Czech Technical University in Prague
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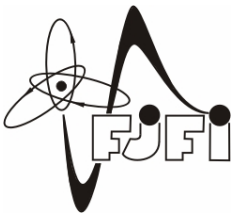

Quantum walks of interacting particles

Kvantové procházky interagujících částic

by

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Thesis submitted to
the Faculty of Nuclear Sciences and Physical Engineering of
Czech Technical University in Prague
in partial fulfillment of the requirements
for the degree of

Bachelor of Science

in the branch of study Mathematical Physics
of the study program Mathematical Engineering

Prague, 2013

Acknowledgement

Foremost, I would like to express my sincere gratitude to Ing. Martin Štefaňák, Ph.D. for his kind guidance, support, motivation and extensive knowledge. I found his insightful comments and intelligible profound answers to my numerous questions most helpful.
My sincere thanks goes also to professor Reinhard F. Werner for permitting me to use part of his work and providing me with the original graphical files.
Last but not least, I would like to thank my family for their endless support during my studies.

Oskar Löw

Declaration

I declare that I wrote my bachelor's thesis independently, and that I used only the sources (literature, projects, *etc.*) acknowledged in the Bibliography.

Prohlášení

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V Praze dne 3.7.2013

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Název práce:
Kvantové procházky interagujících částic

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Obor: Matematické inženýrství
Druh práce: Bakalářská práce

Vedoucí práce: Ing. Martin Štefaňák, Ph.D.
Katedra Fyziky, Fakulta jaderná a fyzikálně inženýrská,
České vysoké učení technické v Praze
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Abstrakt: V první části práce shrneme analytické metody používané ke zkoumání kvantových procházek. Pro objasnění těchto metod je používáme na jednoduchých procházkách v malých dimenzích. V další části tyto metody a získané výsledky použijeme ke studiu kvantových procházek s interagujícími částicemi.
Soustředíme se na bodové interakce, které jsou způsobeny jednodimenzionální perturbací evolučního operátoru. Numericky určíme jeho spektrum a na základě srovnání s procházkou bez interakce najdeme známky toho, že vznikají vázané stavy. Na závěr se zabýváme vlastnostmi těchto stavů. Především zjistíme, že se chovají jako molekuly konající kvantovou procházku a najdeme jejich maximální grupovou rychlost.

Klíčová slova: kvantové procházky, interakce částic, metoda momentů, vázaný stav

Title:
Quantum walks of interacting particles

Author: Oskar Löw

Abstract: In the first part we overview the analytical methods used to study quantum walks. These methods are shown on simple low-dimensional walks for better understanding. In the next part the methods and obtained results are used to study quantum walks of interacting particles.
We focus on point interactions, which are caused by one-dimensional perturbation of the evolution operator. We numerically determine the spectrum of the perturbed operator, and by comparison with the free walk, we find signs of bounded states formation. Finally, we discuss the properties and behaviour of these states – most importantly we find out that they behave as molecules undergoing a quantum walk, and determine their maximum group velocity.

Key words: Quantum walks, interacting particles, moments method, bounded state

Contents

Introduction

Despite many doubts at the beginning, caused by its counter-intuitive nature, quantum mechanics made it way into many scientific fields and brought us new exciting discoveries and possibilities. In a way it has even put the world into a completely different perspective.

Although QM is studied intensively, there are still many of its aspects yet to be discovered. One of the latest fruitful axis of research are Quantum walks – a model first introduced by Aharonov, *et al.* [1] in early nineties. They are promising generalization of random walks — a widely-spread mathematical model with applications in Physics, Computer Science, Biology and many others.

Quantum walk is a unitary, both continuous and discrete, time evolution of a quantum particle on a discrete lattice (useful introductory survey can be found in [8]). Due to the effect of superposition and interference, it can spread significantly faster than the classical one. Furthermore, thanks to the effect of quantum entanglement it shows properties that cannot be observed in the classical case. This may provide radical speed-up over the classical algorithms (even exponential for some black boxes — for example see [6]), when used for quantum computation. (For comprehensive introduction to the main ideas of quantum computation see [14].)

In this thesis we overview some of the methods used for analysing quantum walks and use them to study quantum walks of two interacting particles on a line. Interacting quantum walks can play a crucial role for future development of universal quantum computation [5] and quantum systems simulations. Bounded states are important part of nature, and quantum walks with on-site interactions may help us understand the formation and dynamics of them (especially quasi-particles and collective excitations).

The thesis has the following layout. Although we expect some rudimentary knowledge of quantum mechanics from the reader, we provide an overview of basic quantum mechanics principals and effects in the first chapter.

In the second one we show some of the analytic method on elementary one-dimensional quantum walk with Hadamard coin and its continuously perturbed version. The third chapter offers a straightforward generalization of these methods onto two-dimensional quantum walk, which will be useful in the fourth and final chapter, where we introduce the point interaction and find signatures of molecular binding by numerical determination of the spectrum of the evolution operator.

Chapter 1

Introduction to Quantum theory

In this chapter we briefly review few topics of quantum mechanics. It cannot be in any way considered a comprehensive, general text on quantum theory. We include this chapter merely to clarify the notation used further on, for deeper understanding we recommend [4]. Mathematical issues, concepts and definitions are further discussed in appendix A.

1.1 Dirac formalism

During the time a formalism introduced in 1939 by Paul Dirac has proved to be very convenient and has spread world-wide. Based on the word bracket it is often called Bra-Ket formalism — a connection soon to be understood.

Bra and Ket vectors

Crucial role in formulation of quantum mechanics plays the well-known Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi\,, \tag{1.1}$$

which directs the time evolution of the system. In classical mechanics the state of a particle is fully determined by a point in the phase-space. However, this deterministic approach does not work for quantum mechanics. Instead of it a Hilbert space ($\mathcal{H}$) is assigned to each quantum system and each state is represented by a vector from this space (more precisely a 1D subspace as any multiplication by a complex number does not change the physics). Any linear combination of vectors from the said Hilbert space is also its element and represents a physical state of the system. This formulation is possible due to the linearity of (1.1). We usually choose a suitable basis depending on the problem we want to describe and then every vector can be written as a linear combination of the basis ones ($\{\psi_i\}_{i=1}^N$):

$$\varphi = \sum_{i=1}^{N} a_i\psi_i\,; \quad a_i \in \mathbb{C}\,, \operatorname{Dim}\mathcal{H} = N \tag{1.2}$$

In the case of infinite dimension of $\mathcal{H}$ the sum becomes infinite series.
The notation for vectors from the Hilbert space is $|\psi\rangle$. They are called *Ket* vectors. Different values, which describes the state (for example quantum number[s]), are often used in the Bra-Ket notation instead of ψ.

Important for the formalism is the dual space ($\mathcal{H}^*$) — the space of linear functionals on $\mathcal{H}$, which map $\mathcal{H}$ to $\mathbb{C}$. They are called *Bra* vectors and are denoted $\langle\psi|$.

Inner product

Inner product (denoted: (x,y)) is a structure added to a space allowing rigorous introduction of angles between two vectors and orthogonality (for its axioms see appendix A). It can also induce one of the possible norms.
By the Riesz's theorem every linear functional can be defined by the inner product. Thanks to this we can use very advantageously the bra-ket notation: $\langle\psi|\varphi\rangle$. This inner product induces a norm defined as:

$$\|\psi\|^2 = \langle\psi|\psi\rangle \tag{1.3}$$

Further on we will always use normalized vectors ($\|\psi\| = 1$) if not said otherwise. We call two vector orthogonal if and only if their inner product is zero. We often work with so called orthonormal basis, that means a basis $\{\psi_i\}_{i=1}^N$, for which the following formula is valid:

$$\forall i,j \in \widehat{N};\ \langle\psi_i|\psi_j\rangle = \delta_{ij} \tag{1.4}$$

Let us now consider $M \subseteq \mathcal{H}$, we will denote M with all possible linear combinations Span(M) and call it the linear span of M. The set of all vectors from $\mathcal{H}$ orthogonal to every element of M is called orthogonal complement and is denoted $M^\perp$. Notice that $M^{\perp^\perp} = \text{Span}(M)$. Every vector $|\psi\rangle \in \mathcal{H}$ can be decomposed as:

$$|\psi\rangle = |\psi_M\rangle + |\psi_M^\perp\rangle \tag{1.5}$$

Where $|\psi_M\rangle \in \text{Span}(M)$ and $|\psi_M^\perp\rangle \in M^\perp$. These vectors are called orthogonal projections to the according subspace.

Tensor product

To describe a system composed of several known subsystems, we introduce a tensor product (for mathematical definition see appendix A). Let us consider two systems and their corresponding Hilbert spaces $\mathcal{H}^{(1)}$, $\mathcal{H}^{(2)}$. Then the Hilbert space of the composite system is the tensor product $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$. Let $\{|i\rangle\}_{i=1}^n$ and $\{|j\rangle\}_{j=1}^m$ be the basis of $\mathcal{H}^{(1)}$, $\mathcal{H}^{(2)}$, then we can construct the basis of $\mathcal{H}$ as $\{|i\rangle \otimes |j\rangle\}_{i,j=1}^{n,m}$ (often notation $|i\rangle \otimes |j\rangle \equiv |i\rangle|j\rangle$ is used). The most general state is of the form:

$$|\psi\rangle_{12} = \sum_{i,j=1} c_{ij}|i\rangle|j\rangle \tag{1.6}$$

If $c_{ij} = c_i^{(1)} c_j^{(2)}$, the state is called *separable* and can be written as:

$$|\psi\rangle_{12} = \left(\sum_i c_i^{(1)}|i\rangle\right)\left(\sum_{j=1} c_j^{(2)}|j\rangle\right).$$

Denoting $|\psi\rangle^{(1)} = \sum_i c_i^{(1)}|i\rangle \in \mathcal{H}^{(1)}$ and $|\psi\rangle^{(2)} = \sum_j c_j^{(2)}|j\rangle \in \mathcal{H}^{(2)}$ we see that a separable state is the tensor product of states of the subsystems.

If $c_{ij} \neq c_i^{(1)} c_j^{(2)}$, the state is inseparable and is called *entangled*. Entangled states, among others, have many application in quantum information theory. Of a special interest are the so called *Bell states*, which are the maximally entangled (in the sense of entropy) states of two qubits (quantum bits).
It is straightforward to generalize the concept of tensor product with all its properties to a system composed of multiple subsystems. The Hilbert space is then $\mathcal{H} = \bigotimes_{i=1}^{n} \mathcal{H}^{(i)}$.

1.2 Observables

In classical physics the observable physical quantities are represented by a function on the phase-space and their values are fully determined by a point in that space. Quantum mechanics is, on the other hand, essentially probabilistic.
Observable is a measurable operator or gauge, by which a property of the system is determined. In this section we will describe its mathematical formulation and discuss some of the properties and effects yielding from it.

Linear Operators

Linear operator is a linear map from the Hilbert space to itself. In the Dirac formalism the following simple notation is used: $A|\psi\rangle$. Here A is the operator and $|\psi\rangle$ is a vector from the Hilbert space. An operator acts on the bra vector as: $A(\langle\psi|) = \langle\psi|A$. This allows us to use a convenient notation $\langle\psi|A|\varphi\rangle$.
Using the inner product and Riesz's lemma, we can define a unique continuous operator with following properties:

$$(y, Ax) = \left(A^\dagger y, x\right); \quad \forall x, y \in \mathcal{H} \tag{1.7}$$

We call this operator *adjoint* to A. A densely defined operator that equals to its adjoint one (*i.e.* it is symmetric) is called a self-adjoint operator and will play a crucial role in the mathematical description of observables. Bounded operator for which $A = A^\dagger$ stands true is called a *Hermitian operator*. Note that for bounded operators the terms hermitian and self-adjoint are equivalent and are used interchangeably. The spectrum of a hermitian operator is real.
Another important set of operators are the unitary ones. An operator is *unitary* if and only if both the domain and the rank of the operator are the whole space and it preserves the norm. An equivalent definition is that it is an everywhere defined bounded operator for which $U^{-1} = U^\dagger$.
Often used in quantum mechanics are so called *projectors*, which are hermitian operator for which $P^2 = P$. It projects the vectors to a subspace of $\mathcal{H}$ (more specifically to the rank of the projector). For every vector we can construct a projector that maps to the subspace generated by the vector. It is of the form $P_\psi = |\psi\rangle\langle\psi|$.

Mathematical representation of observables

In quantum mechanics to each observable (*e.g.* position, energy, angular momentum, spin, *etc.*) a self-adjoint operator on the Hilbert space of the system is assigned. The only values that can be measured are the ones from the spectrum of the operator. During the measurement the wavefunction of the system collapses into one of the eigenstates of the operator of the measured observable.

