Asymptotic Behavior of Decoherent and Interacting Quantum Walks

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Abstract

In this thesis we study the propagation behavior of quantum particles which perform discrete-time quantum walks on spatial lattices. By definition, quantum walks are discrete-time evolutions such that a single time step couples only neighboring lattice sites. Additionally, we assume in this thesis that the dynamical law commutes with all translations of the spatial lattice, that is we consider translationally invariant quantum walks. The results presented in the following are separated into two parts: The first part is devoted to the study of single-particle quantum walks, and in the second part we investigate quantum walks of several particles.

Single-particle quantum walks: Our aim is to study the asymptotic behavior of particles undergoing general translationally invariant quantum walks. Employing perturbation theory, we establish a direct method for computing the asymptotic distribution of the particle's position rescaled by an appropriate time-dependent factor. If the time evolution is implemented by a unitary operator commuting with all lattice translations and with empty pure point spectrum, we find linear scaling of the asymptotic position distribution. In this case, the asymptotic distribution of position divided by time is determined by the analog of the group velocity. If, on the other hand, the quantum walk is subject to decoherence, we expect that it behaves like a classical random walk. We provide explicit criteria under which this intuitive statement is true, that is, the asymptotic scaling of the particle's position distribution is that of a diffusion process. We find that the asymptotic distribution of position divided by the square root of time is a mixture of Gaussians in this case. However, we also provide examples of decoherent quantum walks which violate these criteria, and exhibit linear scaling of the asymptotic position distribution.

Many-particle quantum walks: We investigate unitary quantum walks of two particles with collisional interactions. That is, the particles perform independent single-particle quantum walks if they are at distinct lattice sites, and an interaction takes place if both particles occupy the same lattice site. We prove that such quantum walks generically exhibit a molecular binding effect between the particles. More precisely, for a measurement of the particles' positions we have a bound on the probability to obtain a certain result which decays exponentially with the particles' distance. As a preparatory step for this analysis, we consider single-particle quantum walks with point defects, and provide a method to compute their eigenvalues in the spectral gap of the quantum walk without defect. We further generalize our model to arbitrary numbers of particles and study the behavior of local excitations in many-particle quantum walks.

Keywords: quantum walk, decoherence, interaction

Zusammenfassung

Die vorliegende Dissertation behandelt die Propagationseigenschaften von Quantenteilchen welche in konstanten Zeitschritten auf räumlichen Gittern einen Quantenwalk vollführen. Definitionsgemäß verstehen wir als Quantenwalk eine zeitlich diskrete Entwicklung welche in einem einzigen Zeitschritt nur benachbarte Gitterplätze koppelt. Zusätzlich nehmen wir in dieser Arbeit an, dass die Dynamik mit allen Translationen des räumlichen Gitters vertauscht, d.h. wir betrachten translationsinvariante Quantenwalks. Die im Folgenden präsentierten Ergebnisse sind in zwei Abschnitte aufgeteilt: Im ersten Teil behandeln wir Ein-Teilchen Quantenwalks und betrachten Quantenwalks mehrerer Teilchen im zweiten Teil.

Ein-Teilchen Quantenwalks: Unser Ziel ist das asymptotische Verhalten eines Teilchens welches einen beliebigen translationsinvarianten Quantenwalk vollführt zu studieren. Basierend auf Ergebnissen der Störungstheorie entwickeln wir eine Methode um die asymptotische Verteilung des zeitabhängig skalierten Teilchenortes zu berechnen. Für Quantenwalks welche durch einen translationsinvarianten unitären Operator ohne Punktspektrum beschrieben werden zeigen wir dass die asymptotische Ortsverteilung linear skaliert. In diesem Fall ist die asymptotische Verteilung des Teilchenortes geteilt durch die Zeit durch das Analogon zur Gruppengeschwindigkeit bestimmt. Wird der betrachtete Quantenwalk hingegen durch einen dekohärenten Prozess beschrieben, so erwarten wir ein Verhalten ähnlich dem eines klassischen Random Walk. Wir geben explizite Kriterien an unter denen diese intuitive Aussage wahr ist, sodass die Ortsverteilung des Teilchens asymptotisch wie ein Diffusionsprozess skaliert. Wir zeigen dass in diesem Fall die asymptotische Verteilung des Teilchenortes geteilt durch die Wurzel der Zeit durch eine Mischung Gaußscher Funktionen gegeben ist. Weiterhin konstruieren wir Beispiele dekohärenter Quantenwalks welche diese Kriterien verletzen und lineare Skalierung der asymptotischen Ortsverteilung zeigen.

Viel-Teilchen Quantenwalks: Wir studieren unitäre Quantenwalks zweier Teilchen mit Kollisionswechselwirkungen. Befinden sich beide Teilchen auf verschiedenen Gitterplätzen so vollführen sie unabhängig voneinander einen unitären Ein-Teilchen Quantenwalk, wohingegen bei Kollision an einem Gitterplatz eine Wechselwirkung stattfindet. Wir zeigen dass solche Quantenwalks im allgemeinen einen molekularen Bindungseffekt zeigen. Dieser zeigt sich dadurch, dass bei einer Ortsmessung die Wahrscheinlichkeit für ein bestimmtes Resultat exponentiell mit dem Abstand beider Teilchen abfällt. Als vorbereitenden Schritt analysieren wir Ein-Teilchen Quantenwalks mit Punktstörungen und entwickeln eine Methode um Eigenwerte in der spektralen Lücke des Quantenwalk ohne Defekt zu berechnen. Weiterhin verallgemeinern wir unser Modell auf den Fall beliebiger Teilchenzahlen und studieren das Verhalten lokaler Anregungen in Viel-Teilchen Quantenwalks.

Schlagwörter: Quantenwalk, Dekohärenz, Wechselwirkung

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1. Notation

In the following we list some notation we are going to use throughout this thesis.

$\langle .\|. \rangle$	scalar product
$\|\|.\|\|$	Hilbert space norm
$\|\|.\|\|_{op}$	operator norm
$\|\|.\|\|_1$	trace norm
$\|.\|_\infty$	maximum norm of vectors
$\|.\|_1$	ℓ^1-norm of vectors
$\|.\|$	modulus of a number
$\otimes$	tensor product
$\oplus$	direct sum
∇_p	gradient with respect to p
$[.,.]$	commutator
$\mathbb{1}$	identity operator
id	identity map

$\mathcal{B}(\mathcal{H})$	bounded operators on Hilbert space $\mathcal{H}$
$\mathbb{C}$	complex numbers
δ_{xy}	Kronecker-delta
$\text{dist}(z, X)$	distance of $z \in \mathbb{C}$ to set $X \subset \mathbb{C}$
$\mathbb{E}(.)$	expectation value
$\ell^2(\mathbb{Z})$	square-summable sequences $\{c_x\}_{x\in\mathbb{Z}^s}$, $c_x \in \mathbb{C}$
$\mathcal{L}^1(\mathbb{R}^s)$	functions f from $\mathbb{R}^s$ to $\mathbb{C}$ such that $\|f\|$ is integrable
$\mathcal{L}^2(s, \mathcal{K})$	square-integrable functions from $\mathbb{R}^s$ to $\mathcal{K}$
$\mathcal{L}^\infty(\Gamma)$	bounded functions on Γ
$\mathcal{L}(\mathcal{H})$	linear operators on Hilbert space $\mathcal{H}$
$\mathbb{N}$	natural numbers without zero
$\mathbb{N}_0$	$\mathbb{N}_0 = \mathbb{N} \cup \{0\}$
$\mathcal{O}(.), o(.)$	big- and little-o notation
$\text{Prob}(A)$	probability for the event A to occur
$\mathbb{R}$	real numbers
$\mathbb{S}$	$\mathbb{S} = \{z \in \mathbb{C} : \|z\| = 1\}$
$\mathcal{SU}(\mathcal{K})$	special unitary group on finite dimensional Hilbert space $\mathcal{K}$

$\sigma_0, \sigma_1, \sigma_2, \sigma_3$	Pauli-operators
tr	trace of an operator
$\mathcal{T}(\mathcal{H})$	trace-class operators on Hilbert space $\mathcal{H}$
$\mathcal{U}(\mathcal{H})$	unitary operators on Hilbert space $\mathcal{H}$
$\mathbb{Z}$	integer numbers
$\mathbb{Z}_d$	$\mathbb{Z}_d = \{1, \ldots, d\}$

2. Motivation

In the following chapters we study the propagation behavior of translationally invariant discrete-time quantum walks on infinite lattices of arbitrary dimensions. However, before we deepen the analysis of discrete-time quantum walks, we illustrate the concept of general quantum walks in the subsequent paragraphs.

The origin of quantum walks is at least two-fold, we can either regard them as quantum counterpart of random walks, or as a discretized version of a quantum particle's time evolution. Both points of view attracted a lot of attention, the first because random walks provide a versatile framework for the study of processes with inherent randomness. Moreover, random walks are also successfully used to study large deterministic systems by describing complex behavior through a random process. Indeed, applications of random walks range from modeling the movement of animals, micro-organisms, and cells [CPB08], to the simulation of the stock market [Fam65], or algorithmic analysis of the world wide web [HHMN99] as well as social networks [BL11]. An intuitive interpretation of a random walk is that of a particle hopping on a spatial structure, e.g. a discrete graph or some continuous space such as $\mathbb{R}^s$. If the time interval in between two jumps of the particle is constant this is called a discrete-time random walk. However, this time interval can be a random variable as well. In this case we have to describe the movement of the particle by a continuous time parameter, and such time evolutions are called continuous-time random walks. For both models quantum generalizations have been introduced, see e.g. [ADZ93] and [FG98], and, not surprisingly, quantum walks quickly found applications as well. In fact, quantum walks can even outperform random walks in algorithms for searching [SKW03, CG04], oracle problems [CCD$^+$03], and are even proven to be universal for quantum computation [Chi09, LCE$^+$10].

The second perspective, which is to consider quantum walks as quantum mechanical time evolutions that happen in discrete steps, focuses on the fundamental differences between classical and quantum mechanical dynamical systems evolving in discrete time steps. In fact, quantum walks constitute a rich platform for the simulation of quantum mechanical phenomena such as Anderson localization [JM10, ASW11, KLMW07], Klein's paradox [Mey97a, Kur08], Landau-Zener tunneling [RBH$^+$11], and topological phases [KRBD10]. Some of these effects can be understood as being inherited from particular dynamics in continuous space and time via an appropriate continuum limit of the quantum walk. For instance, it has been shown that such a limit construction may yield the Dirac, Klein-Gordon, or Weyl equation [BB94, Str06, CBS10]. Naturally, this triggered an immense effort to im-

plement quantum walks experimentally. Successful realizations of quantum walks have been reported with neutral atoms [KFC+09], trapped ions [SMS+09, ZKG+10], and photons in optical fibers [SCP+10].

Of course, any experimental implementation of a quantum walk is subject to decoherence since complete isolation of the system from its environment is an idealization which cannot be realized. For small time scales the decoherence might be negligible, but physical intuition suggests that ultimately decoherence will force the suppression of quantum effects. In other words, we expect that a quantum walk subject to decoherence will behave like a diffusion process in the long-time limit. This intuition has been confirmed by numerous authors investigating particular decoherence models for quantum walks. However, although the quantum walk introduced by Aharonov et al. [ADZ93] includes measurement induced decoherence, it nevertheless shows faster propagation in comparison to random walks. Later it was even found that a small amount of decoherence may enhance properties of quantum walks which are useful for algorithmic applications [KT03]. It is hence desirable to understand the influence of general decoherence mechanisms on quantum walks. This is achieved in the first part of this thesis by establishing a method to study the asymptotic behavior of discrete-time decoherent quantum walks on infinite lattices.

In the second part of this thesis we treat quantum walks involving many particles. The growing complexity of the system with the number of particles and interactions between these particles opens new perspectives for applications. It has been pointed out recently that many-particle quantum walks are of potential use for quantum algorithms [RSŠ+12, RGW+12]. If the interactions between the particles performing the quantum walk can be engineered in a controllable way, the system is essentially a quantum simulator, and we may study other complex many-body quantum systems by means of quantum walks. In fact, even quantum walks with only two particles already exhibit interesting many-particle dynamics. For example, it has been shown in [AAM+12] that two-particle quantum walks with interactions can display a molecular binding effect between the particles, and experiments which confirm the prediction of this effect have been conducted by Schreiber et al. [SGR+12]. These quantum walks are unitary and time is discretized, hence we cannot describe the dynamical behavior of the system by a unique Hamiltonian. This implies that the quasi-energy of the two particles is only defined modulo a constant. Consequently, this binding effect cannot be explained by an attractive potential, but is rather an interference effect.

The remaining part of this thesis is organized as follows: In Chapter 3 we introduce basic concepts which are necessary for subsequent chapters. The first part of our analysis, which is presented in Chapter 4, treats the asymptotic behavior of single-particle quantum walks. Subsequently, in Chapter 5, we study propagation effects of quantum walks involving several particles. Chapters 4 and 5 can be read

independently, and both chapters have their own introductory sections and concluding remarks.

3. Preliminaries

This chapter provides introductory material for several topics of principal interest for later parts of this thesis. We start with a brief account of the basic concepts of quantum theory. Subsequently, we turn our attention to the Fourier transform on Hilbert spaces of the form $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$, and we focus on translationally invariant bounded operators on $\mathcal{H}$. In the third section of this chapter we give a short introduction to the spectral theory of unitary operators. We close this chapter with a survey on the perturbation theory of analytic families of bounded linear operators.

3.1. Quantum theory in a nutshell

In this section we introduce the basic concepts underlying quantum mechanics as far as needed in this thesis. To begin with, let us introduce some notation. In the following we denote vectors in a Hilbert space $\mathcal{H}$ by greek letters, e.g. $\psi \in \mathcal{H}$, and we use Dirac notation for certain operators on $\mathcal{H}$, for instance $|\phi\rangle\langle\psi| \in \mathcal{L}(\mathcal{H})$ for $\phi, \psi \in \mathcal{H}$. The symbol $\mathcal{L}(\mathcal{H})$ stands for the set of all linear operators on $\mathcal{H}$, and since $\mathcal{H}$ is a Hilbert space, $A \in \mathcal{L}(\mathcal{H})$ defines an adjoint operator, which we denote by $A^* \in \mathcal{L}(\mathcal{H})$. For the sets of all bounded and unitary operator on $\mathcal{H}$ we use the notation $\mathcal{B}(\mathcal{H})$ and $\mathcal{U}(\mathcal{H})$, respectively.

A physical system is specified by a separable Hilbert space $\mathcal{H}$, and states on the system are described by positive and normalized trace-class operators ρ, which we also call density operators for short. The state space of $\mathcal{H}$ will be denoted by

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{T}(\mathcal{H}) : \rho > 0, \operatorname{tr}\rho = 1\}, \tag{3.1}$$

where $\mathcal{T}(\mathcal{H})$ denotes the trace-class operators on $\mathcal{H}$. A state $\rho \in \mathcal{S}(\mathcal{H})$ is called pure iff it satisfies $\rho^2 = \rho$, in which case ρ is a rank-one projector on $\mathcal{H}$, i.e. there exists a vector $\psi \in \mathcal{H}$ such that $\rho = |\psi\rangle\langle\psi|$. States for which $\rho^2 \neq \rho$ are called mixed states, which can be written as $\rho = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k|$ with positive numbers $\lambda_k < 1$ summing up to one and pairwise orthogonal vectors $\psi_k \in \mathcal{H}$.

We identify measurements of physical quantities, performed on a system $\mathcal{H}$, with positive operator valued measures, POVMs for short. Mathematically, a POVM is a map F, assigning to each element A in the σ-algebra Σ of a set X a positive operator $F(A)$ on $\mathcal{H}$. Moreover, F is countably additive, i.e. for disjoint sets $A_n \in \Sigma$ we have $F(\cup_n A_n) = \sum_n F(A_n)$, and it satisfies the normalization condition $F(X) = \mathbb{1}$. The set

X represents the possible measurement outcomes, and the probability to obtain a result from the set $A \in \Sigma$ when measuring F on a state ρ is given by $\operatorname{tr} F(A)\rho$. A particular subclass of all POVMs is the set of projection valued measures, PVMs for short. A PVM P takes values in the set of orthogonal projections on $\mathcal{H}$, i.e. for each $A \in \Sigma$ the operator $P(A)$ is an orthogonal projection. Since P is countably additive and projection valued, it fulfills $P(A)P(B) = P(B)P(A) = 0$ for disjoint $A, B \in \Sigma$. Such measures are also known as spectral measures, cf. Definition 3.3.2. A particular example of a PVM which we consider in Chapter 4 is the position measurement of a quantum particle with system Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$. Here, the first subsystem $\ell^2(\mathbb{Z}^s)$ represents the position, while $\mathcal{K}$ is identified with some internal degrees of freedom. More precisely, the position of the particle is defined by choosing an orthonormal basis $\{|x\rangle\}_{x\in\mathbb{Z}^s}$ in $\ell^2(\mathbb{Z}^s)$, and the corresponding PVM is defined by $X = \mathbb{Z}^s$ with the σ-algebra of all subsets of X and $P(x) = |x\rangle\langle x| \otimes \mathbb{1}_{\mathcal{K}}$ for $x \in \mathbb{Z}^s$. Commonly, X is a subset of $\mathbb{R}^n$, such that the expectation value of the POVM F is well-defined[1]. Then we may construct the operator valued vector $\mathcal{F} = \int_{x\in X} xF(x)$ and the expectation value in state ρ is given by $\langle F\rangle_\rho = \operatorname{tr} \mathcal{F}\rho$, cf. the spectral theorem for self-adjoint operators [Tes09].

In the coming parts of this thesis we study time evolutions of quantum systems which happen in discrete steps. Such a time evolution can be formulated in two equivalent ways, we can either regard it as a transformation of the states of $\mathcal{H}$ or as a transformation of the measurement operators. The first point of view, known as the Schrödinger picture, corresponds to a linear map T_* on $\mathcal{S}(\mathcal{H})$[2]. In the Heisenberg picture, which is the second point of view, the time evolution is represented by a linear map T on the set of POVMs on $\mathcal{H}$. By linearity, both T_* and T extend to maps on $\mathcal{T}(\mathcal{H})$ and $\mathcal{B}(\mathcal{H})$, respectively. They are equivalent representations of the same physical transformation if and only if all probabilities for measurement operators $F(A)$ and states ρ coincide after application of T and T_*, respectively. Hence, the representations in Heisenberg and Schrödinger picture are connected by the duality relation

$$\operatorname{tr}(T_*(\rho)A) = \operatorname{tr}(\rho\, T(A)), \quad \forall \rho \in \mathcal{S}(\mathcal{H}), A \in \mathcal{B}(\mathcal{H}) \tag{3.2}$$

In order to represent physical transformations, the maps T_* and T have to satisfy certain properties. Both have to be completely positive, that is, the extended maps $T_* \otimes \mathrm{id}_n$ and $T \otimes \mathrm{id}_n$, where id_n denotes the identity map on n-dimensional matrices, preserve positivity of operators. Additionally, it is often assumed that the quantum channel always generates an output state when it is fed with a state of the input system. Mathematically, this is expressed by the assumption that T_* is trace-preserving, i.e. $\operatorname{tr} T_*(\rho) = \operatorname{tr}\rho$ for all $\rho \in \mathcal{T}(\mathcal{H})$, and T is unital, that is $T(\mathbb{1}) = \mathbb{1}$. Note

[1] If $\mathcal{H}$ is e.g. the Fock-space of different species of particles and F represents a measurement of the particle-type, there is no notion of an expectation value for F.

