis of space $\mathcal{H}_w$ reads,

$$L = \sum_{m\in\mathbb{Z}} m\,|m\rangle\langle m|\,,\;\; E_\pm = \sum_{m\in\mathbb{Z}} |m\pm 1\rangle\langle m|\,. \tag{147}$$

The step operators $E_{\pm}$ admits basis vectors $|\phi\rangle \in \mathcal{H}_w^*$, as eigenvectors i.e. $E_{\pm}|\phi\rangle = e^{\pm i\phi}|\phi\rangle$. Furthermore, the position operator L acts on these vectors via a differential operator, i.e.

$$L|\phi\rangle = \frac{1}{i}\frac{\vartheta}{\vartheta\phi}|\phi\rangle. \tag{148}$$

Therefore, the matrix representation of $ISO(2)$ generators in the continous $\phi-$basis of space $\mathcal{H}_w^*$ reads,

$$E_{\pm} = \int_0^{2\pi} e^{\pm i\phi}|\phi\rangle\langle\phi|\frac{d\phi}{2\pi}, L|\phi\rangle = \int_0^{2\pi}\frac{1}{i}\frac{\vartheta}{\vartheta\phi}|\phi\rangle\langle\phi|\frac{d\phi}{2\pi}. \tag{149}$$

Proposition 27 *Given the interrelation between the $m-$basis and the $\phi-$basis vectors and additional the step-wise action of $E_{\pm}$ on the $\phi-$basis vectors, we show that the $\phi-$basis vectors are eigenvectors of $E_{\pm}$ and furthermore, that they form a conjugate unitary pair.*

Proof. *Firstly, we prove that the $\phi-$basis is eigenbasis of $E_{\pm}$. We have to prove that $E_{\pm}|\phi\rangle = e^{\pm i\phi}|\phi\rangle$. We begin with the action $E_{\pm}$ on $|\phi\rangle$ and we expand $|\phi\rangle$ to the $|m\rangle$ basis.*

$$\begin{aligned} E_{\pm}|\phi\rangle &= E_{\pm}[\frac{1}{(2\pi)}\sum_{m\in\mathbb{Z}} e^{-im\phi}|m\rangle] \\ &= \frac{1}{(2\pi)}\sum_{m\in\mathbb{Z}} e^{-im\phi}E_{\pm}|m\rangle \\ &= \frac{1}{(2\pi)}\sum_{m\in\mathbb{Z}} e^{-im\phi}|m\pm 1\rangle. \end{aligned} \tag{150}$$

by setting $m \pm 1 = l \in \mathbb{Z}$ and substituting for $|m\rangle$ we obtain that

$$\begin{aligned} E_{\pm}|\phi\rangle &= \frac{1}{(2\pi)}\sum_{l\in\mathbb{Z}} e^{-i(l\pm 1)\phi}|l\rangle \\ &= e^{\pm i\phi}[\frac{1}{(2\pi)}\sum_{l\in\mathbb{Z}} e^{-il\phi}|l\rangle] \\ &= e^{\pm i\phi}|\phi\rangle. \end{aligned} \tag{151}$$

Next, we prove the existence of the conjugate unitary pair $E_{\pm}E_{\mp} = \mathbf{1}_{\mathcal{H}_w}$ by using the above relation,

$$\begin{aligned} E_{+}|\phi\rangle &= e^{+i\phi}|\phi\rangle \\ E_{-}E_{+}|\phi\rangle &= e^{-i\phi}e^{+i\phi}|\phi\rangle \\ E_{-}E_{+}|\phi\rangle &= |\phi\rangle, \end{aligned} \tag{152}$$

and in the same way $E_{+}E_{-}|\phi\rangle = |\phi\rangle$. Thus, $E_{\pm}E_{\mp} = \mathbf{1}_{\mathcal{H}_w}$. ■

3.5 Quantization of the CRW

We transform a CRW to a QW by introducing a non trivial unitary rotation matrix that acts locally in the coin vector space. This action operating on the density matrix ρ_c, is in the form of an adjoint action, i.e. $\rho_c \to U\rho_c U^\dagger$ (to be called the U quantization rule); or in the form of a convex combination of such unitary actions, i.e. $\rho_c \to \lambda U_1\rho_c U_1^\dagger + (1-\lambda)U_2\rho_c U_2^\dagger$, $0 \leq \lambda \leq 1$ (to be called the E quantization rule).

The rules that we use, will be called quantization rules, and they assume a kind of interaction between the walker and the coin systems. We can consider that the source of the quantization is an underlying quantum or classical noise that is larking in the background of these two physical systems.

Definition 28 (Quantization of a CRW) *The quantization of a random walk is the incorporation of a unitary operator U in the coin space called the coin ressufling matrix.*

3.5.1 U quantization rule and Original Tracing Scheme

The density matrix of the n step for the walker is defined as

$$\rho_w^{(n)} = \mathcal{E}_{V_q^n}(\rho_w) = Tr_c\left\{\left(V_q^n\right)(\rho_c \otimes \rho_w)\left(V_q^n\right)^\dagger\right\}. \qquad (U \text{ rule Original Scheme})$$

We observe that n is transformed as a power of the matrix V_q.The action of $V_q = V_{cl}U \otimes \mathbf{1}$ on $\rho_c \otimes \rho_w$ is described below

Example 29

$$\begin{aligned}
\rho_w^{(n)} &= \mathcal{E}_{V_q^n}(\rho_w) = Tr_c\left\{\left(V_q^n\right)(\rho_c \otimes \rho_w)\left(V_q^n\right)^\dagger\right\} \\
&= Tr_c\left\{(V_{cl}U \otimes \mathbf{1})^n(\rho_c \otimes \rho_w)(V_{cl}U \otimes \mathbf{1})^{n\dagger}\right\} \\
&= Tr_c\left\{(V_{cl}U)^n\,\rho_c(V_{cl}U)^{n\dagger} \otimes \rho_w\right\} \\
&= \rho_w Tr\left\{Adj^n(V_{cl})(U)(\rho_c)\right\} \qquad (153)
\end{aligned}$$

3.5.2 U quantization rule and V^k model

The density matrix of the n step for the walker is defined as

$$\rho_w^{(n)} = \mathcal{E}_{V_q^k}(\rho_w^{(n-1)}) = Tr_c\left\{\left(V_q^k\right)(\rho_c \otimes \rho_w^{(n-1)})\left(V_q^k\right)^\dagger\right\} \qquad (U \text{ rule } V^k \text{ model})$$

We observe that n remains in its position, i.e. as a power of ρ_w. The transformation of ρ_c at each step by the unitary matrix U is

$$\rho_c \to U\rho_c U^\dagger = Adj(U)(\rho_c). \qquad (154)$$

The action of $V_q = V_{cl}U \otimes \mathbf{1}$ on $\rho_c \otimes \rho_w$ is described below

$$
\begin{aligned}
\rho_w^{(n)} &= \mathcal{E}_{V_q^k}(\rho_w^{(n-1)}) = Tr_c\left\{(V_q^k)(\rho_c \otimes \rho_w^{(n-1)})(V_q^k)^\dagger\right\} \\
&= Tr_c\left\{(V_{cl}U \otimes \mathbf{1})^k\,(\rho_c \otimes \rho_w^{(n-1)})\left[(V_{cl}U \otimes \mathbf{1})^k\right]^\dagger\right\} \\
&= \rho_w^{(n-1)} Tr\left\{Adj^k\,(V_{cl}U)\,(\rho_c)\right\}. \qquad (155)
\end{aligned}
$$

3.5.3 ε quantization rule and Original Tracing Scheme

A generalized version for the U quantization rule is the ε quantization rule. The ε quantization rule employs a completely positive trace preserving map (CPTP) ε, which acts on the coin density matrix. The density matirx ρ_c at each step is

$$
\begin{aligned}
\rho_c \xrightarrow{\varepsilon} \varepsilon(\rho_c) &= \\
&= S_1\rho_c S_1^\dagger + ... + S_n\rho_c S_n^\dagger \\
&= Adj(S_1)(\rho_c) + ... + Adj(S_n)(\rho_c) \\
&= \sum_i Adj\,(S_i)\,(\rho_c)\,, \qquad (156)
\end{aligned}
$$

where $(S_1, ..., S_n)$ are Kraus generators. The CPTP map that we use, is not necessary unital

$$\varepsilon(\mathbf{1}) \neq \mathbf{1}. \qquad (157)$$

Then we applicate $Adj(V_{cl})$ on $\rho_c \otimes \rho_w$ for the accomplishment of the action of

$$Adj(V_{cl})(\varepsilon \otimes \mathbf{1}), \qquad (158)$$

on the combined system. The density matrix of the n step for the walker is defined as

$$
\begin{aligned}
\rho_w^{(n)} &= \mathcal{E}_{V_q^n}(\rho_w) = Tr_c\left\{[V_{cl}\,(\varepsilon \otimes \mathbf{1})]^n\,(\rho_c \otimes \rho_w)\left[V_{cl}^\dagger\right]^n\right\} \\
&= Tr_c\left\{\left[V_{cl}\left(\sum_i Adj(S_i) \otimes \mathbf{1}\right)\right]^n (\rho_c \otimes \rho_w)\left[V_{cl}^\dagger\right]^n\right\} \\
&= \rho_w Tr\left\{\left(V_{cl}\sum_i Adj(S_i)\right)^n \rho_c\left[V_{cl}^\dagger\right]^n\right\} \\
&= \rho_w Tr\left\{\sum_i Adj^n(V_{cl}S_i)\,(\rho_c)\right\}. \qquad (159)
\end{aligned}
$$

3.5.4 ε quantization rule and V^k model

The density matrix of the n step for the walker is defined as

$$
\begin{aligned}
\rho_w^{(n)} &= \mathcal{E}_{V_q^k}(\rho_w^{(n-1)}) = \\
&= Tr_c\{V_{cl}(\varepsilon_k \otimes \mathbf{1})...V_{cl}((\varepsilon_1 \otimes \mathbf{1})(\rho_c \otimes \rho_w^{(n-1)})V_{cl}^{\dagger}...V_{cl}^{\dagger})\} \\
&= \rho_w^{(n-1)} Tr\left\{Adj\left(V_{cl}^k\right)(\varepsilon_k...\varepsilon_1(\rho_c))\right\}, \qquad (160)
\end{aligned}
$$

where $\varepsilon_1, ..., \varepsilon_k$ are different CPTP maps, that are not necessary unital.

3.5.5 Quantization Rules Summary

The quantization rules are summarized on the following table

	Original Scheme	V^k model
U rule	$\rho_w^{(n)} = \rho_w Tr\left\{Adj^n(V_{cl})(U)(\rho_c)\right\}$	$\rho_w^{(n)} = \rho_w^{(n-1)} Tr\left\{Adj^k\left(V_{cl}U\right)(\rho_c)\right\}$
ε rule	$\rho_w^{(n)} = \rho_w Tr\left\{\sum_i Adj^n(V_{cl}S_i)(\rho_c)\right\}$	$\rho_w^{(n)} = \rho_w^{(n-1)} Tr\left\{Adj\left(V_{cl}^k\right)(\varepsilon_k...\varepsilon_1(\rho_c))\right\}$

(161)

3.6 Density Matrix of the QWer

If we express the density matrix in the discrete basis $|m\rangle$ then

$$
\rho_w = \sum_{m,m' \in \mathbb{Z}} \rho_{mm'} |m\rangle \langle m'| . \qquad (162)
$$

Alternative, if we express the density matrix in the continuous basis $|\phi\rangle$ then

$$
\rho_w = \int_0^{2\pi}\int_0^{2\pi} \left\{\rho\left(\phi, \phi'\right)|\phi\rangle\langle\phi'|\right\} \frac{d\phi d\phi'}{(2\pi)^2}. \qquad (163)
$$

We search the density matrix of the walker. The walker performs a QW. Firstly, the density matrix ρ_w must satisfy three conditions i)

$$
Tr\{\rho_w\} = 1, \qquad (164)
$$

ii) Hermitian $\rho_w = \rho_w^{\dagger}$ iii) Positive Definite

$$
\forall \underline{x} \in \mathbb{C}_{nxn}, \;\; (\underline{x})\,\rho_w\,(\underline{x})^T \geq 0. \qquad (165)
$$

We calculate the density matrix ρ_w using a certain base. We will use the basis $|\phi\rangle$, for $\phi \in [0, 2\pi)$ which is the set of the eigenvectors of the two step operators E_+, E_-. We suppose that using the above basis, the ρ_w density operator will have the form

$$
\rho_w = \int_0^{2\pi}\left\{\int_0^{2\pi} \rho(\phi, \phi')|\phi\rangle\langle\phi'|\right\} \frac{d\phi d\phi'}{(2\pi)^2}. \qquad (166)
$$

The limits of the integrals are 0 and 2π because the ϕ basis lives in the space $[0,2\pi)$. We have divided the integral with 2π to succeed the normalization of the integral. The basis $|\phi\rangle$ is a continous basis because it represents an angle. Thus, we use integral $\int$ instead of using a sum $\sum$ which is used in discrete basis. The $|\phi\rangle\langle\phi'|$ locates the elements of which are in the matrix ρ_w. We consider that we expand the density matrix ρ_w using the discrete basis $|m\rangle$

$$\rho_w = \sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} |m\rangle\langle m'| . \tag{167}$$

By means of the intertransformation betwwen $|m\rangle$ and $|\phi\rangle$ basis. We obtain

$$\begin{aligned}\rho_w &= \sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} |m\rangle\langle m'| \\ &= \sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} [\frac{1}{2\pi}\int_0^{2\pi} e^{im\phi} |\phi\rangle\, d\phi][\frac{1}{2\pi}\int_0^{2\pi} e^{-im'\phi'} \langle\phi'|\, d\phi'], \end{aligned}\tag{168}$$

then finally

$$\rho_w = \int_0^{2\pi}\int_0^{2\pi} \underbrace{\sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} e^{i(m\phi-m'\phi)'}}_{\rho(\phi,\phi')} |\phi\rangle\langle\phi'| \frac{d\phi d\phi}{(2\pi)^2}. \tag{169}$$

We have find now the function $\rho(\phi,\phi')$, which is the kernel of the ρ_w density matrix in the continuous basis. The first step of the walk means that we will apply the evolution operator $\mathcal{E}_{V^2}$ (we use V^2 tracing scheme) to the density matrix ρ_w such that

$$\mathcal{E}_{V^2}(\rho_w) = \int_0^{2\pi}\int_0^{2\pi} \underbrace{\sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} e^{i(m\phi-m'\phi)'}}_{\rho(\phi,\phi')} \mathcal{E}_{V^2}(|\phi\rangle\langle\phi'|) \frac{d\phi d\phi}{(2\pi)^2}, \tag{170}$$

where the kernel can be expressed as the Fourier transform of the matrix elements

$$\rho(\phi,\phi') = \sum_{m,m'\in\mathbb{Z}} (\rho_w)_{mm'} e^{i(m\phi-m'\phi')}, \tag{171}$$

$$= \mathcal{F}[(\rho_w)_{mm'}]. \tag{172}$$

Therefore, to compute the action of $\mathcal{E}_{V^2}(\rho_w)$ we need to compute $\mathcal{E}_{V^2}(|\phi\rangle\langle\phi'|)$. The map $\mathcal{E}_{V^2}$ is representing the ε quantization rule using the tracing scheme V^2. The V^k QW model is described by the map

$$\mathcal{E}_{V^k}(\rho_w) = Tr_c\{V_{cl}[\varepsilon_k \otimes \mathbf{1}]...[V_{cl}[\varepsilon_1 \otimes \mathbf{1}](\rho_c \otimes \rho_w)V_{cl}^\dagger]...V_{cl}^\dagger\}. \tag{173}$$

The V^2 QW model is

$$\begin{aligned}
\mathcal{E}_{V^2}(\rho_w) &= Tr_c\{Adj(V_{cl}) \cdot (\varepsilon_\tau \otimes \mathbf{1})Adj(V_{cl}) \cdot (\varepsilon_t \otimes \mathbf{1}) \cdot (\rho_c \otimes \rho_w)\} \\
&= Tr_c\{Adj(V_{cl}) \cdot (\varepsilon_\tau \otimes \mathbf{1})Adj(V_{cl}) \cdot \varepsilon_t(\rho_c) \otimes \rho_w)\} \\
&= Tr_c\{V_{cl}(\varepsilon_\tau \otimes \mathbf{1})[V_{cl}[\cdot\varepsilon_t(\rho_c) \otimes \rho_w)]V_{cl}^\dagger)V_{cl}\}. \qquad (174)
\end{aligned}$$

For $\rho_w = |\phi\rangle\langle\phi'|$, we have that

$$\begin{aligned}
\mathcal{E}_{V^2}(|\phi\rangle\langle\phi'|) &= Tr_c\{V_{cl}(\varepsilon_\tau \otimes \mathbf{1})[V_{cl}[\varepsilon_t(\rho_c) \otimes |\phi\rangle\langle\phi'|)]V_{cl}^\dagger)V_{cl}^\dagger\} \\
&= |\phi\rangle\langle\phi'| \, Tr\{V_{cl}\varepsilon_\tau[V_{cl}[\varepsilon_t(\rho_c))]V_{cl}^\dagger)V_{cl}^\dagger\} \\
&= |\phi\rangle\langle\phi'| \, Tr\left\{Adj^2\left(V_{cl}\right)\left(\varepsilon_{\tau+t}\left(\rho_c\right)\right)\right\}. \qquad (175)
\end{aligned}$$

Thus, $\mathcal{E}_{V^2}(\rho_w)$ is described as

$$\mathcal{E}_{V^2}(\rho_w) = \int_0^{2\pi}\int_0^{2\pi} \mathcal{F}[(\rho_w)_{mm'}]Tr\left\{Adj^2\left(V_{cl}\right)\left(\varepsilon_{\tau+t}\left(\rho_c\right)\right)\right\}|\phi\rangle\langle\phi'| \frac{d\phi d\phi}{(2\pi)^2}. \tag{176}$$

Example 30 *We consider the following density matrix of the walker in the discrete basis* $|m\rangle$.

$$\rho_w = 0.3\,|{-1}\rangle\langle{-1}| + 0.7\,|{+1}\rangle\langle{+1}| + (3+2i)\,|{-1}\rangle\langle{+1}| + (3-2i)\,|{+1}\rangle\langle{-1}| \tag{177}$$

The matrix representation of ρ_w will be

$$\rho_w = \begin{array}{c} \\ ... \\ -1 \\ 0 \\ +1 \\ ... \end{array} \begin{array}{c} \begin{array}{ccccc} ... & -1 & 0 & +1 & ... \end{array} \\ \begin{bmatrix} ... & ... & ... & ... & .. \\ ... & 0.3 & 0 & 3+2i & ... \\ ... & 0 & 0 & 0 & ... \\ ... & 3-2i & 0 & 0.7 & ... \\ ... & 0 & 0 & 0 & ... \end{bmatrix} \end{array}. \tag{178}$$