Throughout the thesis the Copenhagen interpretation is used. It states that the description of nature given by QM is essentially probabilistic, and that the wafefunction is the amplitude of probability, while the probability itself is given by its squared magnitude.
For the sake of simplicity let us assume that the operator has only point spectrum with eigenvalues a_i and corresponding eigenvectors $|a_i\rangle$. Then, assuming that the vectors are normalized, the probability of measuring a given value of the observable is:

$$P_{A=a_i} = |\langle\psi|a_i\rangle|^2 \tag{1.8}$$

It works for the continuous spectrum as well, but there are some mathematical technicalities, which we will omit here, as they are not necessary for the understanding of the topics discussed further in the thesis.
Now that we have established what the probability looks like, we can introduce the *expectation value* of the observable. We make use of the classical definition of expected value (see appendix A) and the quantum mechanical probability as well as the eigendecomposition of the operator.

$$\langle A\rangle_\psi = \sum_{i=1} a_i|\langle\psi|a_i\rangle|^2 = \sum_{i=1}\langle\psi|a_i\rangle a_i\langle a_i|\psi\rangle = \langle\psi|\left(\sum_{i=1}|a_i\rangle a_i\langle a_i|\right)|\psi\rangle = \langle\psi|A|\psi\rangle \tag{1.9}$$

It is important for the probabilistic interpretation that the wafefunction is properly normalized and that this normalization does not change with time. Fortunately it was shown that for a closed system the time evolution is unitary and thus does not change the norm.
We often encounter a situation in which the system is composed of several subsystems. We have dealt with this problem in section 1.1. We will now describe how the observables are treated. Let us consider a Hilbert space $\mathcal{H} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$. Linear operator $A^{(1)}$ defined on the space $\mathcal{H}^{(1)}$ does not act on the other one. Hence, we extend the operator to the whole space $\mathcal{H}$ as $A^{(1)} \otimes I$, where I is the identical operator. It is worth noting that the operators defined on different subsystems thus commute.

Chapter 2

One-dimensional Quantum walk

2.1 Quantum walk and its mathematical formulation

A simple description of a classical random walk (for comprehensive introduction we recommend [12]) on a line is a particle tossing a fair coin before each step. According to the result of the tossing it goes either to the right or to the left.
In the case of quantum walk on line this idea is generalized to a quantum particle, with added degree of freedom called simply *coin*. The coin takes two values – right and left ($|L\rangle$, $|R\rangle$) and determines the motion of the particle. Thanks to this added chirality we use a two-component wavefunction to describe the particle. The dynamics of the walk is then following – before each step the coin undergoes a unitary transformation and then the particle moves accordingly. The main distinction between classical and quantum walk is that in the quantum one every path is not assigned a probability but merely an amplitude of probability. This results in interference of different paths. In addition the particle may be in the superposition of the states of the coin.
We will now describe the walk using the notation and concepts from previous chapter. The Hilbert space of the walk consists of the position and the coin space as follows

$$\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_c$$

Here $\mathcal{H}_p = Span\{|m\rangle, m \in \mathbb{Z}\}$ is the position space and $\mathcal{H}_c = Span\{|L\rangle, |R\rangle\}$ is the coin one. The walk is driven by the single step unitary operator

$$U = S(I \otimes C) = \left(\sum_{m=-\infty}^{m=+\infty} |m-1\rangle\langle m| \otimes |L\rangle\langle L| + |m+1\rangle\langle m| \otimes |R\rangle\langle R| \right)(I \otimes C) \tag{2.1}$$

where C denotes the unitary coin operator. Let $\psi(m,t) = \begin{pmatrix} \psi_L(m,t) \\ \psi_R(m,t) \end{pmatrix}$ be the vector of amplitudes of probability of the particle being at the point m after t steps with the coin having the left (upper component) or the right (lower component) value. Suppose that a particle begins its walk from the origin with the coin state being $|\psi_C\rangle = \psi_L|L\rangle + \psi_R|R\rangle$. Thus the initial state is $|\psi(0)\rangle = |O\rangle \otimes |\psi_C\rangle$. By successive application of the unitary operator U we obtain the state of the particle after t steps, that means

$$|\psi(t)\rangle = U^t|\psi(0)\rangle = \sum_m \psi_L(m,t)|m\rangle|L\rangle + \psi_R(m,t)|m\rangle|R\rangle.$$

We see that the walk is fully deterministic. On the other hand, the position is a random variable with the probability of finding a particle at the point m after t steps being

$$p(m,t) = |\psi_L(m,t)|^2 + |\psi_R(m,t)|^2,$$

yielding following condition for the initial state of the coin

$$|\psi_L|^2 + |\psi_R|^2 = 1\,.$$

2.2 Fourier analysis

As the above described walk is translation invariant, Fourier transformation to momentum picture is a powerful method often used to analyse it. We introduce it on the so called *Hadamard walk* - a walk for which Hadamard operator is chosen to perform the unitary transformation of the coin. In our particular case of quantum walk on line it is given by

$$C_H = \frac{1}{\sqrt{2}}(|L\rangle\langle L| + |L\rangle\langle R| + |R\rangle\langle L| - |R\rangle\langle R|) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

The function $\psi(m,t)$ is a complex valued function over the integers and so its Fourier transform ($\widetilde{\psi}(k,t) : (-\pi,\pi)\times\mathbb{Z} \longmapsto \mathbb{C}^2$) is defined as

$$\widetilde{\psi}(k,t) = \sum_m \psi(m,t)e^{ikm} \tag{2.2}$$

Before proceeding any further we examine the dynamics of each component of the vector ψ using the previously defined step operator:

$$\psi_L(m,t+1) = \frac{1}{\sqrt{2}}\psi_L(m+1,t) + \frac{1}{\sqrt{2}}\psi_R(m+1,t) \tag{2.3}$$

$$\psi_R(m,t+1) = \frac{1}{\sqrt{2}}\psi_L(m-1,t) - \frac{1}{\sqrt{2}}\psi_R(m-1,t) \tag{2.4}$$

Denoting $M^+ = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ 0 & 0\end{pmatrix}$, $M^- = \begin{pmatrix}0 & 0\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix}$ and using (2.2), (2.3) and (2.4), we obtain the following for $\widetilde{\psi}$

$$\begin{aligned}\widetilde{\psi}(k,t+1) &= \sum_m (M^+\psi(m+1,t) + M^-\psi(m-1,t))e^{ikm}\\ &= M^+e^{-ik}\sum_m \psi(m+1,t)e^{ik(m+1)} + M^-e^{ik}\sum_m \psi(m-1,t)e^{ik(m+1)}\\ &= (M^+e^{-ik} + M^-e^{ik})\widetilde{\psi}(k,t)\,.\end{aligned}$$

We have obtained a recurrence

$$\widetilde{\psi}(k,t+1) = \widetilde{U}(k)\widetilde{\psi}(k,t), \tag{2.5}$$

where

$$\widetilde{U}(k) = Diag\left(e^{-ik}, e^{ik}\right)C_H\,. \tag{2.6}$$

Note that as both the diagonal and the Hadamard matrices are unitary the $\widetilde{U}(k)$ operator is also unitary and the dynamics can be rewritten as $\widetilde{\psi}(k,t) = \widetilde{U}^t(k)\widetilde{\psi}(k,0)$. $\widetilde{U}^t(k)$ can be easily calculated by diagonalising $\widetilde{U}(k)$, this is readily done by finding its eigensystem. Let us assume that $\widetilde{U}(k)$ has eigenvalues $\alpha_k^{(1)}$, $\alpha_k^{(2)}$ and corresponding eigenvectors $\Theta_k^{(1)}$, $\Theta_k^{(2)}$. Then using the eigendecomposition we can write:

$$\widetilde{U}(k) = \alpha_k^{(1)}|\Theta_k^{(1)}\rangle\langle\Theta_k^{(1)}| + \alpha_k^{(2)}|\Theta_k^{(2)}\rangle\langle\Theta_k^{(2)}|.$$

It is now straightforward to show that the time evolution matrix is:

$$\widetilde{U}^t(k) = (\alpha_k^{(1)})^t |\Theta_k^{(1)}\rangle\langle\Theta_k^{(1)}| + (\alpha_k^{(2)})^t |\Theta_k^{(2)}\rangle\langle\Theta_k^{(2)}|.$$

The Fourier transform we are looking for is then

$$\widetilde{\psi}(k,t) = (\alpha_k^{(1)})^t \langle\Theta_k^{(1)}|\widetilde{\psi}(k,0)\rangle|\Theta_k^{(1)}\rangle + (\alpha_k^{(2)})^t \langle\Theta_k^{(2)}|\widetilde{\psi}(k,0)\rangle|\Theta_k^{(2)}\rangle, \tag{2.7}$$

and at the end we return to the initial basis using the inverse Fourier transformation:

$$\psi(m,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \widetilde{\psi}(k,t)e^{-ikm}dk$$

We do not calculate specifically the eigensystem and the wavefunction here because it will be done for a perturbed Hadamard matrix in the next section. We acknowledge that these results were already obtained by Ashwin Nayak, *et al.* (presented in [3]).

2.3 Moments method and asymptotic behaviour

We will now use the weak theorems, introduced by Grimmett,*et al.* [7] and further developed by Konno,*et al.* [17] to calculate the probability distribution of the particles position for large number of steps. We demonstrate the method on a quantum walk on a line with continuously perturbed Hadamard coin operator. The step operator will be the same as in (2.1), except that the coin will be transformed by the continuously perturbed Hadamard matrix

$$C_{Hp} = \begin{pmatrix} \rho & \sqrt{1-\rho^2} \\ \sqrt{1-\rho^2} & -\rho \end{pmatrix}; \quad \rho \in (0,1).$$

First we will perform the Fourier analysis as shown in the previous section. According to the formula (2.6) the Fourier transform of the evolution operator is

$$\widetilde{U}(k) = Diag\left(e^{-ik}, e^{ik}\right) C_{Hp}. \tag{2.8}$$

We observe that the evolution operator gives a momentum kick $+k$ with probability ρ^2 and $-k$ with probability $1-\rho^2$ to the first component. The opposite states true for the second one. We can thus conclude that the walk is biased except for the Hadamard case ($\rho = \frac{1}{\sqrt{2}}$).

The second step is to find its eigensystem. The eigenvalues are $\lambda_2 = e^{i(\omega_k+\pi)} = -e^{i\omega_k}$, $\lambda_1 = e^{-i\omega_k}$, where ω_k satisfies the *dispersion relation* (we use the wave approach, see [9])

$$\sin\omega_k = \rho\sin k. \tag{2.9}$$

The corresponding eigenvectors for λ_1 and λ_2 are respectively

$$\Phi_1 = \frac{1}{\sqrt{1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k}-\rho\cos k\right)^2}}\begin{pmatrix}\sqrt{1-\rho^2}e^{-ik} \\ e^{-i\omega_k}-\rho e^{-ik}\end{pmatrix}$$

$$\Phi_2 = \frac{1}{\sqrt{1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k}+\rho\cos k\right)^2}}\begin{pmatrix}\sqrt{1-\rho^2}e^{-ik} \\ -e^{i\omega_k}-\rho e^{-ik}\end{pmatrix}.$$

Denoting the normalization N_1 and N_2 and using the dispersion relation they can be rewritten in the terms of the wavenumber k only:

$$\begin{aligned}\Phi_1 &= N_1\begin{pmatrix}\sqrt{1-\rho^2}e^{-ik}\\ \sqrt{1-\rho^2\sin^2 k}-\rho\cos k\end{pmatrix}\\ \Phi_2 &= N_2\begin{pmatrix}\sqrt{1-\rho^2}e^{-ik}\\ -\sqrt{1-\rho^2\sin^2 k}-\rho\cos k\end{pmatrix}.\end{aligned} \tag{2.10}$$

We are now ready to calculate the moments of the particle's position. The easiest way to do so is again to express them in the Fourier picture:

$$\langle x^n\rangle = \langle\psi(t)|X^n|\psi(t)\rangle = \langle\widetilde{\psi}(t)|FX^nF^\dagger|\widetilde{\psi}(t)\rangle = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\widetilde{\psi}^\dagger(k,t)\left(i\frac{d}{dk}\right)^n\widetilde{\psi}(k,t) \tag{2.11}$$

Here the function

$$\widetilde{\psi}(k,t) = \widetilde{U}^t(k)\psi_C \tag{2.12}$$

is the state in the momentum representation, provided that the initial state is $\psi_C = (\psi_L,\psi_R)^T$. Following (2.7) the solution of the above mentioned time-evolution equation reads

$$\widetilde{\psi}(k,t) = e^{-i\omega_k t}f_1(k)v_1(k) + (-1)^t e^{i\omega_k t}f_2(k)v_2(k), \quad f_j = (v_j(k),\psi_C)$$

To calculate the integrand of (2.11) we differentiate the above relation n times with respect to k using the general Leibniz rule[1]. We obtain the following expression

$$\left(i\frac{d}{dk}\right)\widetilde{\psi}(k,t) = t^n\left(\frac{d\omega}{dk}\right)^n e^{-i\omega_k t}f_1(k)v_1(k) + (-1)^{n+t}t^n\left(\frac{d\omega}{dk}\right)^n e^{i\omega_k t}f_2(k)v_2(k) + O(t^{n-1}),$$

where $O(t^{n-1})$ are the terms that come from lower derivations of $e^{\pm i\omega_k t}$, and which are of a degree $m \le n-1$. As the eigenvectors are orthonormal and the exponents sum up to zero, the integrand takes up the form

$$\widetilde{\psi}^\dagger(k,t)\left(i\frac{d}{dk}\right)^n\widetilde{\psi}(k,t) = t^n\left(\frac{d\omega}{dk}\right)^n|f_1|^2 + (-1)^n t^n\left(\frac{d\omega}{dk}\right)^n|f_2|^2 + O(t^{n-1})$$

At this point we introduce the *pseudo-velocity* defined as $\frac{x}{t}$. The moments of the pseudo-velocity are then

$$\left\langle\left(\frac{x}{t}\right)^n\right\rangle = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\left(\frac{d\omega}{dk}\right)^n(|f_1|^2 + (-1)^n|f_2|^2) + O(t^{-1})$$

We change the integration variable to a new one — *the group velocity* — defined subsequently

$$v = \frac{d\omega}{dk} = \frac{\rho\cos k}{\sqrt{1-\rho^2\sin^2 k}}, \text{ yeilding } dk = \frac{\sqrt{1-\rho^2}}{\rho}\frac{dv}{(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}}$$