[2] We only consider time evolutions where input and output are represented by identical quantum systems.

that one property is a consequence of the other together with the duality relation (3.2).

We will mostly consider the time evolution of quantum systems in the Heisenberg picture, and the following definition singles out the linear maps on $\mathcal{B}(\mathcal{H})$ representing physical transformations of the system, which we refer to as quantum channels.

Definition 3.1.1. *A quantum channel T on a Hilbert space $\mathcal{H}$ is a completely positive and unital map on $\mathcal{B}(\mathcal{H})$.*

There are several useful representation theorems for quantum channels, the most prominent one by Stinespring [Sti55]. We present a version of this theorem for quantum channels T which are defined on all of $\mathcal{B}(\mathcal{H})$. For a more general statement which also covers the case where T is only defined on a subset of $\mathcal{B}(\mathcal{H})$ see [Pau02].

Theorem 3.1.2. *Each quantum channel T on $\mathcal{H}$ can be written as*

$$T(A) = \mathcal{V}^*(A \otimes \mathbb{1}_{\mathcal{D}})\mathcal{V} \quad , \forall A \in \mathcal{B}(\mathcal{H}), \tag{3.3}$$

where $\mathcal{V} : \mathcal{H} \to \mathcal{H} \otimes \mathcal{D}$ is an isometry, i.e. $\mathcal{V}^*\mathcal{V} = \mathbb{1}_{\mathcal{H}}$. The Hilbert space $\mathcal{D}$ is called the dilation space for T.

The Stinespring representation is essentially unique if $\mathcal{D}$ is chosen minimal. That is, if $\mathcal{D}$ is chosen such that the closure of $\{(A \otimes \mathbb{1}_{\mathcal{D}})\mathcal{V}\psi \,:\, A \in \mathcal{B}(\mathcal{H}), \psi \in \mathcal{H}\}$, equals $\mathcal{H} \otimes \mathcal{D}$, then any two isometries $\mathcal{V}_1$ and $\mathcal{V}_2$ satisfying Equation (3.3) are related by a unitary operator U on $\mathcal{D}$ via $(\mathbb{1}_{\mathcal{H}} \otimes U)\mathcal{V}_1 = \mathcal{V}_2$.

By choosing an orthonormal basis $\{e_i\}_i$ in $\mathcal{D}$ and writing $\mathbb{1}_{\mathcal{D}} = \sum_i |e_i\rangle\langle e_i|$ we immediately get the Kraus representation [Kra83] of a quantum channel T.

Corollary 3.1.3. *Let T be a quantum channel on the separable Hilbert space $\mathcal{H}$. From any orthonormal basis $\{e_i\}_i$ of $\mathcal{D}$ we get a representation of T of the form*

$$T(A) = \sum_i K_i^* A K_i \quad \forall A \in \mathcal{B}(\mathcal{H}),$$

with $K_i \in \mathcal{B}(\mathcal{H})$, and the relation between the K_i and the isometry $\mathcal{V}$ is

$$\langle \phi | K_i \psi \rangle = \langle \phi \otimes e_i | \mathcal{V}\psi \rangle \quad \phi, \psi \in \mathcal{H}.$$

3.2. Fourier transform and momentum space

In the following we provide some background on translationally invariant operators acting on a Hilbert space $\mathcal{H}$ with lattice structure, by which we mean that the

underlying Hilbert space is a tensor product $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$. Here, $\mathcal{K}$ is assumed to be a finite dimensional Hilbert space, i.e. $\mathcal{K} \cong \mathbb{C}^d$. The idea is to consider vectors $\psi \in \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ as $\mathcal{K}$-valued functions on $\mathbb{Z}^s$ and apply the Fourier transform to these functions. More precisely, we consider $\psi = \sum_{x \in \mathbb{Z}^s} |x\rangle \otimes \psi_x$ as a function $\psi : x \mapsto \psi_x$ and map ψ to a function on $[-\pi, \pi)^s$ via

$$(\mathcal{F}\psi)(p) := \sum_{x \in \mathbb{Z}^s} \psi_x e^{\mathrm{i}x \cdot p} . \tag{3.4}$$

We will refer to p as the momentum variable and the space of vector-valued functions $(\mathcal{F}\psi)$ is called momentum space. A linear map acting on vectors ψ may be converted to a linear map acting on the corresponding functions $(\mathcal{F}\psi)$. This induces a Fourier transform on the level of operators on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$, and the benefit of our approach is that operators which are invariant under all translations of the lattice $\mathbb{Z}^s$ have a simple Fourier transformed version, see Lemma 3.2.2.

To begin with, we note some basic properties and relations regarding the map $\mathcal{F}$ defined in Equation (3.4). By $\mathcal{L}^2(s, \mathcal{K})$ we denote the $\mathcal{K}$-valued functions on $[-\pi, \pi)^s$ which are square-integrable with respect to Lebesgue measure. This means $\widehat{\psi} \in \mathcal{L}^2(s, \mathcal{K})$ is a function $p \mapsto \widehat{\psi}(p) \in \mathcal{K}$, which satisfies

$$\frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \left\| \widehat{\psi}(p) \right\|_{\mathcal{K}}^2 < \infty . \tag{3.5}$$

To be precise, the elements of $\mathcal{L}^2(s, \mathcal{K})$ are equivalence classes of square-integrable functions on $[-\pi, \pi)^s$ with respect to the semi-norm induced by the integral in (3.5). In fact, this semi-norm is generated by the sesqui-linear form

$$\langle \widehat{\psi} | \widehat{\phi} \rangle_{\mathcal{L}^2} = \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \langle \widehat{\psi}(p) | \widehat{\phi}(p) \rangle_{\mathcal{K}} \tag{3.6}$$

and hence $\mathcal{L}^2(s, \mathcal{K})$ is a Hilbert space which is isomorphic to $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$.

Lemma 3.2.1. *The Fourier transform* (3.4) *is a unitary map from $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ to $\mathcal{L}^2(s, \mathcal{K})$. That is, $\mathcal{F}$ is invertible and*

$$\langle \phi | \psi \rangle_{\mathcal{H}} = \langle \mathcal{F}\psi | \mathcal{F}\phi \rangle_{\mathcal{L}^2} . \tag{3.7}$$

The inverse map $\mathcal{F}^{-1}$ is defined via

$$\psi_x = \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \, e^{-\mathrm{i}x \cdot p} (\mathcal{F}\psi)(p) . \tag{3.8}$$

Proof. For $\mathcal{K}=\mathbb{C}$ the statement is well-known in Fourier-analysis. Equation (3.7) is a simple generalization of Parseval's theorem to vector-valued functions and Equation (3.8) also emerges from the case $\mathcal{K}=\mathbb{C}$ in a straightforward way. □

Due to Lemma 3.2.1 there is a one-to-one correspondence between vectors $\psi \in \ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ and elements $\widehat{\psi}$ in $\mathcal{L}^2(s,\mathcal{K})$. Hence, a vector $\psi \in \ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ may be regarded as a representative of an equivalence class of functions in $\mathcal{L}^2(s,\mathcal{K})$ via Equation (3.4), and vice versa. To shorten notation we will from now on often write $\psi(p)$ instead of $(\mathcal{F}\psi)(p)$ and keep in mind that a representative $\psi(p)$ uniquely determines ψ.

The Fourier transform $\mathcal{F}:\psi\mapsto(\mathcal{F}\psi)$ induces a map $A\mapsto\mathcal{F}A\mathcal{F}^{-1}$ on the space of linear operators $\mathcal{L}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$. In a slight abuse of terminology we will also refer to this map as Fourier transform. A simple example is a rank one operator $A=|\phi\rangle\langle\psi|$ for which we get using Equation (3.6)

$$A\eta=\langle\psi|\eta\rangle\cdot\phi \quad\Leftrightarrow\quad (A\eta)(p)=\phi(p)\frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p'\langle\psi(p')|\eta(p')\rangle_{\mathcal{K}},$$

and hence $\mathcal{F}A\mathcal{F}^{-1}$ is defined by the operator-valued integral kernel $|\phi(p)\rangle\langle\psi(p')|$. In fact, Schwartz's kernel theorem assures that bounded operators A on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ can be represented on momentum space by integral operators $A(p,p')$ via

$$\mathcal{F}A\mathcal{F}^{-1}\psi(p)=(A\psi)(p)=\int\limits_{[-\pi,\pi)^s} d^s p' A(p,p')\psi(p').$$

As we will see below, the integral kernel $A(p,p')$ may have to be taken in the distributional sense, by which we mean that the integral kernel does not exist as integrable function but as a generalized function or distribution. A case where this generically happens is when the operator A commutes with translations of the lattice $\mathbb{Z}^s$. Such a translation by $x\in\mathbb{Z}^s$ is represented by a unitary operator $\mathcal{T}_x$ acting on $\mathcal{H}$ defined via

$$(\mathcal{T}_x\psi)_y=\psi_{y-x}. \tag{3.9}$$

The Hilbert space $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ is isomorphic to $\ell^2(\mathbb{Z})^{\otimes s}\otimes\mathcal{K}$ and hence $\mathcal{T}_x$ can be written in terms of elementary translations

$$\mathcal{T}_x=t_1^{x_1}\otimes\ldots\otimes t_s^{x_s}\otimes\mathbb{1}_{\mathcal{K}} \quad\text{for}\quad x=(x_1,\ldots,x_s)\in\mathbb{Z}^s \tag{3.10}$$

where each t_i is isomorphic to a translation operator on $\ell^2(\mathbb{Z})$. An operator A on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ may be translated by a lattice vector $x\in\mathbb{Z}^s$ via

$$\tau_x(A)=\mathcal{T}_x A\mathcal{T}_x^* \tag{3.11}$$

and the following lemma concerns operators A which are invariant with respect to τ_x.

Lemma 3.2.2. *For bounded operators A on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ the following statements are equivalent:*

i) A is translationally invariant, that is, $\tau_x(A)=A$ for all $x\in\mathbb{Z}^s$.

ii) The integral kernel $A(p,p')$ corresponding to $\mathcal{F}A\mathcal{F}^{-1}$ is a multiplication operator, that is, $(A\phi)(p)=A(p)\phi(p)$.

Proof. If $i)$ is true, i.e. A is translationally invariant, the action of A is completely determined by the images of vectors $|0\rangle\otimes\psi_0$. Indeed, let A_{xy} be the operator on $\mathcal{K}$ defined by

$$\langle\phi_x|A_{xy}|\psi_y\rangle=\langle x\otimes\phi_x|A|y\otimes\psi_y\rangle\quad\forall\,\phi_x,\psi_y\in\mathcal{K},$$

then translation invariance implies $A_{x,y}=A_{x-y,0}$ and it is straightforward to see that the Fourier transform $\mathcal{F}A\mathcal{F}^{-1}$ coincides with the $\dim\mathcal{K}$-dimensional matrix

$$A(p)=\sum_{x\in\mathbb{Z}^s}e^{\mathrm{i}x\cdot p}A_{x,0}\,.$$

If, on the other hand, the integral kernel corresponding to A is a multiplication operator, one verifies directly that A is translationally invariant by observing that $\mathcal{T}_x$ acts in momentum space by multiplication with $e^{\mathrm{i}x\cdot p}\,\mathbb{1}_{\mathcal{K}}$. □

Considered as bivariate integral kernel, $A(p,p')$ has to be considered in the distributional sense if A is translationally invariant. However, the multiplication operator $A(p)$ exists as ordinary function since its matrix elements are given by uniformly convergent and bounded Fourier series.

Lemma 3.2.3. *Let A be a translationally invariant bounded operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. The multiplication operator $A(p)$ is a $\dim\mathcal{K}$-dimensional matrix with uniformly continuous matrix elements and $\|A\|_{op}=\max\limits_{p\in[-\pi,\pi)^s}\big\|A(p)\big\|_{op}$.*

Proof. We use once again the expansion

$$A(p)=\sum_{x\in\mathbb{Z}^s}e^{\mathrm{i}x\cdot p}A_{x,0}\,,$$

and note that for A to be bounded we must have

$$\sum_{\|x\|>r}\big\|A_{x,0}\psi\big\|_{\mathcal{K}}^2\to 0$$

for $r\to\infty$ and all $\psi\in\mathcal{K}$. Hence, for $\varepsilon>0$ and $\psi\in\mathcal{K}$ there exists $r_{\varepsilon,\psi}\in\mathbb{N}$ such that $\sum_{\|x\|>r_{\varepsilon,\psi}}\big\|A_{x,0}\psi\big\|^2<\varepsilon$. Since $\mathcal{K}$ is finite-dimensional we can use a compactness argument to prove the existence of $R_\varepsilon\in\mathbb{N}$ such that $r_{\varepsilon,\psi}<R_\varepsilon$ for all normalized

$\psi \in \mathcal{K}$. This already implies uniform convergence of the Fourier series for $A(p)$, which entails that $A(p)$ is uniformly continuous on $[-\pi,\pi)^s$.

To verify the formula for the operator norm of A we first note that

$$\|A\|_{op} \leq \max_{p\in[-\pi,\pi)^s} \left\|A(p)\right\|_{op}$$

since we have the inequality

$$\begin{aligned} \left\|A\psi\right\|_{\mathcal{H}}^2 &= \frac{1}{(2\pi)^s}\int_{[-\pi,\pi)^s} \left\|A(p)\psi(p)\right\|_{\mathcal{K}}^2 \\ &\leq \max_{p\in[-\pi,\pi)^s} \left\|A(p)\right\|^2 \frac{1}{(2\pi)^s}\int_{[-\pi,\pi)^s} \left\|\psi(p)\right\|^2 . \end{aligned}$$

On the other hand, there exists $p_* \in [-\pi,\pi)^s$ such that $\left\|A(p_*)\right\| = \max_{p\in[-\pi,\pi)^s} \left\|A(p)\right\|_{op}$, and for $\varepsilon > 0$ we can construct a vector ψ whose momentum distribution is peaked around p_* and satisfies $\left|\left\|A\psi\right\| - \max_{p\in[-\pi,\pi)^s} \left\|A(p)\right\|_{op}\right| < \varepsilon$. □

It is well-known that the set of all linear operators on a finite dimensional Hilbert space constitutes a Hilbert space with respect to the Hilbert-Schmidt scalar product. However, for infinite dimensional Hilbert spaces this scalar product is only well-defined for Hilbert-Schmidt class operators. Translationally invariant operators are rarely trace class, but there is another construction to turn the set of all translationally invariant bounded operators on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, which we denote by $\mathcal{T}_{\mathcal{K},s}$, into a Hilbert space. Let $A, B \in \mathcal{T}_{\mathcal{K},s}$ and denote their Fourier transforms, which, by Lemma 3.2.2, are multiplication operators, by $A(p)$ and $B(p)$. On these operators we define the sesqui-linear form

$$\langle A|B\rangle = \frac{1}{(2\pi)^s}\int_{[-\pi,\pi)^s} d^s p\, \frac{1}{\dim\mathcal{K}} \mathrm{tr}_{\mathcal{K}} A(p)^* B(p). \tag{3.12}$$

It is straightforward to see that Equation (3.12) is positive definite on $\mathcal{T}_{\mathcal{K},s}$, so, in fact, it defines a scalar product on $\mathcal{T}_{\mathcal{K},s}$.

Lemma 3.2.4. *The set of all translationally invariant bounded operators on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, denoted by $\mathcal{T}_{\mathcal{K},s}$, is a Hilbert space with scalar product* (3.12).

Proof. Clearly, Equation (3.12) defines a scalar product on $\mathcal{T}_{\mathcal{K},s}$. Now suppose the elements $A_n(p)$ constitute a Cauchy sequence in $\mathcal{T}_{\mathcal{K},s}$, i.e. the matrix elements of $A_n(p)$ converge in quadratic mean to square integrable functions. Clearly, the operator defined by these functions induces a translationally invariant bounded operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, hence, $\mathcal{T}_{\mathcal{K},s}$ is complete with respect to Equation (3.12). □

In the proof of Lemma 3.2.2 we already used that translationally invariant operators $A \in \mathcal{T}_{\mathcal{K},s}$ are fully characterized by their matrix elements at the origin, i.e. if we expand A in position basis as $A = \sum_{x,y\in\mathbb{Z}^s} |x\rangle\langle y| \otimes A_{x,y}$ with $A_{x,y} \in \mathcal{B}(\mathcal{K})$ then $A_{x,y} = A_{x-y,0}$. The corresponding multiplication operator in Fourier space is now given by $A(p) = \sum_{x\in\mathbb{Z}^s} e^{\mathrm{i}p\cdot x} A_{x,0}$ and therefore we get the alternative expression

$$\langle A|B\rangle = \tfrac{1}{\dim\mathcal{K}} \sum_{x\in\mathbb{Z}^s} \operatorname{tr}_{\mathcal{K}} A^*_{x0} B_{x0} \tag{3.13}$$

for the scalar product (3.12). We denote the norm on $\mathcal{T}_{\mathcal{K},s}$ induced by this scalar product by $\|.\|$, thus, $\|A\|^2 = \langle A|A\rangle$ for all $A \in \mathcal{T}_{\mathcal{K},s}$.

Of course, there are large classes of operators, e.g. density operators, which fail to be translationally invariant. As stated before, the integral kernel corresponding to a general bounded operator A may only exist in the distributional sense. However, for certain classes of operators, e.g. all compact operators, the integral kernels $A(p,p')$ are well-described by integrable functions. An important subset of all compact operators is the set of all trace-class operators. Consequently, density operators are described by integrable functions as integral kernels. In fact, if a density operator is supported on a finite subset of the lattice $\mathbb{Z}^s$, its integral kernel is just a Fourier polynomial. Given the integral kernels of an observable A and a density operator ρ it is easy to compute their expectation value.