I will calculate the above $\rho(\phi, \phi')$ and the representation of the above ρ_w on the continuous basis $|\phi\rangle$. We will use the following formulae

$$\begin{aligned}
\rho(\phi,\phi') &= \sum_{n,n'\in\mathbb{Z}} (\rho_w)_{nn'} e^{i(n\phi - n'\phi')} \\
&= \rho_{(-1),(-1)} \exp\{i[(-1)\phi - (-1)\phi']\} \\
&\quad \times + \rho_{(+1),(+1)} \exp\{i[(+1)\,\phi - (+1)\,\phi']\} \\
&\quad \times + \rho_{(-1),(+1)} \exp\{[(-1)\phi - (+1)\phi']\} \\
&\quad \times + \rho_{(+1),(-1)} \exp\{i[(+1)\phi - (-1)\phi']\} \\
&= 0.3 \exp\{i(\phi' - \phi)\} + 0.7 \exp\{i(\phi - \phi')\} \\
&\quad \times + (3+2i) \exp\{-\phi - \phi'\} + (3-2i) \exp\{\phi - \phi'\}. \qquad (179)
\end{aligned}$$

3.7 Asymptotics of QW and the double horn Distribution

Limit probability distribution of a double horn shape evaluates its asymptotic behaviour. The statistical correlations between the random coin and walker of a CRW are replaced by quantum correlations and this is achieved by appropriate quantization of the coin walker system and by their dynamic interaction between them in the course of time evolution of the walk. We construct an asymptotic probability function of the walk. This limit probabilty density function is obtained and has a distinct double horn shape. We use $\mathcal{H}_w = span\,\{|m\rangle\}_{m\in\mathbb{Z}}$, $\mathcal{H}_c = span\,\{|+\rangle\,,|-\rangle\}$ and $\rho_w^{(0)} = |0\rangle\,\langle 0|$. Then a general density matrix for the walker is written as

$$\rho_w = \int_0^{2\pi}\int_0^{2\pi} \rho\left(\phi,\phi'\right) |\phi\rangle\,\langle\phi'|\, \frac{d\phi d\phi'}{(2\pi)^2}. \qquad (180)$$

For initial state $\rho_w^{(0)} = |0\rangle\,\langle 0|$, we take that $\rho_w^{(0)}\left(\phi,\phi'\right) = 1$. To start investigating the dynamics of the walk we suppose that initially a pure coin density matrix $\rho_c = |c\rangle\,\langle c|$, and that its first evolution step involves k applications of the V_q before tracing out the coin system. This choice specifies the V_q^k QW model. Then the once evolved matrix $|\phi\rangle\,\langle\phi'|$ is

$$|\phi\rangle\,\langle\phi'| \xrightarrow{\mathcal{E}} \mathcal{E}_{V_q^k}\left(|\phi\rangle\,\langle\phi'|\right) = Tr_c\left\{\left(V_q^k\right)\left(\rho_c \otimes |\phi\rangle\,\langle\phi'|\right)\left(V_q^k\right)^\dagger\right\}, \qquad (181)$$

which is written by means of the Kraus generators, defined as

$$A_\pm\left(k,\Phi;c\right) = \langle\pm|\, V^k\left(\Phi\right)|c\rangle\,, \qquad (182)$$

as follows

$$\begin{aligned}
\mathcal{E}_{V^k}\left(|\phi\rangle\left\langle\phi'\right|\right) &= A_+\left(k,\Phi;c\right)|\phi\rangle\left\langle\phi'\right|A_+\left(k,\Phi;c\right)^\dagger \\
&\quad +A_-\left(k,\Phi;c\right)|\phi\rangle\left\langle\phi'\right|A_-\left(k,\Phi;c\right)^\dagger \\
&= \left(A_+\left(k,\phi;c\right)A_+\left(k,\phi';c\right)^* \right.\\
&\quad \left.+A_-\left(k,\phi;c\right)A_-\left(k,\phi';c\right)^*\right)|\phi\rangle\left\langle\phi'\right| \\
&= A\left(k,\phi,\phi';c\right)|\phi\rangle\left\langle\phi'\right|. \qquad (183)
\end{aligned}$$

This means, that the n th-step evolution map operates multiplicative on $|\phi\rangle\langle\phi|'$ viz.

$$\mathcal{E}^n_{V^k_q}\left(|\phi\rangle\left\langle\phi'\right|\right)=A\left(k,\phi,\phi';c\right)^n|\phi\rangle\left\langle\phi'\right|, \qquad (184)$$

with $A\left(k,\phi,\phi';c\right)$ to be referred as the *characteristic function* of the walk. Then the walker desnity matrix evolves as

$$\begin{aligned}
\mathcal{E}^n_{V^k_q}\left(\rho_w\right) &= \mathcal{E}^{(n-1)}_{V^k_q}\left(\sum_{i=\pm}A_i\left(k,\Phi;c\right)\rho_w A_i\left(k,\Phi;c\right)^\dagger\right) \\
&= \int_0^{2\pi}\int_0^{2\pi}\rho\left(\phi,\phi'\right)A\left(k,\phi,\phi';c\right)^n|\phi\rangle\left\langle\phi'\right|d\phi d\phi'. \qquad (185)
\end{aligned}$$

Next, we proceed to evaluate the quantum moment of the walker's position operator L for the n-step evolved density matrix

$$\begin{aligned}
\left\langle L^s\right\rangle_n &= Tr\left\{L^s\mathcal{E}^n_{V^k}\left(\rho_w\right)\right\} \\
&= \frac{1}{2\pi i^s}\int_0^{2\pi}d\phi\vartheta^s_\phi\left[\rho\left(\phi,\phi'\right)A^n\left(k,\phi,\phi';c\right)\right]_{\phi'=\phi} \\
&= \sum_{m\in\mathbb{Z}}m^sP^{(n)}_m\equiv\left\langle m^s\right\rangle_n. \qquad (186)
\end{aligned}$$

In last equation,

$$P^{(n)}_m=\langle m|\,\mathcal{E}^n_{V^k}\left(\rho_w\right)|m\rangle \qquad (187)$$

is the classical probability distribution for the walker to be in position m after n evolution steps and $\left\langle m^s\right\rangle_n$ are the classical statistical moments of the walker position. The asymptotic behaviour of these moments for large n is

$$\begin{aligned}
\left\langle L^s\right\rangle_n &= \left\langle n^s\right\rangle_n \\
&= \frac{n^s}{2\pi i^s}\int_0^{2\pi}h\left(2\phi;t\right)d\phi\left[\rho\left(\phi,\phi'\right)\left(\frac{\vartheta}{\vartheta\phi}A\left(k,\phi,\phi';c\right)\right)^s\right]_{\phi'=\phi} \\
&\quad +O\left(n^{s-1}\right). \qquad (188)
\end{aligned}$$

Hence, $\frac{m}{n}$ converges weakly to

$$h\left(\phi;k,c\right)=-i\left[\frac{\vartheta}{\vartheta\phi}A\left(k,\phi,\phi';c\right)\right]_{\phi=\phi'}, \qquad (189)$$

and ϕ assumes the role of a random variable with probability measure $\frac{\rho(\phi,\phi)}{2\pi}$.

An alternative expression for the function h, useful in our further investigations is given below

$$h\left(\phi';k,c\right) = Tr\{(\sigma + V\left(\phi\right)^{\dagger}\sigma V\left(\phi\right) + \cdots + V\left(\phi\right)^{\dagger(k-1)}\sigma V\left(\phi\right)^{(k-1)})\rho_c\},$$

where $\sigma := U_0^{\dagger}\sigma_3 U_0$.

We proceed to evaluate the asymptotic probability density function of the walk. Firstly, we must resort the concept of the dual of completely trace preserving map. Consider the dual map

$$\mathcal{E}_{V_q^k}^{*} : B\left(\mathcal{H}_w\right) \longrightarrow B\left(\mathcal{H}_w\right), \tag{190}$$

defined on the set of bounded operators acting on the walker Hilbert space $\mathcal{H}_w$ of some given CPTP map

$$\mathcal{E}_{V_q^k} : D\left(\mathcal{H}_w\right) \longrightarrow D\left(\mathcal{H}_w\right), \tag{191}$$

operating on the desnity matrices $\rho_w \in D\left(\mathcal{H}_w\right)$, with operator sum realization

$$\mathcal{E}_{V^k}\left(\rho_w\right) = \sum_{i=\pm} A_i\left(k,\Phi;c\right)\rho_w A_i\left(k,\Phi;c\right)^{\dagger}. \tag{192}$$

This dual map is defined to act on bounded operators $X \in B\left(\mathcal{H}_w\right)$,as

$$\mathcal{E}_{V_q^k}^{*}\left(X\right) = \sum_{i=\pm} A_i\left(k,\Phi;c\right)^{\dagger} X A_i\left(k,\Phi;c\right). \tag{193}$$

By virtue of the last definition, the expectation value (quantum moments) of the scaled powers of position operator $\left(\frac{L}{n}\right)^s$, evaluated after n steps of the walker which is now in the state

$$\rho_w^{(n)} = \mathcal{E}_{V_q^k}^{n}\left(\rho_w\right), \tag{194}$$

becomes

$$\left\langle\left(\left(\frac{L}{n}\right)^s\right)\right\rangle_n = Tr\left\{\rho_w^{(n)}\left(\frac{L}{n}\right)^s\right\}, \tag{195}$$

or dually is determined by the equation

$$\left\langle\left(\frac{L}{n}\right)^s\right\rangle_n \equiv \left\langle\mathcal{E}_{V_q^k}^{*n}\left(\left(\frac{L}{n}\right)^s\right)\right\rangle_0 = Tr\left(\rho_w \mathcal{E}_{V_q^k}^{*n}\left(\left(\frac{L}{n}\right)^s\right)\right). \tag{196}$$

Specializing to the V_q^2 model and taking the case where initially $\rho_w = |0\rangle\langle 0|$, and $\rho_c = |c\rangle\langle c|$, with

$$|c\rangle = \cos\chi\,|+\rangle + i\sin\chi\,|-\rangle, \tag{197}$$

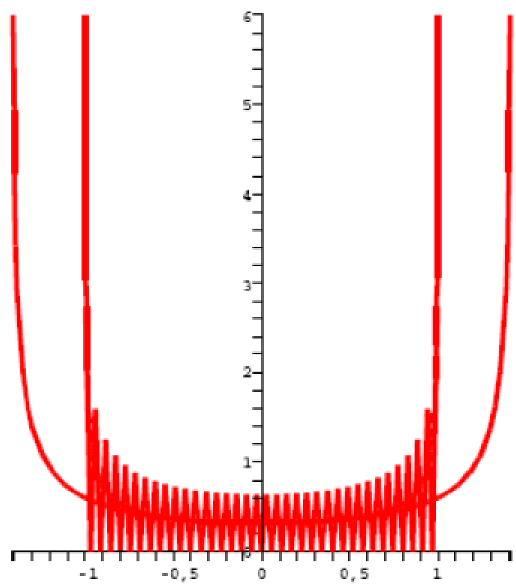
we get the limit

$$\lim_{n\longrightarrow\infty}\left\langle\mathcal{E}_{V_q^2}^{*n}\left(\left(\frac{L}{n}\right)^s\right)\right\rangle_0 = \int_0^{2\pi} h\left(\phi\right)^s \frac{d\phi}{2\pi} = \int_{-1}^{1}\frac{y^s}{\pi\sqrt{1-y^2}}dy. \tag{198}$$

The resulting value of the quantum moment is seen in the last equation to be given as statistical moment of the random variable y^s with respet to the limit probaility density function determined as follows

$$P(y) = \frac{1}{\pi\sqrt{1-y^2}}, -1 \leq y \leq 1 \tag{199}$$

This probability density function determines asymptotically the occupation probabilities for the scaled position variable of our QW. In the figure below we present its graph which has the shape of a double horn peaked at the position $y = \pm 1$. This is very much in difference with the Gaussian shape of the limit probability density function that occurs in a CRW but shares the double horn shape with the limit of another model of QW, although the two distributions differ in their exact functional form. Also, in the figure below we have included the position occupation probabilities of the QW after a large number of steps in order to show their tendency towards asymptotic values.



(200)

The double horn [3] shaped limit probability distribution function for the QW of the V_q^2 model is given in the plot above. Furthermore, superimposed to it are given the occupation probabilities of the walk as evaluated after $n = 36$ evolution steps.

3.8 Miscellaneous Examples

Example 31 *Calculate the density matrix of the walker for the first step, using the U quantization rule and the orginal tracing sheme. Let $\rho_c = |c\rangle\langle c|$ and*

$V_{cl} = \sum_{i=\pm} P_i \otimes E_i.$

Solution 32 *The density matrix of the walker for the first step is*

$$\begin{aligned}
\rho_w^{(1)} &= \mathcal{E}_{V_q^1}(\rho_w) = Tr_c\{V_q(\rho_c \otimes \rho_w)V_q^\dagger\} \\
&\overset{\rho_c=|c\rangle\langle c|}{=} Tr_c\{V_q(|c\rangle\langle c| \otimes \rho_w)V_q^\dagger\} \\
&\overset{V_q=V_{cl}(U\otimes\mathbf{1})}{=} Tr_c\{V_{cl}(U\otimes\mathbf{1})(|c\rangle\langle c| \otimes \rho_w)(U^\dagger\otimes\mathbf{1})V_{cl}^\dagger\} \\
&= Tr_c\{V_{cl}[(U|c\rangle\langle c|U^\dagger) \otimes \rho_w]V_{cl}^\dagger\} \\
&\overset{\substack{V_{cl}=\sum_{i=\pm} P_i\otimes E_i \\ V_{cl}^\dagger=\sum_{j=\pm} P_j\otimes E_j}}{=} Tr_c\{\sum_{i,j=\pm} P_i(U|c\rangle\langle c|U^\dagger)P_j \otimes E_i\rho_w E_j\} \\
&= \sum_{i,j=\pm} Tr\left\{P_i(U|c\rangle\langle c|U^\dagger)P_j\right\} \otimes E_i\rho_w E_j \\
&= \sum_{i=\pm}[\langle i|(U|c\rangle\langle c|U^\dagger)|i\rangle]E_i\rho_w E_i^\dagger \\
&= \sum_{i=\pm}[\langle i|(U|c\rangle\langle i|U^*)|c\rangle]E_i\rho_w E_i^\dagger \\
&= \sum_{i=\pm}[\langle i|(U\circ U^*)|c\rangle]E_i\rho_w E_i^\dagger.
\end{aligned} \tag{201}$$

For the particular case of the reshuffling matrix U being a $SO(2)$ rotation the general formula above, yields

$$\rho_w^{(1)} = \mathcal{E}_{V_q}(\rho_w) = \left(E_+\rho_w E_+^\dagger\right)\cos^2\theta + \left(E_-\rho_w E_-^\dagger\right)\sin^2\theta. \tag{202}$$

Example 33 *Calculate the density matrix of the walker for the first step, using the U quantization rule and the orginal tracing sheme. Let $\rho_c = |0\rangle\langle 0|$, $\rho_w = |m\rangle\langle n|$ and $V_{cl} = E_+ \otimes P_+ + E_- \otimes P_-$.*

Solution 34 *The density matrix of the walker for the first step is*

$$\begin{aligned}
\rho_w^{(1)} &= \mathcal{E}_{V_q^1}(|m\rangle\langle n|) = Tr_c\left\{V_q(|0\rangle\langle 0| \otimes |m\rangle\langle n|)V_q^\dagger\right\} \\
&= Tr_c\left\{\begin{pmatrix} E_+ & E_+ \\ E_- & E_- \end{pmatrix}\begin{pmatrix} |m\rangle\langle n| & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} E_+ & E_+ \\ E_- & E_- \end{pmatrix}^\dagger\right\} \\
&= Tr_c\left\{\begin{pmatrix} |m+1\rangle\langle n|E_- & |m+1\rangle\langle n|E_+ \\ |m-1\rangle\langle n|E_- & |m-1\rangle\langle n|E_+ \end{pmatrix}\right\} \\
&= |m+1\rangle\langle n-1| + |m-1\rangle\langle n+1|.
\end{aligned} \tag{203}$$

Example 35 *Calculate the density matrix of the walker for the first step, using the U quantization rule and the orginal tracing sheme. Let $\rho_c = |0\rangle\langle 0|$, $\rho_w = |\phi\rangle\langle\phi'|$ and $V_{cl} = E_+ \otimes P_+ + E_- \otimes P_-$. After that, calculate the n actions of $\mathcal{E}$ on ρ_w.*

Solution 36 *The density matrix of the walker for the first step is*

$$\begin{aligned}
\rho_w^{(1)} &= \mathcal{E}_{V_q}(|\phi\rangle\langle\phi'|) = Tr_c\{V_q[|0\rangle\langle 0| \otimes |\phi\rangle\langle\phi'|]V_q^\dagger\} \\
&= Tr_c\{\begin{bmatrix} E_+ & E_+ \\ E_- & E_- \end{bmatrix} \begin{bmatrix} |\phi\rangle\langle\phi'| & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} E_+ & E_+ \\ E_- & E_- \end{bmatrix}^\dagger\} \\
&= Tr_c\left\{\begin{pmatrix} e^{i\phi}|\phi\rangle\langle\phi'|E_- & e^{i\phi}|\phi\rangle\langle\phi'|E_+ \\ e^{-i\phi}|\phi\rangle\langle\phi'|E_- & e^{-i\phi}|\phi\rangle\langle\phi'|E_+ \end{pmatrix}\right\} \\
&= 2\cos(\phi - \phi')\,|\phi\rangle\langle\phi'|. \qquad (204)
\end{aligned}$$

Now, we want to calculate the n actions of $\mathcal{E}$ on ρ_w. Firstly, we apply $\mathcal{E}_{V_q}$ another time

$$\begin{aligned}
\mathcal{E}_{V_q}^2(|\phi\rangle\langle\phi'|) &= \mathcal{E}_{V_q}(2\cos(\phi - \phi')\,|\phi\rangle\langle\phi'|) \\
&= 2^2\cos^2(\phi - \phi')\,|\phi\rangle\langle\phi'|. \qquad (205)
\end{aligned}$$

Thus, for n the action $\mathcal{E}_{V_q}^n$ on $\rho_w = |\phi\rangle\langle\phi'|$, we obtain

$$\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|) = 2^n\cos^n(\phi - \phi')\,|\phi\rangle\langle\phi'|. \qquad (206)$$

Next, we express $\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|)$ in terms of Chebychev polynomials [12]. The trigonometric definition of the first kind of Chebychev polynomials is

$$T_n(\cos\vartheta) = \cos(n\vartheta), \qquad (207)$$

and of the second kind is

$$U_n(\cos\vartheta) = \frac{\sin[(n+1)\vartheta]}{\sin\vartheta}. \qquad (208)$$

We know that

$$\mathcal{E}_{V_q^n}(|\phi\rangle\langle\phi'|) = 2^n\cos^n(\phi - \phi')\,|\phi\rangle\langle\phi'|. \qquad (209)$$

We see the term $\cos^n(\phi - \phi')$, thus it can be used the first kind of Chebychev polynomials. We know that

$$T_n(\cos\vartheta) = \cos(n\vartheta), \qquad (210)$$

and

$$\cos(\phi - \phi') = T_1[\cos(\phi - \phi')]. \qquad (211)$$

We take the $n-$th power of $cos\phi$ expressed by the first kind of Chebychev polynomials. We obtain that

$$\cos^n(\phi - \phi') = T_1^n[\cos(\phi - \phi')]. \tag{212}$$

I will express $\cos^n(\phi - \phi')$ in a better form. If n is odd then

$$\cos^n \theta = \frac{2}{2^n} \sum_{k=0}^{\frac{n-1}{2}} \binom{n}{k} \cos[(n-2k)\theta]. \tag{213}$$