It can be easily observed that the group velocity reaches its maximum (minimum) value ρ (-ρ) in $2k\pi$ ($(2k+1)\pi$) and that it is an even function. We calculate the long-time limit

[1] The general Leibniz rule is the generalization of the product rule for differentiating and states:

$$(f\cdot g)^n = \sum_{k=0}^{n}\binom{n}{k}f^k g^{n-k}$$

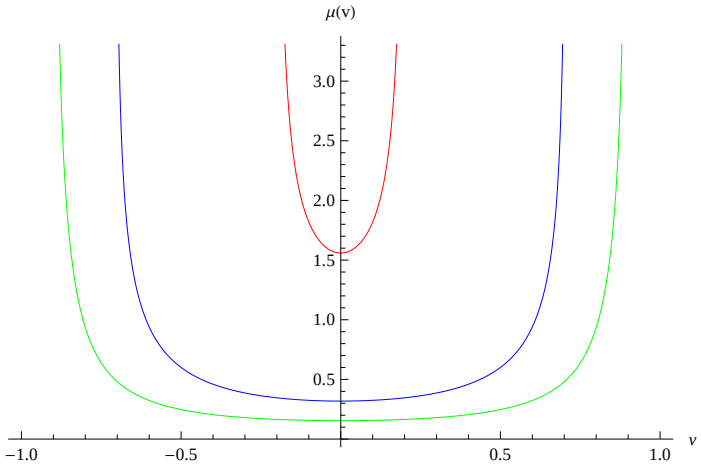


Figure 2.1: Dependence of the fundamental density on the choice of the coin for $\rho = \frac{1}{10}$ (red), $\rho = \frac{1}{\sqrt{2}}$ (blue) and $\rho = \frac{9}{10}$(green)

of the moments separately for odd and even ones.
For even moments we obtain

$$\lim_{t\to+\infty}\left\langle\left(\frac{x}{t}\right)^{2n}\right\rangle = 2\int_{-\rho}^{\rho} v^{2n}\frac{\sqrt{1-\rho^2}}{\rho}\frac{dv}{2\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}},$$

and for the odd ones we conclude that

$$\lim_{t\to+\infty}\left\langle\left(\frac{x}{t}\right)^{2n+1}\right\rangle = -2\int_{-\rho}^{\rho} v^{2n+1}\frac{\sqrt{1-\rho^2}}{\rho}\frac{[|\psi_L|^2-|\psi_R|^2+\frac{\sqrt{1-\rho^2}}{\rho}(\psi_L\bar{\psi}_R+\psi_R\bar{\psi}_L)]v\,dv}{2\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}}.$$

As we integrate even function over symmetric interval we can join these two results into single integral

$$\lim_{t\to+\infty}\left\langle\left(\frac{x}{t}\right)^{n}\right\rangle = \int_{-\rho}^{\rho} v^{n}\frac{\sqrt{1-\rho^2}}{\rho}\frac{1-[|\psi_L|^2-|\psi_R|^2+\frac{\sqrt{1-\rho^2}}{\rho}(\psi_L\bar{\psi}_R+\psi_R\bar{\psi}_L)]v}{\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}}dv,$$

and by the method of moment find that the group velocity density is

$$w_{\psi_C}(v) = \frac{\sqrt{1-\rho^2}}{\rho}\frac{1-[|\psi_L|^2-|\psi_R|^2+\frac{\sqrt{1-\rho^2}}{\rho}(\psi_L\bar{\psi}_R+\psi_R\bar{\psi}_L)]v}{\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}}. \tag{2.13}$$

This result for the Hadamard walk was obtained by Konno [10], [11] using different methods. For better understanding we can divide the result (2.13) into to two terms. First will be the density determined by the coin operator (for illustration of this dependence see Figure 2.1), which is called *fundamental*:

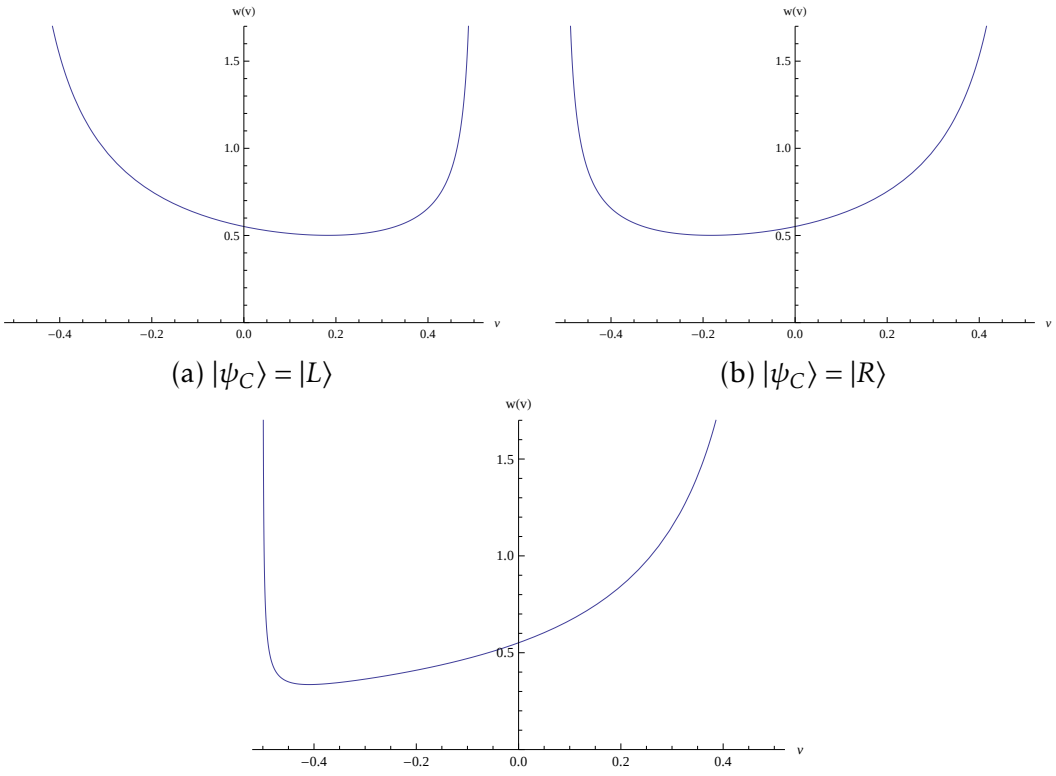
$$\mu = \frac{\sqrt{1-\rho^2}}{\rho}\frac{dv}{\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}}. \tag{2.14}$$

The second one is the *weight function* which express the dependence on the initial state, and which is of the following form

$$M = 1 - [|\psi_L|^2 - |\psi_R|^2 + \frac{\sqrt{1-\rho^2}}{\rho}(\psi_L\bar{\psi_R} + \psi_R\bar{\psi_L})]v\,. \tag{2.15}$$

We can use the group velocity density to evaluate any desired moment of the particle pseudo-velocity in the limit $t \to +\infty$. To illustrate the influence of the initial state on the propagation of the walk we plot the density for the initial states $|\psi_C\rangle = |L\rangle$, $|R\rangle$, $\frac{1}{\sqrt{2}}|L\rangle - \frac{1}{\sqrt{2}}|R\rangle$ in Figure 2.2

This approach can be used, in principle, for every transitionally invariant quantum walk. Unfortunately the dispersion relations are problematic to find for most of the coin operators (especially those with more than two states). Furthermore, even if we know the dispersion relations and group velocities, it is often laborious to find the weight function, which is then very complex and thus not very suitable for further use.



(a) $|\psi_C\rangle = |L\rangle$ (b) $|\psi_C\rangle = |R\rangle$

(c) $|\psi_C\rangle = \frac{1}{\sqrt{2}}|L\rangle - \frac{1}{\sqrt{2}}|R\rangle$

Figure 2.2: Dependence of the group velocity density on the initial state (for $\rho = \frac{1}{2}$)

2.4 Eigenvectors of the coin operator

We observe that the weight function (2.15) is rather complicated. The aim of this section is to express it in a different basis in which the formula has a simpler form, so that the analysis of the influence of the initial state becomes more intuitive. (We follow the idea used in [16].) It is reasonable to assume that the suitable basis will be the one constructed from the eigenvectors of the coin operator. The eigenvectors are

$$|\kappa^+\rangle = \frac{\sqrt{2}}{2}\begin{pmatrix}\sqrt{1+\rho}\\ \sqrt{1-\rho}\end{pmatrix}, \quad |\kappa^-\rangle = \frac{\sqrt{2}}{2}\begin{pmatrix}\sqrt{1+\rho}\\ -\sqrt{1-\rho}\end{pmatrix}.$$

Let us assume that the initial state is $|\psi_C\rangle = h^+|\kappa^+\rangle + h^-|\kappa^-\rangle$. We construct a matrix P with the eigenvectors being the columns. We now express $|\psi_C\rangle$ in the standard basis by left-multiplying it by P

$$P|\psi_C\rangle = \frac{\sqrt{2}}{2}\begin{pmatrix}\sqrt{1+\rho} & \sqrt{1-\rho}\\ \sqrt{1-\rho} & -\sqrt{1+\rho}\end{pmatrix}\begin{pmatrix}h^+\\ h^-\end{pmatrix} = \frac{\sqrt{2}}{2}\begin{pmatrix}h^+\sqrt{1+\rho}+h^-\sqrt{1-\rho}\\ h^+\sqrt{1-\rho}-h^-\sqrt{1+\rho}\end{pmatrix}.$$

The initial state in the standard basis was $|\psi_C\rangle = \psi_L|L\rangle + \psi_R|R\rangle$ and so we can conclude that:

$$\begin{aligned}\psi_L &= \frac{\sqrt{2}}{2}(h^+\sqrt{1+\rho}+h^-\sqrt{1-\rho})\\ \psi_R &= \frac{\sqrt{2}}{2}(h^+\sqrt{1-\rho}-h^-\sqrt{1+\rho})\end{aligned} \tag{2.16}$$

Substituting ψ_L, ψ_R according to (2.16) and using the fact that $|h^+|^2 + |h^-|^2 = 1$, which stems from the probability interpretation, we obtain the weight function in the new basis

$$M(v) = 1 - \frac{1}{\rho}(2|h^+|^2 - 1)v$$

We thus have the following formula for the group velocity density

$$w_{\psi_C}(v) = \frac{\sqrt{1-\rho^2}}{\rho}\frac{1-\frac{1}{\rho}(2|h^+|^2-1)v}{\pi(1-v^2)\sqrt{1-\frac{v^2}{\rho^2}}} \tag{2.17}$$

We can now easily reveal the influence of the initial state. The density diverges for $v = \pm\rho$ where ρ is also the maximum magnitude of the velocity. This is corresponding to the two peaks on both sides of the distribution with few exceptions discussed below (for illustration see Figure 2.1 and 2.2). The maximum velocity is the one of the peaks of probability distribution of the walk. We can also easily see that the right peak vanishes for $|\psi_C\rangle = |\kappa^+\rangle$ as the numerator goes to zero quicker then the denominator for $v \to \rho$(we plot this particular case in Figure 2.3). It is worth noting that the situation is exactly the mirror one for $|\psi_C\rangle = |\kappa^-\rangle$ – meaning that the left peak vanishes.

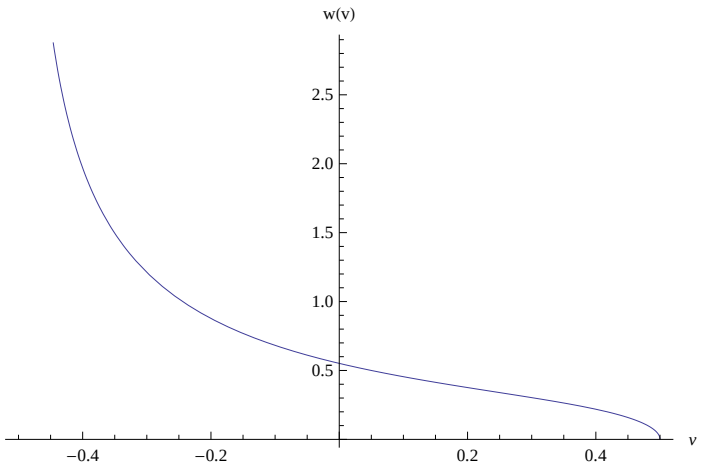


Figure 2.3: The group velocity density for a walk with initial state being the eigenvector $|\kappa^+\rangle$

Chapter 3

Two-dimensional Quantum walk

In this chapter we will use the methods shown in the previous one to analyse a quantum walk on an infinite square lattice. A two-dimensional walk has more interesting topology that has proved to be more suitable than the rather simple one of the walk on a line for many applications.
In addition if the walk is tensor product of two one-dimensional walks it is isomorphic to a walk of two particles on a line. This will be most useful for the description of the walks with interacting particles, at which we are aiming. Furthermore, the entanglement of the two particles provides huge advantage over the classical walk for many applications.