Lemma 3.2.5. *Let ρ be a trace-class operator and A a bounded operator with corresponding integral kernels $\rho(p,p')$ and $A(p,p')$. Then*

$$\operatorname{tr} A\rho = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p\, d^s p'\, \operatorname{tr}_{\mathcal{K}} A(p',p)\rho(p,p'). \tag{3.14}$$

If A is translationally invariant this simplifies to

$$\operatorname{tr} A\rho = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p\, \operatorname{tr}_{\mathcal{K}} A(p)\rho(p,p)\,. \tag{3.15}$$

Proof. To begin with, we note that if ρ is trace-class and A is bounded, then $A\rho$ is also trace-class and the integral kernels satisfy

$$(A\rho)(p,p') = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s q\, A(p,q)\rho(q,p')\,.$$

Thus we have to prove that trace-class operators with integral kernel $\rho(p,p')$ satisfy the formula

$$\operatorname{tr}\rho = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p\, \operatorname{tr}_{\mathcal{K}} \rho(p,p).$$

We denote by Γ_L the hypercube of length $2L+1$ in $\mathbb{Z}^s$, i.e.

$$\Gamma_L = \{x \in \mathbb{Z}^s : |x_i| \leq L \quad \forall\, i = 1, \ldots, s\},$$

and by P_L the projection onto Γ_L in $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$

$$P_L |x \otimes \phi\rangle = \begin{cases} |x \otimes \phi\rangle & , \quad x \in \Gamma_L \\ 0 & , \quad \text{else} \end{cases}.$$

Clearly, $\operatorname{tr} \rho = \lim_{L\to\infty} \operatorname{tr} P_L \rho$ and with a basis $|i\rangle$, $i = 1, \ldots, \dim \mathcal{K}$, we obtain

$$\begin{aligned} \operatorname{tr} P_L \rho &= \sum_{i=1}^{\dim \mathcal{K}} \sum_{x \in \Gamma_L} \langle x \otimes i | \rho | x \otimes i \rangle \\ &= \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p\, d^s p' \sum_{x \in \Gamma_L} e^{\mathrm{i}x(p'-p)} \operatorname{tr} \rho(p, p'). \end{aligned}$$

The term $(2\pi)^{-s} \sum_{x\in\Gamma_L} e^{\mathrm{i}x(p'-p)}$ converges for $L \to \infty$ to the Dirac distribution, which proves the assertion. □

Equation (3.15) displays a strong similarity with Equation (3.12), defining $\rho(p) := \rho(p,p)$ yields an equation which, up to division by $\dim \mathcal{K}$, coincides with Equation (3.12). The integral kernel $\rho(p)$ defines a translationally invariant operator, whose relation with $\rho(p,p')$ is clarified in the following lemma.

Lemma 3.2.6. *Let ρ be a trace-class operator and $A \in \mathcal{T}_{\mathcal{K},s}$. The integral kernel $\rho(p) = \rho(p,p)$ represents the translationally invariant bounded operator*

$$\Xi = \sum_{x \in \mathbb{Z}^s} \mathcal{T}_x \rho \mathcal{T}_x^* \tag{3.16}$$

and the trace of $A\rho$ fulfills

$$\operatorname{tr} A\rho = (\dim \mathcal{K}) \cdot \langle A^* | \Xi \rangle \tag{3.17}$$

with the scalar product (3.12).

Proof. If $\rho = \sum_{x,y\in\mathbb{Z}^s} |x\rangle\langle y| \otimes \rho_{x,y}$ is trace-class we get the convergent Fourier series

$$\rho(p,p') = \sum_{x,y\in\mathbb{Z}^s} \rho_{x,y}\, e^{\mathrm{i}x\cdot p} e^{-\mathrm{i}y\cdot p'}$$

as its integral kernel. In fact, since $\sum_{x,y\in\mathbb{Z}^s} \operatorname{tr}_{\mathcal{K}} \rho_{x,y}^* \rho_{x,y} < \infty$ this expression is even uniformly convergent and $\rho(p,p')$ is uniformly continuous on $[-\pi,\pi)^{2s}$. Consequently, $\rho(p) = \rho(p,p)$ is uniformly continuous on $[-\pi,\pi)^s$ and defines a unique

translationally invariant and bounded operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. To compute this operator we use the expression

$$\begin{aligned}\rho(p) &= \int\limits_{[-\pi,\pi)^s} d^s p'\, \rho(p,p')\delta(p-p') \\ &= \int\limits_{[-\pi,\pi)^s} d^s p'\, \rho(p,p')\frac{1}{(2\pi)^s}\sum_{x\in\mathbb{Z}^s} e^{\mathrm{i}x\cdot(p-p')}\end{aligned}$$

and the fact that translation operators $\mathcal{T}_x$ are represented in momentum space by $e^{\mathrm{i}x\cdot p}\mathbb{1}_{\mathcal{K}}$. This proves the formula for Ξ, the operator corresponding to $\rho(p)$, and the expression $\operatorname{tr} A\rho = (\dim\mathcal{K})\cdot\langle A^*|\Xi\rangle$ is a trivial consequence. □

Later on we will calculate the characteristic function of density operators $\rho\in\mathcal{S}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$, that is, we wish to determine the parameter-dependent expectation value

$$C(\lambda) = \operatorname{tr}\rho\, e^{\mathrm{i}\lambda\cdot Q}. \tag{3.18}$$

The unitary operator $e^{\mathrm{i}\lambda\cdot Q}$ has a specific form in momentum space, its action on a vector valued function $\psi(p)$ reads

$$(e^{\mathrm{i}\lambda\cdot Q}\psi)(p) = \sum_{x\in\mathbb{Z}^s} e^{\mathrm{i}x\cdot\lambda}\psi_x e^{\mathrm{i}p\cdot x} = \psi(p+\lambda). \tag{3.19}$$

From the above equation it follows that the Fourier transform of the operator $e^{\mathrm{i}\lambda\cdot Q}$ corresponds to the integral kernel $A(p,p') = \delta(p-p'+\lambda)$. Consequently, evaluation of the characteristic function $C(\lambda)$ in momentum space boils down to the computation of

$$C(\lambda) = \int\limits_{[-\pi,\pi)^s} \operatorname{tr}_{\mathcal{K}}\rho(p,p+\lambda). \tag{3.20}$$

In Equation (3.18) the unitary operator $U_\lambda = e^{\mathrm{i}\lambda\cdot Q}$ plays the role of a Fourier transform of the position distribution corresponding to a quantum state ρ on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. However, there is another interpretation of U_λ. Since it is unitary we may consider U_λ as the discrete time evolution of a quantum system. Clearly, U_λ is not translationally invariant, but

$$\mathcal{T}_x U_\lambda \mathcal{T}_x^* = e^{-\mathrm{i}\lambda\cdot x} U_\lambda,$$

and hence the overall effect of translating the operator U_λ by a lattice vector x is multiplication by the global phase factor $e^{-\mathrm{i}\lambda\cdot x}$. Such global phase factors are usually not observable in quantum mechanics, therefore they are of no particular im-

portance. This fact is best expressed in the Heisenberg picture: let A be any observable in $\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$, then

$$\begin{aligned}\tau_x(U_\lambda^* A U_\lambda) &= \mathcal{T}_x U_\lambda^* \mathcal{T}_x^* \mathcal{T}_x A \mathcal{T}_x^* \mathcal{T}_x U_\lambda \mathcal{T}_x^* \\ &= e^{\mathrm{i}\lambda\cdot x} U_\lambda^* \tau_x(A) U_\lambda e^{-\mathrm{i}\lambda\cdot x} \\ &= U_\lambda^* \tau_x(A) U_\lambda\,.\end{aligned}$$

Hence, in the Heisenberg picture the time evolution generated by U_λ commutes with translations. Motivated by this observation we now define translation invariance in a more general setting.

Definition 3.2.7. *We say that an operator* $\mathbf{W}$ *on* $\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ *is translationally invariant if*

$$\tau_x \circ \mathbf{W} = \mathbf{W} \circ \tau_x\,, \quad \forall x \in \mathbb{Z}^s\,.$$

By converting the time evolution $\mathbf{W}(A) = U_\lambda^* A U_\lambda$ to momentum space we see that it acts on the integral kernel $A(p,p')$ by a shift of the momentum variables, $\mathbf{W}(A)(p,p') = A(p+\lambda, p'+\lambda)$. Surely, $\mathbf{W}$ respects translation invariance, that is, if A is translationally invariant then $\mathbf{W}(A)$ is again a multiplication operator but with a shift of λ in the momentum variable, i.e. $\mathbf{W}(A)(p) = A(p+\lambda)$.

Lemma 3.2.8. *Let* A *be a bounded operator on* $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ *and denote its Fourier kernel by* $A(p,p')$*. Denote by* Q *the position operator on* $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$*, then*

$$(e^{\mathrm{i}\lambda\cdot Q} A e^{-\mathrm{i}\lambda\cdot Q})(p,p') = A(p+\lambda, p'+\lambda)\,.$$

In particular, if A *is translationally invariant we have*

$$(e^{\mathrm{i}\lambda\cdot Q} A e^{-\mathrm{i}\lambda\cdot Q})(p) = A(p+\lambda)\,.$$

Proof. The operator $e^{\mathrm{i}\lambda\cdot Q} A e^{-\mathrm{i}\lambda\cdot Q}$ acts on a vector ψ like

$$\begin{aligned}(e^{\mathrm{i}\lambda\cdot Q} A e^{-\mathrm{i}\lambda\cdot Q}\psi)(p) &= \int_{[-\pi,\pi)^s} d^s p'\, A(p+\lambda, p')\psi(p'-\lambda) \\ &= \int_{[-\pi,\pi)^s} d^s p'\, A(p+\lambda, p'+\lambda)\psi(p')\,,\end{aligned}$$

which proves the assertion. □

3.3. Spectral theory of unitary operators

The aim of this section is to introduce basic notions and ideas from the spectral theory of unitary operators. These concepts will be used in the following chapters to analyze the asymptotic behavior of quantum walks. In particular, we will connect the nature of certain subsets of the spectrum of a quantum walk operator to its propagation properties, see Theorem 3.3.6. Since most statements are well-known results we omit their proofs and refer to [Lax02] or [DS88] for a detailed introduction.

Throughout this section, U denotes a unitary operator on a separable Hilbert space $\mathcal{H}$. Much information about U can be inferred solely from its spectrum, in particular we will see that transport properties associated with U are closely related to the spectral properties of U. The following definition introduces the basic objects of this section and fixes terminology.

Definition 3.3.1. *Let A be a bounded operator on a separable Hilbert space $\mathcal{H}$. The set of all $z \in \mathbb{C}$ such that the inverse $(A - z\,\mathbb{1})^{-1}$ exists as bounded operator is called the resolvent $\rho(A)$ of A. Its complement $\sigma(A) = \mathbb{C}\backslash\rho(A)$ is called the spectrum of A.*

The spectrum of a bounded operator A is always a compact subset of $\mathbb{C}$. If U is unitary we also have $\sigma(U) \subset \mathbb{S} = \{z \in \mathbb{C} : |z| = 1\}$. A core result in the theory of self-adjoint operators is the spectral representation theorem. In order to formulate an adaption of this result to the case of unitary operators we need the notion of a spectral measure.

Definition 3.3.2. *Let X be a set with σ-algebra Σ, i.e. (X, Σ) is a measure space, and $\mathcal{P}(\mathcal{H})$ the set of all orthogonal projections on a separable Hilbert space $\mathcal{H}$. A spectral measure E is a map from Σ to $\mathcal{P}(\mathcal{H})$ which satisfies:*

i) $E(X) = \mathbb{1} \quad , \quad E(\emptyset) = 0$

ii) For a sequence $A_n \in \Sigma$ of disjoint sets we have $E\left(\bigcup_{n\in\mathbb{N}} A_n\right) = \sum_{n\in\mathbb{N}} E(A_n)$ *in the strong operator topology.*

Spectral measures E can be used to construct linear operators by integrating complex valued functions on X with respect to E, see [DS88] for a rigorous treatment. The spectral theorem for unitary operators covers the opposite direction, it states the existence of a spectral measure with $X = [-\pi, \pi)$ and the σ-algebra $\Sigma_{\mathcal{B}}$ of Borel sets of X, which generalizes the eigenbasis representation of finite dimensional unitary matrices.

Theorem 3.3.3. *Let U be a unitary operator on a separable Hilbert space $\mathcal{H}$. There exists a unique spectral measure E on $([-\pi,\pi),\Sigma_{\mathcal{B}})$ such that*

$$U=\int_{[-\pi,\pi)} e^{\mathrm{i}\lambda}E(d\lambda). \tag{3.21}$$

The spectral measure is supported on $\sigma(U)$, i.e. $E(\rho(U)\cap\mathbb{S})=0$ with $\rho(U)\cap\mathbb{S}$ considered as subset of $[-\pi,\pi)$.

Unitary matrices on finite dimensional Hilbert spaces commute if and only if there is an orthonormal basis in which they are simultaneously diagonal. The analogue statement for infinite dimensional $\mathcal{H}$ is the following:

Lemma 3.3.4. *Let U,V be unitary operators on $\mathcal{H}$ and denote their respective spectral measures by E,F. Then U and V commute if and only if $E(\Lambda_1)$ and $F(\Lambda_2)$ commute for all Borel sets $\Lambda_1,\Lambda_2\in\Sigma_{\mathcal{B}}$.*

It is straightforward to see that a spectral measure E and two vectors $\phi,\psi\in\mathcal{H}$ define a unique complex measure $\mu_{\phi,\psi}(d\lambda)=\langle\phi|E(d\lambda)|\psi\rangle$. In fact, the measures $\mu_{\phi,\psi}$ uniquely define the spectral measure E. These measures satisfy the equation

$$\langle\phi|U^n|\psi\rangle=\int_{[-\pi,\pi)} e^{\mathrm{i}n\cdot\lambda}\mu_{\phi,\psi}(d\lambda),\quad \forall n\in\mathbb{N}, \tag{3.22}$$

and a closer analysis of these measures yields a division of the spectrum $\sigma(U)$ into characteristic parts. According to Lebesgue's decomposition theorem for signed measures μ there exists a unique decomposition

$$\mu=\mu_{pp}+\mu_{ac}+\mu_{sc}\,. \tag{3.23}$$

The pure point part, denoted by μ_{pp}, is a discrete counting measure, that is, it is a linear combination of point measures. The measure μ_{ac} is absolutely continuous with respect to Lebesque measure, that is, there exists a positive density function ρ such that $\mu_{ac}(d\lambda)=\rho(\lambda)d\lambda$. The remaining measure μ_{sc} is singularly continuous, its cumulative distribution function is continuous but not absolutely continuous, hence, there is no density function with respect to Lebesgue measure. By applying this decomposition theorem to the signed measures $\mu_{\phi,\phi}$ we may define the following subsets of $\mathcal{H}$

$$\begin{aligned}
\mathcal{H}_{pp} &= \{\phi\in\mathcal{H}:\mu_{\phi,\phi}\text{ is pure point}\}\\
\mathcal{H}_{ac} &= \{\phi\in\mathcal{H}:\mu_{\phi,\phi}\text{ is absolutely continuous}\}\\
\mathcal{H}_{sc} &= \{\phi\in\mathcal{H}:\mu_{\phi,\phi}\text{ is singularly continuous}\}\,.
\end{aligned}$$

These sets are in fact orthogonal subspaces which generate $\mathcal{H}$, that is,

$$\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}\,.$$

Moreover, these are invariant subspaces for U, that is, $U\mathcal{H}_{pp} \subset \mathcal{H}_{pp}$ and equally for $\mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$. The spectra of the restrictions of U to these subspaces yields a characteristic refinement of $\sigma(U)$.

Definition 3.3.5. *Let U be a unitary operator on a separable Hilbert space $\mathcal{H}$ and denote the restrictions of U to the subspaces $\mathcal{H}_{pp}$, $\mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$ by U_{pp}, U_{ac} and U_{sc}. The pure point, absolutely continuous and singularly continuous part of $\sigma(U)$ are defined by $\sigma_{pp}(U) := \sigma(U_{pp})$, $\sigma_{ac}(U) := \sigma(U_{ac})$ and $\sigma_{sc}(U) := \sigma(U_{sc})$.*

Whilst the subspace $\mathcal{H}_{pp}$ consists of all eigenvectors of U, the remaining subspaces $\mathcal{H}_{ac}$ and $\mathcal{H}_{sc}$ have no such simple interpretation. Each set $\sigma_{pp}(U)$, $\sigma_{ac}(U)$, and $\sigma_{sc}(U)$ coincides with the union of the support of all measures of the corresponding subclass, i.e.

$$\sigma_{pp} \quad = \quad \bigcup_{\phi \in \mathcal{H}_{pp}} \operatorname{supp} \mu_{\phi,\phi} \tag{3.24}$$

and likewise for $\sigma_{ac}(U)$ and $\sigma_{sc}(U)$. Hence, $\sigma_{pp}(U)$ is a set of discrete points, $\sigma_{ac}(U)$ is a union of closed proper intervals, and $\sigma_{sc}(U)$ is a Cantor set. Due to a theorem by Ruelle, Amrein, Georgescu and Enss, known as RAGE theorem, we can characterize the subspaces $\mathcal{H}_{pp}$ and $\mathcal{H}_c = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$ by propagation properties of U.

Theorem 3.3.6 (RAGE)**.** *Let U be a unitary operator on a separable Hilbert space $\mathcal{H}$ and P_n a sequence of compact operators converging strongly to the identity. The pure point subspace $\mathcal{H}_{pp}$ and the continuous subspace $\mathcal{H}_c = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$ are given by*

$$\begin{aligned} \mathcal{H}_{pp} &= \{\psi \in \mathcal{H} : \lim_{n\to\infty} \sup_{t\geq 0} \left\| (\mathbb{1} - P_n) U^t \psi \right\|^2 = 0\} \\ \mathcal{H}_c &= \{\psi \in \mathcal{H} : \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T+1} \sum_{t=0}^{T} \left\| P_n U^t \psi \right\|^2 = 0\}\,. \end{aligned}$$

This theorem is well-known in the setting of self-adjoint operators and its proof for unitary operators is essentially the same. For a proof of the theorem for self-adjoint operators we refer to [Tes09], a proof for the unitary version can be found in [AVWW11]. The interpretation of this theorem is straightforward, vectors which can be written as linear combination of eigenvectors of U are exactly those vectors which remain in a finite section of the Hilbert space $\mathcal{H}$ up to asymptotically vanishing corrections and vectors in the continuous subspace $\mathcal{H}_c$ leave all finite subspaces

almost surely. We will come back to an interpretation of this theorem in the context of quantum walks in Chapter 4.