If n is even then

$$\cos^n \theta = \frac{1}{2^n} \binom{n}{\frac{n}{2}} + \frac{2}{2^n} \sum_{n=0}^{\frac{n}{2}-1} \binom{n}{k} \cos[(n-2k)\theta]. \tag{214}$$

Let $\theta = (\phi - \phi')$ be a change of variables. If n is odd then

$$\cos^n(\phi - \phi') = \frac{2}{2^n} \sum_{k=0}^{\frac{n-1}{2}} \binom{n}{k} \cos[(n-2k)(\phi - \phi')]. \tag{215}$$

The Chebyshev polynomial of first kind is defined as

$$T_n(\cos\vartheta) = \cos(n\vartheta). \tag{216}$$

Thus,

$$\begin{aligned} \cos^n(\phi - \phi') &= \frac{2}{2^n} \sum_{k=0}^{\frac{n-1}{2}} \binom{n}{k} \cos[(n-2k)(\phi - \phi')] \\ &= \frac{2}{2^n} \sum_{k=0}^{\frac{n-1}{2}} \binom{n}{k} T_{(n-2k)}[\cos(\phi - \phi')] \end{aligned} \tag{217}$$

Considering all the above, we can express $\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|)$ in two different ways. In the first way, for every n the map $\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|)$ is expressed as

$$\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|) = 2^n \cos^n(\phi - \phi')\,|\phi\rangle\langle\phi'| = T_1^n[\cos(\phi - \phi')]\,|\phi\rangle\langle\phi'|. \tag{218}$$

In the second way, we for n odd

$$\mathcal{E}_{V_q}^n(|\phi\rangle\langle\phi'|) = 2^n \cos^n(\phi - \phi')\,|\phi\rangle\langle\phi'|, \tag{219}$$

where

$$\cos^n(\phi - \phi') = \frac{2}{2^n} \sum_{k=0}^{\frac{n-1}{2}} \binom{n}{k} T_{(n-2k)}[\cos(\phi - \phi')], \tag{220}$$

and for n even

$$\mathcal{E}^{n}_{V_q}(|\phi\rangle\langle\phi'|) = 2^n \cos^n(\phi-\phi')\,|\phi\rangle\langle\phi'|\,, \tag{221}$$

where

$$\cos^n(\phi-\phi') = \frac{1}{2^n}\binom{n}{\frac{n}{2}} + \frac{2}{2^n}\sum_{n=0}^{\frac{n}{2}-1}\binom{n}{k}T_{(n-2k)}[\cos(\phi-\phi')]\,|\phi\rangle\langle\phi'|\,. \tag{222}$$

3.9 Quantum Optical Walk: An Application of QW

An application of the quantization rule on a CRW is a quantum optical walk [1]. Firstly, we consider a continuous family of Completely Positive Trace Preserving Maps (CPTP)

$$\mathbf{E} = \{t \to \varepsilon_t \in \mathcal{H}_c, \varepsilon_0 = id, t \geq 0\}\,, \tag{223}$$

acting on the $\mathcal{H}_c$ space and the semigroup composition law defined as

$$\varepsilon_{t_1} \circ \varepsilon_{t_1} = \varepsilon_{(t_1+t_2)}, \tag{224}$$

where t denotes time. We have to describe what a quantum optical walk is. It is a physical phenomenon in which a two level atom beam, the coins, cross a quantum optical cavity which maintain a quantum mode identified as the walker system. Thus, the beam is the coin and the cavity is the walker system. The beam "walks" on the cavity. The coin+walker interaction is realized with a V^2 (ε rule) QW model. It takes account the interaction of the coin with some external enviroment that is mathematically described as a CPTP time independent map ε_t. This interaction begins at time $t = 0$ and it continues while the beam crosses the cavity. The evolution of the walk of the beam is described as follows. The beam enters the cavity at some time t with state $\varepsilon(\rho_c)$. The atom is the coin part of the QW. It interacts with the walker cavity mode. For the V^2 model two successive coin+walker ineractions occur. The interaction at time t and a second at time $t+\tau$.

$$\begin{aligned} & \varepsilon_t(\rho_c)\otimes\rho_w \xrightarrow{t} V_{cl}\left[\varepsilon_t(\rho_c)\otimes\rho_w\right]V_{cl}^{\dagger} \\ & \xrightarrow{(t+\tau)} V_{cl}\left(\varepsilon_\tau\otimes\mathbf{1}\right)\left\{V_{cl}\left[\varepsilon_t(\rho_c)\otimes\rho_w\right]V_{cl}^{\dagger}\right\}V_{cl}^{\dagger} \\ = \; & (V_{cl})^2\left[\varepsilon_{\tau+t}(\rho_c)\otimes\rho_w\right]\left(V_{cl}^{\dagger}\right)^2 \end{aligned} \tag{225}$$

One step of the QW consists of two external enviroment interactions taken together with two V_{cl} actions in appropriate order. After that, the atom leaves the cavity, the atom clock is reset and a new atom enters tha cavity. The total change of the walker's density matrix between two successive steps is

$$\begin{aligned} \rho_w^{(n)} &= \mathcal{E}_{V^2}(\rho_w^{(n-1)}) \\ &= Tr_c\left\{[Adj(V_{cl})(\varepsilon_\tau\otimes\mathbf{1})Adj(V_{cl})\varepsilon_t]\otimes\mathbf{1}(\rho_c\otimes\rho_w^{(n-1)})\right\} \end{aligned} \tag{226}$$

for $n = 1, 2$ or more explicitly

$$\begin{aligned} \rho_w^{(n)} &= \mathcal{E}_{V^2}\left(\rho_w^{(n-1)}\right) \\ &= \sum_{ijk=\pm 1} \langle i| \varepsilon_t(\rho_c) |j\rangle \langle k| \varepsilon_\tau(|i\rangle\langle j|) |k\rangle E_{i+k} \rho_w^{(n-1)} E_{j+k} \end{aligned} \tag{227}$$

where $E_k |l\rangle = |l+k\rangle$. For $k > 0$, $E_k = E_+^k$ and for $k < 0$, $E_k = E_-^{-k}$. The quantized V^2 walk proceeds with steps of length 0 and 2.

Suppose now, that in the basis of $|\phi\rangle$ the walker density matrix has the form

$$\begin{aligned} \rho_w &= \sum_{k,l\in\mathbb{Z}} d_{kl} |k\rangle\langle l| \\ &= \sum_{k,l\in\mathbb{Z}} d_{kl} \left(\int_0^{2\pi} e^{-ik\phi} |\phi\rangle \frac{d\phi}{2\pi}\right)\left(\int_0^{2\pi} e^{il\phi'} \langle\phi'| \frac{d\phi'}{2\pi}\right) \\ &= \int_0^{2\pi}\int_0^{2\pi} \left\{\sum_{k,l\in\mathbb{Z}} d_{kl} e^{-i\left(k\phi - l\phi'\right)}\right\} |\phi\rangle\langle\phi'| . \end{aligned} \tag{228}$$

We set $\rho(\phi,\phi') = \sum_{k,l\in\mathbb{Z}} d_{kl} e^{-i\left(k\phi - l\phi'\right)}$, thus

$$\rho_w = \int_0^{2\pi}\int_0^{2\pi} \left\{\rho(\phi,\phi') |\phi\rangle\langle\phi'|\right\} \frac{d\phi d\phi'}{(2\pi)^2}. \tag{229}$$

We want to calculate the action of $\mathcal{E}$ on ρ_w matrix $\rho_w \xrightarrow{\mathcal{E}} \mathcal{E}_{V^2}(\rho_w)$. First, we caculate the action of $\mathcal{E}$ on $|\phi\rangle\langle\phi'|$

$$\begin{aligned} \mathcal{E}_{V^2}\left(|\phi\rangle\langle\phi'|\right) &= Tr_c\left\{V_{cl}(\phi)(\varepsilon_\tau\otimes\mathbf{1})\left[V_{cl}(\phi)\left(\varepsilon_t(\rho_c)\otimes|\phi\rangle\langle\phi'|\right)V_{cl}^\dagger(\phi')\right]V_{cl}^\dagger(\phi')\right\} \\ &= Tr_c\left\{V_{cl}^2(\phi)\,\varepsilon_{\tau+t}(\rho_c)\left(V_{cl}^\dagger(\phi')\right)^2\right\}|\phi\rangle\langle\phi'| , \end{aligned} \tag{230}$$

and setting

$$A\left(\phi,\phi'\right) = Tr_c\left\{V_{cl}^2(\phi)\,\varepsilon_{\tau+t}(\rho_c)\left(V_{cl}^\dagger(\phi')\right)^2\right\}, \tag{231}$$

results for the 1st step into

$$\mathcal{E}_{V^2}\left(|\phi\rangle\langle\phi'|\right) = A\left(\phi,\phi'\right)|\phi\rangle\langle\phi'| , \tag{232}$$

and for the n th step into

$$\mathcal{E}_{V^2}^{(n)}\left(|\phi\rangle\langle\phi|'\right) = A^n\left(\phi,\phi'\right)|\phi\rangle\langle\phi|' . \tag{233}$$

For the n th step the action of $\mathcal{E}$ on ρ_w is

$$\mathcal{E}_{V^2}^{(n)}(\rho_w) = \int_0^{2\pi}\int_0^{2\pi} \rho\left(\phi, \phi'\right) A^n\left(\phi, \phi'\right) |\phi\rangle \left\langle \phi' \right| \frac{d\phi d\phi'}{(2\pi)^2}. \tag{234}$$

The discrete probability distribution that determines the occupation probability of the site m on walker's ladder, after n steps reads

$$\begin{aligned} p_m^{(n)} &= \langle m| \mathcal{E}_{V^2}^{(n)}(\rho_w)|m\rangle \\ &= \int_0^{2\pi}\int_0^{2\pi} \left\{A^{(n)}\left(\phi, \phi'\right) \langle m|\phi\rangle \left\langle \phi'|m\right\rangle\right\} \frac{d\phi d\phi'}{(2\pi)^2} \\ &= \int_0^{2\pi}\int_0^{2\pi} \left\{A^{(n)}\left(\phi, \phi'\right) e^{-im\phi} e^{im\phi'}\right\} \frac{d\phi d\phi'}{(2\pi)^2} \\ &= \int_0^{2\pi}\int_0^{2\pi} \left\{A^{(n)}\left(\phi, \phi'\right) e^{-im\left(\phi-\phi'\right)}\right\} \frac{d\phi d\phi'}{(2\pi)^2}. \end{aligned} \tag{235}$$

By a change of variable

$$\phi, \phi' \longrightarrow \begin{cases} \phi_+ = \phi + \phi' \\ \phi_- = \phi - \phi' \end{cases} \iff \begin{cases} \phi = \frac{\phi_+ + \phi_-}{2} \\ \phi' = \frac{\phi_+ - \phi_-}{2} \end{cases}, \tag{236}$$

we see that if $A\left(\phi_+, \phi_-\right)$ is a function of the ϕ_- only, i.e.

$$A\left(\phi_+, \phi_-\right) = A\left(\phi_-\right), \tag{237}$$

then $p_m^{(n)}$ is a classical probability distribution and it is defined as

$$p_m^{(n)} = \frac{1}{(2\pi)} \int_0^{2\pi} A^{(n)}\left(\phi_-\right) e^{-im\phi_-} d\phi_-. \tag{238}$$

3.10 Classicality Criterion

Criterion 37 *Sufficient and necessary condition [1] for quantum effects in V^2 QW model on $\mathbb{Z}$ is that the characteristic function $A\left(\phi, \phi'\right)$ occuring in one step evolution*

$$\mathcal{E}_{V^2}\left(|\phi\rangle \left\langle \phi' \right|\right) = A\left(\phi, \phi'\right) |\phi\rangle \left\langle \phi' \right|, \tag{239}$$

expressed in terms of coordinates

$$\phi \pm \phi' = \phi_\pm, \tag{240}$$

i.e. $A\left(\phi_+,\phi_-\right)$ *should be a function of variables. If*

$$A_V\left(\phi_+,\phi_{\_}\right)=A_V\left(\phi_-\right), \tag{241}$$

then the occupation probability distribution $p_m^{(n)}$ *is a classical probability distribution and it describes a CRW.*

Proof. We know that

$$A^n\left(\phi,\phi'\right)e^{-im\left(\phi-\phi'\right)}=\frac{1}{2\pi}\int_0^{2\pi}A^n\left(\phi_-\right)e^{-im\phi_-}d\phi_-, \tag{242}$$

$(\Longrightarrow)$

$$\mathcal{F}\left(p_m^{(n)}\right)=A^{(n)}\left(\phi_-\right)=A^1\left(\phi_-\right)A^{(n-1)}\left(\phi_-\right), \tag{243}$$

then

$$p_m^{(n)}=\mathcal{F}^{-1}\left(A^1\left(\phi_-\right)A^{n-1}\left(\phi_-\right)\right). \tag{244}$$

Thus,

$$p_m^{(n)}=\sum_{m'}p_{m-m'}^{(1)}p_{m'}^{(n-1)}. \tag{245}$$

A recurrence relation describing a CRW.
$(\Longleftarrow)$ Given a recurence relation of the form

$$p_m^{(n)}=\sum_{m'}p_{m-m'}^{(1)}p_{m'}^{(n-1)}. \tag{246}$$

If we assume that initially $m=0$ then

$$\mathcal{F}\left(p_m^{(n)}\right)=A^n\left(\phi_-\right). \tag{247}$$

■

3.10.1 Examples U-rule

Example 38 *Let V model with density matrix*

$$\mathcal{E}_{V_q}\left(\rho_w^{(n)}\right)=Tr_c\left\{V_q\left(\rho_c\otimes\rho_w^{(n-1)}\right)V_q^\dagger\right\}, \tag{248}$$

where

$$A_{V_q}\left(\phi_+,\phi_-\right)=\langle+|\,\rho_c\,|+\rangle\,e^{i\phi_-}+\langle-|\,\rho_c\,|-\rangle\,e^{-i\phi_-}. \tag{249}$$

I observe that

$$A_{Vq}\left(\phi_+,\phi_-\right)=A_{Vq}\left(\phi_-\right). \tag{250}$$

The classicality criterion is satisfied . Thus, the occupation probability distribution is classical and it'doesnt give a QW.

Example 39 *Let V^2 model with density matrix*

$$\rho_c = \left|+\right\rangle \left\langle +\right| \tag{251}$$

and resufling matrix is the matrix

$$U_{\frac{\pi}{4}} = e^{i\left(\frac{\pi}{4}\right)\sigma_2}. \tag{252}$$

The density matrix of the n step is

$$\mathcal{E}_{V_q^2}\left(\rho_w^{(n)}\right) = Tr_c\left\{\left(V^2\right)\left(\rho_c \otimes \rho_w^{(n-1)}\right)\left(V^2\right)^\dagger\right\}, \tag{253}$$

where

$$A_{V_q^2}\left(\phi_+, \phi_-\right) = \cos^2\phi_- - i\cos\phi_+ \sin\phi_-. \tag{254}$$

I obsreve that

$$A_{V_q^2}\left(\phi_+, \phi_-\right) \neq A_{V_q^2}\left(\phi_-\right). \tag{255}$$

The classicality criterion is not satisfied. Thus, the occupation probability distribution is not classical and gives a QW.

3.10.2 Examples ε-rule

Let

$$\rho_c = diag\left(q, 1-q\right), 0 \leq q \leq 1 \tag{256}$$

density matrix, for $q = \frac{1}{2}, \rho_c = \frac{1}{2}\mathbf{1}$ then

$$\varepsilon_t\left(\rho_c\right) = S_0\left(t\right)\rho_c S_0^\dagger + S_1\left(t\right)\rho_c S_1^\dagger\left(t\right), \tag{257}$$

where

$$S_0\left(t\right) = \begin{pmatrix} \cos\left(\lambda t\right) & 0 \\ 0 & 1 \end{pmatrix} \tag{258}$$

and

$$S_1\left(t\right) = \begin{pmatrix} 0 & 0 \\ \sin\left(\lambda t\right) & 0 \end{pmatrix}, \tag{259}$$

We know that

$$\cos\left(\lambda t\right) = \sqrt{1 - e^{-2\lambda t}} \tag{260}$$

and

$$\begin{aligned} A_{V_q^2}\left(\phi_+, \phi_-\right) &= e^{-i2\phi_-}\left(1 - q\cos^2\lambda t\right) \\ &\quad + e^{i2\phi_-} q\cos^2\lambda t\cos^2\lambda\tau + q\cos^2\lambda t\sin^2\lambda\tau \\ &= A_{V^2}\left(\phi_-\right). \end{aligned} \tag{261}$$

$$\varepsilon_t\left(\rho_c\right) = diag\left(q\cos^2\lambda t, -q\cos^2\lambda t + 1\right) \tag{262}$$

I observe that

$$A_{V_q^2}\left(\phi_+,\phi_-\right)=A_{V_q^2}\left(\phi_-\right). \tag{263}$$

The classicality criterion is satifsfied. Thus, the occupation probability distribution is classical and it doesn't give a QW.

Example 40 *We consider the density matrix*

$$\rho_c=diag\left(q,1-q\right),0\leq q\leq 1,q\neq\frac{1}{2}, \tag{264}$$

where

$$\varepsilon\left(\rho_c\right)=R_0\rho_c R_0^\dagger+R_1\rho_c R_1^\dagger, \tag{265}$$

$$R_0=\frac{1}{\sqrt{2}}\mathbf{1},R_1=\frac{1}{\sqrt{2}}U_{\frac{\pi}{4}}, \tag{266}$$

and

$$\begin{aligned} A_{V_q^2}\left(\phi_+,\phi_-\right) &= \frac{3\left(1+2q\right)}{16}e^{i2\phi_-}+\frac{3\left(1-2q\right)}{16}e^{-i2\phi_-} \\ &\quad +\frac{i\left(1-2q\right)\sin\phi_-\cos\phi_+}{4}+\frac{1}{4}. \end{aligned} \tag{267}$$

I observe that

$$A_{V_q^2}\left(\phi_+,\phi_-\right)\neq A_{V_q^2}\left(\phi_-\right). \tag{268}$$

The classicality criterion is not satisfied. Thus, the occupation probability distribution is not classical and it gives a QW.