3.1 Mathematical formulation

We choose the walk as the tensor product of two walks on a line described in previous chapter. The Hilbert space is then

$$\mathcal{H}_2 = \mathcal{H}_1 \otimes \mathcal{H}_1\,; \qquad \mathcal{H}_1 = Span(|m\rangle;\, m \in \mathbb{Z}) \otimes Span(|L\rangle,\, |R\rangle).$$

We can also rewrite the Hilbert space as

$$\mathcal{H}_2 = Span(|m,n\rangle;\, m,n \in \mathbb{Z}) \otimes Span(|LL\rangle,\, |LR\rangle,\, |RL\rangle,\, |RR\rangle).$$

We will use the unitary step operator (2.1) (U_1) to construct the operator for our two-dimensional walk:

$$U_2 = U_1 \otimes U_1 = S_1 \otimes S_1[I \otimes (C(\rho) \otimes C(\rho))], \tag{3.1}$$

where

$$\begin{aligned} S_1 \otimes S_1 = \sum_{m,n=-\infty}^{\infty} & |m-1,n-1\rangle\langle m,n| \otimes |LL\rangle\langle LL| + |m-1,n+1\rangle\langle m,n| \otimes |LR\rangle\langle LR| + \\ & + |m+1,n-1\rangle\langle m,n| \otimes |RL\rangle\langle RL| + |m+1,n+1\rangle\langle m,n| \otimes |RR\rangle\langle RR|. \end{aligned}$$

Following the rules for tensor product of matrices, the coin operator is

$$\begin{aligned} C_2(\rho) = C(\rho) \otimes C(\rho) &= \begin{pmatrix} \rho & \sqrt{1-\rho^2} \\ \sqrt{1-\rho^2} & -\rho \end{pmatrix} \otimes \begin{pmatrix} \rho & \sqrt{1-\rho^2} \\ \sqrt{1-\rho^2} & -\rho \end{pmatrix} \\ &= \begin{pmatrix} \rho^2 & \rho\sqrt{1-\rho^2} & \rho\sqrt{1-\rho^2} & 1-\rho^2 \\ \rho\sqrt{1-\rho^2} & -\rho^2 & 1-\rho^2 & -\rho\sqrt{1-\rho^2} \\ \rho\sqrt{1-\rho^2} & 1-\rho^2 & -\rho^2 & -\rho\sqrt{1-\rho^2} \\ 1-\rho^2 & -\rho\sqrt{1-\rho^2} & -\rho\sqrt{1-\rho^2} & \rho^2 \end{pmatrix} \end{aligned} \tag{3.2}$$

Except for the dimensionality everything works the same as in chapter 2. We choose the initial state to be $|\psi_C\rangle = \psi_{LL}|LL\rangle + \psi_{LR}|LR\rangle + \psi_{RL}|RL\rangle + \psi_{RR}|RR\rangle$. The state of the particle after t steps will then be obtained by successive application of the operator U_2. Note that as the walk is the tensor product of two walks, the particle must move simultaneously in both the horizontal and the vertical direction - meaning that it is moving along the diagonals of the lattice.

3.2 Fourier transformation

The walk is as well as the one from chapter 2 translation invariant and so we use the Fourier transformation to simplify its analysis. The Fourier transform ($\widetilde{\psi}(k_x, k_y, t) : (-\pi, \pi) \times (-\pi, \pi) \times \mathbb{Z} \longmapsto \mathbb{C}^4 \times \mathbb{Z}$) is defined by

$$\widetilde{\psi}(k_x, k_y, t) = \sum_{x,y} \psi(x, y, t) e^{i(k_x x + k_y y)} \tag{3.3}$$

We will denote

$$M^{--} = \begin{pmatrix} \rho^2 & \rho\sqrt{1-\rho^2} & \rho\sqrt{1-\rho^2} & 1-\rho^2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad M^{-+} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \rho\sqrt{1-\rho^2} & -\rho^2 & 1-\rho^2 & -\rho\sqrt{1-\rho^2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$M^{+-} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \rho\sqrt{1-\rho^2} & 1-\rho^2 & -\rho^2 & -\rho\sqrt{1-\rho^2} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \; M^{++} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1-\rho^2 & -\rho\sqrt{1-\rho^2} & -\rho\sqrt{1-\rho^2} & \rho^2 \end{pmatrix} \tag{3.4}$$

Assuming that $\psi(x, y, t) = (\psi_{LL}(x, y, t), \psi_{LR}(x, y, t), \psi_{RL}(x, y, t), \psi_{RR}(x, y, t))^T$ and using the notation (3.4), we obtain following relations:

$$\begin{aligned} \psi_{LL}(x, y, t+1) &= M^{--}\psi(x+1, y+1, t), \quad \psi_{LR}(x, y, t+1) = M^{-+}\psi(x+1, y-1, t) \\ \psi_{RL}(x, y, t+1) &= M^{+-}\psi(x-1, y+1, t), \quad \psi_{RR}(x, y, t+1) = M^{++}\psi(x-1, y-1, t). \end{aligned} \tag{3.5}$$

Using (3.3) and (3.5) we find subsequent formula for the Fourier transform

$$\widetilde{\psi}(k_x, k_y, t+1) = (e^{-i(k_x+k_y)}M^{--} + e^{i(-k_x+k_y)}M^{-+} + e^{i(k_x-k_y)}M^{+-} + e^{i(k_x+k_y)}M^{++})\widetilde{\psi}(k_x, k_y, t).$$

This formula yields the recurrence

$$\widetilde{\psi}(k_x, k_y, t+1) = \widetilde{U}(k_x, k_y)\widetilde{\psi}(k_x, k_y, t); \; \widetilde{U}(k_x, k_y) = Diag(e^{-i(k_x+k_y)}, e^{i(-k_x+k_y)}, e^{i(k_x-k_y)}, e^{i(k_x+k_y)})C_2$$

The next step is to examine the eigensystem of $\widetilde{U}(k_x, k_y)$. The eigenvalues are $\lambda_1 = e^{i(\omega_x+\omega_y)}$, $\lambda_2 = e^{-i(\omega_x+\omega_y)}$, $\lambda_3 = -e^{i(\omega_x-\omega_y)}$, $\lambda_1 = -e^{i(-\omega_x+\omega_y)}$, where ω_x and ω_y satisfy the dispersion relations

$$\begin{aligned} \sin\omega_x &= \rho \sin k_x \\ \sin\omega_y &= \rho \sin k_y \end{aligned} \tag{3.6}$$

We find that the corresponding eigenvectors are the ones listed below.

$$
\begin{aligned}
v_1(k_x,k_y) &= N_1\begin{pmatrix} e^{-i(k_x+k_y)}(1-\rho^2) \\ -e^{-ik_x}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y) \\ -e^{-ik_y}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x) \\ (\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x)(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y) \end{pmatrix} \\
v_2(k_x,k_y) &= N_2\begin{pmatrix} e^{-i(k_x+k_y)}(1-\rho^2) \\ e^{-ik_x}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_y}-\rho\cos k_y) \\ e^{-ik_y}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_x}-\rho\cos k_x) \\ (\sqrt{1-\rho^2\sin^2 k_x}-\rho\cos k_x)(\sqrt{1-\rho^2\sin^2 k_y}-\rho\cos k_y) \end{pmatrix} \\
v_3(k_x,k_y) &= N_3\begin{pmatrix} e^{-i(k_x+k_y)}(1-\rho^2) \\ e^{-ik_x}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_y}-\rho\cos k_y) \\ -e^{-ik_y}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x) \\ (\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x)(-\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y) \end{pmatrix} \\
v_4(k_x,k_y) &= N_4\begin{pmatrix} e^{-i(k_x+k_y)}(1-\rho^2) \\ -e^{-ik_x}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y) \\ e^{-ik_y}\sqrt{1-\rho^2}(\sqrt{1-\rho^2\sin^2 k_x}-\rho\cos k_x) \\ (-\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x)(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y) \end{pmatrix}
\end{aligned}
\tag{3.7}
$$

We find the appropriate normalisations $N_j;\quad j\in\{1,2,3,4\}$ to be

$$
\begin{aligned}
N_1 &= \left[\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x\right)^2\right)\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y\right)^2\right)\right]^{-\frac{1}{2}} \\
N_2 &= \left[\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_x}-\rho\cos k_x\right)^2\right)\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_y}-\rho\cos k_y\right)^2\right)\right]^{-\frac{1}{2}} \\
N_3 &= \left[\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_x}+\rho\cos k_x\right)^2\right)\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_y}-\rho\cos k_y\right)^2\right)\right]^{-\frac{1}{2}} \\
N_1 &= \left[\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_x}-\rho\cos k_x\right)^2\right)\left(1-\rho^2+\left(\sqrt{1-\rho^2\sin^2 k_y}+\rho\cos k_y\right)^2\right)\right]^{-\frac{1}{2}}
\end{aligned}
$$

As the walk is a tensor product of two walks, the above eigensystem can be found by using the one obtained in chapter 2 and the matrix theory (see Appendix A). The just found eigenvectores are tensor products of the vectors listed in (2.10). The eigenvalues are then multiples of the ones corresponding to these vectors. This approach does not work for more general walks.

3.3 Moment method

Using the moment method we will now find the joint group velocities density and discuss the resulting behaviour of the walk.

We will again use the Fourier transformation to calculate the moments:

$$\langle X^\alpha Y^\beta \rangle = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} \int_{-\pi}^{\pi} \frac{dk_y}{2\pi} \widetilde{\psi}^\dagger(k_x,k_y,t) \left(i\frac{\partial}{\partial k_x}\right)^\alpha \left(i\frac{\partial}{\partial k_y}\right)^\beta \widetilde{\psi}(k_x,k_y,t) \tag{3.8}$$

Utilising the eigendecomposition we can write the Fourier transform of the state as

$$\widetilde{\psi}(k_x,k_y,t) = \sum_{j=1}^{4} \lambda_j^t f_j(k_x,k_y) v_j(k_x,k_y); \qquad f_j(k_x,k_y) = (v_j(k_x,k_y), \psi_C). \tag{3.9}$$

Because the eigenvectors are orthonormal, and because $\omega_x = \omega_x(k_x)$ and $\omega_y = \omega_y(k_y)$ we find the following for the integrand

$$\begin{aligned} &\widetilde{\psi}^\dagger(k_x,k_y,t) \left(i\frac{\partial}{\partial k_x}\right)^\alpha \left(i\frac{\partial}{\partial k_y}\right)^\beta \widetilde{\psi}(k_x,k_y,t) \\ &= t^{\alpha+\beta} \left(\frac{d\omega_x}{dk_x}\right)^\alpha \left(\frac{d\omega_y}{dk_y}\right)^\beta \left((-1)^{\alpha+\beta}|f_1|^2 + |f_2|^2 + (-1)^\alpha |f_3|^2 + (-1)^\beta |f_4|^2 + O\left(t^{\alpha+\beta-1}\right)\right) \end{aligned} \tag{3.10}$$

We will now change the variables to the group velocities defined as

$$\begin{aligned} v_x &= \frac{d\omega_x}{dk_x} = \frac{\rho \cos k_x}{\sqrt{1-\rho^2 \sin^2 k_x}}; \qquad & dk_x &= \frac{\sqrt{1-\rho^2}}{\rho} \frac{dv_x}{(1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}} \\ v_y &= \frac{d\omega_y}{dk_y} = \frac{\rho \cos k_y}{\sqrt{1-\rho^2 \sin^2 k_y}}; \qquad & dk_y &= \frac{\sqrt{1-\rho^2}}{\rho} \frac{dv_y}{(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}} \end{aligned}$$

Equation (3.8) for the pseudo-velocity $V = \left(\frac{X}{t}, \frac{Y}{t}\right)$ in long-time limit thus reads

$$\lim_{t\to\infty} \left\langle \left(\frac{X}{t}\right)^\alpha \left(\frac{Y}{t}\right)^\beta \right\rangle = \int_{-\rho}^{\rho} dv_x \int_{-\rho}^{\rho} dv_y v_x^\alpha v_y^\beta \frac{1-\rho^2}{\rho^2} \frac{\left((-1)^{\alpha+\beta}|f_1|^2 + |f_2|^2 + (-1)^\alpha |f_3|^2 + (-1)^\beta |f_4|^2\right)}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}} \tag{3.11}$$

We now determine the moments for all possible combinations of even and odd α, β with the initial state $\psi_C = (q_1, q_2, q_3, q_4)$ (because of the complexity of the terms we will write only the integrands as function $f(\alpha,\beta)$):

$$f(2m,2n) = v_x^{2m} v_y^{2n} \frac{1-\rho^2}{\rho^2} \frac{1}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}},$$

$$\begin{aligned} &f(2m+1,2n) = \\ &= -v_x^{2m+1} v_y^{2n} \frac{1-\rho^2}{\rho^2} \frac{v_x \left[|q_1|^2 + |q_2|^2 - |q_3|^2 - |q_4|^2 + \frac{\sqrt{1-\rho^2}}{\rho}(\bar{q}_1 q_3 + q_1 \bar{q}_3 + \bar{q}_2 q_4 + q_2 \bar{q}_4)\right]}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}}, \end{aligned}$$

$$
\begin{aligned}
&f(2m,2n+1) = \\
&= -v_x^{2m} v_y^{2n+1} \frac{1-\rho^2}{\rho^2} \frac{v_y \left[|q_1|^2 - |q_2|^2 + |q_3|^2 - |q_4|^2 + \frac{\sqrt{1-\rho^2}}{\rho} (\bar{q}_1 q_2 + q_1 \bar{q}_2 + \bar{q}_3 q_4 + q_3 \bar{q}_4) \right]}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}}, \\
&f(2m+1,2n+1) = \\
&= v_x^{2m+1} v_y^{2n+1} \frac{1-\rho^2}{\rho^2} \frac{v_x v_y \left[|q_1|^2 - |q_2|^2 - |q_3|^2 + |q_4|^2 + \frac{1-\rho^2}{\rho^2} (\bar{q}_1 q_4 + q_1 \bar{q}_4 + \bar{q}_2 q_3 + q_2 \bar{q}_3) \right]}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}} + \\
&+ v_x^{2m+1} v_y^{2n+1} \frac{1-\rho^2}{\rho^2} \frac{v_x v_y \frac{\sqrt{1-\rho^2}}{\rho} (\bar{q}_1 q_2 + q_1 \bar{q}_2 + \bar{q}_1 q_3 + q_1 \bar{q}_3 - \bar{q}_2 q_4 - q_2 \bar{q}_4 - \bar{q}_3 q_4 - q_3 \bar{q}_4)}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}}.
\end{aligned}
\tag{3.12}
$$