Theorem 3.3.6 distinguishes the pure point spectrum from the continuous spectrum, but it makes no statement about the difference between singularly and absolutely continuous spectrum. Thus we provide next a necessary condition for the absolutely continuous part of the spectrum. A condition which exactly separates the absolutely continuous part from the singular continuous spectrum for unitary operators U can be found in [GVWW12].

Theorem 3.3.7. *Let U be a unitary operator on a separable Hilbert space $\mathcal{H}$, P a compact operator and $\psi \in \mathcal{H}_{ac}$. Then*

$$\lim_{t\to\infty} \left\| PU^t \psi \right\| = 0 . \tag{3.25}$$

The proof of this statement is essentially the same as the one for Theorem 5.6 in [Tes09] in the self-adjoint setting.

We conclude this section with an example to visualize the concepts introduced.

Interlude 1: Translation Operators

One of the main topics of Chapter 4 are translationally invariant unitary operators W on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ and their spectral properties. That is, we are given a unitary operator W which satisfies $[W,\mathcal{T}_x]=0$ for all $x\in\mathbb{Z}^s$ and $\mathcal{T}_x$ as defined in Equation (3.9). As a warm up we will now determine the spectral measure of $\mathcal{T}_x$.

By definition, each operator $\mathcal{T}_x$ is translationally invariant, hence, by Lemma 3.2.2, they act as a multiplication operator in momentum space. Indeed, it can be directly verified that $\mathcal{T}_x$ possesses the momentum representation $\mathcal{T}_x(p) = e^{\mathrm{i}p\cdot x}\,\mathbb{1}_{\mathcal{K}}$, i.e.

$$\left(\mathcal{T}_x\psi\right)(p) = e^{\mathrm{i}p\cdot x}\psi(p).$$

For any interval $A\subset[-\pi,\pi)$ we denote by χ_A the characteristic function of A, which is defined by $\chi_A(\lambda)=1$ if $\lambda\in A$ and $\chi_A(\lambda)=0$ if $\lambda\notin A$. The map $\psi(p)\mapsto\chi_A(x\cdot p)\psi(p)$ defines a translationally invariant bounded operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. This map, which we denote by $E_x(A)$, is an orthogonal projection, i.e. $E_x(A)=E_x(A)^2=E_x(A)^*$. Considered as map from the Borel sets of $[-\pi,\pi)$ to orthogonal projections on $\mathcal{H}$, $E_x(.)$ defines a spectral measure. This spectral measure indeed gives a representation of $\mathcal{T}_x$, that is,

$$\mathcal{T}_x = \int_{[-\pi,\pi)} e^{\mathrm{i}\lambda} E_x(d\lambda).$$

For $x \neq 0$ it follows from the RAGE Theorem 3.3.6 that $\mathcal{H} = \mathcal{H}_c = \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$, thus $\sigma(\mathcal{T}_x) = \sigma_c(\mathcal{T}_x) = \sigma_{ac}(U) \cup \sigma_{sc}(U)$. In fact, as a consequence of Proposition 4.5.7 we have $\sigma(\mathcal{T}_x) = \sigma_{ac}(\mathcal{T}_x)$ for $x \neq 0$.

The measures $\mu_{\phi,\psi}$ satisfy

$$\mu_{\phi,\psi}(A) = \langle \phi | E_x(A) | \psi \rangle = \frac{1}{2\pi} \int\limits_{[-\pi,\pi)^s} \chi_A(x \cdot p) \langle \phi(p) | \psi(p) \rangle_{\mathcal{K}} \, dp \,,$$

which proves $\sigma(\mathcal{T}_x) = \sigma_{ac}(\mathcal{T}_x) = \mathbb{S}$ for $x \neq 0$.

3.4. Analytic perturbation theory

The purpose of this section is to provide some background on analytic perturbation theory for linear operators. For a profound introduction to this topic we refer the reader to the encyclopedic books by Kato [Kat95] and Baumgärtel [Bau85]. Our intention is to convey the underlying ideas and give a survey of the theory presented in these books instead of proving their results in a rigorous way.

The object we consider in the following is a map assigning to $\varepsilon \in G$, where G is an open subset of $\mathbb{C}^s$, a bounded operator T_ε acting on a separable Hilbert space $\mathcal{H}$. Our main assumption about this map is analyticity in a sense which is specified below, and the object of interest is the spectral representation of T_ε. More precisely, we wish to study the behavior of the eigenvalues and eigenvectors of T_ε under small changes of ε. We divide the following section into two parts, of which the first deals with finite dimensional $\mathcal{H}$, and the second part generalizes some results to the infinite dimensional case. In both cases, the set of bounded operators $\mathcal{B}(\mathcal{H})$ on $\mathcal{H}$ is a Banach space, thus, it is sufficient to define analyticity of a map $\varepsilon \mapsto T_\varepsilon$ with values in a Banach space $\mathcal{B}$. In our definition of analyticity we use the fact that holomorphy and analyticity of maps from G to $\mathcal{B}$ are equivalent concepts. That is, a map $f : G \to \mathcal{B}$ is complex differentiable in a neighborhood of a point $\varepsilon \in G$ if and only if it can be represented as a convergent power series in a neighborhood of ε.

Definition 3.4.1. *A map $\varepsilon \mapsto T_\varepsilon \in \mathcal{B}$ defined for all $\varepsilon \in G$, where G is an open subset of $\mathbb{C}^s$ and $\mathcal{B}$ is a Banach space, is said to be analytic or holomorphic at ε if there exists a $\mathcal{B}$-valued map T'_ε such that*

$$\left\| \frac{T_{\varepsilon+\delta} - T_\varepsilon}{|\delta|} - T'_\varepsilon \right\| \to 0 \tag{3.26}$$

for $\delta \to 0$.

3.4.1. Finite dimensional Hilbert spaces

In this section we consider the case $\dim \mathcal{H} = d < \infty$, such that T_ε is a family of finite dimensional matrices with matrix elements which are analytic functions of $\varepsilon \in G \subset \mathbb{C}^s$. The starting point of our analysis is the characteristic polynomial $\chi_\varepsilon(z) = \det T_\varepsilon - z\,\mathbb{1}$, from which we determine the eigenvalue-functions $\lambda_k(\varepsilon)$. For a better understanding of the further approach, let us fix $\varepsilon = \varepsilon_0$ and assume for the moment that the eigenvalue $\lambda_1(\varepsilon_0)$ is non-degenerate. By the implicit function theorem we can find a neighborhood of ε_0 such that $\lambda_1(\varepsilon)$ is analytic. Consequently, if all eigenvalues of T_{ε_0} are non-degenerate, there exists a neighborhood of ε_0 on which the eigenvalues are given by analytic functions. Of course, this is still true if the characteristic polynomial is of the form $\chi_\varepsilon(z) = g_\varepsilon(z)^m$ with a function g which is analytic in ε, polynomial in z and has non-degenerate roots $z_1, \ldots, z_r$ at ε_0. Therefore, our first step is to eliminate such multiplicities from the characteristic polynomial $\chi_\varepsilon(z)$. To this end we note that collecting terms in $\chi_\varepsilon(z)$ with respect to powers of z yields

$$\chi_\varepsilon(z) = c_d(\varepsilon) z^d + \ldots + c_1(\varepsilon) z + c_0(\varepsilon), \tag{3.27}$$

with analytic functions $c_j(\varepsilon)$. We define the set $\mathbb{M}_\varepsilon[z]$ of all polynomials in z with coefficients which are meromorphic functions in ε, i.e. $g \in \mathbb{M}_\varepsilon[z]$ is of the form (3.27), but with $c_j(\varepsilon)$ meromorphic. The crucial property for our purpose is the fact that $\mathbb{M}_\varepsilon[z]$ is an Euclidean ring[3], such that we may uniquely decompose $g \in \mathbb{M}_\varepsilon[z]$ into irreducible elements. That is, we can write $g = g_1^{m_1} \cdot \ldots \cdot g_r^{m_r}$ and the g_j have no non-trivial divisors in $\mathbb{M}_\varepsilon[z]$. Applying these ideas to the characteristic polynomial results in

$$\chi_\varepsilon(z) = \zeta_1(\varepsilon, z)^{r_1} \cdot \ldots \cdot \zeta_\ell(\varepsilon, z)^{r_\ell}, \tag{3.28}$$

with irreducible elements $\zeta_j \in \mathbb{M}_\varepsilon[z]$, from which we construct the polynomial

$$\gamma_\varepsilon(z) = \zeta_1(\varepsilon, z) \cdot \ldots \cdot \zeta_\ell(\varepsilon, z). \tag{3.29}$$

The coefficients $c_j(\varepsilon)$ of the elements ζ_j are at least meromorphic functions of ε. In fact, it follows from the analyticity of the coefficients of $\chi_\varepsilon(z)$ that the coefficients of ζ_j as well as those of γ_ε are analytic functions of ε, see [Bau85].

We reduced the problem of finding the eigenvalue functions of T_ε to the task of finding functions $\lambda_j(\varepsilon)$ such that $\gamma_\varepsilon(\lambda_j(\varepsilon)) \equiv 0$, which may be further simplified to the computation of all functions $\lambda_{j,k}(\varepsilon)$ such that $\zeta_j(\varepsilon, \lambda_{j,k}(\varepsilon)) \equiv 0$. Exploiting again the implicit function theorem we see that a simple root $z = \lambda_j(\varepsilon_0)$ of γ_{ε_0} gives rise to an analytic eigenvalue function $\lambda_j(\varepsilon)$ at ε_0, and all eigenvalues of T_ε are analytic at ε_0 if all roots of $\gamma_{\varepsilon_0}(z)$ are non-degenerate. Non-degeneracy of these roots is equivalent

[3] An Euclidean ring is a ring without zero divisors, hence, one can define a Euclidean algorithm for such rings.

to non-vanishing of the discriminant $D_\gamma(\varepsilon_0)$ of γ_ε considered as polynomial in z. Hence, points at which some eigenvalues are non-analytic are contained in the set $M = \{\varepsilon \in G : D_\gamma(\varepsilon) = 0\}$. Since $D_\gamma(\varepsilon)$ can be expressed as a polynomial in the coefficients $c_j(\varepsilon)$ of γ_ε it must be an analytic function of ε. Moreover, D_γ is not the zero function, see [Bau85], so M is the zero set of a non-vanishing analytic function. The points ε_0 at which $D_\gamma(\varepsilon_0) \neq 0$ are called simple points and if ε_0 is simple we can choose the eigenvalues of T_ε analytic at ε_0. Points ε_0 at which the discriminant vanishes, that is $D_\gamma(\varepsilon_0) = 0$, are called multiple points.

Our second point of interest is the spectral decomposition of T_ε. We do not assume T_ε to be a family of normal operators, the appropriate normal form of T_ε is thus the Jordan normal form [Kat95]. We denote by $\lambda_j(\varepsilon)$ the eigenvalues and by $\mathbf{P}_j(\varepsilon)$ and $\mathbf{D}_j(\varepsilon)$ the corresponding eigenprojections and eigennilpotents of T_ε. These operators satisfy $\mathbf{P}_j(\varepsilon)\mathbf{P}_k(\varepsilon) = \delta_{jk}\mathbf{P}_j(\varepsilon)$, $\mathbf{P}_j(\varepsilon)\mathbf{D}_k(\varepsilon) = \mathbf{D}_k(\varepsilon)\mathbf{P}_j(\varepsilon) = \delta_{jk}\mathbf{D}_j(\varepsilon)$, and $\mathbf{D}_j(\varepsilon)^{r_j} = 0$ for some integer $r_j \leq \dim \mathcal{H}$, and in terms of these operators we can write T_ε as

$$T_\varepsilon = \sum_j \lambda_j(\varepsilon)\mathbf{P}_j(\varepsilon) + \mathbf{D}_j(\varepsilon), \tag{3.30}$$

and our aim is to verify analyticity of the operators $\mathbf{P}_j(\varepsilon)$ and $\mathbf{D}_j(\varepsilon)$. We start with the eigenprojections $\mathbf{P}_j(\varepsilon)$ and note that if $z = \lambda_j(\varepsilon_0)$ is a simple root of γ_{ε_0}, we may find a neighborhood $\mathcal{N}_{\varepsilon_0}$ of ε_0 and a positively oriented closed curve $\mathcal{C}_j$ enclosing $\lambda_j(\varepsilon)$ and no other eigenvalues of T_ε for all ε in this neighborhood. Using such a curve $\mathcal{C}_j$ we can compute the eigenprojection corresponding to $\lambda_j(\varepsilon)$ via the well-known integral-formula

$$\mathbf{P}_j(\varepsilon) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}_j} dz\, (z\mathbb{1} - T_\varepsilon)^{-1}. \tag{3.31}$$

We may choose the curve $\mathcal{C}_j$ and $\mathcal{N}_{\varepsilon_0}$ such that the distance of any point on $\mathcal{C}_j$ to the spectrum of T_ε is lower bounded by a strictly positive constant which is independent of $\varepsilon \in \mathcal{N}_{\varepsilon_0}$. This choice ensures that the operator norm of the resolvent $(T_\varepsilon - z\mathbb{1})$ is uniformly upper bounded on $\mathcal{C}_j$. With these choices we get an expression for $\mathbf{P}_j(\varepsilon)$ which is analytic in ε. For the eigennilpotents we use the formula $\mathbf{D}_j(\varepsilon) = (T_\varepsilon - \lambda_j(\varepsilon)\mathbb{1})\mathbf{P}_j(\varepsilon)$ to verify that these are analytic if the $\lambda_j(\varepsilon)$ and $\mathbf{P}_j(\varepsilon)$ are. Before we turn our attention to the behavior of the Jordan normal form at multiple points let us summarize:

Lemma 3.4.2. *Let T_ε for $\varepsilon \in G \subset \mathbb{C}^s$ be an analytic family of operators on $\mathcal{H} = \mathbb{C}^d$, γ_ε according to Equation* (3.29)*, and $\varepsilon_0 \in G$. Then we have the following statements:*

i) If $z = \lambda_j(\varepsilon_0)$ is a simple root of γ_{ε_0} the eigenvalue $\lambda_j(\varepsilon)$, eigenprojection $\mathbf{P}_j(\varepsilon)$ and eigennilpotent $\mathbf{D}_j(\varepsilon)$ are analytic in a neighborhood of ε_0.

ii) If ε_0 is a simple point all eigenvalues $\lambda_j(\varepsilon)$, eigenprojections $\mathbf{P}_j(\varepsilon)$ and eigennilpotents $\mathbf{D}_j(\varepsilon)$ are analytic in a neighborhood of ε_0

iii) The set of all multiple points is the zero set of an analytic function on G.

The behavior of the eigenvalues λ_j and spectral projections $\mathbf{P}_j$ and $\mathbf{D}_j$ at multiple points is more complicated. Whilst the eigenvalues are still continuous but possibly non-analytic, the spectral projections may even be singular at multiple points. In Chapter 4 we deal with analytic operators T_ε with $\varepsilon \in G \subset \mathbb{C}$, i.e. the perturbation parameter ε is one-dimensional. Of course, the theory outlined so far applies to this case, but additionally we may also make statements about the behavior in the neighborhood of multiple points. So let G be an open subset of $\mathbb{C}$ and denote the set of all multiple points of T_ε by M. Then, for any compact subset $K \subset \mathbb{C}$, the intersection $K \cap M$ is a finite set since M is the zero set of the non-vanishing analytic function D_γ, i.e. multiple points are always isolated. Hence we may assume without loss that ε_0 is the only multiple point of T_ε in G. We denote the different roots of Equation (3.29) at ε_0 by $x_1, \ldots, x_k$. At least one of these roots is a multiple root of Equation (3.29), say x_1, and we denote its multiplicity by $m_1 > 1$. This root gives rise to m_1 possible eigenvalue functions $\lambda_1(\varepsilon), \ldots, \lambda_{m_1}(\varepsilon)$ of T_ε, which may have multiplicities larger than one if $r_j > 1$ for some factors in Equation (3.28). The functions λ_j are analytic functions at every $\varepsilon \in G \backslash \{\varepsilon_0\}$, and we can analytically continue each eigenvalue on a circle enclosing ε_0. After analytic continuation of, say, λ_1 around ε_0 we may end up with another function λ_j, which is again an eigenvalue of T_ε. Thus we can relabel and group the eigenvalues into sets $\Lambda_s = \{\lambda_{s,t} : t = 1, \ldots, d_s\}$, with $s = 1, \ldots, n$, such that analytic continuation around ε_0 cyclically permutes the elements of each Λ_s. Clearly, we must have $d_1 + \ldots + d_n = m_1$. A deeper analysis of the characteristic polynomial shows that each Λ_s can be represented by convergent Puiseux-series around ε_0, that is

$$\lambda_{s,t}(\varepsilon) = r_1 + \sum_{k=1}^{\infty} c_{s,k} \left(e^{\mathrm{i}\frac{2\pi t}{d_s}} (\varepsilon - \varepsilon_0)^{\frac{1}{d_s}} \right)^k , \quad t = 1, \ldots, d_s , \tag{3.32}$$

with a fixed branch of the d_s^{th} root, see [Bau85]. Consequently, the eigenvalue functions are analytic at ε_0 if and only if $d_s = 1$.

For the eigenprojections $\mathbf{P}_{s,t}$ and eigennilpotents $\mathbf{D}_{s,t}$ we encounter the problem that the curves $\mathcal{C}_{s,t}$ in Equation (3.31) have to be chosen smaller with ε approaching ε_0, so we fail to obtain a uniform bound for the norm of the resolvent. Hence, these operator may be singular in this limit, and in fact, if $d_s > 1$ the corresponding operators $\mathbf{P}_{s,t}$ and $\mathbf{D}_{s,t}$ are guaranteed to be singular at ε_0 [Bau85, Kat95]. However, these operators can still be expressed as convergent Laurant-Puiseux-series at ε_0, more precisely,

$$\mathbf{P}_{s,t}(\varepsilon) = (\varepsilon - \varepsilon_0)^{-n_s} \sum_{k=0}^{\infty} P_{s,t,k} (\varepsilon - \varepsilon_0)^{\frac{k}{d_s}} , \tag{3.33}$$

with $n_s \in \mathbb{N}$ and $P_{s,t,k} \in \mathrm{Mat}(\mathbb{C}^d)$. Consequently, the singularities are at most algebraic, i.e. $\left\| \mathbf{P}_{s,t}(\varepsilon) \right\| = \mathcal{O}(|\varepsilon - \varepsilon_0|^{-n_s})$. Nevertheless, we may choose the total eigenpro-

jection $\mathbf{P}_j(\varepsilon)$ corresponding to $\lambda_1,\dots,\lambda_{m_1}$ analytic as in the case of a simple eigenvalue. In summary we have:

Lemma 3.4.3. *Let T_ε for $\varepsilon \in G \subset \mathbb{C}$ be an analytic family of operators on $\mathcal{H} = \mathbb{C}^d$ and $\varepsilon_0 \in G$ a multiple point for T_ε. The eigenvalues are continuous at ε_0 and the eigenprojections and eigennilpotents have at most algebraic singularities at ε_0, i.e. we have the estimates $\left\|\mathbf{P}_j(\varepsilon)\right\| = \mathcal{O}(|\varepsilon-\varepsilon_0|^{-k})$ and $\left\|\mathbf{D}_j(\varepsilon)\right\| = \mathcal{O}(|\varepsilon-\varepsilon_0|^{k})$ for some $k \in \mathbb{N}$.*

A particular case where all objects in the spectral representation of T_ε can be chosen analytic is when these operators are normal, see [Kat95, §1. Thm 1.10]. Since $d_s > 1$ implies a pole of the eigenprojections, we immediately conclude that $d_s = 1$ for all s since $\left\|\mathbf{P}_{s,t}(\varepsilon)\right\| = 1$ for all ε. Thus all eigenvalues are analytic at ε_0 and $\mathbf{D}_{s,t} \equiv 0$. The eigenprojections $\mathbf{P}_{s,t}$ have Laurant-Puiseux series expressions with $d_s = 1$ and no poles, i.e. $n_s = 0$. So in fact, these are Taylor expansions and the eigenprojections are also analytic.