3.11 Memory Effects in QWs

Example 41 *Let* $\mathcal{H}_c=\mathbb{C}^2=span\left\{|0,|1\rangle\rangle\right\}$, *the coin space with dimension* $d_c=2$ *and* $\mathcal{H}_w=span\left\{|m\rangle\right\}_{m\in\mathbb{Z}}$, *the walker space. We use the matrix*

$$V_q=V_{cl}\left(U\otimes\mathbf{1}\right)=\left(P_0\otimes E_++P_1\otimes E_-\right)U\otimes\mathbf{1}. \tag{269}$$

We consider as

$$U=U_p=\begin{pmatrix}\sqrt{p} & \sqrt{1-p}\\ \sqrt{1-p} & -\sqrt{p}\end{pmatrix}, \tag{270}$$

thus for $p=\frac{1}{2}$ *we get the* 2×2 *Hadamard matrix*

$$U_{p=\frac{1}{2}}=H_{2x2}=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}. \tag{271}$$

Furthermore, we consider the coin density matrix as $\rho_c=|0\rangle\langle 0|$*.The QW density matrix for the first step is*

$$\begin{aligned} \rho_w^{(1)} &= \mathcal{E}_{V_q}\left(\rho_w\right)=Tr_c\left\{V_q\left(\rho_c\otimes\rho_w^{(0)}\right)V_q^\dagger\right\}= \\ &= Tr_c\left\{\begin{pmatrix}pE_+\rho_w E_- & 0\\ 0 & \left(1-p\right)E_-\rho_w E_+\end{pmatrix}\right\}, \end{aligned} \tag{272}$$

thus,

$$\rho_w^{(1)} = pE_+\rho_w E_+^\dagger + (1-p)\,E_-\rho_w E_-^\dagger.$$

We calculate now the occupation probability distribution for the first step

$$\begin{aligned} p_m^{(1)} &= \langle m|\,\rho_w^{(1)}\,|m\rangle \\ &= \sum_i \left(pE_+ \circ E_+ + (1-p)\,E_- \circ E_-\right)_{mi} \left(\rho_w^{(0)}\right)_{ii}, \end{aligned} \tag{273}$$

thus,

$$diag\left(\rho_w^{(1)}\right) = \Delta diag\left(\rho_w^{(0)}\right) \tag{274}$$

where

$$\Delta = pE_+ \circ E_+ + (1-p)\,E_- \circ E_- \tag{275}$$

and $diag\left(\rho_w^{(1)}\right)$, $diag\left(\rho_w^{(0)}\right)$ *are diagonal matrices with elements the diagonal elements of matrices* $\rho_w^{(1)}, \rho_w^{(0)}$ *respectively. Matrix* Δ *is double stochastic matrix since it admits the all-ones vector* $e = (1,1,...)$, *as left and right eigenvector i.e.* $\Delta e = e$ *and* $e^T\Delta = e^T$.

We obtain that

$$\Delta_c e = pE_+ e + (1-p)\,E_- = pe + (1-p)\,e = e \tag{276}$$

and

$$e^T\Delta_c = pe^T E_+ + (1-p)\,E_- = pe^T\,(1-p)\,e^T = e^T. \tag{277}$$

Thus, the matrix Δ_c is double stochastic. Finally the density matrix of the walker for the n step is

$$\rho_w^{(n)} = \mathcal{E}_{V_q^n}\left(\rho_w\right) = Tr_c\left\{\left(V_q^n\right)\left(\rho_c \otimes \rho_w\right)\left(V_q^n\right)^\dagger\right\} \tag{278}$$

and the diagonal elements are satisfying the following

$$diag\left(\rho_w^{(n)}\right) = \Delta_c diag\left(\rho_w^{(n-1)}\right). \tag{279}$$

[4], [5].

3.12 QW Applications in Quantum Information Science and Technology

A basic and important application of the QW are the quantum algorithms [7]. Qws give new methods for the designing of quantum algorithms. A famous category of algorithms affected by QWs is the search algorithms. In 1996 Lov Grover was the inventor of a very important quantum search algorithm, which increased the speed of searching in very difficult search problems. Grover's algorithm solves any search problem with N possible solutions in time $O\left(\sqrt{N}\right)$. We will mention some quantum algorithms that use QWs. Firstly, we have the QW on the "glued trees" graph. "Glued trees" are graphs of exponential size. We consider that we have a "glued tree" graph with two particular vertices, the entrance and the exit. Our problem is to find the exit if we begin from the entrance. A classical algorithm would require exponential time for the solution contrary to a quantum algorithm that require polynomial time. One more quantum algorithm is for searching on grids. We have N items placed on a d-dimensional grid. Our problem is to find an item with a certain property. In one unit of time step we can control if the item in the location that we are is the one that we search or we can move to an adjacent location of the grid. It should be noted that this problem is more difficult than the Grover's search problem because we are able to transpose only to an adjacent location in each step in the unit of time contrary to Grover's algorithm that we can go everywhere we want. This problem can be solved with a discrete or with a continuous time QW. Another application of QWs is the simulation of stochastic unitary CPTP maps.

4 Estimation Theory

4.1 Fundamentals of Statistical Inference

Let $(\Omega, \mathcal{A}, P)$ a probability space with unknown the likely function $P \in \mathcal{P}$ (a family of likely functions). Within the parametric statistics we suppose the family

$$\mathcal{P} = \{P_\theta : \theta \in \Theta\}, \tag{280}$$

with $\Theta \subseteq \mathbb{R}^k, k \in \mathbb{N}$, where every likely function P_θ depends from the unknown parameter $\theta \in \Theta$ but it is a known function.

Example 42 *The following*

$$P_\theta(B) = \int\limits_B \left(2\pi\sigma^2\right)^{-1} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} dx, \tag{281}$$

is a likely function, where $B \in \mathcal{B}$, $\theta = \left(\mu, \sigma^2\right) \in \Theta = \mathbb{R} \times (0, +\infty) \subseteq \mathbb{R}^2$.

One of the basic purposes of parametric statistics is the estimation of the unknown parameter $\theta_0 \in \Theta \subseteq \mathbb{R}^k$. The estimators of the parameter $\theta \in \Theta$ are statistical functions and thus generally random variables themselves.

In the estimation we are interested to identify the real unknown value θ_0 of the parameter $\theta \in \Theta$. Let $\underset{\sim}{x} = (x_1, ..., x_r)$ be a r dimensional random variable ($r.v.$) which follows a probability distribution with a probability density function $f\left(\underset{\sim}{x}; \bar{\theta}\right)$, where $\bar{\theta} \in \Omega \subseteq \mathbb{R}^s, s \geq 1$ is an s dimensional parameter. In probability theory and its applications we consider that the parameter $\bar{\theta}$ is known and theoretically we can calculate any probability that involves the random variable x and the parameter $\bar{\theta}$. In more practical problems the parameter $\bar{\theta}$ is considered as unkonwn. The need of searching the parameter $\bar{\theta}$ creates some of the most important problems of the statistical inference called estimation of the parameter $\bar{\theta}$. This estimation is leaned in experimental data and there are many methods for its realization.

Definition 43 (estimator) *Every statistical function $\tilde{\bar{\theta}} : \mathcal{X} \subseteq \mathbb{R}^{mn} \longrightarrow \mathcal{A} \subseteq \mathbb{R}^k$, that is used for the estimation of the unknown parameter $\bar{\theta} \in \Theta$ is called estimator of $\bar{\theta}$.*

There are two types of estimators. The estimators at point and the estimators at set. The estimators at point give us the specific value of the estimator while the estimator at set give us the set in which the estimator will be.

Definition 44 *Let $\underset{\sim}{x}_1, \underset{\sim}{x}_2, ..., \underset{\sim}{x}_n$ independent and identically distributed random variables with probability density function $f\left(\underset{\sim}{x}_i; \bar{\theta}\right)$, for every $i \in \{1, ..., n\}$ and let $\bar{\theta} \in \Omega \subseteq \mathbb{R}^s, s \geq 1$ be an s dimensional parameter. Estimator $\tilde{\bar{\theta}}$ of the parameter $\bar{\theta}$ is called any statistical function of the variables $\underset{\sim}{x}_1, \underset{\sim}{x}_2, ..., \underset{\sim}{x}_r \in \mathbb{R}^r$ which is used for the estimation of the parameter $\bar{\theta}$.*

The choice of the estimator is based on some criterions. The criterion of bias, minimum dispersion, Bayes, minimum squares, tendecy and maximum likelihood are some of them. We will examine the criterion of the maximum likelihood in this thesis.

4.2 Maximum Likelihood Estimation

Maximum likelihood estimation [24] is one of the most preferred method of parameter estimation in statistics and it is used to many statistical methods, such as non-linear modeling with non-normal data. In classical statistics we have probability density functions. We have discrete and continuous probability distributions. We are interested in continuous probability distributions which are defined as $f\left(\underline{\mathrm{x}};\bar{\theta}\right)$. The variable $\underline{\mathrm{x}}$ is "following" the probability distribution, for example a Gaussian, and $\bar{\theta}$ is the so called parameter. The parameter estimation problem is described as the problem of finding an appropriate value of the parameter θ under some cirmumstances. The parameter $\bar{\theta}$ belongs to the set of parameters Θ.

Let $\underline{\mathrm{x}}= (x_1, ..., x_n)$ independent and identically distributed random variables with probability density function $p_x\left(\underline{\mathrm{x}}|\bar{\theta}\right), \bar{\theta} \in \Theta$, and we suppose that the result ϖ_0 of an experiment, gave the sample $\underline{\mathrm{X}}(\varpi_0) = \underline{\mathrm{x}}^0$,whereby we want to estimate the real value $\bar{\theta}_0$ of the unknown parameter $\bar{\theta} \in \Theta$, i.e. the real distribution $p\left(...|\theta_0\ \right)$ which created the sample. If the value of the unknown parameter was θ, then the probability of observing this specific sample $\underline{\mathrm{X}}^0$ is

$$P_\theta\left(\underline{\mathrm{X}}=\underline{\mathrm{x}}_0\right) = \prod_{i=1}^{n} p_x\left(x_i^0|\bar{\theta}\right). \tag{282}$$

Since where from all the elements of the sample space $\mathcal{X}$, the unknown $p\left(...|\bar{\theta}_0\right)$, i.e. $\bar{\theta}_0$ elected the $\underline{\mathrm{x}}^0$, it is intuitively satisfactory estimator of the unknown $\bar{\theta}_0$, that $\tilde{\bar{\theta}} \in \Theta$ from which is maximized the observation probability $P_\theta\left(\underline{\mathrm{X}}=\underline{\mathrm{x}}^0\right)$ of this specific sample $\underline{\mathrm{x}}^0$ that really happened, i.e. the $\tilde{\bar{\theta}} \in \Theta$ is satisfying that

$$P_{\tilde{\bar{\theta}}}\left(\underline{\mathrm{X}}=\underline{\mathrm{x}}^0\right) = \max_{\bar{\theta}\in\Theta} p_\theta\left(\underline{\mathrm{X}}=\underline{\mathrm{x}}^0\right), \tag{283}$$

if of course such a maximum exists. If the sample comes from a continuous distribution $f\left(...|\bar{\theta}\right), \bar{\theta} \in \Theta$ then the above equality will be

$$P_\theta\left(x_i^0 - \varepsilon < x_i \leq x_i^0 + \varepsilon\right) = (2\varepsilon)^n \prod_{i=1}^{n} f\left(x_i^0|\bar{\theta}\right), \forall\varepsilon > 0, \tag{284}$$

where $i = 1, ..., n$ and $\bar{\theta} \in \Theta = \Theta$. Thus, the estimator $\tilde{\bar{\theta}}$ of $\bar{\theta}_0$, must satisfying the following

$$f\left(\underline{\mathrm{x}}^0|\tilde{\bar{\theta}}\right) = \max_{\theta\in\Theta} f\left(\underline{\mathrm{x}}^0|\tilde{\bar{\theta}}\right), \tag{285}$$

if of course such a maximum exists. We are interested in the estimators found using the criterion of the maximum likelihood. Firstly, we define the likelihood function.

Definition 45 *Let $x_1, ..., x_n$ independent and identically distributed random variables with probability density functions $p_x\left(..|\bar{\theta}\right)$ if they are discrete, or $f_x\left(...|\bar{\theta}\right)$ if they are continuous and $\bar{\theta} \in \Theta$. The stochastic function $L : \Theta \longrightarrow \mathbb{R}$ with*

$$L\left(\bar{\theta}|\underline{x}\right) = \begin{cases} \prod_{i=1}^{n} p_x\left(x_i|\bar{\theta}\right), \text{if } x_i \text{ is discrete} \\ \prod_{i=1}^{n} f_x\left(x_i|\bar{\theta}\right), \text{if } x_i \text{ is continuous} \end{cases}, \tag{286}$$

is called Stochastical Function of Likelihood or Likelihood Function of the parameter $\bar{\theta} \in \Theta$.

We observe that for each $\underline{\mathrm{x}} \in \mathcal{X}$, the likelihood of $\bar{\theta}$ on $\underline{\mathrm{x}}$, i.e. $L\left(\underline{\mathrm{X}}=\underline{\mathrm{x}}|\bar{\theta}\right)$, is exactly the probability density function of the stochastical sample X on the point $\underline{\mathrm{x}}$, calculated with the parameter $\bar{\theta}$. We observe likelihood as a function of $\bar{\theta}$ for a given sample rather than a function of the sample.

4.3 Construction of the Maximum Likelihood Estimators

Suppose that for each $\bar{\theta} \in \Theta \subseteq \mathbb{R}^k$, with probability density function $p_x\left(x|\bar{\theta}\right)$ or $f_x\left(x|\bar{\theta}\right)$, then there is a maximum

$$\max_{\bar{\theta}\in\Theta} L\left(\bar{\theta}\right) \equiv \max_{\bar{\theta}\in\Theta} L\left(\underline{\mathrm{x}}|\bar{\theta}\right). \tag{287}$$

This happens because $L\left(\bar{\theta}\right)$ is a concave function of $\bar{\theta} \in \Theta$. Then each statistical function

$$\tilde{\bar{\theta}}_n \equiv \tilde{\bar{\theta}}\left(\underline{\mathrm{x}}\right) : \varpi \in \Omega \longmapsto \tilde{\bar{\theta}}\left(\underline{\mathrm{X}}\left(\varpi\right)\right) = \tilde{\bar{\theta}}\left(\underline{\mathrm{x}}\right) \in \Theta, \tag{288}$$

such that

$$L\left(\tilde{\bar{\theta}}_n\right) = \max_{\bar{\theta}\in\Theta} L\left(\bar{\theta}\right), \tag{289}$$

is called maximum likelihood estimator of the parameter $\bar{\theta} \in \Theta$. A maximum likelihood estimator, if it exists is not necessary unique. Let $k = \dim \Theta = 1$ such that $\theta \in \Theta \subseteq \mathbb{R}$, and we suppose that the likelihood function $L\left(\theta\right)$ exists, then if exists the maximimum likelihood estimator $\tilde{\theta}_n$, it must

$$L'\left(\tilde{\theta}_n\right) = 0. \tag{290}$$

Thus, we have to solve the equation $L'\left(\theta\right) = 0$. Let θ^* a solution of the equation

$$L'\left(\theta\right) = 0, \tag{291}$$

and in addition

$$L''(\theta^*) < 0, \tag{292}$$

then $\widetilde{\theta}_n = \theta^*$ is one (not necessary unique) maximum likelihood estimator. If generally $k \in \mathbb{N}$, the equations

$$L'\left(\bar{\theta}\right) = 0, \tag{293}$$

and

$$L''\left(\bar{\theta}^*\right) < 0, \tag{294}$$

must be substituted respectively from

$$\bigtriangledown L\left(\bar{\theta}\right) = \left(\frac{\vartheta}{\vartheta\theta_1} L\left(\bar{\theta}\right), ..., \frac{\vartheta}{\vartheta\theta_1} L\left(\bar{\theta}\right)\right) = \underline{0}. \tag{295}$$

A solution θ^* of the above system with Hessian defined as follows

$$H'(\theta^*) = \left[\frac{\vartheta^2}{\vartheta\theta_i\vartheta\theta_j} L\left(\bar{\theta}\right)\right]_{\bar{\theta}=\bar{\theta}^*} < 0, \tag{296}$$

is a maximum likelihood estimator $\widetilde{\bar{\theta}}_n$,where $H' < 0$ means that the $k \times k$ matrix $H'(\theta^*)$ is negative definite, i.e. for each $\underline{\mathrm{a}} \in \mathbb{R}^k \setminus \{\underline{0}\}$

$$\underline{\mathrm{a}}^T H' \underline{\mathrm{a}} < 0. \tag{297}$$

Considering the fact that for independent samples the likelihood is a product of probability density functions, it is easier and equivalent to maximize the logarithm of the likelihood which is defined as

$$l_n = l_n\left(\bar{\theta}|\underline{\mathrm{x}}\right) = \log L_n\left(\bar{\theta}\right) = \log L_n\left(\bar{\theta}|\underline{\mathrm{x}}\right) = \begin{cases} \sum\limits_{i=1}^{n} \log p_x\left(x_i|\bar{\theta}\right), \text{if } x_i \text{ is a discrete variable} \\ \sum\limits_{i=1}^{n} \log f_x\left(x_i|\bar{\theta}\right), \text{if } x_i \text{ is a continuous variable} \end{cases}. \tag{298}$$

We know that the function log is ascending. Thus, the points of maximum of the likelihood function L, if they exists are the same with the points of maximum of the function l_n. We search the maximum likelihood estimation $\tilde{\bar{\theta}}_n$to the solutions $\bar{\theta}^*$ of the system

$$\bigtriangledown l_n\left(\bar{\theta}\right) = \sum_{i=1}^{n} \bigtriangledown \log f_x\left(x_i|\bar{\theta}\right) = \underline{0}. \tag{299}$$

The above set of equations are called maximum likelihood equations and they widow the Hessian negative definite

$$H\left(\bar{\theta}^*\right) = \left[\frac{\vartheta^2}{\vartheta\theta_i\vartheta\theta_j} l_n\left(\bar{\theta}\right)\right] = \left[\sum_{i=1}^{n} \frac{\vartheta^2}{\vartheta\theta_i\vartheta\theta_j} \log f_x\left(x_i|\bar{\theta}\right)\right]_{\bar{\theta}=\bar{\theta}^*} < 0. \tag{300}$$

If the variables x_i are discrete, we simply substitute $f_x\left(x_i|\bar{\theta}\right)$ with $p_x\left(x_i|\bar{\theta}\right)$. Summing, if the relevant derivatives exists we will find the maximum likelihood estimators $\tilde{\bar{\theta}}_n$using the equations

$$\triangledown\, l_n\left(\theta\right) = 0, \tag{301}$$

and

$$H\left(\bar{\theta}^*\right) < 0. \tag{302}$$

4.4 Procedure Step by Step

First Step. We find the first derivative of $L(\bar{\theta})$

$$\triangledown\, L(\bar{\theta}). \tag{303}$$

Second Step. We set

$$\triangledown\, L(\bar{\theta}) = 0, \tag{304}$$

and we solve the equation to locate extrema.
Third Step. We search the appropriate extrema such that

$$H(\tilde{\bar{\theta}}) < 0, \tag{305}$$

where $\tilde{\bar{\theta}}$ is the solution of the equation

$$\triangledown\, L(\bar{\theta}) = 0. \tag{306}$$

Finally, the $\tilde{\bar{\theta}}$ is the maximum likelihood estimator.