Again by the argument of the evenness of the group velocities and symmetry of the intervals over which we integrate, we can rewrite the four integrals as one and thus obtain the group velocities joint density. For further usage we split the density into the fundamental one (for illustration see its plot in Figure 3.1) and the weight function. The formula for the fundamental density is

$$
\mu(v_x, v_y) = \frac{1-\rho^2}{\rho^2} \frac{1}{\pi^2 (1-v_x^2)\sqrt{1-\frac{v_x^2}{\rho^2}}(1-v_y^2)\sqrt{1-\frac{v_y^2}{\rho^2}}}.
$$

3.4 Weight function and analysis of the walk

We have not stated the weight function in the previous section, because it is very complex and thus of little interest for the purpose of analysis. However, it can be simplified by the change of basis. (Again we are following the method from [16].) In the previous chapter the basis consisting of the eigenvectors of the coin operator proved to be the most advantageous one. Therefore we will proceed likewise.
According to the theory of matrices the eigenvectors of the coin operator will be the tensor product of those found for the one-dimensional case. They are hence of the form

$$
|\kappa^{++}\rangle = \frac{1}{2}\begin{pmatrix} 1+\rho \\ \sqrt{1-\rho^2} \\ \sqrt{1-\rho^2} \\ 1-\rho \end{pmatrix}, \; |\kappa^{--}\rangle = \frac{1}{2}\begin{pmatrix} 1-\rho \\ -\sqrt{1-\rho^2} \\ -\sqrt{1-\rho^2} \\ 1+\rho \end{pmatrix}, \; |\kappa^{+-}\rangle = \frac{1}{2}\begin{pmatrix} \sqrt{1-\rho^2} \\ -1-\rho \\ 1-\rho \\ -\sqrt{1-\rho^2} \end{pmatrix}, \; |\kappa^{-+}\rangle = \frac{1}{2}\begin{pmatrix} \sqrt{1-\rho^2} \\ 1-\rho \\ -1-\rho \\ -\sqrt{1-\rho^2} \end{pmatrix}.
\tag{3.13}
$$

Let us denote the new basis $\chi = (|\kappa^{++}\rangle, |\kappa^{--}\rangle, |\kappa^{-+}\rangle, |\kappa^{+-}\rangle)$. The initial state expressed in this basis will be $(\psi_c)_\chi = (h^{++}, h^{--}, h^{+-}, h^{-+})$. We find the components of the initial state

in the standard basis to be:

$$\begin{aligned}
q_1 &= \frac{1}{2}\left(h^{++}(1+\rho)+h^{--}(1-\rho)+h^{+-}\sqrt{1-\rho^2}+h^{-+}\sqrt{1-\rho^2}\right)\\
q_2 &= \frac{1}{2}\left(h^{++}\sqrt{1-\rho^2}-h^{--}\sqrt{1-\rho^2}-h^{+-}(1+\rho)+h^{-+}(1-\rho)\right)\\
q_3 &= \frac{1}{2}\left(h^{++}\sqrt{1-\rho^2}-h^{--}\sqrt{1-\rho^2}+h^{+-}(1-\rho)-h^{-+}(1+\rho)\right)\\
q_4 &= \frac{1}{2}\left(h^{++}(1-\rho)+h^{--}(1+\rho)-h^{+-}\sqrt{1-\rho^2}-h^{-+}\sqrt{1-\rho^2}\right)
\end{aligned} \tag{3.14}$$

Substituting (3.14) into the integrands (3.12) we obtain the weight function:

$$M(v_x, v_y) = 1 - K_1 v_x - K_2 v_y + K_{12} v_x v_y \tag{3.15}$$

The coefficients K_1, K_2, K_{12} depend on the initial state subsequently

$$\begin{aligned}
K_1 &= \frac{1}{\rho}\left(|h^{++}|^2+|h^{+-}|^2-|h^{-+}|^2-|h^{--}|^2\right)\\
K_2 &= \frac{1}{\rho}\left(|h^{++}|^2-|h^{+-}|^2+|h^{-+}|^2-|h^{--}|^2\right)\\
K_{12} &= \frac{1}{\rho^2}\left(|h^{++}|^2-|h^{+-}|^2-|h^{-+}|^2+|h^{--}|^2\right)
\end{aligned}$$

Let us now discuss the properties of the group velocities joint density. We see that the fundamental density, which depends entirely on the choice of the coin operator, diverges as $v_x \to \pm\rho$ and $v_x \to \pm\rho$. In addition we can observe that it diverges much faster for v_x, v_y going to $\pm\rho$ simultaneously, hence the peaks on the diagonals in Figure 3.1.

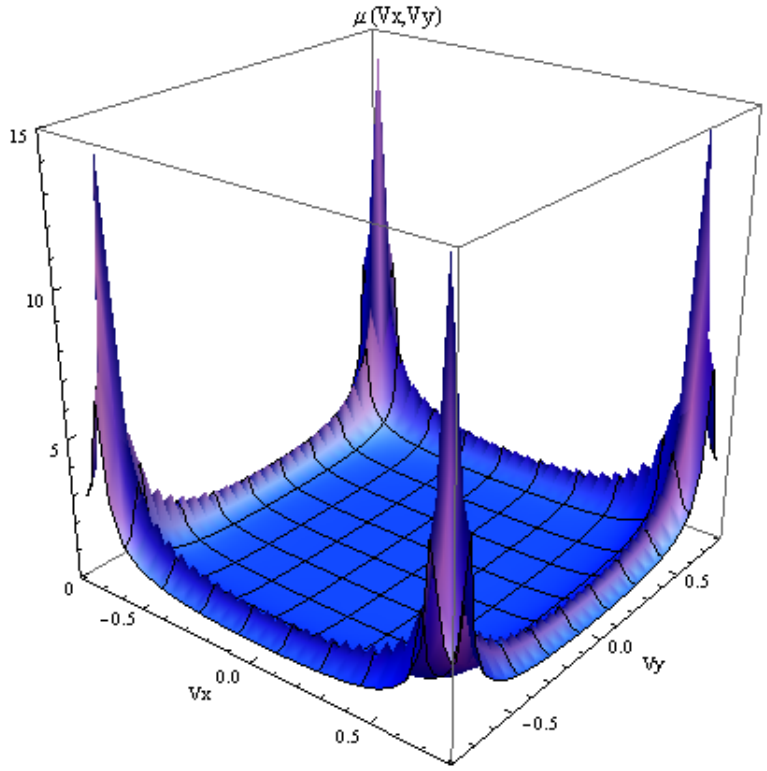
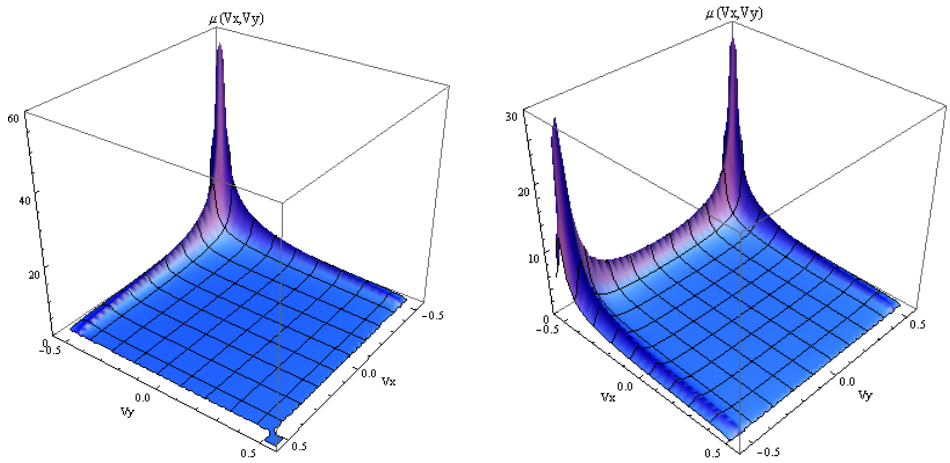
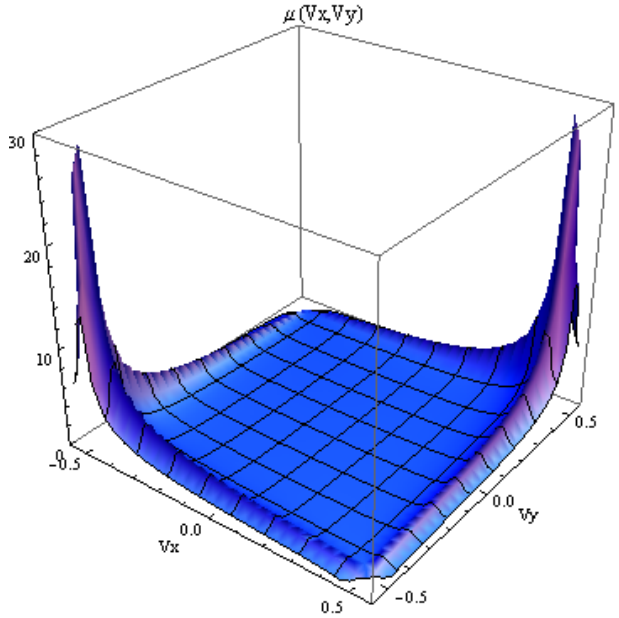


Figure 3.1: Fundamental joint density for $\rho = \frac{1}{\sqrt{2}}$.



(a) $|\psi_C\rangle = |\kappa^{++}\rangle$ (b) $|\psi_C\rangle = \frac{1}{\sqrt{2}}(|\kappa^{++}\rangle + |\kappa^{+-}\rangle$



(c) $|\psi_C\rangle = \frac{1}{\sqrt{2}}(|\kappa^{++}\rangle + |\kappa^{--}\rangle$

Figure 3.2: Dependence of the group velocities joint density on the initial state (for $\rho = \frac{1}{2}$)

The weight function on the other hand depends solely on the initial state. Thanks to its simplified form (3.15) we can easily analyse this dependence and find many extremal results. In particular some of the divergences can be eliminated by choosing a proper basis state or suitable combination of states, because then the numerator goes to zero faster then the denominator.
For example:

1. Only the peak for $v_x, v_y \to -\rho$ remains for the state $|\psi_C\rangle = |\kappa^{++}\rangle$
2. Divergence on the diagonal $v_x = -v_y$ is eliminated for $|\psi_C\rangle = \frac{1}{\sqrt{2}}(|\kappa^{++}\rangle + |\kappa^{--}\rangle)$
3. Divergence for $v_x \to \rho$ vanishes for $|\psi_C\rangle = \frac{1}{\sqrt{2}}(|\kappa^{++}\rangle + |\kappa^{+-}\rangle)$

For illustration we plot these three examples in Figure 3.2. We can partially predict these results by focusing on the initial state and results from previous chapter. We observe that in the first case we have a separable state of two walks with behaviour shown in Figure 2.3, hence the one peak. The other two are entangled in the coin space. This entanglement provides otherwise unlikely results.
Please note that the above analysed walk, however perfectly sufficient for our purpose, is rather specific as it is a tensor product of two walks. Many difficulties can occur for more general ones (among others finding the dispersion relations).