Lemma 3.4.4. *Let T_ε for $\varepsilon \in G \subset \mathbb{C}$ be an analytic family of normal operators on $\mathcal{H} = \mathbb{C}^d$. Then all eigenvalues and eigenprojections are analytic at all $\varepsilon \in G$ and $\mathbf{D}_j(\varepsilon) \equiv 0$.*

3.4.2. Infinite dimensional Hilbert spaces

Some results from the case $\dim \mathcal{H} < \infty$ are straightforward to generalize to infinite dimensional $\mathcal{H}$ if the family of operators T_ε satisfies certain requirements. We assume in the following that T_ε is bounded and analytic for all ε in a sufficiently small neighborhood of ε_0. This means the limit (3.26) exists, with the norm given by the operator norm on $\mathcal{H}$. Moreover, we assume that at ε_0 we have a finite set of isolated eigenvalues, and we are interested in the behavior of these eigenvalues and the corresponding eigenvectors for ε close to ε_0.

We denote the finite system of eigenvalues by $\lambda_1,\dots\lambda_r$ and since these are assumed to be isolated we have $\sigma(T_{\varepsilon_0}) = \{\lambda_1,\dots,\lambda_r\} \cup \sigma_0$ with a closed set σ_0 and $\lambda_j \notin \sigma_0$ for all j. Thus we can find a positively oriented curve $\mathcal{C}$ in the resolvent set $\rho(T_{\varepsilon_0})$ which separates $\{\lambda_1,\dots,\lambda_r\}$ from σ_0 in the sense that it winds around each eigenvalue λ_j once without enclosing points from σ_0. The crucial point is now that $\mathcal{C}$ may be chosen such that it lies in the resolvent set of T_ε for ε close to ε_0, and the projection

$$P_\varepsilon = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} dz\, (z\mathbb{1} - T_\varepsilon)^{-1} \tag{3.34}$$

is analytic in ε, see [Bau85]. Clearly, P_ε projects onto the eigenspace corresponding to the perturbed eigenvalues $\lambda_1(\varepsilon),\dots,\lambda_r(\varepsilon)$, and we can use this projection to

construct the operator

$$S_\varepsilon = P_\varepsilon P_{\varepsilon_0} + (\mathbb{1} - P_\varepsilon)(\mathbb{1} - P_{\varepsilon_0}). \tag{3.35}$$

This operator satisfies $S_\varepsilon P_{\varepsilon_0} = P_\varepsilon S_\varepsilon$ and it is proven in [Bau85] that both, S_ε and its inverse S_ε^{-1}, exist as bounded and analytic operator valued maps in a sufficiently small neighborhood of ε_0. Thus we may rewrite this equation equivalently as

$$P_\varepsilon = S_\varepsilon P_{\varepsilon_0} S_\varepsilon^{-1}. \tag{3.36}$$

This reduces the study of the eigenvalues $\lambda_1(\varepsilon), \ldots, \lambda_r(\varepsilon)$ of T_ε and corresponding eigenvectors to the analysis of the spectral decomposition of the operator $S_\varepsilon^{-1} T_\varepsilon S_\varepsilon$ acting on the finite dimensional Hilbert space $P_{\varepsilon_0}\mathcal{H}$, which immediately yields the following statement.

Lemma 3.4.5. *Let T_ε for $\varepsilon \in G \subset \mathbb{C}^s$ be an analytic family of bounded operators on a separable Hilbert space $\mathcal{H}$. Suppose for $\varepsilon_0 \in G$ there is a finite set of isolated and non-degenerate eigenvalues $\lambda_1, \ldots, \lambda_r$ for T_{ε_0}. There exists a neighborhood of ε_0 such that T_ε has r analytic, isolated and non-degenerate eigenvalues $\lambda_1(\varepsilon), \ldots, \lambda_r(\varepsilon)$ with analytic eigenvectors which approach the eigenvalues and eigenvectors of T_{ε_0} in the limits $\varepsilon \to \varepsilon_0$*

4. Asymptotic Time Evolution of Translationally Invariant Quantum Walks

Loosely speaking, quantum walks model the time evolution of a quantum particle moving in discrete time steps on a spatial lattice. The particle is endowed with an internal degree of freedom, which is described by a finite dimensional Hilbert space, and in the course of one time step the particle is translated by a finite step size depending on its internal state. Two common assumptions about the time evolution are space and time homogeneity, that is, the dynamical map commutes with translations and is fixed for all times. A further idealization is to assume that the time evolution of the quantum particle is unitary. However, in real-world experiments there is always interaction with the environment which leads to decoherence. Quantum systems exposed to decoherence generically suffer the loss of their genuine quantum features and start to behave classically. Unitary quantum walks are distinguished from their classical counterparts by their asymptotic behavior for large numbers of time steps t. It is well-known that coherent, i.e. unitary, quantum walks exhibit ballistic behavior, meaning that the asymptotic position distribution in $1/t$-scaling has a well-defined meaning. Under the influence of decoherence this is, in general, no longer true, the appropriate scaling for the limiting position distribution is now given by $1/\sqrt{t}$. In other words, decoherent quantum walks behave like a classical diffusion process. Consequently, we expect to see a crossover from ballistic to diffusive behavior if a former unitary quantum walk is subject to decoherence.

The aim of this chapter is to provide a general method suitable to determine the asymptotic behavior of translationally invariant quantum walks. Our method is based on perturbation theory and yields automatically the appropriate asymptotic scaling together with complete information about the limiting position distribution of the quantum walk. We also prove that the intuitive statement that decoherent quantum walks behave diffusively is true under rather mild assumptions about the kind of decoherence, while we also provide examples of decoherent quantum walks which exhibit ballistic transport.

We start this chapter with an overview of literature concerned with the asymptotic analysis of translationally invariant quantum walks. After giving a general def-

inition of a translationally invariant quantum walk, we provide a structure theorem for time evolutions compatible with this definition in Section 4.2. This structure theorem entails a classification of translationally invariant quantum walks according to the properties of their Fourier space representation. In what follows, we distinguish between translationally invariant quantum walks without and with momentum transfer. In order to give the notion of asymptotic behavior a well-defined mathematical meaning, we introduce the concept of asymptotic position distributions in Section 4.3. Finally, in Section 4.4, we present a sketch of our method to determine the asymptotic position distribution, which we apply to translationally invariant quantum walks without and with momentum transfer in Section 4.5 and Section 4.6, respectively. We conclude this chapter with a summary of our results and some open questions in Section 4.7.

4.1. Literature overview and related work

The aim of the following sections is to provide a literature overview together with connections of the results presented in this thesis to other work. The subject of this chapter are translationally invariant quantum walks in discrete time, thus, the following overview will be biased towards this direction. For the sake of brevity we will mostly use the term quantum walk for the remainder of this chapter, and it is understood that this implies translation invariance of the time evolution.

4.1.1. Historical survey

With the intention to quantize a classical random walk, Aharonov, Davidovich and Zagury introduced a scheme, for which they coined the term quantum random walk, in [ADZ93]. In the presentation of their model, the authors took spatial discreteness rather as an approximation of a continuum, and their construction was based on a repeated measure-and-prepare scheme instead of a fully coherent quantum evolution. Nevertheless, the comparison with a classical random walk already showed a faster spreading of the position distribution with time. Since then, there has been an immense scientific effort to investigate the propagation behavior of quantum walks, a question which is clearly triggered by the manifold applications of classical random walks in various scientific areas, such as randomized algorithms in computer science [MR95], modeling of biological processes [CPB08], or diffusion processes in statistical physics [SF12]. This brought together many different concepts and approaches from the respective fields which had to be quantized.

In the beginning, theoretical work focused primarily on unitary quantum walks

of a particular form, called coined quantum walks[1]. The structure of these quantum walks is similar to that of a classical random walk in the sense that the toss of a coin is replaced by a unitary operator acting locally on the particle's internal degree of freedom. This local operator is then followed by a transport of the particle, where the displacement depends on the internal state of the particle. The analysis of quantum walks on a variety of graphs showed a generic behavior. Based on many different figures of merit, it was found that quantum walks perform faster than classical random walks. An incomplete list of examples of such quantities are mixing times [AAKV01, ABN$^+$01, MR02], hitting times [Kem05], absorption probabilities [BCG$^+$04, YKI03] and standard deviation [MBSS02]. A common observation is that, as shown by many of these figures of merit, quantum walks exhibit a quadratically faster propagation than classical random walks. In the case of infinite periodic graphs, as for example $\mathbb{Z}^s$, this can be explained by investigating the asymptotic scaling of the position distribution. It is well-known that classical random walks behave diffusively, i.e. they scale asymptotically as $\sqrt{t}$, where t denotes the number of time steps. Mathematically, this is expressed by the fact that the random variable $X_t/\sqrt{t}$, where X_t denotes the random variable obtained from a measurement of the particle's position after t time steps, converges weakly for t going to infinity, see Section 4.3 for a precise definition of weak convergence. Based on different techniques, it was shown by several authors that unitary quantum walks behave ballistically, i.e. the correct scaling for weak convergence of the position distribution is $1/t$, thus, quantum walks generically scale like t in the asymptotic sense. In fact, Nayak et al. [NV01, ABN$^+$01] completely solved the question of asymptotic scaling for one-dimensional coined quantum walks. Their method is based on Fourier analysis and was subsequently generalized by Grimmett et al. [GJS04b] in order to cope also with more general quantum walks. A different technique, inspired by path integrals, was devised by Konno [Kon02, IKS05]. Another method, which gives more information about the behavior for large but finite times, is due to Carteret et al. [CIR03, CRT05]. This technique relies heavily on Jacobi polynomials and the steepest-descent method, and gives additional information about the behavior outside the asymptotic propagation region. The form of this propagation region, which is the support of the asymptotic position distribution, as well as the shape of this distribution, can be analyzed using the differential-geometric approach introduced by Bressler et al. [BGPP09, BBBP10].

The significant difference in propagation speed is indeed a characteristic fingerprint of the coherent evolution of a quantum walk. Intuitively, one would expect that, the system, as it is subject to decoherence, begins to behave classically and the spreading of the position distribution occurs on a $\sqrt{t}$-scale. And indeed, this behavior has been observed for numerous examples, where the different types of

[1] Note that a general definition of a unitary nearest neighbor quantum walk on an arbitrary graph, without necessity of such a coin structure, is already contained in [AAKV01].

decoherence can be classified as measurement induced [BCA03b, BCA03a, KS05, KT04, Zha08], fluctuations of the coin operator [KT04, SBH03, KBH06], more general interactions of the internal degree of freedom with the environment [CSB07, LB05, LP03], randomly distributed impurities [RSA+05] or imperfect shift operators [DRKB02]. The study of these models was often performed numerically or on a basis of the asymptotic behavior of the first moments of the probability distribution. Analytic methods to obtain the asymptotic distribution of the particle's position in $\sqrt{t}$-scaling for large classes of decoherent quantum walks were independently introduced by Joye et al. [Joy11, HJ12] and Ahlbrecht et al. [AVWW11, ACM+12].

4.1.2. Related work

Parts of the statements presented in Sections 4.2 and 4.5 are already contained in the thesis [Vog09]. However, our results constitute a proper extension of [Vog09] and we clarify the relation to the work done in [Vog09] at the appropriate places in these sections.

The results presented in Section 4.5 have been published in [AVWW11]. Our results concerning unitary quantum walks in Section 4.5.1 are partially covered by the analysis done by Grimmett et al. [GJS04b], see also [GJS04a], but go beyond. Firstly our approach to quantum walks is more general, as we do not assume a decomposition of the unitary quantum walks into a shift operator and a coin operator. Secondly we prove that a technical assumption left unproven in [GJS04b, GJS04a] is indeed true. This assumption concerns the Fourier transform $W(p)$ of the unitary quantum walk operator W, which is a finite dimensional unitary matrix depending on a momentum variable p. An important property of $W(p)$ is that the momenta at which different eigenvalues of $W(p)$ cross constitute a set of zero Lebesgue measure in momentum space. Based on a perturbation theory approach, we prove the soundness of this assumption for a more general model of quantum walks as compared to [GJS04b, GJS04a]. Similar results as the ones presented in Section 4.5.2 for decoherent quantum walks have been derived by Joye et al. in [Joy11, HJ12] where the authors considered a particular class of quantum walks with a shift and coin decomposition and derived the asymptotic limit of the position distribution in diffusive scaling.

Unitary quantum walks as considered in Section 4.6.1 have been studied numerically in [WŁK+04, BB04, BNP+06]. We give an explanation for the propagation behavior observed in these references by connecting these quantum walks to simpler versions without momentum transfer and sketch a connection to Bloch-oscillations as known from solid state physics. Parts of the results on decoherent quantum walks in Section 4.6.2 have been published in [ACM+12]. Numerical studies of related models can be found in [RSA+05, LKBK10].

4.2. General structure of translationally invariant quantum walks

As already mentioned in the beginning of this chapter, our aim is to model the dynamics of a quantum particle with internal degree of freedom moving on a spatial lattice in discrete time steps. For simplicity we will always assume the quantum particle's internal state space to be described by a finite dimensional Hilbert space $\mathcal{K} \cong \mathbb{C}^d$. In principle, one could also allow for infinite dimensional $\mathcal{K}$ and most results of this section are straightforward to generalize. However, the derivations of the results in later sections would be more involved, as this would require to step from finite dimensional perturbation theory to the infinite dimensional case. The underlying lattice of the quantum walk will always be the cubic lattice $\mathbb{Z}^s$ with $s \in \mathbb{N}$. Of course, one can imagine quantum walks on more general periodic lattices, e.g. a Kagome lattice as shown in Figure 4.1, but this situation can always be mapped to a cubic lattice by similarity transforms and grouping several cells into a super-cells, which effectively enlarges the state space of the internal degree of freedom. Such a grouping of finitely many lattice sites into a super-cell leaves the results of the asymptotic analysis unchanged since this local modification will always vanish in the asymptotic scaling, and a similarity transform can easily be inverted given the asymptotic distribution for a cubic lattice. Consequently, the combined Hilbert space $\mathcal{H}$, describing spatial and internal degree of freedom, is given by the square summable sequences with values in $\mathcal{K}$, that is, $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$.

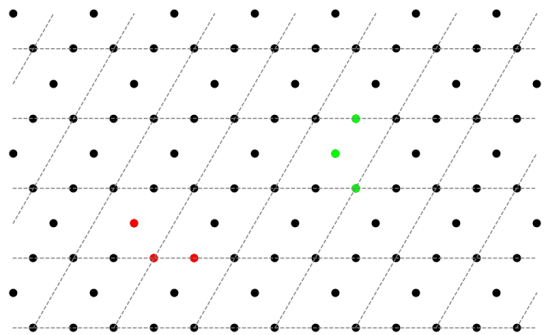


Figure 4.1.: The green and red points indicate two different regroupings of the Kagome lattice which yield a tilted cubic super-lattice.

Our aim is to analyze decoherent quantum walks, therefore it is necessary to describe the state of the quantum particle by a density operator $\rho \in \mathcal{S}(\mathcal{H})$ rather than a pure state represented by a vector $\psi \in \mathcal{H}$. We choose to work in the Heisenberg

picture, which means the time evolution generated by a quantum walk acts on the observables $\mathcal{M}(\mathcal{H})$. The most general form of a physical transformation applied to a quantum system, including decoherent processes, is mathematically formulated by the concept of completely positive maps on $\mathcal{B}(\mathcal{H})$, which we also call quantum channels, see Chapter 3. Quantum walks in all their variety are also well described within this framework, but of course there exist transformations one would not regard as quantum walks. The two basic restrictions we impose on the time evolution are translation invariance and finite propagation speed or finite step size of the process.

Definition 4.2.1. *A translationally invariant quantum walk on $\mathbb{Z}^s$ with internal state space $\mathcal{K}$ is a completely positive unital map $\mathbf{W}$ acting on $\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$, which satisfies*

$$\mathbf{W}\circ\tau_x = \tau_x\circ\mathbf{W} \quad \forall\, x\in\mathbb{Z}^s\,, \tag{4.1}$$

with τ_x defined in Equation (3.11)*, and for which there exists a finite set $\mathcal{N}\subset\mathbb{Z}^s$, called the neighborhood scheme of $\mathbf{W}$, such that for arbitrary $A\in\mathcal{B}(\mathcal{K})$ and $\phi,\psi\in\mathcal{K}$*

$$\langle x\otimes\phi|\mathbf{W}(|k\rangle\langle l|\otimes A)|y\otimes\psi\rangle = 0 \quad \textit{if} \quad k-x\notin\mathcal{N} \quad \textit{or} \quad l-y\notin\mathcal{N}\,. \tag{4.2}$$

We assume $\mathcal{N}$ to be chosen minimal in the sense that there is no strict subset of $\mathcal{N}$ for which Equation (4.2) *is also valid.*

Before we analyze the structure of such quantum walks, let us note some immediate consequences of this definition. First, it is obvious that the concatenation of two quantum walks $\mathbf{W}_1$ and $\mathbf{W}_2$ is again a valid quantum walk with neighborhood scheme obeying $\mathcal{N}(\mathbf{W}_1\circ\mathbf{W}_2)\subset\mathcal{N}(\mathbf{W}_1)+\mathcal{N}(\mathbf{W}_2)$ with the set theoretic sum of $\mathcal{N}(\mathbf{W}_1)$ and $\mathcal{N}(\mathbf{W}_2)$. The same is true for the convex combination of two quantum walks, where the neighborhood scheme of the convex combination is given by $\mathcal{N}(r\mathbf{W}_1+(1-r)\mathbf{W}_2)=\mathcal{N}(\mathbf{W}_1)\cup\mathcal{N}(\mathbf{W}_2)$, for $r\in(0,1)$. The third basic combination of two quantum walks is given by their tensor product. If $\mathbf{W}_{1,2}$ are quantum walks on $\mathbb{Z}^{s_{1,2}}$ with internal state spaces $\mathcal{K}_{1,2}$ then $\mathbf{W}_1\otimes\mathbf{W}_2$ is a translationally invariant quantum walk on $\mathbb{Z}^{s_1+s_2}$ with internal state space $\mathcal{K}_1\otimes\mathcal{K}_2$ and neighborhood scheme $\mathcal{N}(\mathbf{W}_1\otimes\mathbf{W}_2)=\mathcal{N}(\mathbf{W}_1)\times\mathcal{N}(\mathbf{W}_2)$.