4.5 Examples

Example 46 *We have a coin. We execute n independent coin tosses and we have k heads. The toss of the coin is following a Binominal Distribution with parameter r. Likelihood is given as*

$$L\left(x_1, ..., x_n; r\right) = \prod_n p_X\left(x_i; r\right) = \frac{n!}{(n-k)!r!} r^k \left(1-r\right)^{(n-k)}. \tag{307}$$

For $n = 100$ trials and $k = 56$ heads the likelihood will be

$$L\left(x_1, ..., x_n; r\right) = \frac{100!}{44!56!} r^{56} \left(1-r\right)^{44}. \tag{308}$$

We natural log both sides

$$\begin{aligned} \ln\left(L\left(\underset{\sim}{x}; r\right)\right) &= \ln\left(\frac{n!}{(n-k)!r!} r^k \left(1-r\right)^{(n-k)}\right) \text{ or} \\ &= \ln\left(\frac{n!}{(n-k)!r!}\right) + k\ln r + (n-k)\ln\left(1-r\right) \\ &= 2464 + 56\ln r + 44\ln\left(1-r\right). \end{aligned} \tag{309}$$

We differentiate for θ

$$\begin{aligned}
\frac{\partial}{\partial\theta}\left\{2464+56\ln r+44\ln(1-r)\right\} &= 0 \ or \\
\frac{56}{r} &= \frac{44}{1-r} \ or \\
r &= \frac{56}{100}. \qquad (310)
\end{aligned}$$

We verify that the second derivative is negative for $p = \frac{56}{100}$ *with the following calculation*

$$\frac{\partial^2}{\partial^2\theta}\left\{\ln\left(L\left(\underline{x};\frac{56}{100}\right)\right)\right\} = -100 < 0. \qquad (311)$$

Example 47 *Let* $x_1, ..., x_n$ *independent and identically distributed variables from a (stochastical sample) that are following the Gamma*(a, λ) *distribution, with a known and probability distibution with parameter* λ*. Find the maximum likelihood estimator of the parameter* λ*.*

Solution 48 *We know that the probability density function of the Gamma* (a, λ) *probability distribution is*

$$f\left(x_i|\left(a,\lambda\right)\right) = \frac{\lambda^a}{\Gamma(a)} x_i^{a-1} e^{-\lambda x_i} 1\left(x_i > 0\right). \qquad (312)$$

We set as the parameter for estimation

$$\theta = \lambda. \qquad (313)$$

Thus, the probability density function is

$$f\left(x_i|\left(a,\theta\right)\right) = \frac{\theta^a}{\Gamma(a)} x_i^{a-1} e^{-\theta x_i} 1\left(x_i > 0\right). \qquad (314)$$

The stochastic likelihood function is

$$L(\theta) = L(\theta|x_i) = \prod_{i=1}^{n} f\left(x_i|\left(a,\theta\right)\right). \qquad (315)$$

The logarithm of the likelihood function is

$$\begin{aligned}
l(\theta) &= l(\theta|x_i) \\
&= \log L(\theta|x_i) \\
&= \log\left\{\prod_{i=1}^{n} f\left(x_i|\left(a,\theta\right)\right)\right\} \\
&= \sum_{i=1}^{n}\log\left\{\frac{\theta^a}{\Gamma(a)} x_i^{a-1} e^{-\theta x_i}\right\} \\
&= na\log\theta - n\log\left(\Gamma(a)\right) + \log\left(\prod_{i=1}^{n} x_i^{a-1}\right) + \log\left(e^{-\theta\sum_{i=1}^{n} x_i}\right) \qquad (316)
\end{aligned}$$

We differentiate $l(\theta)$

$$
\begin{aligned}
\frac{\vartheta}{\vartheta\theta}\{l(\theta)\} &= \\
&= \frac{na}{\theta} - \frac{\left(\sum_{i=1}^{n} x_i\right)\left(e^{-\theta\sum_{i=1}^{n} x_i}\right)}{e^{-\theta\sum_{i=1}^{n} x_i}} \\
&= \frac{na}{\theta} - \sum_{i=1}^{n} x_i. \qquad (317)
\end{aligned}
$$

We verify that

$$\frac{\vartheta^2}{\vartheta^2\theta}\{l(\theta)\} = -\frac{na}{\theta^2} < 0. \qquad (318)$$

Thus, there is maximum value of θ*.We solve the equation*

$$\frac{\vartheta}{\vartheta\theta}\{l(\theta)\} = 0, \qquad (319)$$

to find critical points.

$$
\begin{aligned}
\frac{\vartheta}{\vartheta\theta}\{l(\theta)\} &= 0 \text{ or} \\
\frac{na}{\theta} - \sum_{i=1}^{n} x_i &= 0. \qquad (320)
\end{aligned}
$$

Thus,

$$\theta = \frac{na}{\sum_{i=1}^{n} x_i} = \frac{a}{\frac{\sum_{i=1}^{n} x_i}{n}} = \frac{a}{\bar{x}}, \qquad (321)$$

where $\bar{x}$ is the arithmetic mean. The estimator $\tilde{\lambda}$ of the parameter λ is

$$\tilde{\lambda} = \frac{a}{\bar{x}}. \qquad (322)$$

Example 49 *We will present a more difficult problem. We must find the estimator of a two dimensional parameter* θ*. Let* $\binom{x_1}{y_1}, ..., \binom{x_n}{y_n}$ *independent and identically distributed variables from a (stochastical) sample following the dis-*

tribution called $N_1\left(\binom{\mu_1}{\mu_2}, \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}\right)$ *with probability density function*

$$
\begin{aligned}
f\left(\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}\right) &= \frac{1}{\pi\sqrt{3}} \\
&\quad \times \exp\{-\frac{2}{3}[(x-\mu_1)^2 \\
&\quad + (y-\mu_2)^2 - (x-\mu_1)(y-\mu_2)]\}. \quad (323)
\end{aligned}
$$

Find the maximum likelihood estimator of the two dimensional parameter $\binom{\mu_1}{\mu_2} \in \Theta \equiv \mathbb{R}^2$.

Solution 50 *We set*

$$\bar{\theta} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}. \quad (324)$$

The logarithm of the likelihood is

$$
\begin{aligned}
l\left(\bar{\theta}\right) &= \log L\left(\bar{\theta}\right) \\
&= \sum_{i=1}^{n} \log\left\{f\left(\begin{pmatrix} x_i \\ y_i \end{pmatrix}; \bar{\theta}\right)\right\} \\
&= \sum_{i=1}^{n} \\
&\quad \log\{\frac{1}{\pi\sqrt{3}} \\
&\quad \times \exp\left\{-\frac{2}{3}\left[(x_i-\mu_1)^2 + (y_i-\mu_2)^2 - (x_i-\mu_1)(y_i-\mu_2)\right]\right\}\} \\
&= \log\left\{\frac{1}{\pi\sqrt{3}}\right\}^n \\
&\quad -\frac{2}{3}\sum_{i=1}^{n}\left\{(x_i-\mu_1)^2 + (y_i-\mu_2)^2 - (x_i-\mu_1)(y_i-\mu_2)\right\} \\
&= -n\log\left(\pi\sqrt{3}\right) \\
&\quad -\frac{2}{3}\sum_{i=1}^{n}\left\{(x_i-\mu_1)^2 + (y_i-\mu_2)^2 - (x_i-\mu_1)(y_i-\mu_2)\right\}. \quad (325)
\end{aligned}
$$

We differentiate $l\left(\bar{\theta}\right)$ *as follows*

$$\begin{aligned}
\frac{\vartheta}{\vartheta\bar{\theta}}\left\{l\left(\bar{\theta}\right)\right\} &= \\
&= l\left(\begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix}\right) \\
&= \begin{pmatrix}\frac{\vartheta}{\vartheta\mu_1}\left\{l\left(\bar{\theta}\right)\right\}\\ \frac{\vartheta}{\vartheta\mu_2}\left\{l\left(\bar{\theta}\right)\right\}\end{pmatrix} \\
&= -\frac{2}{3}\begin{pmatrix}\sum_{i=1}^{n}\left[-2\left(x_i-\mu_1\right)+\left(y_i-\mu_2\right)\right]\\ \sum_{i=1}^{n}\left[-2\left(y_i-\mu_2\right)+\left(x_i-\mu_1\right)\right]\end{pmatrix} \\
&= -\frac{2}{3}\begin{pmatrix}A\left(\mu_1,\mu_2\right)\\ B\left(\mu_1,\mu_2\right)\end{pmatrix}. \qquad (326)
\end{aligned}$$

We differentiate $\frac{\vartheta}{\vartheta\bar{\theta}}\left\{l\left(\bar{\theta}\right)\right\}$ *one more time*

$$\begin{aligned}
&\frac{\vartheta^2}{\vartheta^2\bar{\theta}}\left\{l\left(\bar{\theta}\right)\right\} \\
&= \begin{pmatrix}\frac{\vartheta}{\vartheta\mu_1^2}\left\{l\left(\bar{\theta}\right)\right\} & \frac{\vartheta}{\vartheta\mu_2\vartheta\mu_1}\left\{l\left(\bar{\theta}\right)\right\}\\ \frac{\vartheta}{\vartheta\mu_1\vartheta\mu_2}\left\{l\left(\bar{\theta}\right)\right\} & \frac{\vartheta}{\vartheta\mu_2^2}\left\{l\left(\bar{\theta}\right)\right\}\end{pmatrix} \\
&= \begin{pmatrix}\frac{\vartheta}{\vartheta}\left\{A\left(\mu_1,\mu_2\right)\right\} & \frac{\vartheta}{\vartheta}\left\{A\left(\mu_1,\mu_2\right)\right\}\\ \frac{\vartheta}{\vartheta}\left\{B\left(\mu_1,\mu_2\right)\right\} & \frac{\vartheta}{\vartheta}\left\{B\left(\mu_1,\mu_2\right)\right\}\end{pmatrix} \\
&= \begin{pmatrix}-\frac{4}{3}n & \frac{2}{3}n\\ \frac{2}{3}n & -\frac{4}{3}n\end{pmatrix} \\
&= -\frac{2}{3}\begin{pmatrix}2n & -n\\ -n & 2n\end{pmatrix}. \qquad (327)
\end{aligned}$$

We must check now that the matrix

$$-\frac{2}{3}\begin{pmatrix}2n & -n\\ -n & 2n\end{pmatrix}, \qquad (328)$$

is negative definite. For every vector

$$\underset{\sim}{a} = \begin{pmatrix}a_1 & a_2\end{pmatrix} \qquad (329)$$

we verify that

$$\begin{aligned}
\underset{\sim}{a}^T\left\{-\frac{2}{3}\begin{pmatrix}2n & -n\\ -n & 2n\end{pmatrix}\right\}\underset{\sim}{a} &< 0 \textit{ or} \\
-\begin{pmatrix}a_1 & a_2\end{pmatrix}\frac{2}{3}\begin{pmatrix}2n & -n\\ -n & 2n\end{pmatrix}\begin{pmatrix}a_1\\ a_2\end{pmatrix} &< 0 \textit{ or} \\
-\frac{2}{3}\left(2na_1^2-2na_1a_2+2na_2^2\right) &< 0. \qquad (330)
\end{aligned}$$

Thus, there is a maximum value for $\binom{\mu_1}{\mu_2}$. *I search now the critical values of* $\frac{\vartheta}{\vartheta\,\vec{\theta}}\left\{l\left(\bar{\theta}\right)\right\}$. *We solve the equation*

$$\frac{\vartheta}{\vartheta\bar{\theta}}\left\{l\left(\bar{\theta}\right)\right\} = 0. \tag{331}$$

The above equation consists of two other equations,

$$\begin{aligned}
\frac{\vartheta}{\vartheta\mu_1}\left\{\bar{\theta}\right\} &= 0 \textit{ or} \\
A\left(\mu_1,\mu_2\right) &= 0 \textit{ or} \\
\frac{4}{3}\sum_{i=1}^{n} x_i + \frac{4}{3}n\mu_1 + \frac{2}{3}\sum_{i=1}^{n} y_i - \frac{2}{3}n\mu_2 &= 0 \textit{ or} \\
\mu_1 &= \frac{\sum_{i=1}^{n} x_i}{n} = \bar{x},
\end{aligned} \tag{332}$$

and

$$\begin{aligned}
\frac{\vartheta}{\vartheta\mu_2}\left\{l\left(\bar{\theta}\right)\right\} &= 0 \textit{ or} \\
B\left(\mu_1,\mu_2\right) &= 0 \textit{ or} \\
\frac{4}{3}\sum_{i=1}^{n} y_i + \frac{4}{3}n\mu_2 + \frac{2}{3}\sum_{i=1}^{n} x_i - \frac{2}{3}n\mu_1 &= 0 \textit{ or} \\
\mu_2 &= \frac{\sum_{i=1}^{n} y_i}{n} = \bar{y}.
\end{aligned} \tag{333}$$

Thus, the maximum likelihood estimator of

$$\bar{\theta} = \begin{pmatrix}\mu_1 \\ \mu_2\end{pmatrix}, \tag{334}$$

is

$$\bar{\bar{\theta}} = \begin{pmatrix}\bar{x} \\ \bar{y}\end{pmatrix}. \tag{335}$$

5 Parametric Estimation via QW

Firstly, we determine the probability density function from the QW and then follow the procedure of the maximum likelihood estimation.

5.1 The Density Matrix Discrete Time Evolution

The density matrix of the walker for a CRW is,

$$\mathcal{E}_{V_{cl}}(\rho_w) = Tr_c\{V_{cl}(\rho_c \otimes \rho_w)V_{cl}^\dagger\} \tag{336}$$

where

$$V_{cl} = P_0 \otimes E_+ + P_1 \otimes E_-. \tag{337}$$

We quantize the CRW using the U rule, which introduces the quantization map

$$V_{cl} \to V_q = (U \otimes \mathbf{1})V_{cl}, \tag{338}$$

where the unitary reshuffling matrix operating in coin space is used

$$U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \in SU(2), \tag{339}$$

where $SU(2) = \{U \in M_{2x2}, s.t. UU^\dagger = \mathbf{1} = U^\dagger U \text{ and } \det U = \mathbf{1}\}$. More specifically, $U(\theta)$ is a real matrix and belongs to the subgroup of orthogonal matrices i.e. $U \in SO(2) \subset SU(2)$.

The density matrix of the walker after one step of QW is

$$\begin{aligned} \mathcal{E}_{V_q}(\rho_w) &= Tr_c\{V_q(\rho_c \otimes \rho_w)V_q^\dagger\} \\ &= Tr_c\{[\underbrace{(U \otimes \mathbf{1})V_{cl}}_{V_q}](\rho_c \otimes \rho_w)[\underbrace{V_{cl}^\dagger(U^\dagger \otimes \mathbf{1})}_{V_q^\dagger}]\}. \end{aligned} \tag{340}$$

Next we calculate explicitly the matrix V_q, starting with the CRW unitary evolution operator

$$V_{cl} = \int_0^{2\pi} \left\{ \begin{pmatrix} e^{i\phi_1} & 0 \\ 0 & e^{-i\phi_1} \end{pmatrix} \otimes |\phi_1\rangle \langle\phi_1| \right\} \frac{d\phi_1}{2\pi}, \tag{341}$$

and obtaining

$$
\begin{aligned}
V_q &= (U \otimes \mathbf{1})V_{cl} \\
&= (\begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}) \\
&\quad \times \int\limits_0^{2\pi} \left\{ \begin{bmatrix} e^{i\phi_1} & 0 \\ 0 & e^{-i\phi_1} \end{bmatrix} \otimes |\phi_1\rangle \langle\phi_1| \right\} \frac{d\phi_1}{2\pi} \\
&= \int\limits_0^{2\pi} \left\{ \begin{bmatrix} e^{i\phi_1}\cos\theta & e^{-i\phi_1}\sin\theta \\ -e^{i\phi_1}\sin\theta & e^{-i\phi_1}\cos\theta \end{bmatrix} \otimes |\phi_1\rangle \langle\phi_1| \right\} \frac{d\phi_1}{2\pi}.
\end{aligned} \tag{342}
$$

Setting

$$
M(\phi) = U(\theta)V_{cl}(\phi) = \begin{pmatrix} e^{i\phi_1}\cos\theta & e^{-i\phi_1}\sin\theta \\ -e^{i\phi_1}\sin\theta & e^{-i\phi_1}\cos\theta \end{pmatrix}, \tag{343}
$$

we obtain for V_q

$$
V_q = \int\limits_0^{2\pi} [M(\phi_1) \otimes |\phi_1\rangle \langle\phi_1|] \frac{d\phi_1}{2\pi}. \tag{344}
$$

Due to the delta-function orthogonality of the ϕ-basis vectors i. e. $\underbrace{\langle\phi_1| \, |\phi_2\rangle} = \delta(\phi_1 - \phi_2)$, the evaluation of kth step density operator of QW requires the evaluation of the kth power of matrix V_q, which will be next derived inductively as follows:

(Initialization Step) For $n = 1$, the decomposition of V_q previously obtained reads

$$
V_q = \int\limits_0^{2\pi} [M(\phi_1) \otimes |\phi_1\rangle \langle\phi_1|] \frac{d\phi_1}{2\pi}. \tag{345}
$$

For $n = 2$,

$$
\begin{aligned}
V_q^2 &= V_q V_q \\
&= [\int_0^{2\pi} \{M(\phi_1) \otimes |\phi_1\rangle \langle\phi_1|\} \frac{d\phi_1}{2\pi}][\int_0^{2\pi} \{M(\phi_2) \otimes |\phi_2\rangle \langle\phi_2|\} \frac{d\phi_2}{2\pi}] \\
&= \int_0^{2\pi}\int_0^{2\pi} \left\{ M(\phi_1)M(\phi_2) \otimes |\phi_1\rangle \underbrace{\langle\phi_1| |\phi_2\rangle}_{\delta(\phi_1-\phi_2)} \langle\phi_2| \right\} \frac{d\phi_1}{2\pi}\frac{d\phi_2}{2\pi} \\
&\overset{*}{=} \int_0^{2\pi} \left\{ \int_0^{2\pi} M(\phi_1)M(\phi_2) \otimes |\phi_1\rangle \langle\phi_2| \, \delta(\phi_1-\phi_2)\frac{d\phi_1}{2\pi} \right\} \frac{d\phi_2}{2\pi} \\
&= \int_0^{2\pi} \{M(\phi_2)M(\phi_2) \otimes |\phi_2\rangle \langle\phi_2|\} \frac{d\phi_2}{2\pi} \\
&= \int_0^{2\pi} M(\phi_2)^2 \otimes |\phi_2\rangle \langle\phi_2| \frac{d\phi_2}{2\pi}, \qquad (346)
\end{aligned}
$$

(where the *reproducing kernel* property of delta function viz. $\int_0^{2\pi} F(\phi_1)\delta(\phi_1 - \phi_2)\frac{d\phi_1}{2\pi} = F(\phi_2)$).