Chapter 4

Interacting particles

4.1 The interaction

In this section we will use the quantum walk analysed in the previous chapter with the choice of $\rho = \frac{1}{\sqrt{2}}$ — *i.e.* the Hadamard walk — to introduce the point interaction as described by Andre Albrecht *et al.* in [2].
Although we approached the walk as if it was a single particle in two dimensions in chapter 3, we noted that as a tensor product of two walks it can be regarded as a walk of two non-interacting particles on a line. To each particle we simply assign one of the x, y-coordinates of the single particle on the square lattice ($x \mapsto x_1, y \mapsto x_2$).
The interaction is introduced by implementing a dependence of the coin on the particles coordinates. We will provide such dependence by changing the evolution operator to $U_{in} = U_2 G$, where G is a space dependent coin operator described in the following paragraph.
Let us denote the basis vector as $|x_1, c_1, x_2, c_2\rangle$, where x_1, x_2 are the positions of the particles and c_1, c_2 are their coin states. We will add a phase factor in the subspace generated by basis vectors for which the particles are at the same position ($x_1 = x_2$) — the set of *collision points* . The operator G will hence be:

$$G|x_1, c_1, x_2, c_2\rangle = \begin{cases} |x_1, c_1, x_2, c_2\rangle & \text{if } x_1 \neq x_2 \\ e^{ig}|x_1, c_1, x_2, c_2\rangle & \text{if } x_1 = x_2 \end{cases} \tag{4.1}$$

Denoting the fixed operator $\Gamma = e^{ig} I_C$ and the projector to the set of collision points N, we can rewrite the evolution operator as:

$$U_{in} = U_2 \left((I - N) \otimes I_C + N \otimes \Gamma\right) \tag{4.2}$$

We can easily note that the walk has following symmetries:

- From the construction of $U_2 = U_1 \otimes U_1$ stems, that it is invariant under permutation of the particles. This leads to the invariance of the symmetric and antisymmetric subspaces.
- We know that the free walk is invariant under both joint and separate translation. The invariance under the joint translation remains as Γ is the same for all the collision points; however, the separate translation invariance is broken by the perturbation.
- As we have established in the previous chapter, the shift operator changes the positions of the particles simultaneously by ± 1. This means that the parity of $x_1 - x_2$

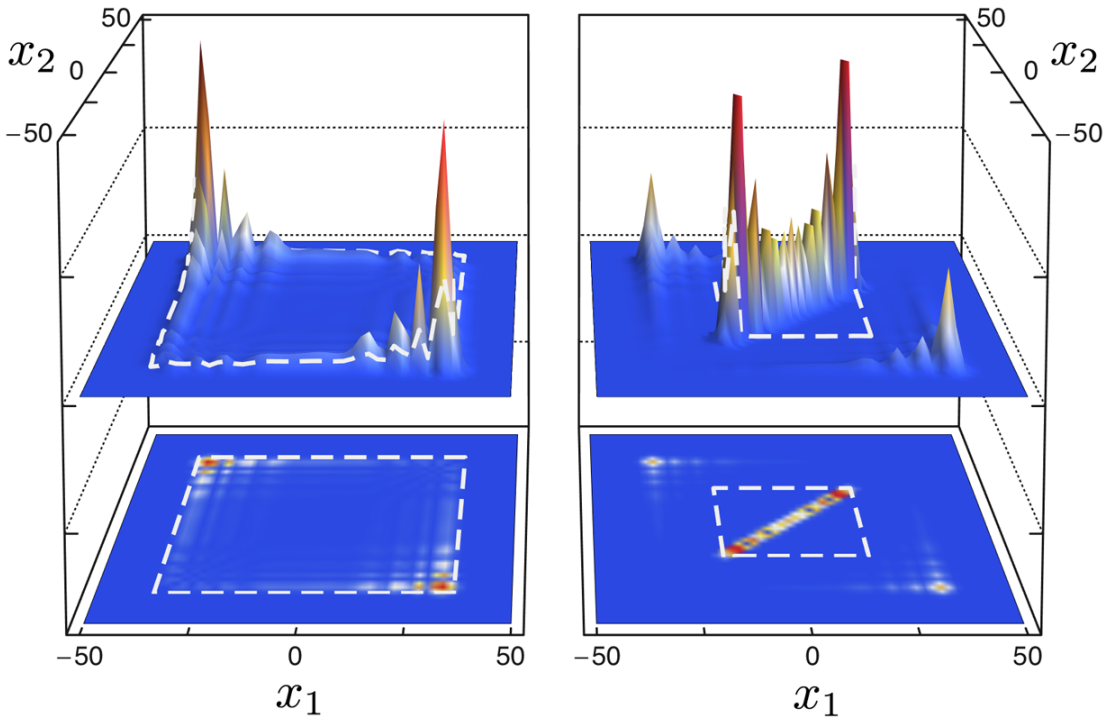


Figure 4.1: Simulation of the walk in position space. The left panel is the joint probability density of the position for free walk (compare with figure 3.2 (b) from chapter 3 — the peaks are on the other diagonal because we chose the "symmetric singlet"). The right panel is then the joint probability density for the walk with interaction (for $g = \pi$). The peaks of the free walk, however significantly smaller, remains, and new peaks occur along the diagonal $x_1 = x_2$. These correspond to the walk of the molecule. The white squares are for comparison with the theoretically calculated group velocities. (Picture adapted from [2] with permission from authors.)

is preserved. We will hence always choose the initial state such that $x_1 - x_2$ is even so that the interaction is permissible.

- Due to the discreet-time translation invariance, and as we apply the operator periodically, the energy is preserved up to $2k\pi$; $\quad k \in \mathbb{Z}$.

Bearing in mind what we have just said about the symmetries, let us discuss possible changes of coordinates. We have already defined the coordinates x_1, x_2. Unfortunately these are not very suitable for the analysis. Therefore, we use the Fourier transformation and obtain the momentums p_1, p_2. As we have found out in previous chapters, these are well defined coordinates for the free walk, because it is invariant under both joint and separate translation. However, the perturbation obviously break the invariance under separate translation and neither of the momentum is conserved.
We can solve this problem by introducing the center of mass momentum $p = \frac{p_1+p_2}{2}$ and the relative momentum $k = p_1 - p_2$. We can instantly see that the center of mass momentum is invariant under the joint translation, because the perturbation preserves this symmetry. The relative momentum, on the other hand, is invariant only for the free walk.

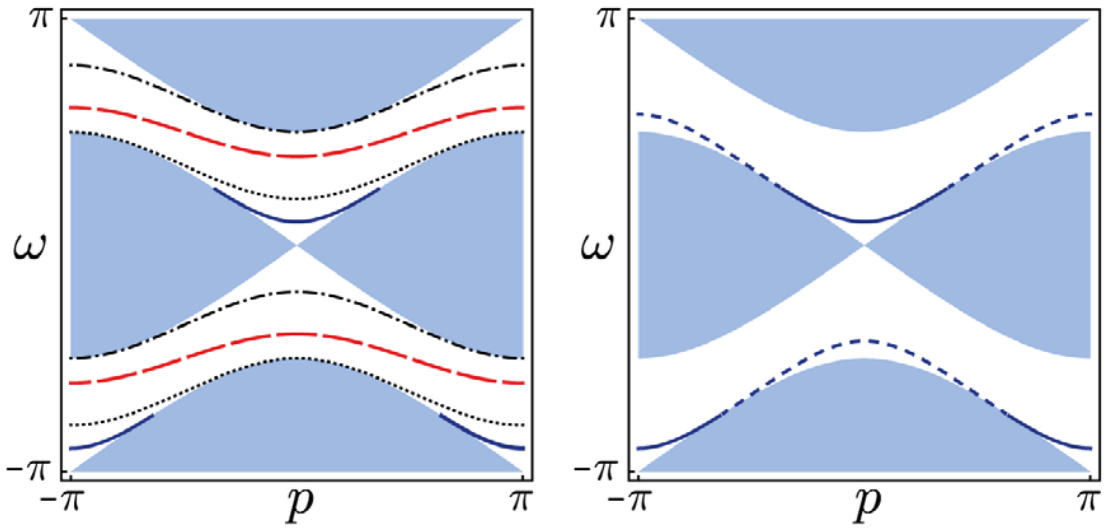


Figure 4.2: The spectrum of the evolution operator in dependence of center of mass momentum p. The lines founded in the white gaps are the dispersion relations for the molecule. The blue continuous parts are the bands of the free walk. In the left panel dispersion relations for several choice of g are plotted (Especially important for us is the red one with $g = \pi$). In the right panel there is the spectrum for the choice of $g = \pi/4$. The dashed parts are so called *virtual bands* – bands that do not satisfy the additional condition (4.4) and so have no physical meaning. (Picture adapted from [2]with permission from authors.)

4.2 Analytical solutions

This section is mostly based on the work of Andre Albrecht *et al.* as presented in [2] and we include it mainly to support our numerical results. Please note that everything in this section is restricted to the fermions case and thus to the singlet inner state (This is further discussed in section 4.3).
It is a fundamental result of the theory of perturbation of linear operators that as the operator $U_{in} - U_2 = U_2 N \otimes (\Gamma - I_C)$ has a finite rank, the continuous spectra of U_{in}, U_2 are the same. In addition it can be shown that for one dimensional perturbation which is our case the eigenvalues of U_{in} are not embedded in the spectrum of U_2.
We will call the continuous spectrum of the unperturbed operator *the bands* and the resolvent set *the gaps*. From what was said in previous paragraph, we can expect the eigenvalues of U_{in} that appear due to the interaction to occur in the gaps.
It shows that it is possible to find the dispersion relation for the subspace $x_1 = x_2$ for which the relative momentum k is constant, and that in our case a walk determined by the eigenvalues and corresponding eigenvectors is indeed a quantum walk on line — actually the walk of the molecule formed due to the perturbation.
The dispersion relation that can be found in [2] is

$$e^{i\omega} = \frac{e^{ig}}{2e^{ig} - 1}\left(\cos p \pm i\sqrt{\sin^2 p + 4(1 - \cos g)}\right) \tag{4.3}$$

with further condition

$$\sin\omega \cdot \sin(g - \omega) > 0\,. \tag{4.4}$$

For graphical representation of the dispersion relation see figure 4.2.
We can easily find the molecule's group velocity, which is the derivative of the disper-

sion relation. For $g = \pi$ it reads

$$v(p) = \frac{d\omega}{dp} = \frac{\sin p}{\sqrt{\sin^2 p + 8}}\,. \tag{4.5}$$

It is straightforward to find out that the maximum velocities are $v(p_0) = \pm\frac{1}{3}$ for $\cos p_0 = 0$. This is corresponding to the peaks that can be observed on the diagonal $x_1 = x_2$ in the left panel of figure 4.1.
The main result is that the wavefunction of the molecule decays exponentially in terms of $|x_1 - x_2|$ and hence indeed is a bounded state. For detailed and much more general analysis see [2].

4.3 Spectrum of the evolution operator

We numerically determine the spectral properties of the operator U_{in}, and look for signs of bounded states formation. The Mathematica code with commentaries is provided in appendix B.
In the previous section we have established, that the center of mass momentum (p) and for the free walk also the relative momentum (k) is conserved. It is thus useful to rotate the standard coordinates by 45°.
For the purpose of numerical computation we close the system to a ring with a finite number (N) of sites (a finite lattice with periodic boundary conditions). By doing so we discretize the momentums as well. Notice that as the boundaries are periodic and we want to approximate infinite lattice we need $N = 2n + 1$ because otherwise the Fourier transformation will not be injective.

Free walk

Although we have already examined the spectrum of the free walk analytically, we will use the numerical method as well for later comparison with the interacting case.

We can block-diagonalize the operator U_2 into blocks $4x4$ by the unitary discreet Fourier transformation:

$$F = \frac{1}{\sqrt{N}} \begin{pmatrix} \omega_N^{0\cdot 0} & \omega_N^{0\cdot 1} & \cdots & \omega_N^{0\cdot N-1} \\ \omega_N^{1\cdot 0} & \omega_N^{1\cdot 1} & \cdots & \omega_N^{1\cdot N-1} \\ \vdots & \vdots & \ddots & \vdots \\ \omega_N^{N-1\cdot 0} & \omega_N^{N-1\cdot 1} B & \cdots & \omega_N^{N-1\cdot N-1} \end{pmatrix}; \qquad \omega_N = e^{\frac{2i\pi}{N}}$$

Then for each fixed p, k we obtain operator $U_2(p,k)$ with eigenvalues $e^{i\omega(p,k)}$, which we can compute. Technically we have jointly diagonalized translation operators with the evolution operator. As they are all unitary, the eigenvalues are on unit circle. For graphical representation (Figure 4.3) we unwrap these circles and describe the eigenvalues via triplets (p, k, ω).

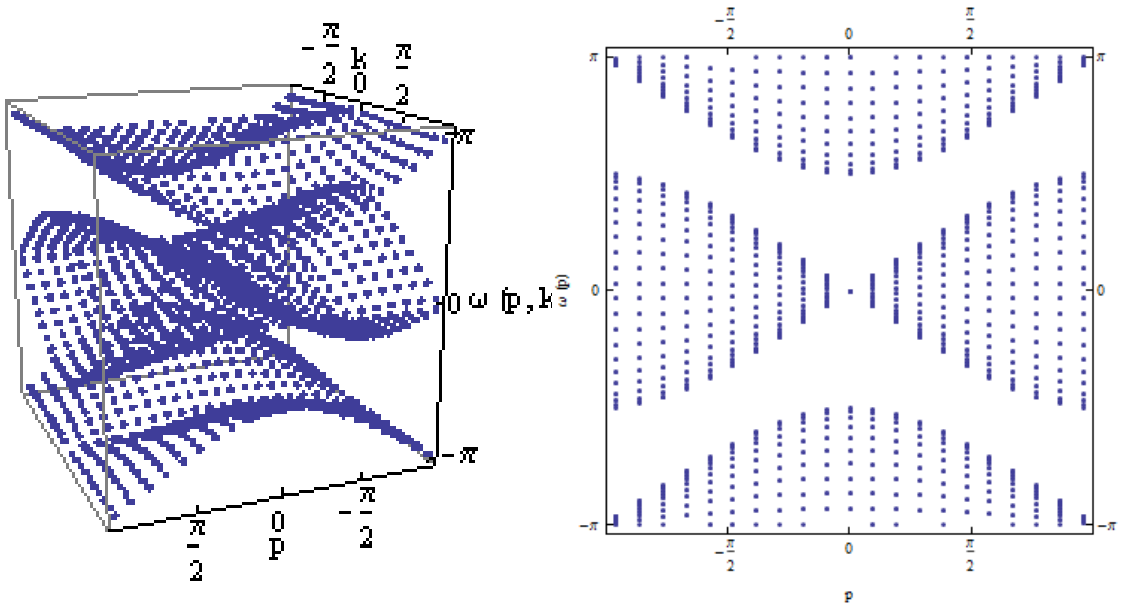


Figure 4.3: Numerically determined spectrum of the evolution operator for the free walk with the length of the ring $N = 21$(corresponding to the choice of $n = 10$ in appendix B). In the left figure the dependence of ω on the center of mass momentum as well as the relative momentum (axis orthogonal to the paper) is shown. Note that the points constitute three surfaces which will be filled for infinite lattice as the spectrum of the walk is continuous. The bands in the right figure are projections of the left one into the p, ω-plane.

Interacting fermions

We would like to determine numerically the spectrum of the walk operator (4.2) for two interacting fermions and compare it with the results obtained for the free walk to find marks of molecular binding.