As described in Chapter 3, the Stinespring dilation grants us a convenient way to describe a completely positive map in terms of an isometry $\mathcal{V}$. A striking consequence of Definition 4.2.1 is the following structure theorem which characterizes the isometries $\mathcal{V}$ which yield completely positive maps corresponding to quantum walks on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. We stress that a similar version of this theorem already appeared in [Vog09] where it was implicitly assumed that the number of Kraus operators, which are necessary to represent $\mathbf{W}$, is finite. This, however, is a restriction we do not impose on our model as it would exclude the type of decoherent quantum walks we consider in Section 4.6.

Theorem 4.2.2. *Let $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ and $\mathbf{W} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ be a translationally invariant quantum walk according to Definition 4.2.1. There exists a dilation space $\mathcal{D}$ and a unitary representation $\{U_x\}_{x\in\mathbb{Z}^s}$ of $\mathbb{Z}^s$ on $\mathcal{D}$ together with operators $v_y : \mathcal{K} \to \mathcal{K} \otimes \mathcal{D}$, $y \in \mathcal{N}$, such that an isometry $\mathcal{V} : \mathcal{H} \to \mathcal{H} \otimes \mathcal{D}$ representing $\mathbf{W}$ is given by*

$$\mathcal{V}|x \otimes \phi\rangle = \sum_{y\in\mathcal{N}} |x+y\rangle \otimes |(\mathbb{1}_{\mathcal{K}} \otimes U_x) v_y \, \phi\rangle\,, \quad x \in \mathbb{Z}^s\,, \phi \in \mathcal{K}\,. \tag{4.3}$$

Conversely, a dilation space $\mathcal{D}$ and a unitary representation $\{U_x\}_{x\in\mathbb{Z}^s}$ of $\mathbb{Z}^s$ on $\mathcal{D}$ together with a set of operators $v_y : \mathcal{K} \to \mathcal{K} \otimes \mathcal{D}$, $y \in \mathcal{N}$, satisfying the normalization condition

$$\sum_{y\in\mathcal{N}\cap(\mathcal{N}-x)} v_{x+y}^*(\mathbb{1}_{\mathcal{K}} \otimes U_x) v_y = \mathbb{1}_{\mathcal{K}} \cdot \delta_{x0}\,, \tag{4.4}$$

define a translationally invariant quantum walk $\mathbf{W}$ via Equation (4.3).

In practice, quantum channels are often represented by a Kraus decomposition. The relation between the Kraus operators K_j and the isometry $\mathcal{V}$ is given in Corollary 3.1.3. By expressing $\mathcal{V}$ through the representation U_x of $\mathbb{Z}^s$ and operators v_y associated with $\mathbf{W}$ we get the following corollary.

Corollary 4.2.3. *By choosing orthonormal bases $e_j \in \mathcal{D}$ and $e_\alpha \in \mathcal{K}$ we obtain the Kraus operators $K_j \in \mathcal{B}(\ell^2(\mathbb{Z}^s) \otimes \mathcal{K})$ corresponding to the isometry $\mathcal{V}$ of Theorem 4.2.2 via*

$$\langle z \otimes e_\beta | K_j | x \otimes e_\alpha \rangle = \langle e_\beta \otimes e_j | (\mathbb{1} \otimes U_x) v_{z-x} | e_\alpha \rangle\,.$$

Proof of Theorem 4.2.2. A general isometry $\mathcal{V}$ is given by the relation

$$\mathcal{V}|x \otimes \phi\rangle = \sum_{y\in\mathbb{Z}} |x+y\rangle \otimes |v_y(x)\,\phi\rangle\,,$$

with operators $v_y(x) : \mathcal{K} \to \mathcal{K} \otimes \mathcal{D}$. If we choose the Stinespring pair $\mathcal{V}, \mathcal{D}$ minimal, invariance under translation by $x \in \mathbb{Z}^s$ requires $\mathcal{V}\mathcal{T}_x = \mathcal{T}_x \otimes U_x \mathcal{V}$, where $\mathcal{T}_x$ is the translation operator on $\mathcal{H}$, see Equation (3.9), and the U_x form a unitary representation of $\mathbb{Z}^s$ on $\mathcal{D}$ since all minimal Stinespring pairs are unitarily equivalent on $\mathcal{D}$. The intertwining relation of $\mathcal{V}$ leads to $v_y(x) = U_x v_y(0) =: U_x v_y$. The locality condition (4.2) assures $v_y = 0$ if $y \notin \mathcal{N}$ and the normalization condition is a consequence of the isometry condition $\delta_{xy} \cdot \langle \phi | \psi \rangle = \langle x \otimes \phi | \mathcal{V}^* \mathcal{V} | y \otimes \psi \rangle$. □

Equipped with Theorem 4.2.2 we can further divide the class of all translationally invariant quantum walks according to Definition 4.2.1 into two subclasses, and the defining property of each class is due to the particular structure of the Kraus decomposition, see also Table 4.1. If this decomposition of $\mathbf{W}$ is given by a set of Kraus operators K_j which are translationally invariant in their own right, we say that $\mathbf{W}$ has no momentum transfer. Using Corollary 4.2.3 we can equivalently phrase this

condition in terms of the isometry $\mathcal{V}$ by saying that the operators U_x do not depend on x, hence, $U_x = \mathbb{1}$ for all $x \in \mathbb{Z}^s$. Quantum walks **W** which fail to satisfy this condition are said to have momentum transfer. This means there is no Kraus decomposition such that all Kraus operators are translationally invariant or, equivalently, $U_x \neq \mathbb{1}$ for some $x \in \mathbb{Z}^s$.

The following proposition motivates our terminology of momentum transfer by expressing the isometry $\mathcal{V}$ and the associated Kraus operators K_j by their momentum space representation and connecting this to the spectral representations of the U_x.

Proposition 4.2.4. *Let* **W** *be a translationally invariant quantum walk according to Definition 4.2.1 and e_j an orthonormal basis of the dilation space $\mathcal{D}$. For $p \in [-\pi,\pi)^s$ we define $\mathcal{V}_0(p) = \sum_{y\in\mathcal{N}} e^{\mathrm{i}p\cdot y} v_y$. If* **W** *is without momentum transfer we have*

$$(\mathcal{V}\psi)(p) = \mathcal{V}_0(p)\psi(p)$$

$$(K_j\psi)(p) = K_j(p)\psi(p) \quad \text{with} \quad \langle\eta|K_j(p)|\gamma\rangle = \langle\eta\otimes e_j|\mathcal{V}_0(p)|\gamma\rangle \quad \eta,\gamma\in\mathcal{K}.$$

If **W** *exhibits momentum transfer there exists a spectral measure E on $[-\pi,\pi)^s$ with values in $\mathcal{D}$ such that*

$$(\mathcal{V}\psi)(p) = \int_{q\in[-\pi,\pi)^s} \mathbb{1}_{\mathcal{K}}\otimes E(dq)\mathcal{V}_0(p)\psi(p+q)$$

$$(K_j\psi)(p) = \int_{q\in[-\pi,\pi)^s} \widehat{K}_j(p,dq)\psi(p+q)$$

with the operator valued measure $\widehat{K}_j$ defined by

$$\langle\eta|\widehat{K}_j(p,dq)|\gamma\rangle = \langle\eta\otimes e_j|\mathbb{1}_{\mathcal{K}}\otimes E(dq)\mathcal{V}_0(p)|\gamma\rangle \quad \eta,\gamma\in\mathcal{K}.$$

Proof. The first part, where **W** has no momentum transfer, follows directly from applying the Fourier transform on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}\otimes\mathcal{D}$ to Equation (4.3).

For the second part we note that U_x can be written as a product of powers of s elementary commuting generators U_i, where each U_i corresponds to a translation by one lattice site along the direction of the i^{th} coordinate axis. We denote the spectral measure of U_i by E_i, that is, each E_i is a map from the Borel sets of $[-\pi,\pi)$ to the set of orthogonal projections on $\mathcal{D}$ such that $U_i = \int_{[-\pi,\pi)} e^{\mathrm{i}q_i} E_i(dq_i)$, see Theorem 3.3.3. Then we have

$$U_x = \prod_i U_i^{x_i} = \int_{q\in[-\pi,\pi)^s} \cdots \int_{q\in[-\pi,\pi)^s} e^{\mathrm{i}(x_1q_1+\ldots+x_sq_s)} E_1(dq_1)\cdot\ldots\cdot E_s(dq_s).$$

For a rectangular subset $\square_{p_i,q_i} = [p_1,q_1)\times\ldots\times[q_s,p_s)\subset[-\pi,\pi)^s$, where we assume $p_i \le q_i$, we define

$$E(\square_{p_i,q_i}) := \prod_{i=1}^{s} E_i([p_i,q_i)).$$

As the U_i commute, this defines a projection valued measure E on the rectangular subsets of $[-\pi,\pi)^s$ and since the U_i are unitary this defines a spectral measure on the Borel sets of $[-\pi,\pi)^s$ [BVS78]. Thus we can express U_x as

$$U_x = \int\limits_{q\in[-\pi,\pi)^s} e^{\mathrm{i}x\cdot q} E(dq),$$

which finally yields

$$\begin{aligned}(\mathcal{V}\psi)(p) &= \int\limits_{q\in[-\pi,\pi)^s} \mathbb{1}_{\mathcal{K}}\otimes E(dq)\sum_{y\in\mathcal{N}} e^{\mathrm{i}p\cdot y} v_y \psi(p+q)\\ &= \int\limits_{q\in[-\pi,\pi)^s} \mathbb{1}_{\mathcal{K}}\otimes E(dq)\mathcal{V}_0(p)\psi(p+q).\end{aligned}$$

□

Table 4.1.: The table summarizes the structure of the Kraus operators K_j and the representation $\{U_x\}_{x\in\mathbb{Z}^s}$ of $\mathbb{Z}^s$ for quantum walks with and without momentum transfer.

Momentum transfer	Kraus operators K_j	$\{U_x\}_{x\in\mathbb{Z}^s}$
No	translationally invariant $K_j(p)$	$U_x = \mathbb{1} \quad \forall x$
Yes	non-translationally invariant $\widehat{K}_j(p,dq)$	$\exists x : U_x \neq \mathbb{1}$

To illustrate the classification of quantum walks according to their momentum transfer properties let us briefly consider the characteristic differences if **W** is unitarily implemented or decoherent:

Unitary quantum walks:
The simplest class of quantum walks is the set of unitary quantum walks without momentum transfer. In this case **W** is given by conjugation with a translationally invariant unitary W, i.e. $\mathbf{W}(A) = W^*AW$, and we will see in Section 4.5.1 how the

asymptotic behavior of $\mathbf{W}$ is determined by W. In particular, it will turn out that the generic propagation behavior of such quantum walks is ballistic, which means that the expected distance of the quantum particle from its initial position scales linearly with the number of time steps.

A basic example of a unitary quantum walk on $\mathbb{Z}^s$ with momentum transfer is given by the unitary operator $W_\varphi = e^{\mathrm{i}\varphi\cdot Q}$, already introduced in Equation (3.19), where $\varphi \in [-\pi,\pi)^s$ and Q denotes the position operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. As already argued at the end of Section 3.2, $\mathbf{W}_\varphi$ defined via $\mathbf{W}_\varphi(A) = W_\varphi^* A W_\varphi$ is translationally invariant, which is also true for the product $W\cdot W_\varphi$ if W is any unitary quantum walk without momentum transfer. In fact, the product of W_φ and a translationally invariant W is the most general form of unitary quantum walks with momentum transfer, see Proposition 4.6.1. We will see in Section 4.6.1 that $\mathbf{W}_\varphi$ can be mapped to a unitary quantum walk without momentum transfer iff the phase φ is rational modulo π. For irrational phases φ the propagation behavior is more complicated.

Decoherent quantum walks:
A prototype of a decoherent quantum walk without momentum transfer is given by a classical mixture of unitary quantum walks W_ω without momentum transfer, that is, $\mathbf{W}$ can be written as

$$\mathbf{W}(A) = \int_{\omega\in\Omega} \mu(d\,\omega) W_\omega^* A W_\omega\,,$$

where μ is a probability measure on some probability space Ω. This can be generalized by replacing the unitary W_ω by non-unitary Kraus operators but keeping the translation invariance.

Decoherent quantum walks exhibit a wider range of possible momentum transfer mechanisms. For example, one could take a classical mixture of finitely many unitary quantum walks W_i with different momentum transfer $\varphi_i \in [-\pi,\pi)^s$ to obtain a decoherent quantum walk with discrete momentum transfer. In general, we cannot even exclude continuous momentum transfer by means of a spectral measure E on $[-\pi,\pi)^s$, cf. Proposition 4.2.4. The spectral measure E is related to the spectral measures of the U_x acting on $\mathcal{D}$, in particular, for $s=1$ both coincide. Hence, the presence of continuous spectrum for U_x will lead to a quantum walk $\mathbf{W}$ with continuous momentum transfer. The following example describes a quantum walk where the U_x exhibit continuous spectrum.

Interlude 2: Continuous momentum transfer quantum walk

Consider $\mathcal{H} = \ell^2(\mathbb{Z})$, that is, a particle with no internal degree of freedom moving on a one dimensional lattice. As a further simplification we assume $\mathcal{D} = \mathcal{H}$ and

$\mathcal{N}=\{-1,1\}$. We have to choose a representation $\{U_x\}_{x\in\mathbb{Z}}$ of $\mathbb{Z}$ on the dilation space $\mathcal{D}=\ell^2(\mathbb{Z})$ and two operators $v_{-1,1}:\mathbb{C}\to\ell^2(\mathbb{Z})$ such that the normalization condition (4.4) is fulfilled. If we identify the operators $v_{-1,1}$ with vectors $|v_{-1,1}\rangle$ in $\mathcal{D}$, Equation (4.4) leads to the conditions

$$\langle v_{-1}|v_{-1}\rangle+\langle v_1|v_1\rangle=1 \quad \text{and} \quad \langle v_1|U_2|v_{-1}\rangle=0\,.$$

The first condition can trivially be assured and for the second condition we choose vectors v_i which are supported on subsets Λ_i of the lattice $\mathbb{Z}^s$ with the property that there exists $z\in\mathbb{Z}$ such that $\Lambda_{-1}\cap(\Lambda_1\pm 2z)=\emptyset$. As the final step we set $U_1=\mathcal{T}_z$, see Equation (3.9) for a definition of $\mathcal{T}_z$. This entails $\langle v_1|U_2|v_{-1}\rangle=\langle v_1|\mathcal{T}_z^2|v_{-1}\rangle=0$ such that $\mathbf{W}(A)=\mathcal{V}^*(A\otimes\mathbb{1}_{\mathcal{D}})\mathcal{V}$, with $\mathcal{V}$ according to Equation (4.3), defines a quantum walk with continuous momentum transfer. The action of the operator $\mathbf{W}$ corresponding to $\mathcal{V}$ is

$$\mathbf{W}(|x\rangle\langle y|)=\sum_{k,l=\pm1}\langle v_{-k}|\mathcal{T}_z^{y-x+l-k}|v_{-l}\rangle\cdot|x+k\rangle\langle y+l|\,.$$

By introducing a Fourier transform on $\mathcal{D}=\ell^2(\mathbb{Z})$ we can express the scalar product in this equation by the integral

$$\langle v_{-k}|\mathcal{T}_z^{y-x+l-k}|v_{-l}\rangle=\frac{1}{2\pi}\int\limits_{[-\pi,\pi)}dq\,e^{\mathrm{i}q\cdot z(y-x+l-k)}\overline{v_{-k}(q)}v_{-l}(q),$$

with the Fourier transform $v_j(p)$ of v_j. Of particular interest to us is the action of $\mathbf{W}$ on translationally invariant operators $A\in\mathcal{B}(\mathcal{H})$, which, by Lemma 3.2.2, are represented in momentum space by multiplication with square integrable functions $A(p)=\sum_{x\in\mathbb{Z}}e^{\mathrm{i}xp}A_{x0}$. A straightforward computation shows that the action of $\mathbf{W}$ in momentum space reads

$$\mathbf{W}(A)(p)=\frac{1}{2\pi}\int\limits_{[-\pi,\pi)}dq\,A(p+zq)\left(|v_{-1}(q)|^2+|v_1(q)|^2+2\Re(e^{\mathrm{i}2(p-zq)}\overline{v_{-1}(q)}v_1(q))\right)$$

which nicely illustrates that momentum is not conserved by $\mathbf{W}$.

As a concrete example we choose $\Lambda_{-1}=2\mathbb{N}_0$ and $\Lambda_1=2\mathbb{N}_0+1$. The vectors v_i are defined by

$$\langle\delta_{2x}|v_{-1}\rangle=\frac{1}{\sqrt{2}}\sqrt{1-r^2}\,r^x \quad \text{and} \quad \langle\delta_{2x+1}|v_1\rangle=\frac{1}{\sqrt{2}}\sqrt{1-r^2}\,r^x$$

for $x\in\mathbb{N}_0$, $0<r<1$ and δ_x the unit vector in $\ell^2(\mathbb{Z})$ supported on lattice site $x\in\mathbb{Z}$. The quantum walk $\mathbf{W}$ acts like

$$\mathbf{W}(|x\rangle\langle y|)=C_r\cdot\begin{cases}|x+1\rangle\langle y+1|+|x-1\rangle\langle y-1| & , \quad x-y\in2\mathbb{Z}\\ q|x-1\rangle\langle y+1|+q^{-1}|x+1\rangle\langle y-1| & , \quad x-y\in2\mathbb{Z}+1\end{cases}$$

with

$$C_r = \frac{\sqrt{r}^{|y-x|}}{2} \quad \text{and} \quad q = \sqrt{r}^{\operatorname{sgn}(y-x)}.$$

One verifies directly that this quantum walk behaves exactly like an unbiased classical random walk: The Schrödinger picture representation $\mathbf{W}_*$ coincides with $\mathbf{W}$ except that the roles of q and q^{-1} are exchanged. Hence, for an arbitrary density operator ρ, the position distribution of $\mathbf{W}_*^t(\rho)$ and $\mathbf{W}_*^t(\rho_D)$ coincide, where ρ_D denotes the density operator obtained from ρ by a projective position measurement, i.e. a projection of ρ onto its diagonal elements. Since ρ_D is only affected by the transition rule for $0 = x - y \in 2\mathbb{Z}$, which is the time evolution of an unbiased classical random walk, we conclude that the position distribution of $\mathbf{W}_*^t(\rho)$ is indeed that of a classical random walk.