(Inductive Step) For $n = k+1$,

$$
\begin{aligned}
V_q^{k+1} &= V_q ... V_q \\
&= \{\int_0^{2\pi} [M(\phi_1) \otimes |\phi_1\rangle \langle\phi_1|] \frac{d\phi_1}{2\pi}\} ... \{\int_0^{2\pi} [M(\phi_{k+1}) \otimes |\phi_{k+1}\rangle \langle\phi_{k+1}|] \frac{d\phi_{k+1}}{2\pi}\} \\
&= \int_0^{2\pi} ... \int_0^{2\pi} \{[M(\phi_1)...M(\phi_{k+1})] \otimes [|\phi_1\rangle \langle\phi_1| ... |\phi_{k+1}\rangle \langle\phi_{k+1}|]\} \frac{d\phi_1}{2\pi} ... \frac{d\phi_{k+1}}{2\pi} \\
&= \int_0^{2\pi} ... \int_0^{2\pi} \{[M(\phi_1)...M(\phi_{k+1})] \otimes [|\phi_1\rangle \langle\phi_{k+1}| \, \delta(\phi_1-\phi_2)...\delta(\phi_k-\phi_{k+1})]\} \frac{d\phi_1}{2\pi} ... \frac{d\phi_{k+1}}{2\pi} \\
&= \int_0^{2\pi} [M(\phi_{k+1})...M(\phi_{k+1}) \otimes |\phi_{k+1}\rangle \langle\phi_{k+1}|] \frac{d\phi_{k+1}}{2\pi} \\
&= \int_0^{2\pi} [M(\phi_{k+1})^{k+1} \otimes |\phi_{k+1}\rangle \langle\phi_{k+1}|] \frac{d\phi_{k+1}}{2\pi}. \qquad (347)
\end{aligned}
$$

(Final step) Therefore by induction we have shown that

$$V_q^k = \int_0^{2\pi} \left\{ M^k(\phi_1) \otimes |\phi_1\rangle \langle\phi_1| \right\} \frac{d\phi_1}{2\pi}. \tag{348}$$

To explicitly determine operator V_q^k we proceed to calculate the kth power of matrix $M(\phi_1)$,

$$M(\phi_1) = \begin{pmatrix} e^{i\phi_1}\cos\theta & e^{-i\phi_1}\sin\theta \\ -e^{i\phi_1}\sin\theta & e^{-i\phi_1}\cos\theta \end{pmatrix}. \tag{349}$$

To this end, we study the characteristic equation of M, which via the difference

$$\begin{aligned} M(\phi_1) - \lambda\mathbf{1} &= \begin{pmatrix} e^{i\phi_1}\cos\theta & e^{-i\phi_1}\sin\theta \\ -e^{i\phi_1}\sin\theta & e^{-i\phi_1}\cos\theta \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} e^{i\phi_1}\cos\theta - \lambda & e^{-i\phi_1}\sin\theta \\ -e^{i\phi_1}\sin\theta & e^{-i\phi_1}\cos\theta - \lambda \end{pmatrix} \end{aligned} \tag{350}$$

, reads $x_{M(\phi_1)}(\lambda) := \det\left(M(\phi_1) - \lambda\mathbf{1}\right) = 0$, where

$$\begin{aligned} x_{M(\phi_1)}(\lambda) &= \left(e^{i\phi_1}\cos\theta - \lambda\right)\left(e^{-i\phi_1}\cos\theta - \lambda\right) + e^{i\phi_1}e^{-i\phi_1}\sin^2\theta \\ &= \lambda^2 - \lambda\cos\theta\cos\phi_1 + 1 \\ &= \lambda^2 - \lambda Tr\left\{M(\phi_1)\right\} + \det M(\phi_1) \\ &= 0. \end{aligned} \tag{351}$$

We set $\xi = \frac{1}{2}Tr\left\{M(\phi_1)\right\}$, to obtain

$$x_{M(\phi_1)}(\lambda) = \lambda^2 - 2\xi\lambda + 1 = 0. \tag{352}$$

Utilizing the Cayley-Hamilton theorem [6] which states that any finite matrix satisfies its own characteristic equation, we obtain

$$x_{M(\phi_1)}(M(\phi_1)) = M^2(\phi_1) - 2\xi M(\phi_1) + \mathbf{1} = 0,$$

or

$$M^2(\phi_1) = 2\xi M(\phi_1) - \mathbf{1}. \tag{353}$$

Last equation implies that any higher power of $M(\phi_1)$ can be expressed as a linear combination of $M(\phi_1)$ and the identity matrix $\mathbf{1}$, i.e.

$$M^k(\phi_1) = M(\phi_1)U_{k-1}(\xi) - \mathbf{1}U_{k-2}(\xi), \tag{354}$$

where $U_k(\xi)$ is a polynomial of degree k in ξ, to be specified shortly.

Multipling last equation by $M(\phi_1)$ yields

$$
\begin{aligned}
M^{k+1}(\phi_1) &= M^2(\phi_1)U_{k-1}(\xi) - M(\phi_1)U_{k-2}(\xi) \\
&\overset{(353)}{=} [2\xi M(\phi_1) - \mathbf{1}]U_{k-1}(\xi) - M(\phi_1)U_{k-2}(\xi) \qquad (355)
\end{aligned}
$$

and from eq.(354) by substitution $k \to k+1$, we obtain

$$M^{k+1}(\phi_1) = M(\phi_1)U_k(\xi) - \mathbf{1}U_{k-1}(\xi), \tag{356}$$

and then by equating eqs.(355)(356) and elaborating, we obtain

$$[2\xi M(\phi_1) - \mathbf{1}]U_{k-1}(\xi) - M(\phi_1)U_{k-2}(\xi) = M(\phi_1)U_k(\xi) - \mathbf{1}U_{k-1}(\xi), \tag{357}$$

$$2\xi M(\phi_1)U_{k-1}(\xi) - \mathbf{1}U_{k-1}(\xi) - M(\phi_1)U_{k-2}(\xi) = M(\phi_1)U_k(\xi) - \mathbf{1}U_{k-1}(\xi), \tag{358}$$

and

$$M(\phi_1)[2\xi U_{k-1}(\xi) - U_{k-2}(\xi) - U_k(\xi)] = 0. \tag{359}$$

which, given that $M(\phi_1) \neq 0$, yields the recurrence relation

$$2\xi U_{k-1}(\xi) - U_{k-2}(\xi) - U_k(\xi) = 0, \tag{360}$$

which by substituting $k \to k+2$, and multipling by (-1), becomes

$$U_{k+2}(\xi) - 2\xi U_{k+1}(\xi) + U_k(\xi) = 0, \tag{361}$$

which is identified with the two step recursion relation defining Chebyshev polynomials [12]. This relation is initialized by the first two polynomials which are determined by first setting $k = 1$ in eq.(354),

$$M^2(\phi_1) = M(\phi_1)U_1(\xi) - \mathbf{1}U_0(\xi) \tag{362}$$

and then using eq.(353), to obtain equation

$$2\xi M(\phi_1) - \mathbf{1} = M(\phi_1)U_1(\xi) - \mathbf{1}U_0(\xi), \tag{363}$$

which provides the two initial polynomials

$$U_0(\xi) = 1, \quad U_1(\xi) = 2\xi. \tag{364}$$

Thus summarizing $\{U_k(\xi)\}_{k=0}^{\infty}$ are the second kind Chebyshev polynomials, and by means of eq. (354) would determine the density matrix of QW at any step k via. eq.(348).

5.2 QW and Maximum Likelihood Parametric Estimation

Having explicit knowledge of the evolution operator V_q^k for any time step k for the bipartite system of QWer and coin we proceed to determine the distribution of occupation probabilities on the integer lattice. To this end we recall that the density matrix of the QWer after traccing out the coin degrees of freedome reads

$$\mathcal{E}_{q;k}(\rho_w) = Tr_c \left\{ \int_0^{2\pi}\int_0^{2\pi} \left\{ (M^k(\phi_1;\theta)\rho_c M^k(\phi_2;\theta)^\dagger) \otimes |\phi_1\rangle \langle\phi_1| \rho_w |\phi_2\rangle \langle\phi_2| \right\} \frac{d\phi_1}{2\pi}\frac{d\phi_2}{2\pi} \right\}. \tag{365}$$

We now compute the trace in the coin space,

$$\begin{aligned} Tr_c\left\{M^k(\phi_1;\theta)\rho_c M^k(\phi_2;\theta)^\dagger\right\} &= Tr_c\{(M(\phi_1;\theta)U_{k-1}(\xi_1) \\ &\quad -\mathbf{1}U_{k-2}(\xi_1))\rho_c(M(\phi_2;\theta)U_{k-1}(\xi_2) \\ &\quad -\mathbf{1}U_{k-2}(\xi_2))^\dagger\} \\ &= Tr_c\{(M(\phi_1;\theta)U_{k-1}(\xi_1) \\ &\quad -\mathbf{1}U_{k-2}(\xi_1))\rho_c(M(\phi_2;\theta)^\dagger U_{k-1}(\xi_2) \\ &\quad -\mathbf{1}U_{k-2}(\xi_2))\} \\ &= U_{k-1}(\xi_1)U_{k-1}(\xi_2)Tr_c\left\{M(\phi_1;\theta)\rho_c M(\phi_2;\theta)^\dagger\right\} \\ &\quad -U_{k-1}(\xi_1)U_{k-2}(\xi_2)Tr_c\left\{M(\phi_1;\theta)\rho_c\right\} \\ &\quad -U_{k-2}(\xi_1)U_{k-1}(\xi_2)Tr_c\left\{\rho_c M(\phi_2;\theta)^\dagger\right\} \\ &\quad +U_{k-2}(\xi_1)U_{k-2}(\xi_2), \end{aligned} \tag{366}$$

where

$$\begin{aligned} \xi_i &= \xi(\phi_i;\theta) = \frac{1}{2}Tr\left[M(\phi_i;\theta)\right] \\ &= \cos\theta\cos\phi_i, i = 1, 2. \end{aligned} \tag{367}$$

Next, we calculate the occupation probability distribution $P[X_k = x]$, for the walker to be at position $x \in \mathbb{Z}$ in step k. This distribution can be described by X_k, a classical random variable that determines walker's position on the integer lattice i.e. $X_k \in \mathbb{Z} \in \{..., -1, 0, +1, ...\}$, after k steps.

Denoting the time evolved density matrix by

$$\rho_w^{(k)} = \mathcal{E}_{q;k}(\rho_w^{(0)}), \tag{368}$$

and introducing the position projection operator at the $k-$th step,

$$L^{(k)} = |x\rangle\langle x|, \tag{369}$$

where $|x\rangle$, $x \in \mathbb{Z}$, is a positition eigenestate, i.e. $L|x\rangle = x|x\rangle$. Projection $L^{(k)}$ is taken as the observable of interest at time k, the expectation value of which provides the occupation probability distribution, as

$$\begin{aligned} P[X_k &= x] = Tr\left[L^{(k)}\mathcal{E}_{q;k}(\rho_w^{(0)})\right] \\ &= Tr\left\{|x\rangle\langle x|\,\rho_w^{(k)}\right\} = \langle x|\,\rho_w^{(k)}\,|x\rangle \\ &\equiv p^{(k)}(x|\theta). \end{aligned} \tag{370}$$

The likelihood function define for a set of lattice position denoted by a vector as $\underline{\mathrm{x}}$=$(x_1, ..., x_n)$, reads

$$L_n^{(k)}(\theta|\underline{\mathrm{x}}) \equiv \prod_{j=1}^{n} p^{(k)}(x_j|\theta). \tag{371}$$

The task of maximizing the likelihood is equivalent to the maximization of its logarithm

$$\begin{aligned} l_n^{(k)}(\theta) &\equiv l_n^{(k)}(\theta|\underline{\mathrm{x}}) \\ &= \log L_n^{(k)}(\theta) \\ &\equiv \log L_n^{(k)}(\theta|\underline{\mathrm{x}}) \\ &= \log \prod_{j=1}^{n} p^{(k)}(x_j|\theta) \\ &= \sum_{j=1}^{n} \log p^{(k)}(x_j|\theta). \end{aligned} \tag{372}$$

This leads to the need to solve the equation

$$\frac{\partial}{\partial\theta} l_n^{(k)}(\theta) = 0, \tag{373}$$

i.e.

$$\frac{\partial}{\partial\theta} l_n^{(k)}(\theta) = \sum_{j=1}^{n} \frac{1}{p^{(k)}(x_j|\theta)} \frac{\partial p^{(k)}(x_j|\theta)}{\partial\theta} = 0, \tag{374}$$

i.e. for each j we need to determine the roots of function $p^{(k)}(x_j|\theta) = \langle x_j|\,\mathcal{E}_{q;k}(\rho_w^{(0)})\,|x_j\rangle$.

Let us choose a loop for the QW i.e.

$$L^{(k)}=\rho_w^{(0)} = |x\rangle\langle x|, \tag{375}$$

where $|x\rangle$, $x \in \mathbb{Z}$, a basis vector. This choice implies that the initial and final state for QWer be the same, say some $|x\rangle$, $x \in \mathbb{Z}$; then referring to eq. (365),

we compute

$$\begin{aligned} Tr_w\left\{L^{(k)}\,|\phi_1\rangle\langle\phi_1|\,\rho_w\,|\phi_2\rangle\langle\phi_2|\right\} &= Tr_w\left\{|x\rangle\langle x|(|\phi_1\rangle\langle\phi_1|\,|x\rangle\langle x|\,|\phi_2\rangle\langle\phi_2|)\right\} \\ &= |\langle x|\phi_1\rangle|^2|\langle x|\phi_2\rangle|^2 = \frac{1}{(2\pi)^2}, \end{aligned} \tag{376}$$

i.e. independent from variables ϕ_1, ϕ_2 and x. This choice of the loop implies a drastic simplification for the likelihood function since now we have that

$$l_n^{(k)}\left(\theta|\underline{\mathrm{x}}\right) = \log\left(p^{(k)}\left(\underline{\mathrm{x}}|\theta\right)\right)^n = n\log p^{(k)}(\underline{\mathrm{x}}|\theta). \tag{377}$$

Since for the propabilities $p^{(k)} \in [0,1]$, we obtain $l_n^{(k)} = \log p^{(k)} < 0$, thus likelihood must be negative and the maximization of likelihood requires

$$\frac{\partial^2 l_n^{(k)}\left(\theta|\underline{\mathrm{x}}\right)}{\partial\theta^2} < 0, \tag{378}$$

or by denoting derivative with respect to θ with a prime,

$$\frac{p^{(k)''}p^{(k)} - p^{(k)'2}}{p^{(k)2}} < 0. \tag{379}$$

Therefore the introduction of loop idea, which implies the involvement of return probabilities in the evaluation of the likelihood function, results into a factorization of $l_n^{(k)}$ into two factors depending separately on n and k, cf. eq. (377). The task of likelihood maximization is then equivalent to the maximization of distribution $p^{(k)}(\underline{\mathrm{x}}|\theta)$ for given $k \in \mathbb{N}$, for those parameters $\theta \in [-\pi, \pi)$ for which the distribution satisfies

$$p^{(k)''}p^{(k)} < p^{(k)'2}. \tag{380}$$

After this important remarks we proceed with the evaluation of $p^{(k)}(\underline{\mathrm{x}}|\theta)$ which via eqs. (365, 376, and 377) reads,

$$\begin{aligned} p^{(k)}(\underline{\mathrm{x}}|\theta) &= \frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} U_{k-1}(\xi_1)U_{k-1}(\xi_2) \\ &\quad \times Tr_c\left\{M(\phi_1;\theta)\rho_c M(\phi_2;\theta)^\dagger\right\}\frac{d\phi_1 d\phi_2}{(2\pi)^2} \\ &\quad -\frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} U_{k-1}(\xi_1)U_{k-2}(\xi_2) Tr_c\left\{M(\phi_1;\theta)\rho_c\right\}\frac{d\phi_1 d\phi_2}{(2\pi)^2} \\ &\quad -\frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} U_{k-2}(\xi_1)U_{k-1}(\xi_2) Tr_c\left\{\rho_c M(\phi_2;\theta)^\dagger\right\}\frac{d\phi_1 d\phi_2}{(2\pi)^2} \\ &\quad +\frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} U_{k-2}(\xi_1)U_{k-2}(\xi_2)\frac{d\phi_1 d\phi_2}{(2\pi)^2}. \end{aligned} \tag{381}$$

To proceed we need to evaluate seperately the following three terms $Tr_c\left\{M(\phi_1;\theta)\rho_c M(\phi_2;\theta)^\dagger\right\}$, $Tr_c\left\{M(\phi_1;\theta)\rho_c\right\}$ and $Tr_c\left\{\rho_c M(\phi_2;\theta)^\dagger\right\}$. To this recalling the M matrix from eq. (349) and choosing the initial coin state to be $|c\rangle = |0\rangle$, we get

$$
\begin{aligned}
Tr_c\left\{M(\phi_1;\theta)\rho_c M(\phi_2;\theta)^\dagger\right\} &= e^{i\phi_1}e^{-i\phi_2},\\
Tr_c\left\{M(\phi_1;\theta)\rho_c\right\} &= \cos\theta e^{i\phi_1},\\
Tr_c\left\{\rho_c M(\phi_2;\theta)^\dagger\right\} &= \cos\theta e^{-i\phi_2}.
\end{aligned} \tag{382}
$$

This results into the next expression for the distribution function, in terms of factorized integrals,

$$
\begin{aligned}
p^{(k)}(\underline{\mathrm{x}}|\theta) &= \frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)e^{i\phi_1}\frac{d\phi_1}{2\pi}\right)\left(\int_0^{2\pi} U_{k-1}(\xi_2)e^{-i\phi_2}\frac{d\phi_2}{2\pi}\right)\\
&-\frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)e^{i\phi_1}\frac{d\phi_1}{2\pi}\right)\left(\int_0^{2\pi} U_{k-2}(\xi_2)\frac{d\phi_2}{2\pi}\right)\\
&-\frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-2}(\xi_1)\frac{d\phi_1}{2\pi}\right)\left(\int_0^{2\pi} U_{k-1}(\xi_2)e^{-i\phi_2}\frac{d\phi_2}{2\pi}\right)\\
&+\frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-2}(\xi_1)\frac{d\phi_1}{2\pi}\right)\left(\int_0^{2\pi} U_{k-2}(\xi_2)\frac{d\phi_2}{2\pi}\right).
\end{aligned} \tag{383}
$$

An explicit form of probability distribution function above, and subsequently its optimization with respect to the parameter θ, requires the evaluation of integrals with respect to argument ϕ of Chebyshev polynomials and also evaluation of derivatives with respect to parameter θ. To accomplish these tasks the following technical lemma will be used, the proof of which is referred to the appendix.

Lemma 51 (Technical Lemma) *Let the Chebyshev polynomials of the second kind $U_k(\cos\phi)$ with respect to $\cos\phi$, then for polynomials with scaled argument*

$$
U_k(\xi) := U_k(\lambda(\theta)\cos\phi), \tag{384}
$$

where $\lambda(\theta) = \cos\theta$ is a function of parameter θ, the relations and definition of functions $Y_{2r}(\lambda(\theta))$, issued in eqs. (385-389), are valid:

$$
\int_0^{2\pi} U_{2r+1}(\lambda(\theta)\cos\phi)\frac{d\phi}{2\pi} = 0, \tag{385}
$$

$$
\int_0^{2\pi} U_{2r}(\lambda(\theta)\cos\phi)\frac{d\phi}{2\pi} =: Y_{2r}(\lambda(\theta)), \tag{386}
$$

and also the integrals involving polynomials and trigonometric functions

$$\int_0^{2\pi} U_{2r}(\lambda(\theta)\cos\phi)\cos\phi\frac{d\phi}{2\pi} = 0, \tag{387}$$

and similarly

$$2\int_0^{2\pi} U_{2r+1}(\lambda(\theta)\cos\phi)\cos\phi\frac{d\phi}{2\pi} = Y_{2r}(\lambda(\theta)) + Y_{2r+2}(\lambda(\theta)). \tag{388}$$

Also $Y_{m=odd}(\lambda(\theta)) = 0,$ *and*

$$Y_{m=even}(\lambda(\theta)) = \frac{1}{\pi}\sum_{l=0}^{\lfloor m/2\rfloor} c_l(\theta)\frac{(m-2l-1)!!}{(m-2l)!!}, \tag{389}$$

where $c_l(\theta) = (-1)^l\binom{m-l}{l}(2\cos\theta)^{m-2l}.$

Having state the content of technical lemma we now proceed with the evaluation of the distribution function. We will evaluate separately the case of odd and even number of steps.