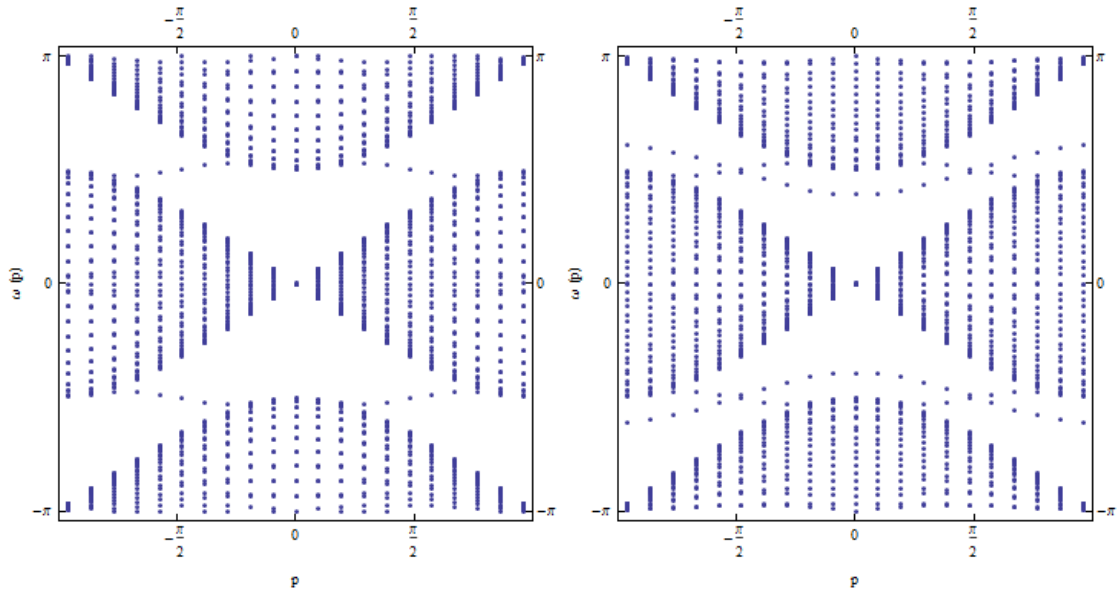
We know from quantum mechanics that the combination of the wavefunctions of two fermions must be antisymmetric. Furthermore, we have found out that the symmetric and antisymmetric subspaces are invariant under the free walk. Due to this we can find the dynamics by simply restricting the interaction to the antisymmetric subspace.

Let us denote the inner state of two particles $|c_1, c_2\rangle$. It is obvious that the only possible inner state of two fermions that are on the same position is the singlet state $\psi_- = \frac{1}{\sqrt{2}}(|-+\rangle - |+-\rangle)$, because the position space part of the wavefunction is symmetric and we need the overall function to be antisymmetric.

From the above said we can see that the operator of the interaction can be written as $\Gamma_f = e^{ig}\Pi_- + (\Pi_+ + \Pi_{++} + \Pi_{--})$. For the description of the interaction operator we have used the following projectors: $\Pi_- = |\psi_-\rangle\langle\psi_-|$, $\Pi_+ = |\psi_+\rangle\langle\psi_+|$, $\Pi_{--} = |--\rangle\langle--|$, $\Pi_{++} = |++\rangle\langle++|$ ($\psi_+ = \frac{1}{\sqrt{2}}(|-+\rangle + |+-\rangle)$).

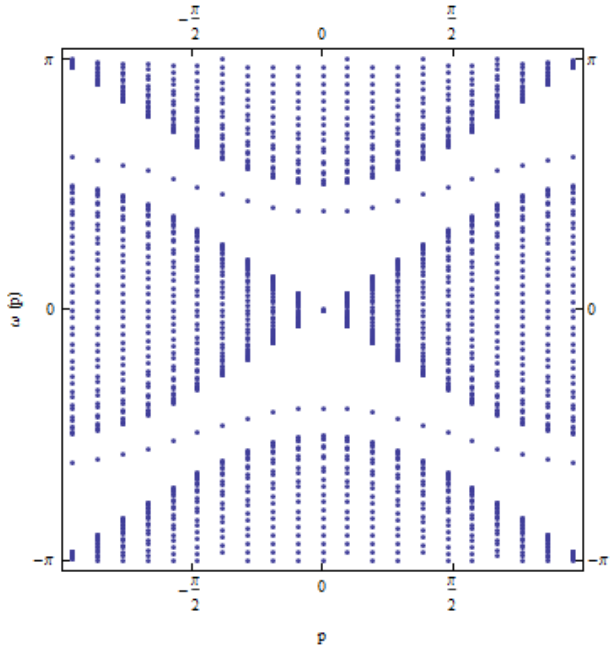
Substituting Γ_f into (4.2) we obtain an operator of the walk of two fermions which we will denote U_{in_f}.

We know that due to the interaction the relative momentum is not conserved and hence the operator U_{in_f} is block-diagonalized only for the center of mass momentum (into N $4N \times 4N$ blocks). Once again we obtain for each fixed p an operator $U_{in_f}(p)$ with eigenvalues $e^{i\omega(p)}$, which we calculate. By the same argument as in the free walk case the eigenvalues are on the unit circle, which we unwrap for the graphical representation (Figure 4.4c).



(a) Bosons

(b) Distinguishable particles



(c) Fermions

Figure 4.4: Numerically determined spectrum of the evolution operators for walks with different types of particles with the interaction factor $g = \pi$. The ring size $N = 21$.

Comparing the graphical representation with the one for the free walk (see right panel of figure 4.3), we notice extra eigenvalues in the gaps - these are the ones analytically predicted that correspond to the walk of the molecule. They are important signs that a bounded state is forming due to the perturbation.

Interacting Bosons

For the interacting bosons the situation is very similar to the fermions. The only difference is that the state of two or more interacting bosons must be symmetric. Therefore, analogously with the fermions case, we restrict the interaction to the symmetric subspace.

Using the same projectors as in the previous case, the interaction operator is defined as

$$\Gamma_b = \Pi_- + e^{ig}(\Pi_+ + \Pi_{++} + \Pi_{--}) \tag{4.6}$$

Once again we numerically determine the spectrum of the evolution operator which is obtained by inserting Γ_b into (4.2). The numerical simulation is exactly the same as for the fermions except for the choice of the operator. Therefore, we omit the details and solely plot the results in figure 4.4a. We notice that again there are new eigenvalues in the gap, although arranged differently then for the fermions. It seems that they are the inverse and that the probability density will be more localized to the origin. However, further calculations and analysis, which are out of the scope of this thesis, are needed to proof that.

Distinguishable particles

For distinguishable particles there are no restrictions as to the symmetries, and we thus use the interaction operator Γ defined in section 4.1. For the last time we determine the spectrum using the above described process and plot the results in figure 4.4b.
We can see that the set of eigenvalues corresponding to the interaction is the union of the sets for fermions and bosons. Hence, we can expect that the walk will show features typical for both the walk of fermions and bosons, and new features stemming from the combination may occur.

Conclusion

We have overviewed the basic formalism and the main ideas of quantum walks. Then we have utilized them for a step by step introduction of the methods used to analyse these walks.
We have started with a simple walk of a single particle on a line to explain the methods in the simplest possible way. Afterwards, understanding the behaviour of 1D walk, we have easily generalized the walk into two dimensions. We have also shown how the slightly modified methods presented for the 1D case can be used to reveal the properties of the 2D one.
Having established that the 2D walk can be represented as a walk of two non-interacting particles on a line, we have introduced a perturbation. We have shown that the perturbation can cause the two particles to form a bounded state – a molecule.
We have used numerical methods to successfully determine the spectrum of the evolution operator, and our results correspond very well with the analytical predictions. Thanks to the knowledge of the spectrum, it has been shown that the bounded state performs a quantum walk, and some of its properties have been examined. In particular we have found the maximum group velocity for the walk.
We admit that the part concerning the analytical solution of the perturbation is rather brief as it is beyond the scope of this thesis. We have also made several presumptions regarding the behaviour of bosons and distinguishable particles that are, in our opinion, worth further examination. Therefore, we would like to focus on these two related topics in our future research.
We belief that the quantum walks with interactions may proof essential for further development of quantum computation and simulation of quantum systems, and that there is a lot yet to be explored.

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Appendices

Appendix A

Mathematics

A.1 Functional analysis

Definition A.1. Axioms of inner product in vector space V over $\mathbb{C}$: $\forall x, y, z \in V, \alpha \in \mathbb{C}$:

1. $(x, \alpha y + z) = \alpha(x, y) + (x, z)$
2. $(x, y) = \overline{(y, x)}$
3. $(x, x) \geq 0 \wedge (x, x) = 0 \Leftrightarrow x = 0$

Theorem A.2 (Riesz's theorem)**.**

$$\forall \varphi \in \mathcal{H}^*, \exists y \in \mathcal{H}; \varphi_y(x) = (y, x), \ \ \forall x \in \mathcal{H}$$

Note A.3. The inner product in space $L^2(M, d\mu)$ is defined as:

$$(f, g) = \int_M \bar{f} g d\mu$$

Definition A.4. Hilbert space is a complete vector space with inner product.

Definition A.5. Let $\mathcal{H}_1$, $\mathcal{H}_2$ be Hilbert spaces. Their tensor product is then every pair $(\mathcal{H}, \varphi)$, where $\mathcal{H}$ is a Hilbert space and $\varphi : \mathcal{H}_1 \times \mathcal{H}_2 \mapsto \mathcal{H}$ is a map $\varphi(x, y) \equiv x \otimes y$, which satisfies following conditions:

1. $\forall x, x' \in \mathcal{H}_1, \forall y, y' \in \mathcal{H}_2; \quad (x \otimes y, x' \otimes y') = (x, x')_1 (y, y')_2$
2. the set $\{x \otimes y | x \in \mathcal{H}_1 y \in \mathcal{H}_2\}$ is total in $\mathcal{H}$

Definition A.6. Schwartz space is the following function space:

$$\mathfrak{S}(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) | \sup_{x \in \mathbb{R}^n} |x^\alpha f^{(\beta)}(x)| < \infty; \quad \forall \alpha, \beta\}$$

Let f be a function from the Schwartz space. we define:

$$\hat{f}(y) = \frac{1}{\left(\sqrt{(2\pi)}\right)^n} \int e^{-ix \cdot y} f(x) dx, \quad y \in \mathbb{R}^n \tag{A.1}$$

It is proved that $|y^\alpha f^{(\beta)}(y)| < \infty$ for all α, β, hence $\hat{f}(y) \in (\mathfrak{S}(\mathbb{R}^n)$. Relation A.2 define a continuous linear operator on the Schwartz space, which we will denote $\mathcal{F}_0$, *i.e.* $\mathcal{F}_0 f = \hat{f}$. We will define $\mathcal{F}_0^{-1} : \hat{f} \mapsto f$ as

$$f(y) = \frac{1}{\left(\sqrt{(2\pi)}\right)^n} \int e^{ix \cdot y} f(x) dx, \quad y \in \mathbb{R}^n \tag{A.2}$$

It can be easily shown that $\mathcal{F}_0^{-1}\mathcal{F}_0 = I$. We will now interpret the above defined map and extend it. It is known, that the Schwartz space is subset of the space of smooth function ($\mathcal{S}(\mathbb{R}^n) \subset C_\infty(\mathbb{R}^n)$). We can see from relation A.2 that $\|\hat{f}\|_\infty \leqq (2\pi)^{-\frac{n}{2}}\|\hat{f}\|_1$. Thus it is possible to interpret $\mathcal{F}_0$ as bounded map $\mathcal{F}_0 : \mathcal{S}(\mathbb{R}^n) \mapsto C_\infty(\mathbb{R}^n)$. We continuously extend it to obtain $\mathcal{F} : L^1(\mathbb{R}^n) \mapsto C_\infty(\mathbb{R}^n)$.

Definition A.7. The above constructed map $\mathcal{F}$ is called the Fourier transformation. It acts on a function $f \in L^1$ as:

$$(\mathcal{F}f)(y) = \hat{f}(y) = \frac{1}{\left(\sqrt{(2\pi)}\right)^n} \int e^{-ix\cdot y} f(x)dx.$$

Note A.8. The Fourier transformation can be defined alternatively according to the function we would like to transform. In this thesis we deal with a discreetly defined function $f : Z^n \mapsto \mathbb{C}^n$. The Fourier transformation is defined by

$$(\mathcal{F}f)(y) = \tilde{f}(m) = \sum_m f(m)e^{im\cdot y}; \quad y \in [-\pi, \pi]^{\times n}.$$

We also make use of the inverse Fourier transformation of a function $\tilde{f} : [-\pi, \pi]^{\times n} \mapsto \mathbb{C}^n$:

$$(\mathcal{F}^{-1}\tilde{f})(m) = f(m) = \frac{1}{(2\pi)^n} \int_{[-\pi,\pi]^{\times n}} \tilde{f}(y)e^{-iy\cdot m}dy$$

For proofs and further reading see [15]

A.2 Probability

Definition A.9. Let us consider a random variable X with absolute continuous distribution. It has density function f_x if and only if

$$Pr[a \leq X \leq b] = \int_a^b f_x(x)dx$$

Note A.10. Important property of the probability density function is that

$$\int_{-\infty}^{\infty} f_x(x)dx = 1$$

Definition A.11. Expected value or equivalently mean of a discrete distribution is calculated as sum over all possible values of the variable weighted by probabilities of them

$$\langle X \rangle = \sum_i x_i P(x_i)$$

For the continuous case we define

$$\langle X \rangle = \int_{-\infty}^{\infty} x f_x(x)dx$$

Definition A.12. The nth moment of a distribution is

$$\langle X^n \rangle = \sum_i x_i^n P(x_i)$$

for the discreet case and

$$\langle X^n \rangle = \int_{-\infty}^{\infty} x^n f_x(x)dx$$

for the continuous one.