We will see in Example 6 in Section 4.6.3 that these quantum walks behave classically for any non-zero choice of the vectors v_{-1} and v_1.

4.3. Asymptotic position distribution

In general, a measurement of the position of a quantum particle moving in s spatial dimensions yields a random variable X which takes values in $\mathbb{R}^s$. Complete information about X is contained in its cumulative distribution function F_X, which is a map from $\mathbb{R}^s$ to the positive reals defined via

$$F_X(x) = \mathbb{P}(X_i \leq x_i \,\forall\, i)\,. \tag{4.5}$$

The function F_X is by construction non-decreasing and right-continuous in each coordinate x_i and its limiting behavior is clearly given by

$$\begin{aligned} \lim_{x_i \to -\infty} F_X(x) &= 0 \\ \lim_{x_i \to \infty} F_X(x) &= F_{\widehat{X}_i}(\widehat{x}_i), \end{aligned}$$

where $\widehat{X}_i$ denotes the random variable obtained from X by ignoring the i^{th} coordinate and similarly for vectors $x \in \mathbb{R}^s$.

Another way to describe the distribution of a random variable X with values in $\mathbb{R}^s$ is via its characteristic function

$$C_X(\lambda) = \mathbb{E}\left(e^{\mathrm{i}\lambda\cdot X}\right) = \int_{\mathbb{R}^s} e^{\mathrm{i}\lambda\cdot x}\, d\,F_X(x), \quad \lambda \in \mathbb{R}^s\,. \tag{4.6}$$

The characteristic function C_X always exists since it can be expressed as Stieltjes-integral of $e^{i\lambda\cdot X}$ with respect to the cumulative distribution function F_X of X. If X has a density function[2] then C_X is nothing but the Fourier transform of this density function. In fact, the characteristic function is an equivalent description of the random variable X. Let us note some basic properties of C_X we will use later.

Lemma 4.3.1. *Let X denote a random variable taking values in $\mathbb{R}^s$ and C_X its characteristic function according to Equation* (4.6)*. Then:*

i) C_X is a uniformly continuous function from $\mathbb{R}^s$ to $\mathbb{C}$.

ii) The correspondence $X \longleftrightarrow C_X$ is one-to-one, that is, if $C_X = C_Y$ then $X = Y$.

iii) If the moments $\mathbb{E}\left(X_1^{k_1}\cdot\ldots\cdot X_s^{k_s}\right)$ of X associated with the numbers $k_1,\ldots,k_s$ exist for all $k_i \leq K_i$ then for those k_i all partial derivatives of C_X exist and the moments obey

$$\mathbb{E}\left(X_1^{k_1}\cdot\ldots\cdot X_s^{k_s}\right) = (-\mathrm{i})^{k_1+\ldots+k_s}\frac{\partial^{k_1+\ldots+k_s}}{\partial^{k_1}\ldots\partial^{k_s}}C_X(\lambda)\bigg|_{\lambda=0}.$$

iv) If the random variable X is supported on $\mathbb{Z}^s$, then C_X is 2π-periodic in each variable λ_i.

Proof. For a proof of statements *i)-iii)* we refer to [Chu01]. Statement *iv)* is a trivial consequence. □

Our aim in the following sections is to distinguish between ballistic and diffusive behavior of quantum walks. Commonly, this is done by computing the standard deviation of the position distribution and then extracting its asymptotic scaling with the number of time steps t. If the standard deviation scales like t ($\sqrt{t}$), the asymptotic behavior is called ballistic (diffusive). This approach, however, has a deficiency, it cannot reveal all information about the propagation behavior. There are several examples of quantum walks where an asymptotic analysis of the position distribution's first two moments yields an incomplete answer. In higher lattice dimensions $s > 1$ one can easily construct quantum walks which behave differently along the coordinate axes. For example, the quantum particle may move ballistically along one axis but be prevented from moving along the others or move in diffusive fashion. In all these cases, the standard deviation would grow linearly with the number of time steps, concealing the detailed propagation effects. A way to overcome these obstacles is to consider the random variables corresponding to a position measurement of a quantum particle after t time steps, denoted by X_t, after an appropriate scaling $t^{-\alpha}X_t$ with $\alpha > 0$. Indeed, much information about the

[2] The term density function is meant to imply that the probability measure corresponding to X is absolutely continuous with respect to the Lebesgue measure.

nature of the quantum walk can be inferred from the asymptotic behavior of the random variables $t^{-\alpha}X_t$. In order to give this vague statement a concrete mathematical meaning we need to introduce the concept of weak convergence of random variables.

Definition 4.3.2. *Let $Y_t, t \in \mathbb{N}$ and Y be random variables taking values in $\mathbb{R}^s$. We say that the sequence Y_t converges weakly to Y for $t \to \infty$, in formulas $Y_t \xrightarrow{w} Y$, if*

$$F_{Y_t}(y) \to F_Y(y) \tag{4.7}$$

at all points y where F_Y is continuous.

An immediate consequence of weak convergence of random variables is that the expectation values of continuous functions of the random variables also converge to a well-defined limit. In fact, convergence of all continuous function expectation values is an equivalent definition for weak convergence.

Now consider the scaled random variable $t^{-\alpha}X_t$ for $\alpha > 0$ and assume for the moment that for some α these random variables converge weakly to some random variable V. Then it is clear that the standard deviation $\sigma_t = \sqrt{\mathbb{E}\left(X_t^2\right) - \mathbb{E}(X_t)^2}$, scales for large t like t^α, that is, $\sigma_t = o(t^\alpha)$, cf. Figure 4.2. Of course, the minimal exponent $\alpha_{\min}$ for which the scaled random variables converge is the crucial one as for $\alpha > \alpha_{\min}$ the random variables converge to a point measure at the origin. Hence, this $\alpha_{\min}$ determines the asymptotic scaling of the expected position of the particle and we say that the particle behaves ballistically or diffusively if $\alpha_{\min}$ equals 1 or $1/2$, respectively.

By Levy's continuity theorem, weak convergence of a family of random variables is equivalent to point wise convergence of the corresponding characteristic functions. Hence, we may alternatively determine the minimal α such that the limit of $C_{t^{-\alpha}X_t}$ for t going to infinity exists point wise. For this, it is useful to observe that characteristic functions behave nicely under scaling of the argument λ by a factor μ, for we have the relation

$$C_X(\mu\lambda) = C_{\mu X}(\lambda). \tag{4.8}$$

This rephrases the problem of computing the asymptotic distribution of $t^{-\alpha}X_t$ to finding the limit of the characteristic function $C_{X_t}(t^{-\alpha}\lambda)$.

Let us come back to the case where a quantum particle moves on a lattice $\mathbb{Z}^s$. We denote its initial state by ρ_0 and after t time steps according to the time evolution $\mathbf{W}$ its position distribution is described by the characteristic function

$$C_{X_t}(t^{-\alpha}\lambda) = \operatorname{tr}\mathbf{W}^t(e^{\mathrm{i}t^{-\alpha}\lambda\cdot Q})\rho_0. \tag{4.9}$$

In this case, the convergence of the random variables $t^{-\alpha}X_t$ shows a characteristic feature. For fixed t the probability distribution of $t^{-\alpha}X_t$ is a discrete distribution supported on $t^{-\alpha}\mathbb{Z}^s$. The limiting random variable Y, however, generically has a

continuous distribution supported on $\mathbb{R}^s$. This is not surprising since weak convergence of random variables only demands point wise convergence of the cumulative distribution function, which does not exclude approximations by step functions. Figure 4.2 illustrates weak convergence for the position distribution of an unbiased classical random walk.

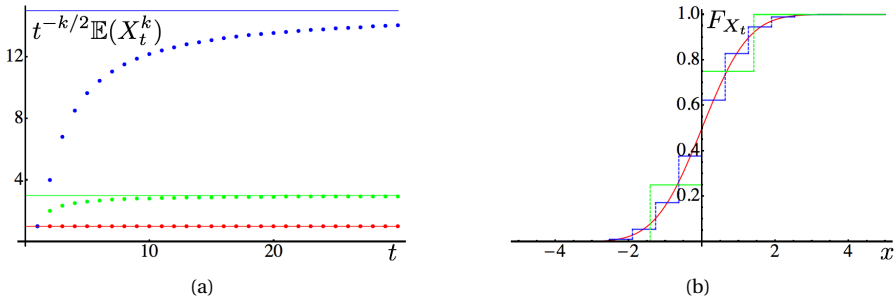


Figure 4.2.: The position distribution of a classical unbiased random walk starting at $x = 0$ after t time steps is a binomial distribution. In diffusive scaling $t^{-1/2}$ these distributions converge weakly to a normal distribution. Plot (a) visualizes convergence of the moments $t^{-k/2}\mathbb{E}\left(X_t^k\right)$ of the position distribution in diffusive scaling for $k = 2$ (red), $k = 4$ (green), and $k = 6$ (blue). Straight lines indicate the value for the asymptotic distribution. Plot (b) compares the cumulative distribution functions of X_t for $t = 2$ (green) and $t = 10$ (blue) with the asymptotic cumulative distribution function (red).

Now suppose we have determined the characteristic function $C_X(\lambda)$ of some random variable X. How can we infer the distribution of X from $C_X(\lambda)$? If $C_X \in \mathcal{L}^1(\mathbb{R}^s)$ we can compute the distribution of X by applying inverse Fourier transform to C_X. This yields a bounded function $P_X \in \mathcal{L}^1(\mathbb{R}^s)$ as probability density for X. However, the characteristic functions we are going to consider in the following sections often fail to share this property. In fact, as we will see in Section 4.5.1, a generic feature of unitary quantum walks is the existence of points $x \in \mathbb{R}^s$ at which the asymptotic position distribution P_X has a singularity. Thus P_X is in general unbounded which means that the corresponding C_X cannot be in $\mathcal{L}^1(\mathbb{R}^s)$ and we have to apply Fourier transform in the distributional sense to obtain P_X. Fortunaltely, we will often encounter the case where $C_X(\lambda)$ itself is given by a Fourier transform. The following Lemma provides a tool to determine P_X in this case.

Lemma 4.3.3. *Let X be a random variable with values in $\mathbb{R}^s$ and assume its characteristic function C_X can be written as*

$$C_X(\lambda) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \; e^{i\lambda\cdot v(p)} \rho(p),$$

with $\rho : [-\pi,\pi)^s \to \mathbb{R}$ and $v : [-\pi,\pi)^s \to \mathbb{R}^s$. Moreover assume v is continuously differentiable, and the set of points where $\det \partial v_i/\partial p_j = 0$, which we denote by R, has zero Lebesgue measure. Then X has a probability density $P_X \in \mathcal{L}^1(\mathbb{R})$, and for $x \in \mathbb{R}^s$ such that its pre-image $v^{-1}(x)$ in $[-\pi,\pi)^s$ satisfies $v^{-1}(x) \cap R = \emptyset$ we have

$$P_X(x) = \frac{1}{(2\pi)^s} \sum_{q\in v^{-1}(x)} \rho(q) \cdot \left|\det \frac{\partial v_i}{\partial p_j}\right|^{-1}(q). \tag{4.10}$$

The sum in Equation (4.10) *is finite, and the probability density P_X diverges when approaching points in R.*

Proof. By the inverse function theorem, we can invert the map v locally at all points where $\det \partial v_i/\partial p_j \neq 0$. Hence, if the pre-image of a point $x \in \mathbb{R}$ satisfies $v^{-1}(x) \cap R = \emptyset$ then $v^{-1}(x)$ is actually of finite cardinality. Indeed, assume there are infinitely many points q_n in the pre-image of x, then there is a limiting point q of a subsequence of $\{q_n\}_n$ since $[-\pi,\pi)^s$ is compact. Because v is differentiable, thus continuous, we must have $v(q) = x$. For each point p in the pre-image of x there exists a neighborhood of p such that v is invertible. But every neighborhood of q contains infinitely many points of the sequence q_n, thus we have a contradiction and $v^{-1}(x)$ must be of finite cardinality.

Even if $C_X \notin \mathcal{L}^1(\mathbb{R}^s)$ it still defines a tempered distribution, thus it makes sense to apply inverse Fourier transform to C_X to determine the probability distribution P_X of X. For any test function f we have

$$\begin{aligned} \int\limits_{\mathbb{R}^s} d^s x \, f(x) P_X(x) &= \int\limits_{\mathbb{R}^s} d^s \lambda \, \widehat{f}(\lambda) C_X(\lambda) \\ &= \frac{1}{(2\pi)^s} \int\limits_{\mathbb{R}^s} d^s \lambda \int\limits_{[-\pi,\pi)^s} d^s p \, \widehat{f}(\lambda) e^{\mathrm{i}\lambda\cdot v(p)} \rho(p), \end{aligned}$$

with the Fourier transform $\mathcal{F} f = \widehat{f}$ of f. By the definition of the Fourier transform for tempered distributions we have

$$\int\limits_{\mathbb{R}^s} d^s \lambda \, \widehat{f}(\lambda) e^{\mathrm{i}\lambda\cdot v(p)} = \int\limits_{\mathbb{R}^s} d^s x \, f(x) \delta(x - v(p))$$

with the Dirac distribution δ. This finally yields

$$\int_{\mathbb{R}^s} d^s x\, f(x) P_X(x) \quad = \quad \frac{1}{(2\pi)^s} \int_{\mathbb{R}^s} d^s x \int_{[-\pi,\pi)^s} d^s p\, f(x) \delta(x - v(p)\rho(p))$$

and Equation (4.10) follows from a substitution of the integration variable p by v. □

Now we have all necessary tools at hand to tackle the asymptotic analysis of quantum walks. Before we turn to the different classes of quantum walks we sketch the general approach in the next section.

4.4. General method

The position distribution of a quantum state ρ_0, evolved for t time steps, with a scaling of the position operator Q by a factor of ε, is equivalently described by the characteristic function

$$C_{t,\varepsilon}(\lambda) = \mathrm{tr}(\rho_0 \mathbf{W}^t(e^{\mathrm{i}\varepsilon\lambda\cdot Q})). \tag{4.11}$$

For the asymptotic analysis of the quantum walk $\mathbf{W}$ we choose a scaling $\varepsilon = t^{-\alpha}$ of the position operator Q and compute the weak limit of the probability measures corresponding to position measurements after t time steps. Of course, the existence of this limit depends on the exponent α. In particular, we are interested in the minimal exponent $\alpha_{\min}$ for which this limit exists. This then determines the type of asymptotic behavior of $\mathbf{W}$. It will turn out that for the models we consider the correct scalings are either given by $\alpha_{\min} = 1$, which we call ballistic scaling, or $\alpha_{\min} = 1/2$, referred to as diffusive scaling.

The weak limit of these probability measures can be computed from the point wise limit of the characteristic functions (4.11) with $\varepsilon = t^{-\alpha}$ and t going to infinity, see Section 4.3. Thus, slightly more abstract, the task is to compute the limiting characteristic function

$$C(\lambda) = \lim_{t\to\infty} C_{t,\varepsilon}(\lambda), \tag{4.12}$$

for some function $\varepsilon = \varepsilon(t)$ with the property $\varepsilon(t) \underset{t\to\infty}{\longrightarrow} 0$.

The method we are going to incorporate is based on results from the perturbation theory of bounded linear operators [Kat95, Bau85]. The idea is to introduce a similarity transform

$$\begin{aligned} \phi_\varepsilon : \mathcal{B}(\mathcal{H}) &\longrightarrow \mathcal{B}(\mathcal{H}) \\ A &\longmapsto \phi_\varepsilon(A) = A e^{i\varepsilon\lambda\cdot Q} \end{aligned} \tag{4.13}$$

and define the operator

$$\mathbf{W}_\varepsilon := \phi_\varepsilon^{-1} \circ \mathbf{W} \circ \phi_\varepsilon \tag{4.14}$$

on $\mathcal{B}(\mathcal{H})$. Thus, for any $A \in \mathcal{B}(\mathcal{H})$ the action of $\mathbf{W}_\varepsilon$ is given by

$$\mathbf{W}_\varepsilon(A) := \mathbf{W}(Ae^{\mathrm{i}\varepsilon\lambda\cdot Q})e^{-\mathrm{i}\varepsilon\lambda\cdot Q}, \tag{4.15}$$

from which it follows inductively that

$$\mathbf{W}^t(e^{\mathrm{i}\varepsilon\lambda\cdot Q}) = \mathbf{W}_\varepsilon^t(\mathbb{1})e^{\mathrm{i}\varepsilon\lambda\cdot Q}, \quad \forall\, t \in \mathbb{N}. \tag{4.16}$$

When inserting this into the characteristic function $C(\lambda)$ we can neglect the factor $e^{\mathrm{i}\varepsilon\lambda\cdot Q}$ on the right hand side, for we have the estimate

$$\begin{aligned} \left|\mathrm{tr}\left(\rho_0\mathbf{W}_\varepsilon^t(\mathbb{1})\right) - \mathrm{tr}\left(\rho_0\mathbf{W}_\varepsilon^t(\mathbb{1})e^{\mathrm{i}\varepsilon\lambda\cdot Q}\right)\right| &= \left|\mathrm{tr}\left((\mathbb{1}-e^{\mathrm{i}\varepsilon\lambda\cdot Q})\rho_0\mathbf{W}_\varepsilon^t(\mathbb{1})\right)\right| \\ &\leq \left\|(\mathbb{1}-e^{\mathrm{i}\varepsilon\lambda\cdot Q})\rho_0\right\|_1 \cdot \left\|\mathbf{W}_\varepsilon^t(\mathbb{1})\right\|_{op} \\ &\leq \left\|(\mathbb{1}-e^{\mathrm{i}\varepsilon\lambda\cdot Q})\rho_0\right\|_1 \cdot \left\|\mathbf{W}^t(e^{\mathrm{i}\varepsilon\lambda\cdot Q})\right\|_{op}, \end{aligned} \tag{4.17}$$

where $\|.\|_1$ denotes the trace-norm. Since $\|\mathbf{W}(A)\|_{op} \leq \|A\|_{op}$ we conclude that the second factor in the last inequality is bounded by one for all t and the first factor converges to zero with $\varepsilon \to 0$. Consequently, the characteristic function of the asymptotic position distribution in ε-scaling, if it exists, is given by the formula

$$C(\lambda) = \lim_{t\to\infty} \mathrm{tr}\left(\rho_0\mathbf{W}_\varepsilon^t(\mathbb{1})\right). \tag{4.18}$$

If $\mathbf{W}$ is unitarily implemented and without momentum transfer it is straightforward to determine the large time limit of $\mathbf{W}_\varepsilon^t(\mathbb{1})$ directly from the momentum space representation $W(p)$ of the translationally invariant unitary operator W. Generically, $\varepsilon = 1/t$ will turn out to be the right scaling for the asymptotic position distribution in this case. Here the main tool is a p-dependent spectral decomposition of the unitary matrix $W(p)$. The p-dependent eigenvalues of $W(p)$ lead us to the notion of dispersion relations and the structure of these dispersion relations can be analyzed in great detail by using results from perturbation theory. If $\mathbf{W}$ exhibits momentum transfer there are special cases which can easily be mapped to the setting without momentum transfer. However, for some cases this is not possible and there is no notion of dispersion relations. These quantum walks defy applicability of our method.