5.2.1 Odd number of steps

For $k = odd, \quad k-1 = even, k-2 = odd$, by means of the lemma, all lines exept the first one is zero, and these yields

$$p(\underline{\mathrm{x}}|\theta) = \frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)e^{i\phi_1}\frac{d\phi_1}{2\pi}\right)\left(\int_0^{2\pi} U_{k-1}(\xi_2)e^{-i\phi_2}\frac{d\phi_2}{2\pi}\right), \tag{390}$$

or

$$\begin{aligned} p(\underline{\mathrm{x}}|\theta) &= \frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)\cos\phi_1\frac{d\phi_1}{2\pi} + i\int_0^{2\pi} U_{k-1}(\xi_1)\sin\phi_1\frac{d\phi_1}{2\pi}\right) \\ &\times\left(\int_0^{2\pi} U_{k-1}(\xi_2)\cos\phi_2\frac{d\phi_2}{2\pi} - i\int_0^{2\pi} U_{k-1}(\xi_2)\sin\phi_2\frac{d\phi_2}{2\pi}\right), \end{aligned} \tag{391}$$

which leads to

$$p^{(k)}(\underline{\mathrm{x}}|\theta) = \frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi)\sin\phi\frac{d\phi}{2\pi}\right)^2 = 0, \tag{392}$$

which then implies $l_n^{(k=odd)}(\theta|\underline{\mathrm{x}}) = 0$.

5.2.2 Even number of steps

For $k = even, \quad k-1 = odd, k-2 = even$, by means of the lemma, we obtain

$$\begin{aligned}
p^{(k)}(\underline{\mathrm{x}}|\theta) &= \frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)\cos\phi_1 \frac{d\phi_1}{2\pi} + i\int_0^{2\pi} U_{k-1}(\xi_1)\sin\phi_1 \frac{d\phi_1}{2\pi}\right) \\
&\times \left(\int_0^{2\pi} U_{k-1}(\xi_2)\cos\phi_2 \frac{d\phi_2}{2\pi} - i\int_0^{2\pi} U_{k-1}(\xi_2)\sin\phi_2 \frac{d\phi_2}{2\pi}\right) \\
&-\frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-1}(\xi_1)\cos\phi_1 \frac{d\phi_1}{2\pi} + i\int_0^{2\pi} U_{k-1}(\xi_1)\sin\phi_1 \frac{d\phi_1}{2\pi}\right) \\
&\times \left(\int_0^{2\pi} U_{k-2}(\xi_2)\frac{d\phi_2}{2\pi}\right) \\
&-\frac{1}{2\pi}\left(\int_0^{2\pi} U_{k-2}(\xi_1)\frac{d\phi_1}{2\pi}\right) \\
&\times \left(\int_0^{2\pi} U_{k-1}(\xi_2)\cos\phi_2 \frac{d\phi_2}{2\pi} - i\int_0^{2\pi} U_{k-1}(\xi_2)\sin\phi_2 \frac{d\phi_2}{2\pi}\right) \\
&+\frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi} U_{k-2}(\xi_1)U_{k-2}(\xi_2)\frac{d\phi_1 d\phi_2}{(2\pi)^2}. \qquad (393)
\end{aligned}$$

Furtherore, by virtue of the lemma the integrals with cosine terms in the integrand give zero, and this results in

$$\begin{aligned}
p(\underline{\mathrm{x}}|\theta) &= \frac{1}{2\pi}\left(\frac{1}{2}\left(Y_{k-2}(\lambda(\theta)) + Y_k(\lambda(\theta))\right) + i\int_0^{2\pi} U_{k-1}(\xi_1)\sin\phi_1 \frac{d\phi_1}{2\pi}\right) \\
&\times \left(\frac{1}{2}\left(Y_{k-2}(\lambda(\theta)) + Y_k(\lambda(\theta))\right) - i\int_0^{2\pi} U_{k-1}(\xi_2)\sin\phi_2 \frac{d\phi_2}{2\pi}\right) \\
&\times - \frac{1}{2\pi}Y_{k-2}(\lambda(\theta))\left(\frac{1}{2}\left(Y_{k-2}(\lambda(\theta)) + Y_k(\lambda(\theta))\right) + i\int_0^{2\pi} U_{k-1}(\xi_1)\sin\phi_1 \frac{d\phi_1}{2\pi}\right) \\
&\times - \frac{1}{2\pi}Y_{k-2}(\lambda(\theta))\left(\frac{1}{2}\left(Y_{k-2}(\lambda(\theta)) + Y_k(\lambda(\theta))\right) - i\int_0^{2\pi} U_{k-1}(\xi_2)\sin\phi_2 \frac{d\phi_2}{2\pi}\right) \\
&\times + \frac{1}{2\pi}Y_{k-2}(\lambda(\theta))Y_{k-2}(\lambda(\theta)), \qquad (394)
\end{aligned}$$

then

$$p^{(k)}(\underline{\mathrm{x}}|\theta) = \frac{1}{8\pi}\left\{Y_{k-2}(\lambda(\theta)) + Y_k(\lambda(\theta)\right\}^2 + \frac{1}{2\pi}\left\{\int_0^{2\pi} U_{k-1}(\xi)\sin\phi \frac{d\phi}{2\pi}\right\}^2, \quad (395)$$

or finally

$$p^{(k)}(\underline{\mathrm{x}}|\theta) = \frac{1}{8\pi}\left(Y_{k-2}(\cos\theta) + Y_k(\cos\theta)\right)^2, \quad (396)$$

which by the realation $l_n^{(k)} = \log(p^{(k)})^n$ yields for the likelihood function

$$l_n^{(k)}(\theta|\underline{\mathrm{x}}) = 2n\log\left\{\frac{1}{\sqrt{8\pi}}\left(Y_{k-2}(\cos\theta) + Y_k(\cos\theta)\right)\right\}. \quad (397)$$

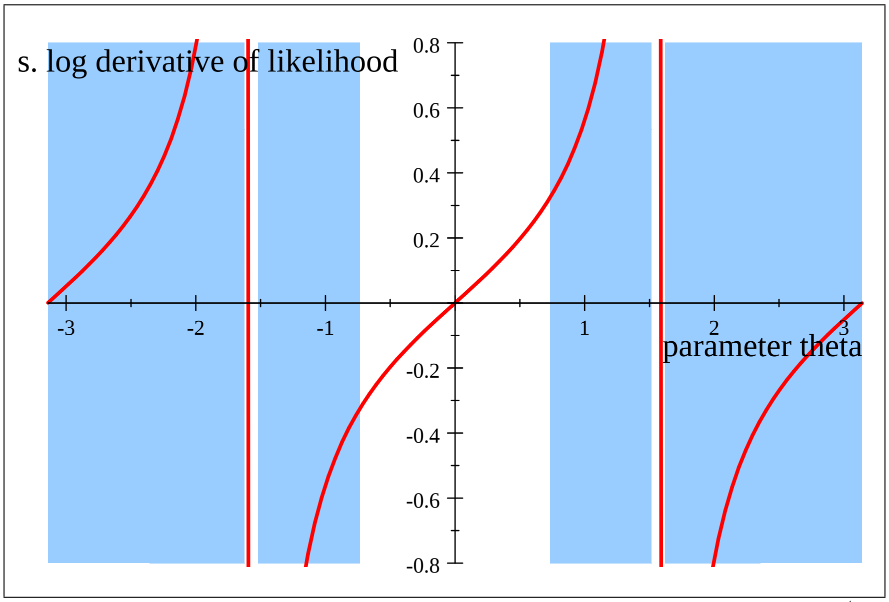
Having determined the distribution of probabilities in eq.(396) we procced to determine parameter θ from inequality of eq. (380), which now reads explicitly

$$\left[(Y_{k-2} + Y_k)^2\right]''(Y_{k-2} + Y_k)^2 < \left[2\left(Y_{k-2} + Y_k\right)\left(Y'_{k-2} + Y'_k\right)\right]^2 . \quad (398)$$

From the explicit form of functions $Y_k(\lambda(\theta))$ we can determine interval of values for the parameter θ, that satisfy the above inequality that amounts to the maximization of likelihood. We proceed with the simplifying case of $k = 2$, which needs only the first two Chebyshev polynomials U_0, U_1 to derive the pertinent functions $Y_0(\theta) = 1$ and $Y_1(\theta) = 2\cos^2\theta - 1$, that lead to the inequality to be satisfied

$$2(\sin\theta)^2(\cos\theta)^2 + (\cos\theta)^3 - 4(\cos\theta)^2(\sin\theta)^2 < 0. \quad (399)$$

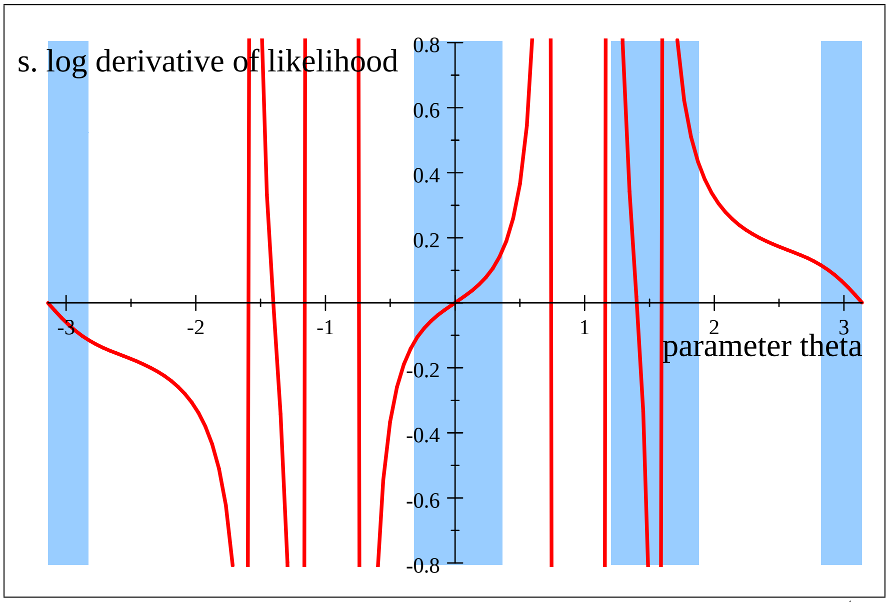
The sets that the optimum value (maximum likelihood estimator) of θ are displayed as shaded bars in the figure below. The line is the graph of $l'(\theta) = 0$. The intersections of this line with the parameter theta axis are the critical points of l'. If an intersection is inside a shaded bar, then this point is a maximum parameter estimator.



(400)

We next repeat the estimation for the cases of more QW steps, namely we deal with the cases of $k = 4$, 6. The respective inequalites and their display are, first for $k = 4$,

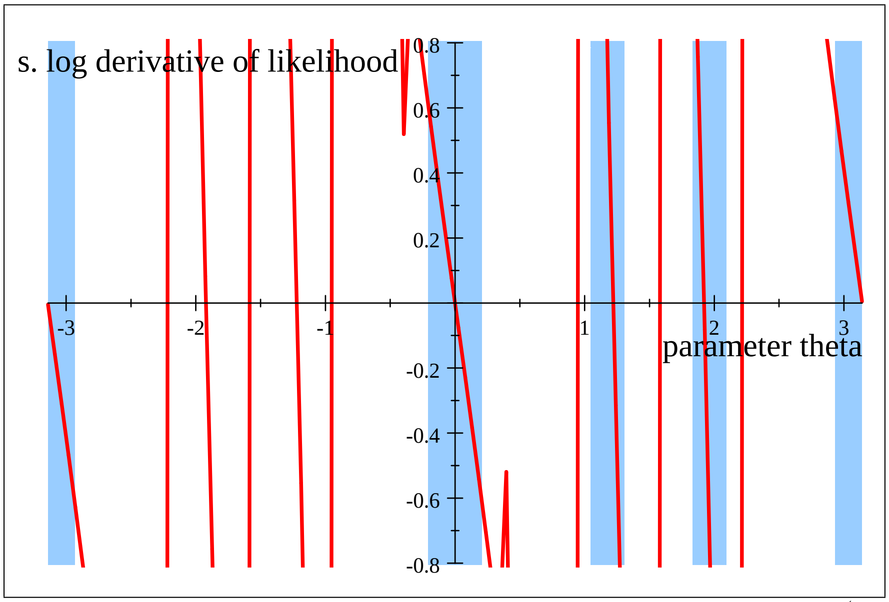
$$\left(-c - 24c^3 s + 12cs\right) + 2\left(c + 6c^4 - 6c^2 + 2\pi\right)\left(-c + 72c^2 s^2 - 24c^4 - 12s^3 + 12c^2\right) < 0$$



(401)

and for $k = 6$,

$$
\begin{aligned}
&\left(120sc^5 - 96sc^3 + 12sc\right)^2 - \left(20c^6 - 24c^4 + 6c^2 + 2\pi - 1\right)^3 \\
&\times(120c^6 - 600c^4s^2 - 96c^4 + 288c^2s^2 + 12c^2 + 12s^3 - 24s^2\theta) \\
&-2\left(120sc^5 - 96sc^3 + 12sc\right)^2 \left(20c^6 - 24c^4 + 6c^2 + 2\pi - 1\right)^2 < 0
\end{aligned}
$$



(402)

5.3 Final remarks on the calculation method for the likelihood

i) The parameter estimation method put forward in this work uses the maximum likelihood problem as a device to accomplish its aim, i.e. the estimation. The likelihood function is constructed by using the return probability for a closed orbit (or loop trip) on integers carried out by a QWer. The closed orbit choice is made solely on the basis of computational simplification it can provide. Within the presumed formalism of QW our choices are possible (i.e. open orbits of so short), for which however some technique of reducing the computation load should be found. Those other type of orbits are expected to give more reliable results for the parameter estimation.

ii) Parameter k denotes the number of steps in which a CRWer diffuses in a range of order $O(\sqrt{k})$, while a QWer is quadratically faster and diffuses in a range of order $O(k)$. This quadratic speed up implies that a MLE of a parameter via QW utilizes a more extended set of points, and in this way renders the QW based estimation algorithm more effective in comparison with its classical counterpart.

iii) The MLE based algorithm uses a set of n QWs to built its likelihood function. Therefore a data box of size $k\times n$, representing the number of steps $\times$ the numbers of QWs constitutes the data resources for the estimation problem in hand. Given that bigger data box is expected to produce better estimations, the standard dilemma: "larger number of steps or larger number of QW?", should be decided efficiently so that the parameter θ is nearly optimal. Both in classical estimation theory and in present quantum like estimation approach, k and n are considered as quantities of two rival resources in scarcity, i.e. the *data box dilemma* transcripts in our context to: "fewer QWs running for longer time, or many QWs running for shorter time?". Notice the significance of the quadratic speed up of QW (faster diffusion rate of a QW), in connection with *data box dilemma*. A QW produces $O(k) \times n$ data points, in comparison to a CRW that could be used instead, which produces $O(\sqrt{k}) \times n$ data points, so it is expected to provide a more efficient parameter estimation.

A Appendix

A.1 Discrete Time Fourier Transform

The Discrete Time Fourier Transform is part of the family of Fourier transforms. It transforms a function $f(n)$ of a discrete time variable $n \in \mathbb{Z}$ into a continuous, periodic spectrum $\mathcal{F}\left(e^{i\varpi}\right)$. Let $f : \mathbb{Z} \longrightarrow \mathbb{C}$ be a complex function over the integers$\Longrightarrow$its discrete fourier transform $\mathcal{F} : [-\pi, \pi] \longrightarrow \mathbb{C}$ is given by

$$\mathcal{F}\left(e^{i\varpi}\right) = \sum_{n=-\infty}^{\infty} f(n)\, e^{-in\varpi} \tag{403}$$

and its inverse is given by

$$f(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathcal{F}\left(e^{i\varpi}\right) e^{in\varpi} d\varpi. \tag{404}$$

A.2 Fourier Transformation Techniques

The discrete Fourier transform of a function $f(x)$ is

$$\tilde{f}(x) = \sum_{l=-\infty}^{+\infty} e^{ixl} f(l). \tag{405}$$

The continuous Fourier transform of a function $f(x)$ is

$$\tilde{f}(x) = \int_{-\infty}^{+\infty} e^{ixt} f(t) dt. \tag{406}$$

The Fourier transforms are often called characteristic functions.

A.3 Fourier Convolution Theorem

Let f be a function. The Fourier transform of f is defined as

$$f \xrightarrow{\mathcal{F}} \hat{f} = \mathcal{F}[f] \tag{407}$$

The inverse Fourier transform of f is defined as

$$\hat{f} \xrightarrow{\mathcal{F}^{-1}} f = \mathcal{F}^{-1}\left[\hat{f}\right]. \tag{408}$$

The linearity of the Fourier transform is defined as

$$f_1 + \beta f_2 \xrightarrow{\mathcal{F}} a\widehat{f_1 + \beta} f_2 = a\hat{f}_1 + \beta \hat{f}_2. \tag{409}$$

The Fourier transform is non commutative because

$$\left[\hat{f}_1, \hat{f}_2\right] \neq 0 \ . \tag{410}$$

Theorem 52 *Convolution Theorem*

$$\widehat{f_1 f_2} = \hat{f}_1 * \hat{f}_2, \tag{411}$$

more explicitly

$$\left(\hat{f}_1 * \hat{f}_2\right)_m = \sum_m \left(\hat{f}_1\right)_m \left(\hat{f}_2\right)_{n-m}, \ \hat{f}_1, \hat{f}_2 \textit{ discrete functions} \tag{412}$$

and

$$\left(\hat{f}_1 * \hat{f}_2\right)(s) = \int \hat{f}_1 (x-s)\, \hat{f}_2 (x)\, dx, \hat{f}_1, \hat{f}_2 \textit{continuous functions} \ . \tag{413}$$

A.4 Chebyshev Polynomials

Chebyshev polynomials [12] are a sequence of orthogonal polynomials which are related to de Moivre's formula and which can be recursively expressed. They are divided into two categories, Chebyshev polynomials of first kind T_n and second kind U_n, and they are polynomials of degree n. Chebyshev polynomials are solutions of the Chebyshev differential equations

$$(1-x^2)y'' - xy' + n^2 y = 0, \tag{414}$$

and

$$(1-x^2)y'' - 3xy' + n(n+2)y = 0. \tag{415}$$

The above equations are special cases of the Sturm Liouville differential equation.