Note A.13. We define the mean separately because of its significant role in physics. It can be otherwise easily observed that it is the first moment of a distribution.

For proofs and further reading see [18]

A.3 Matrix theory

Definition A.14. Let $\mathbb{F}$ be a field. For matrices $A \in \mathbb{F}^{m\times n}$, $B \in \mathbb{F}^{r\times s}$ Kronecker product $A \otimes B$ is defined as a matrix of dimension $mr \times ns$, which is written in the block form as:

$$A \otimes B = \begin{pmatrix} A_{1,1}B & A_{1,2}B & \cdots & A_{1,n}B \\ A_{2,1}B & A_{2,2}B & \cdots & A_{2,n}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1}B & A_{m,2}B & \cdots & A_{m,n}B \end{pmatrix}.$$

Note A.15. Kronecker product of matrices is bilinear, i.e.:

$$A \otimes (\alpha B + C) = \alpha(A \otimes B) + (A \otimes C)$$
$$(\alpha A + B) \otimes C = \alpha(A \otimes C) + (B \otimes C)$$

if the terms on the right sides are defined.

Theorem A.16. *Let x be an eigenvector of a matrix $A \in \mathbb{F}^{m\times m}$ with eigenvalue λ and y an eigenvector of a matrix $B \in \mathbb{F}^{n\times n}$ with eigenvalue μ. Than $x \otimes y \in \mathbb{F}^{mn\times 1}$ is the eigenvector of matrix $A \otimes B$ with eigenvalue $\lambda\mu$.*

Proof. We know that $Ax = \lambda x$ and $By = \mu y$. Using this we derive:

$$(A \otimes B)(x \otimes y) = Ax \otimes By = \lambda x \otimes \mu y = \lambda\mu x \otimes y\,.$$

□

For proofs and further reading see [13]

Appendix B

Numerical simulation

Coin operator

We use the kronecker product of two hadamard operators

In[75]:=
```
H = 1 / Sqrt[2] {{1, 1}, {1, -1}};
H2 = KroneckerProduct[H, H];
```

In[77]:=
```
MatrixForm[H2]
```

Out[77]//MatrixForm=

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Projectors, coin basis and position

We define a function which will be used to construct projectors

In[78]:=
```
pr[u_, v_] := Dot[Transpose[{u}], {v}];
```

We choose the basis of the coin space

In[79]:=
```
LL = {1, 0, 0, 0};
LR = {0, 1, 0, 0};
RL = {0, 0, 1, 0};
RR = {0, 0, 0, 1};
```

and corresponding projectors

In[83]:=
```
prLL = pr[LL, LL];
prLR = pr[LR, LR];
prRL = pr[RL, RL];
prRR = pr[RR, RR];
```

next we set the size of the lattice (the size will be 2num+1)

In[87]:=
```
num = 10;
```

contruction of the position description

In[88]:=
```
vhelp[x_] := Table[KroneckerDelta[x, i], {i, -num, num}];
```

In[89]:=
```
v[x_, y_] := Flatten[Table[vhelp[x][[i]] vhelp[y], {i, 1, 2 num + 1}]];
```

For illustration we show the unflatten version:

In[90]:=
```
MatrixForm[Table[vhelp[1][[i]] vhelp[0], {i, 1, 2 num + 1}]]
```

Out[90]//MatrixForm=
```
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

we see that the rows corresponds to the x coordinate and columns to the y one. (Please note that we use coordinates rotated by 45° to simplify the code as center of mass and relaitve momentum is used further on.)

Evolutuion operator and Fourier transformation

The first step to construct the evolution operator is to introduce the shift operator.
The projector we need to do so is

In[91]:=
```
prpo[x2_, y2_, x1_, y1_] := pr[v[x2, y2], v[x1, y1]];
```

The shift operator S is than

In[92]:=
```
S :=
  Sum[KroneckerProduct[prpo[x + 1, y, x, y], prRR], {x, -num, num - 1}, {y, -num, num}] +
   Sum[KroneckerProduct[prpo[x - 1, y, x, y], prLL], {x, -num + 1, num},
    {y, -num, num}] + Sum[KroneckerProduct[prpo[x, y - 1, x, y], prLR],
    {x, -num, num}, {y, -num + 1, num}] + Sum[
    KroneckerProduct[prpo[x, y + 1, x, y], prRL], {x, -num, num}, {y, -num, num - 1}] +
   Sum[KroneckerProduct[prpo[-num, y, num, y], prRR], {y, -num, num}] +
   Sum[KroneckerProduct[prpo[num, y, -num, y], prLL], {y, -num, num}] +
   Sum[KroneckerProduct[prpo[x, -num, x, num], prRL], {x, -num, num}] +
   Sum[KroneckerProduct[prpo[x, num, x, -num], prLR], {x, -num, num}];
```

The first four terms are the corresponding shifts and the last ones are boundary conditions as we use a circle for the simulation.
The construction of the evolution operator is then straightforward:

In[93]:=
```
U2 := S.KroneckerProduct[IdentityMatrix[(2 num + 1) ^2], H2];
```

Fourier transformation
First we define fourier transformation in one dimension. The two-dimensional will be the Kronecker product of two of those. The Fourier transformation acts only on the position space and so we extend it as usually to the whole space. We will also need the inverse Foureir transformation which is the adjoint one.

In[94]:=
```
F1D = Table[1 / Sqrt[2 num + 1] E^(2 I Pi n m / (2 num + 1)), {m, -num, num}, {n, -num, num}];
```

In[95]:=
```
F2D = KroneckerProduct[F1D, F1D];
```

In[96]:=
```
pF = KroneckerProduct[F2D, IdentityMatrix[4]];
```

In[97]:=
```
F = N[pF];
invF = N[Transpose[Conjugate[pF]]];
```

The evolution operator in the momentum picture will then be block diagonalised

In[99]:=
```
NUmom = Chop[F.N[U2].invF];
```

Finding ω(p,k)

We need to separate individual blocks from the momentum picture of the operator in correct order.

In[100]:=
```
block[x_, y_] :=
  Table[NUmom[[4 (2 num + 1) x + 4 y + i, 4 (2 num + 1) x + 4 y + j]], {i, 1, 4}, {j, 1, 4}];
```

The factor 2 num + 1 stems form the construction of the position describing vector.

We will now unwrap the circle and plot the arguments of the eigenvalues depending on the center of mass and relative momentum. We project the result to the center of mass and ω plain as well for later comparison. We want to generate a scatter plot for which we need a array of points with their coordinates. This will be done subsequently

In[101]:=
```
EigenPlot3D =
  ArrayFlatten[Join[Table[{2 Pi (-num + n) / (2 num + 1), 2 Pi (-num + m) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[2]]]]}, {n, 0, 2 num}, {m, 0, 2 num}],
    Table[{2 Pi (-num + n) / (2 num + 1), 2 Pi (-num + m) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[3]]]]}, {n, 0, 2 num}, {m, 0, 2 num}],
    Table[{2 Pi (-num + n) / (2 num + 1), 2 Pi (-num + m) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[4]]]]}, {n, 0, 2 num}, {m, 0, 2 num}],
    Table[{2 Pi (-num + n) / (2 num + 1), 2 Pi (-num + m) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[1]]]]}, {n, 0, 2 num}, {m, 0, 2 num}]], 1];
EigenPlot2D = ArrayFlatten[Join[Table[{2 Pi (-num + n) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[1]]]]}, {n, 0, 2 num}, {m, 0, 2 num}],
    Table[{2 Pi (-num + n) / (2 num + 1), N[Arg[Eigenvalues[block[n, m]][[2]]]]},
     {n, 0, 2 num}, {m, 0, 2 num}], Table[{2 Pi (-num + n) / (2 num + 1),
      N[Arg[Eigenvalues[block[n, m]][[3]]]]}, {n, 0, 2 num}, {m, 0, 2 num}],
    Table[{2 Pi (-num + n) / (2 num + 1), N[Arg[Eigenvalues[block[n, m]][[4]]]]},
     {n, 0, 2 num}, {m, 0, 2 num}]], 1];
```

Note that only thing that matters is that the blocks and thus ω match the corresponding coordinates, it is not important how the array is ordered.

In[103]:=
```
{ListPointPlot3D[EigenPlot3D, BoxRatios → {1, 1, 1},
  BoxStyle → Gray, Ticks → {{-Pi/2, 0, Pi/2}, {-Pi/2, 0, Pi/2}, {-Pi, 0, Pi}},
  AxesLabel → {"p", "k", "ω (p, k)"}],
 ListPlot[EigenPlot2D, PlotRange → All, Frame → True, AspectRatio → 1, Axes → False,
  FrameTicks → {{-Pi/2, 0, Pi/2}, {-Pi, 0, Pi}}, FrameLabel → {"p", "ω (p)"}]}
```

Interaction

The interaction take place only when the particles are on the same site, thus we will use a projector to this subspace:

In[104]:=
```
PrSame = Sum[prpo[x, 0, x, 0], {x, -num, num}];
```

We will also make use of some other projectors:

Projector to the antisymmetric subspace:

In[105]:=
```
PrAnti = pr[1/Sqrt[2] {0, -1, 1, 0}, 1/Sqrt[2] {0, -1, 1, 0}];
```

Projector to the symmetric subspace

In[106]:=
```
PrSym = pr[1/Sqrt[2] {0, 1, 1, 0}, 1/Sqrt[2] {0, 1, 1, 0}];
```

Projectors to LL and RR

Two distinguishable walkers

The evolution operator will be

In[107]:=
```
U2in = Dot[S, KroneckerProduct[IdentityMatrix[(2 num + 1)^2], H2] -
    2 KroneckerProduct[PrSame, H2]];
```

We perform the Fourier transformation which block-diagonalize the operator only for the center of mass momentum:

In[108]:=
```
NU2inimp = Chop[F.N[U2in].invF];
```

In[109]:=
```
blockin[p_] := Table[NU2inimp[[4 (2 num + 1) (num + p) + i, 4 (2 num + 1) (num + p) + j]],
   {i, 1, 4 (2 num + 1)}, {j, 1, 4 (2 num + 1)}];
```

In[110]:=
```
EigenPlotin =
  ArrayFlatten[Table[Table[{2 Pi i / (2 num + 1), Arg[Eigenvalues[blockin[i]][[j]]},
     {j, 1, 4 (2 num + 1)}], {i, -num, num}], 1];
```

In[111]:=
```
ListPlot[EigenPlotin, Axes → False, AspectRatio → 1, Frame → True,
 FrameTicks → {{-Pi/2, 0, Pi/2}, {-Pi, 0, Pi}}, FrameLabel → {"p", "ω (p)"}]
```

Fermions

We define the interaction Γ

In[112]:=
```
Γf = -PrAnti + PrSym + prLL + prRR;
```

The evolution operator

In[113]:=
```
U2in := Dot[U2, (KroneckerProduct[IdentityMatrix[(2 num + 1)^2], IdentityMatrix[4]] +
     KroneckerProduct[PrSame, Γf - IdentityMatrix[4]])];
```

In[114]:=
```
NU2inimp = Chop[F.N[U2in].invF];
```

In[115]:=
```
blockin[p_] := Table[NU2inimp[[4 (2 num + 1) (num + p) + i, 4 (2 num + 1) (num + p) + j]],
   {i, 1, 4 (2 num + 1)}, {j, 1, 4 (2 num + 1)}];
```

In[116]:=
```
EigenPlotfermi =
  ArrayFlatten[Table[Table[{2 Pi i / (2 num + 1), Arg[Eigenvalues[blockin[i]]][[j]]},
     {j, 1, 4 (2 num + 1)}], {i, -num, num}], 1];
```

In[117]:=
```
ListPlot[EigenPlotfermi, Axes → False, AspectRatio → 1 , Frame → True,
 FrameTicks → {{-Pi/2, 0, Pi/2}, {-Pi, 0, Pi}}, FrameLabel → {"p", "ω (p)"}]
```

Bosons

We define the interaction Γ

In[118]:=
```
rb = PrAnti - (PrSym + prLL + prRR);
```

The evolution operator

In[119]:=
```
U2in := Dot[U2, (KroneckerProduct[IdentityMatrix[(2 num + 1)^2], IdentityMatrix[4]] +
     KroneckerProduct[PrSame, rb - IdentityMatrix[4]])];
```

In[120]:=
```
NU2inimp = Chop[F.N[U2in].invF];
```

In[121]:=
```
blockin[p_] := Table[NU2inimp[[4 (2 num + 1) (num + p) + i, 4 (2 num + 1) (num + p) + j]],
   {i, 1, 4 (2 num + 1)}, {j, 1, 4 (2 num + 1)}];
```

In[122]:=
```
EigenPlotbos =
  ArrayFlatten[Table[Table[{2 Pi i / (2 num + 1), Arg[Eigenvalues[blockin[i]]][[j]]},
     {j, 1, 4 (2 num + 1)}], {i, -num, num}], 1];
```

In[123]:=
```
ListPlot[EigenPlotbos, Axes → False, AspectRatio → 1, Frame → True,
 FrameTicks → {{-Pi/2, 0, Pi/2}, {-Pi, 0, Pi}}, FrameLabel → {"p", "ω (p)"}]
```