A.4.1 The first kind of Chebyshev Polynomial $T_n(x)$

The Chebyshev polynomials of the first kind are defined recursively as

$$T_0(x) = 1,\ T_1(x) = x, \tag{416}$$
$$T_{(n+1)}(x) = 2xT_n(x) - T_{(n-1)}(x). \tag{417}$$

The conventional generating function for T_n is

$$\sum_{n=0}^{+\infty} t^n T_n(x) = \frac{1-tx}{1-2tx+t^2}, \tag{418}$$

or by trigonometric definition

$$T_n(\cos\theta) = \cos(n\theta). \tag{419}$$

A.4.2 The second kind of Chebyshev Polynomial $U_n(x)$

The Chebyshev polynomials of the second kind are defined recursively as

$$U_0(x) = 1,\quad U_1(x) = 2x, \tag{420}$$
$$U_{(n+1)}(x) = 2xU_n(x) - U_{(n-1)}(x), \tag{421}$$

or by trigonometric definition

$$U_n(\cos\theta) = \frac{\sin((n+1)\theta)}{\sin\theta}. \tag{422}$$

A.4.3 Differentiation

Let $n = odd$ and $x = cos\phi$

$$U_n(x) = 2\sum_{j:odd} T_j(x), \tag{423}$$

$$\frac{d}{dx}\{U_n(x)\} = 2\sum_{j:odd}\left(\frac{d}{dx}\{T_j(x)\}\right) = 2\sum_{j:odd} jU_{j-1}(x). \tag{424}$$

We substitute x with λx

$$U_n(\lambda x) = 2\sum_{j:odd} T_j(\lambda x). \tag{425}$$

We differentiate for λx

$$\frac{d}{d(\lambda x)}[U_n(\lambda x)] = 2\sum_{j:odd}\left(\frac{d}{d(\lambda x)}\{T_j(\lambda x)\}\right) = 2\sum_{j:odd} jU_{j-1}(\lambda x). \tag{426}$$

A.4.4 A Lemma about Chebyshev Polynomials

Lemma 53 *Let the Chebyshev polynomials of the second kind* $U_k(\cos\phi)$ *with respect to* $\cos\phi$*, then for polynomials with scaled argument* $U_k(\xi) := U_k(\lambda(\theta)\cos\phi)$*, where* $\lambda(\theta) = \cos\theta$ *is a function of parameter* θ*, the relations issued in eqs. 427,428, and 429-432, are valid*

$$\frac{\partial}{\partial\theta}\ [U_{2r+1}(\xi)] = -\tan\theta \sum_{m:odd}^{2r+1} m[\cos\phi U_{m-2}(\xi) + U_m(\xi)], \tag{427}$$

$$\frac{\partial}{\partial\theta}\ [U_{2r}(\xi)] = -\tan\theta \sum_{m:even}^{2r} m[U_{m-2}(\xi) + U_m(\xi)], \tag{428}$$

regarding derivatives and

$$\int_0^{2\pi} \{U_{2r+1}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} = 0, \tag{429}$$

$$\int_0^{2\pi} \{U_{2r}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} = Y_{2r}(\lambda(\theta)), \tag{430}$$

regarding integrals, and the following integrals involving polynomials and trigonometric functions

$$\begin{aligned} 2\int_0^{2\pi} \{\cos\phi U_{2r}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} &= \int_0^{2\pi} \{U_{2r-1}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} \\ +\int_0^{2\pi} \{U_{2r+1}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} &= 0, \end{aligned} \tag{431}$$

and similarly

$$\begin{aligned} &2\int_0^{2\pi} \{\cos\phi U_{2r+1}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} = \\ =\ & \int_0^{2\pi} \{U_{2r}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} + \int_0^{2\pi} \{U_{2r+2}(\lambda(\theta)\cos\phi)\}\, \frac{d\phi}{2\pi} \\ =\ & : Y_{2r}(\lambda(\theta)) + Y_{2r+2}(\lambda(\theta)), \end{aligned} \tag{432}$$

where the polynomials $Y_{2r}(\lambda(\theta))$ and $Y_{2r+2}(\lambda(\theta))$ wrt parameter θ has been introduced in 430.

Proof

For k odd

$$\begin{aligned}
&\int_0^{2\pi} \left\{ \frac{\partial}{\partial \theta} \ [U_{k-2}(\cos\theta\cos\phi_1)] \right\} \frac{d\phi_1}{2\pi} \\
= &\quad -\tan\theta \sum_{m:odd}^{k-2} m \left(\int_0^{2\pi} \{U_{m-2}(\cos\theta\cos\phi_1) + U_m(\cos\theta\cos\phi_1)\} \frac{d\phi_1}{2\pi} \right).
\end{aligned} \tag{433}$$

Recall the definition

$$U_n(x) = \sum_{l=0}^{\lfloor n/2 \rfloor} (-1)^l \binom{n-l}{l} (2x)^{n-2l}, n > 0, \tag{434}$$

where $x = \cos\phi$. Substituting $x \to \lambda x$,with $\lambda = \cos\theta$, we get

$$U_n(\lambda x) = \sum_{l=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n-l}{l} (2\lambda x)^{n-2l}, n > 0, \tag{435}$$

then e.g. with m odd

$$\begin{aligned}
\int_0^{2\pi} \{U_{m-2}(\cos\theta\cos\phi_1)\} \frac{d\phi_1}{2\pi} &= \int_0^{2\pi} \{U_{m-2}(\lambda\cos\phi_1)\} \frac{d\phi_1}{2\pi} \\
&= \sum_{l=0}^{\lfloor (m-2)/2 \rfloor} (-1)^k \binom{m-2-l}{l} (2\lambda)^{m-2-2l} \\
&\quad \times \left(\int_0^{2\pi} \left\{ (\cos\phi_1)^{m-2-2l} \right\} \frac{d\phi_1}{2\pi} \right) \\
&= 0.
\end{aligned} \tag{436}$$

Next we calculate the derivative wrt θ,

$$\begin{aligned}
\frac{\partial}{\partial \theta} \ U_{k-2}(\cos\theta\cos\phi_1) &= -(\sin\theta\cos\phi_1) 2 \sum_{m:odd}^{k-2} m U_{m-1}(\cos\theta\cos\phi_1) \\
&= -\tan\theta \sum_{m:odd}^{k-2} m[U_{m-2}(\xi_1) + U_m(\xi_1)],
\end{aligned} \tag{437}$$

therefore for k odd

$$\frac{\partial}{\partial \theta} \ U_{k-2}(\xi_1) = -\tan\theta \sum_{m:odd}^{k-2} m[U_{m-2}(\xi_1) + U_m(\xi_1)]. \tag{438}$$

We conclude that

$$Y_{m=odd}(\lambda(\theta)) = 0, \tag{439}$$

and therefore via eq 392, that $p^{(odd)}(x|\theta) = 0$ and $l_n^{(odd)}(\theta|x) = 0$ for odd number of steps.

For k even

$$\begin{aligned}
&\int_0^{2\pi} \left\{ \frac{\partial}{\partial\theta} \; [U_{k-2}(\cos\theta\cos\phi_1)] \right\} \frac{d\phi_1}{2\pi} \\
= \quad & -\tan\theta \sum_{m:even}^{k-2} m \left(\int_0^{2\pi} \{U_{m-2}(\cos\theta\cos\phi_1) + U_m(\cos\theta\cos\phi_1)\} \frac{d\phi_1}{2\pi} \right),
\end{aligned} \tag{440}$$

then by using the explicit expression for Chebyshev polynomials as before we obtain,

$$\begin{aligned}
\int_0^{2\pi} \{U_{m-2}(\cos\theta\cos\phi_1)\} \frac{d\phi_1}{2\pi} &= \int_0^{2\pi} \{U_{m-2}(\lambda\cos\phi_1)\} \frac{d\phi_1}{2\pi} \\
&= \sum_{l=0}^{\lfloor (m-2)/2 \rfloor} (-1)^l \binom{m-2-l}{l} (2\lambda)^{m-2-2l} \\
&\quad \times \left(\int_0^{2\pi} \left\{ (\cos\phi_1)^{m-2-2l} \right\} \frac{d\phi_1}{2\pi} \right) \\
&= \sum_{l=0}^{\lfloor (m-2)/2 \rfloor} (-1)^l \binom{m-2-l}{l} (2\lambda)^{m-2-2l} \\
&\quad \times \left(2\frac{(m-2l-3)!!}{(m-2l-2)!!} \right) \\
&= 2 \sum_{l=0}^{\lfloor (m-2)/2 \rfloor} (-1)^l \binom{m-2-l}{l} \\
&\quad \times (m-2l-2)!(2\cos\theta)^{m-2-2l} \\
&= : Y_{m-2}(\cos\theta).
\end{aligned} \tag{441}$$

Then, similarly

$$\int_0^{2\pi} \{U_m(\cos\theta\cos\phi_1)\} \frac{d\phi_1}{2\pi} = Y_m(\cos\theta), \tag{442}$$

therefore cf. eq. 440, we get

$$\int_0^{2\pi} \left\{ \frac{\partial}{\partial\theta} \; [U_{k-2}(\cos\theta\cos\phi_1)] \right\} \frac{d\phi_1}{2\pi} = -\tan\theta \sum_{m:even}^{k-2} m\left[Y_{m-2}(\cos\theta) + Y_m(\cos\theta)\right], \tag{443}$$

by means of identities

$$\begin{aligned} \int_0^{2\pi} \{\cos^s x\}\, dx &= \begin{cases} = 0, s\ odd \\ \neq 0, s\ even \end{cases}, \\ \int_0^{2\pi} \{\cos^s x\}\, dx &= 2\left(\int_0^{\pi} \{\cos^s x\}\, dx \right) = 2\frac{(s-1)!!}{s!!}\delta_{s,even}. \end{aligned} \tag{444}$$

Next we calculate the derivative wrt θ,

$$\begin{aligned} \frac{\partial}{\partial\theta} \; [U_{k-2}(\cos\theta\cos\phi_1)] &= -(\sin\theta\cos\phi_1)2 \\ &\quad \times \sum_{m:even}^{k-2} mU_{m-1}(\cos\theta\cos\phi_1) \\ &= -\frac{\sin\theta}{\cos\theta}2 \\ &\quad \times \sum_{m:even}^{k-2} m(\cos\theta\cos\phi_1) \\ &\quad \times U_{m-1}(\cos\theta\cos\phi_1) \\ &= -\tan\theta \\ &\quad \times \sum_{m:even}^{k-2} m[U_{m-2}(\cos\theta\cos\phi_1) \\ &\quad + U_m(\cos\theta\cos\phi_1)] \\ &= -\tan\theta \sum_{m:even}^{k-2} m[U_{m-2}(\xi_1) + U_m(\xi_1)], \end{aligned} \tag{445}$$

therefore for k even

$$\frac{\partial}{\partial\theta} \; [U_{k-2}(\xi_1)] = -\tan\theta \sum_{m:even}^{k-2} m[U_{m-2}(\xi_1) + U_m(\xi_1)].\blacksquare \tag{446}$$

Finally, we explicitly compute the integrals determining the Y_m functions,

$$Y_m(\lambda(\theta)) = \int_0^{2\pi} U_m(\lambda(\theta)\cos\phi)\frac{d\phi}{2\pi}, \tag{447}$$

which yields

$$Y_{m=even}(\lambda(\theta)) = \frac{1}{\pi}\sum_{l=0}^{\lfloor m/2 \rfloor} c_l(\theta)\frac{(m-2l-1)!!}{(m-2l)!!}, \tag{448}$$

where

$$c_l(\theta) = (-1)^l \binom{m-l}{l}(2\cos\theta)^{m-2l}. \tag{449}$$

A.5 Tutorial on Maximum Likelihood Estimation

There are two general methods of parameter estimation, least squares estimation and maximum likelihood estimation. Maximum likelihood estimation is a preferred method of parameter estimation in statistics and a basic tool for many statistical modeling techniques. The purpose of the master thesis is to provide a good conceptual understanding of the maximum likelihood method with some concrete examples. The principle of maximum likelihood estimation, originally devoloped by R.A. Fisher in the 1920s, states that the desired probability distribution is the one that makes the observed data "most likely", which means that one must seek the value of the parameter vector that maximizes the likelihood function L. The resulting parameter vector, which is sought by searching the multi dimensional parameter space, is called the maximum likelihood estimate. Maximum likelihood estimates need not exist nor be unique. The maximum likelihood estimates is obtained by maximizing the *log* likelihood function, lnL. This is because the two functions lnL and L are monotically related to each other so the same maximum likelihood estimate is obtained by maximizing either one. Assuming that the *log* of the likelihood function, lnL is differentiable if the maximum likelihood estimate exists, the following partial differential equation known as the likelihood estimation

$$\frac{\vartheta L\left(\theta^*\right)}{\vartheta \theta^*} = 0. \tag{450}$$

This is because the definition of maximum or minimum of a continuous differentiable function implies that its first derivatives vanish at such points. The likelihood equation represents a necessary condition for the existence of a maximum likelihood estimate. An additional condition must also be satisfied to ensure that lnL is maximum and not a minimum, since the first derivative cannot reveal this. To be a maximum the shape of the *log* likelihood function should be convex (it must represent a peak, not a valley) in the neighborhood of θ^*. This can be checked by calculating the second derivatives of the *log* of the likelihoods and showing whether they are all negative at θ^*, i.e.

$$\frac{\vartheta L\left(\theta^*/x_i\right)}{\vartheta \theta^2} < 0. \tag{451}$$

In practice, however it is usually not possible to obtain an analytic form solution for the maximum likelihood estimate, especially when the model involves many parameters and its probability density function is highly non linear. In such situations, the maximum likelihood estimate must be sought numerically using non linear optimization algorithms. The basic idea of non linear optimization is to quickly find optimal parameters that maximize the *log* likelihood. This is done by searching much smaller sub sets of the multi dimensional parameter space rather than exhaustively searching the whole parameter space which becomes intractable as the number of parameters increases.

This section is a small tutorial about maximum likelihood estimation method. We will explain what is a parameter estimation and we will focus on the method of maximum likelihood parameter estimation. Furthermore, we present some examples of the maximum likelihood estimation method, such that the reader understands how the method is applied.

A.6 Euclidean Group $ISO(2)$

The symmetry group of an 2−dimensional Euclidean space is the Euclidean group $E(2)$ or $ISO(2)$ [21]. It consists of two types of transformations, uniform translations $\left(\text{along a certain direction } \hat{b} \text{ by a distance } b\right)$ $T(b)$ and uniform rotations (around a unit vector $\hat{n}$ by some angle θ) $R_{\hat{n}}(\theta)$. We must notice that

$$[T(b), R_{\hat{n}}(\theta)] \neq 0. \tag{452}$$

Definition 54 *The Euclidean group $E(2)$ consists of all continuous linear transformations on the 2 dimensional Euclidean space $R(2)$ which leave the legnth of all vectors invariant.*

The points in $R(2)$ are characterized by their coordinates $\{x_1, x_2\}$. A two dimensional linear transformation $\underline{x} \longrightarrow \underline{x}'$ takes the form

$$\begin{array}{l} x_1' = R_{11}x_1 + R_{12}x_2 + b_1 \\ x_2' = R_{21}x_1 + R_{22}x_2 + b_2 \end{array}. \tag{453}$$

The Euclidean group in the two dimensional space $E(2)$ contains rotations and translations. Rotations are characterized by one angle θ and translations are specified by two parameters (b_1, b_2). The following two equations describe the transformation $\underline{x} \longrightarrow \underline{x}'$

$$\begin{array}{l} x_1' = R_{11}x_1 + R_{12}x_2 + b_1 \\ x_2' = R_{21}x_1 + R_{22}x_2 + b_2 \end{array}. \tag{454}$$

A group element that belongs to $E(2)$ is denoted as $g(\underline{b}, \theta)$. We derive the group multiplication rule of $E(2)$ as follows

$$g(\underline{b}_1, \theta_1)\, g(\underline{b}_2, \theta_2) = g(\underline{b}_3, \theta_3), \tag{455}$$

where

$$\theta_1 + \theta_2 = \theta_3, [R(\theta_2)\ \ \underline{b}_1] + \underline{b}_2 = \underline{b}_3. \tag{456}$$

The inverse element of $g\left(\underline{\mathrm{b}},\theta\right)$ is $g\left(-R\left(-\theta\right)\underline{\mathrm{b}},-\theta\right)$. The matrix representation of the $g\left(\underline{\mathrm{b}},\theta\right)$ is the following 3x3 matrix

$$g\left(\underline{\mathrm{b}},\theta\right)=\begin{pmatrix}\cos\theta & -\sin\theta & b_1\\ \sin\theta & \cos\theta & b_2\\ 0 & 0 & 1\end{pmatrix}. \tag{457}$$

The Euclidean group $E\left(2\right)$ has two subgroups. The group of rotations and the group of translations.

The group of rotations is the subset of elements $\left\{g\left(0,\theta\right)=R\left(\theta\right)\right\}$. The generator of this θ parameter subgroup is the matrix

$$J=\begin{pmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{pmatrix}. \tag{458}$$

A general element of the rotation subgroup is

$$R\left(\theta\right)=e^{-i\theta J}. \tag{459}$$

The second subset of the Euclidean group $E\left(2\right)$ is the subgroup of translations T_2 and it is formed from the subset of elements $\left\{g\left(\underline{\mathrm{b}},0\right)=T\left(\underline{\mathrm{b}}\right)\right\}$. The subgroup of translations has also two independent one parameter subgroups with generators

$$P_1=\begin{pmatrix}0 & 0 & i\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix} \text{ and } P_2=\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & i\\ 0 & 0 & 0\end{pmatrix}, \tag{460}$$

where

$$\left[P_1,P_2\right]=0. \tag{461}$$

A general translation can be expressed as

$$T\left(\underline{\mathrm{b}}\right)=e^{-i\underline{\mathrm{b}}\cdot\underline{\mathrm{P}}}=e^{-ib_1P_1}e^{-ib_2P_2}, \tag{462}$$

where $\underline{\mathrm{P}}$ is the momentum operator. Regarding all the above, the decomposition of an $E\left(2\right)$ element is

$$g\left(\underline{\mathrm{b}},\theta\right)=T\left(\underline{\mathrm{b}}\right)R\left(\theta\right). \tag{463}$$

The generators of the $E\left(2\right)$ group are J,P_1 and P_2. The interactions between them are described by the Lie Algebra of the group. The commutation relations are

$$\begin{gathered}\left[P_1,P_2\right]=0\\ \left[J,P_k\right]=i\varepsilon^{km}P_m, k=1,2\end{gathered}, \tag{464}$$

where ε^{km} is the 2 dimensional unit anti symmetric tensor.

The Euclidean group $E\left(2\right)$ sometimes called $ISO\left(2\right)$ is the symmetry group of the two dimensional Euclidean space. The elements of the group are the isometries associated with the Euclidean metric and are called Euclidean moves. The dimension of the $E(2)$ group is

$$\frac{n(n+1)}{2} \overset{n=2}{\equiv} 3. \tag{465}$$

Thus, $E(2)$ contains three Euclidean moves.

A.7 Adjoint Operator

The adjoint operator of a matrix A is defined as

$$AdA(X) = AXA^{\dagger}. \tag{466}$$

The adjoint operator of the product AB of two matrices A and B equals $Ad(AB)(X) = (AdA)(AdB)(X)$, also the power k of adjoint operator of A equals $Ad^{k}(A)(X) = AdA^{k}(X)$.

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