For decoherent quantum walks $\mathbf{W}$ we interpret ε as a perturbation parameter, so we act with a high power of the perturbed operator $\mathbf{W}_\varepsilon$ on the eigenvector $\mathbb{1}$ of the unperturbed operator $\mathbf{W} = \mathbf{W}_0$. The limit of $\mathbf{W}_\varepsilon^t(\mathbb{1})$ can be computed by expanding perturbed eigenvector and eigenvalue of $\mathbf{W}_\varepsilon$ into power series and equating coefficients of the eigenvalue equation. The crucial point here is that $\mathbf{W}_\varepsilon$, as in the case

of unitary quantum walks, is in fact an endomorphism on the set of translationally invariant bounded operators on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ which are denoted by $\mathcal{T}_{\mathcal{K},s}$. To verify this we have to prove that $\tau_y\circ\mathbf{W}_\varepsilon=\mathbf{W}_\varepsilon\circ\tau_y$ holds for all $y\in\mathbb{Z}^s$, and indeed, although the similarity transform ϕ_ε on $\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ does not preserve translation invariance, more precisely $\tau_y\circ\phi_\varepsilon=e^{\mathrm{i}\varepsilon\lambda\cdot y}\phi_\varepsilon\circ\tau_y$, the operator $\mathbf{W}_\varepsilon=\phi_\varepsilon^{-1}\circ\mathbf{W}\circ\phi_\varepsilon$ commutes with translations τ_y. This is due to the fact that $\mathbf{W}$ preserves translation invariance and the two appearing phase factors cancel each other. It was proven in Section 3.2 that $\mathcal{T}_{\mathcal{K},s}$ is a separable Hilbert space, so we consider $\mathbf{W}_\varepsilon$ as family of bounded operators on $\mathcal{T}_{\mathcal{K},s}$ which we then analyze by means of perturbation theory. Although $\mathbf{W}_\varepsilon$ is similar to $\mathbf{W}$, their respective restrictions to $\mathcal{T}_{\mathcal{K},s}$ do not coincide. Hence, the perturbation theory of $\mathbf{W}_\varepsilon$ is non-trivial, which is expressed by the fact that the similarity transform of the unperturbed eigenvector $\phi_\varepsilon(\mathbb{1})=e^{\mathrm{i}\varepsilon\lambda\cdot Q}$ is no longer an element of $\mathcal{T}_{\mathcal{K},s}$. In this case, the right scaling of the asymptotic position distribution is in general $\varepsilon=1/\sqrt{t}$ regardless of the presence of momentum transfer. However, for the kind of perturbation theory one has to apply the latter plays a crucial role. Without momentum transfer p is a conserved quantity and one can apply finite dimensional perturbation theory to the momentum space representation of $\mathbf{W}_\varepsilon$ for fixed p. This is no longer true if p is not a conserved quantity and one has to apply infinite dimensional perturbation theory to $\mathbf{W}_\varepsilon$.

Table 4.2 summarizes the generic asymptotic behavior of quantum walks.

Table 4.2.: Quantum walks subject to decoherence behave diffusively under rather mild conditions on the kind of decoherence. For unitary quantum walks, the behavior depends on the presence of momentum transfer: Without momentum transfer the quantum walk generically exhibits ballistic spreading, if there is momentum transfer the behavior is more complicated, see Section 4.6.1.

momentum transfer	unitary $\mathbf{W}$	decoherent $\mathbf{W}$
No	ballistic	diffusive
Yes	?	diffusive

4.5. Quantum walks without momentum transfer

Throughout this section we will assume that the considered quantum walks have no momentum transfer. Thus, the momentum variable p is a conserved quantity and one can perform the analysis separately for each p. Consequently, the compu-

tation boils down to a parameter dependent analysis of finite dimensional matrices, where the dimension is determined by the internal state space.

4.5.1. Unitary quantum walks

The quantum channel **W** is now unitarily implemented, hence, it is sufficient to consider its action on pure states. We denote the unitary operator implementing the quantum channel **W** by W, that is $\mathbf{W}(A) = W^*AW$. The assumption of no momentum transfer is equivalent to saying that the single Kraus operator W itself commutes with translations of the lattice. This is expressed by the formula $[\mathcal{T}_x, W] = 0$ for all $x \in \mathbb{Z}^s$, where $\mathcal{T}_x$ denotes the unitary operator implementing spatial translations by a vector $x \in \mathbb{Z}^s$, see Equation (3.9) for the precise definition. This means that the Fourier transform $\mathcal{F}W\mathcal{F}^{-1}$ of W corresponds to a multiplication operator $W(p)$ and the unitarity of W is equivalent to the statement that $W(p)$ is unitary for all $p \in [-\pi, \pi)^s$. The matrix elements of $W(p)$ are functions of p that may be expressed by their Fourier series. Since $W(p)$ has to respect the locality condition (4.2) each matrix element is actually a Fourier polynomial where the maximal degree of these polynomials is exactly the maximal step size of the quantum walk. Indeed, the matrix elements of W obey

$$\langle x \otimes \phi | W | y \otimes \psi \rangle = \langle \phi | W_{xy} | \psi \rangle = \langle \phi | W_{x-y0} | \psi \rangle$$

for all $x, y \in \mathbb{Z}^s$ and $\phi, \psi \in \mathcal{K}$. Since these matrix elements are identically zero if $x - y \notin \mathcal{N}$ we have the following momentum space representation of W

$$W(p) = \sum_{x \in \mathcal{N}} e^{\mathrm{i}x \cdot p} W_{x0}. \tag{4.19}$$

Remark 4.5.1. *Since any translationally invariant unitary quantum walks W on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ is uniquely determined by its Fourier transform $W(p)$, Definition 4.2.1 is equivalent to the condition that W is defined by a $d \times d$ matrix $W(p)$, depending on an s-dimensional momentum vector p, such that $W(p)$ is unitary for all $p \in [-\pi, \pi)^s$ and each matrix element is a finite degree Fourier polynomial in the coordinates p_i.*

Commonly, unitary quantum walks are taken to be compositions of two building blocks, strictly local coin operators and state-dependent shift operators, both of which constitute quantum walks in their own right. The coin operator is strictly local in the sense that it has no non-zero matrix elements between different lattice sites, hence, it can be written in position space as $U_C = \mathbb{1}_{\mathbb{Z}^s} \otimes C$, where $C \in \mathcal{U}(\mathcal{K})$. The shift operator translates the quantum particle according to its internal state, that is, it can be written in terms of translations $\mathcal{T}_{x_i}$ along lattice vectors x_i, and a set of orthonormal vectors $\psi_i \in \mathcal{K}$ as

$$S = \sum_{i=1}^{\dim \mathcal{K}} \mathcal{T}_{x_i} \cdot (\mathbb{1}_{\mathbb{Z}^s} \otimes |\psi_i\rangle\langle\psi_i|). \tag{4.20}$$

Translationally invariant operators which are strictly local correspond to constant operators in momentum space, hence, the Fourier transform of U_C is constant, more precisely, $(\mathcal{F}U_C\mathcal{F}^{-1})(p) = C$. By choosing the ψ_i as orthonormal basis of $\mathcal{K}$, we achieve that the shift operator S becomes a diagonal operator in momentum space

$$\mathcal{F}S\mathcal{F}^{-1}(p) = \begin{pmatrix} e^{\mathrm{i}x_1\cdot p} & & \\ & \ddots & \\ & & e^{\mathrm{i}x_{\dim\mathcal{K}}\cdot p} \end{pmatrix}. \tag{4.21}$$

Clearly, arbitrary products of several coin and shift operators yield valid quantum walks. As the following theorem, which is a result of [Vog09], shows, the converse of this statement is also true if we restrict to quantum walks in one lattice dimension.

Theorem 4.5.2. *Let $W(p)$ be the Fourier transform of a unitary quantum walk W on $\ell^2(\mathbb{Z})\otimes\mathcal{K}$. There exist constant unitaries C_i and p-dependent diagonal unitaries $S_i(p) = \mathrm{diag}(e^{\mathrm{i}x_{i,j}\cdot p})$ such that $W(p)$ can be decomposed as*

$$W(p) = S_1(p)C_1S_2(p)\ldots S_n(p)C_n\,. \tag{4.22}$$

A proof of this theorem can be found in [Vog09]. In any lattice dimension s, we refer to quantum walks W of the form

$$W = S_1\cdot(\mathbb{1}_{\mathbb{Z}^s}\otimes C_1)\cdot\ldots\cdot S_n\cdot(\mathbb{1}_{\mathbb{Z}^s}\otimes C_n), \tag{4.23}$$

with $C_j\in\mathcal{U}(\mathcal{K})$ and S_j according to Equation (4.20), as coined quantum walks. We stress that the common use of this term in the literature is reserved for quantum walks consisting of just a single shift and coin operator. It is an open question whether such a decomposition always exists in higher lattice dimensions, in other words, it is unclear whether the set of coined quantum walks exhausts the set of all unitary quantum walks in any lattice dimension.

Suppose we are given a unitary quantum walk W which we modify by a constant shift along a vector v at each time step. This constant drift of the system is represented in momentum space by multiplication with the operator $e^{\mathrm{i}v\cdot p}\mathbb{1}$. On the other hand, given any unitary quantum walk W we would like to have a simple procedure to determine such a deterministic drift of the system, and to eliminate it from the time evolution. A quantity suitable for this purpose is the index of W, see [GNVW12] for a general definition in the context of quantum walks and quantum cellular automata. Although the general index theory is only applicable for one-dimensional lattices, there is a simpler version for arbitrary lattice dimension if translation invariance is granted. Let $W(p)$ denote the momentum representation of a unitary quantum walk W. The matrix elements of $W(p)$ are Laurent polynomials in the variables $e^{\mathrm{i}p_i}$ and so is the determinant $\det W(p)$. Clearly, $W^* = W^{-1}$ is a translationally invariant unitary quantum walks as well,

hence, $\det W(p)^{-1} = 1/\det W(p)$ is also a Laurent polynomial in the variables e^{ip_i}. This is only possible if $\det W(p)$ is a monomial, that is, $\det W(p) = c\,e^{ip\cdot v}$. The vector v is the desired quantity.

Definition 4.5.3. *Let $W(p)$ be the Fourier transform of a translationally invariant unitary quantum walk W on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. We define the index of W to be the vector*

$$\operatorname{ind} W = -\mathrm{i}\nabla_p \log\det W(p). \tag{4.24}$$

Clearly, the index of strictly local operators $\mathbb{1}_{\mathbb{Z}^s}\otimes C$ equals zero and shift operators S according to Equation (4.21) have index

$$\operatorname{ind} S = \sum_{i=1}^{\dim\mathcal{K}} x_i\,,$$

which is in agreement with our interpretation of the index as a constant and deterministic drift of the system along the direction proportional to the index.

Given a unitary quantum walk W we can infer a lot of information about its propagation properties by looking at the p-dependent spectrum of the unitary matrix $W(p)$. Since $W(p)$ is unitary for all p, we obtain a p-dependent eigendecomposition

$$W(p) = \sum_{j=1}^{\kappa} e^{\mathrm{i}\omega_j(p)}\mathbf{P}_j\,, \tag{4.25}$$

where the $\mathbf{P}_j$ denote the p-dependent projections onto the eigenspace corresponding to the eigenvalues $e^{\mathrm{i}\omega_j(p)}$. The number of eigenvalues κ may actually depend on the momentum p since different eigenvalues can cross at a certain momentum p. Moreover, the ω_j and $\mathbf{P}_j$ can clearly be chosen as continuous functions of p, but if some eigenvalues cross at p there may be some ambiguity in the choice of these functions as the relation between the eigenvalues before and after crossing may not be unique. However, we will see in the next section that for almost all momenta with respect to Lebesgue measure, κ equals a fixed constant. The real valued functions ω_j are called dispersion relations of W. Some properties of the ω_j are evident, they are functions of s coordinates p_k with range $[-\pi,\pi)$, and for each j there exists i such that

$$\lim_{p_k\to\pi}\omega_j(p) = \lim_{p_k\to-\pi}\omega_i(p)$$

for all k. A more subtle point is that the $\operatorname{tr}_{\mathcal{K}}\mathbf{P}_j$-weighted derivatives of the ω_j, if they exist, have to sum up to the index of W. Indeed, from $-\mathrm{i}\log\det W(p) = \sum_j \operatorname{tr}_{\mathcal{K}}\mathbf{P}_j\,\omega_j(p)$ and the definition of the index we obtain the equation

$$\sum_j \operatorname{tr}_{\mathcal{K}}\mathbf{P}_j\nabla_p\omega_j = \operatorname{ind} W\,.$$

Before we turn our attention to the analysis of the asymptotic propagation behavior of W, we investigate the properties of the dispersion relations and their connection to the spectrum of W as an operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ in more detail.

Spectral properties

In this section we shed some light on the close relation between the spectrum of the unitary operator W acting on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ and the functions ω_j. To begin with, it is straightforward to see that each value in the range of the dispersion relations is a point in the spectrum of W, i.e. $e^{\mathrm{i}\omega_j(p)}\in\sigma(W)$ for all j and p. Likewise, if z is a value not in the range of any of the ω_j we can define the inverse of $W-z$ via its Fourier transform

$$(W-z)^{-1}(p)=\sum_{i=1}^{\kappa}(e^{\mathrm{i}\omega_j(p)}-z)^{-1}\mathbf{P}_i\,.$$

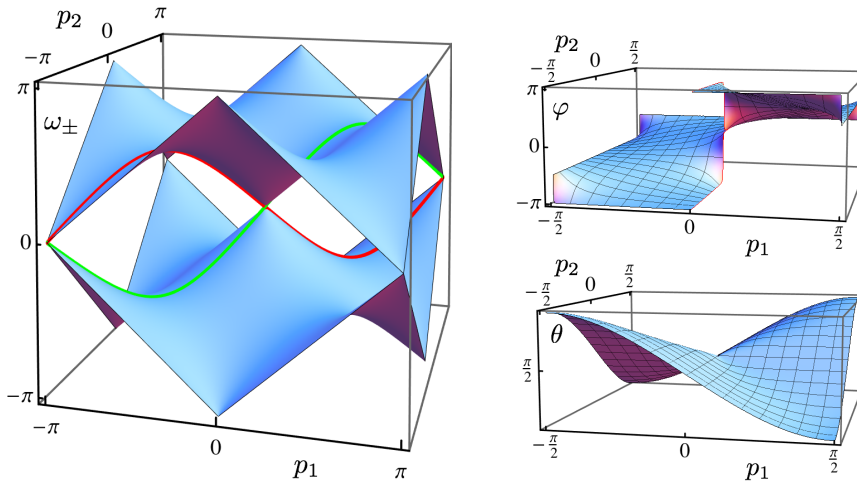
The right hand side clearly defines a translationally invariant operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ with operator norm equal to the reciprocal of $\min_{j,p}|e^{\mathrm{i}\omega_j(p)}-z|$. In fact, from a closer analysis of the functions ω_j we will get a finer picture of the spectrum of W identifying subparts like pure point or continuous spectrum, see Proposition 4.5.7.

Another reason why we are interested in properties of the dispersion relations is that their derivatives $\nabla_p\omega_j$ are the key quantity for the asymptotic behavior of the quantum walk associated with W. More precisely, the derivatives of the one-parameter families $\omega_j(p+\varepsilon\lambda)$ with respect to ε determine the characteristic function of the asymptotic position distribution. We will see that these can always be chosen as analytic functions of ε such that their derivatives are well-defined, see also Figure 4.3. Another statement we prove is that, up to a set of Lebesgue measure zero, the ω_j and $\mathbf{P}_j$ can be chosen as analytic functions of $p\in[-\pi,\pi)^s$. A crucial point is that singular momenta, which are defined as points $p\in[-\pi,\pi)^s$ where some ω_j or $\mathbf{P}_j$ cannot be chosen analytic, have to be momenta at which several dispersion relations cross, cf. Figure 4.3.

Definition 4.5.4. *Let W be a translationally invariant unitary quantum walk and denote its Fourier transform by $W(p)$. A point $q\in[-\pi,\pi)^s$ is called a regular momentum if all dispersion relations ω_j and corresponding eigenprojections $\mathbf{P}_j$ can be chosen as analytic functions in a neighborhood of q.*

Whether or not a point q in momentum space is regular can be analyzed by means of perturbation theory of analytic operators in several variables. A survey of the methods from [Bau85] we are going to use can be found in Section 3.4. The starting point is a decomposition of the characteristic polynomial into irreducible factors

$$\det W(p)-z\,\mathbb{1}=\prod_{j=1}^{r}\zeta_j^{m_j}(p,z). \tag{4.26}$$



(a) (b)

Figure 4.3.: The figure shows the dispersion relations and orientation of eigenprojections of the quantum walk $W(p_1,p_2) = e^{-ip_1\sigma_1}e^{-ip_2\sigma_3}$, where $\sigma_{1,2,3}$ denote the Pauli operators, cf. Interlude 3 and Example 1. Figure (a): The dispersion relations display a singularity at the origin and at the corners of $[-\pi,\pi)^2$. The red and green line visualize analytic choices in one dimension. Figure (b): The eigenprojection corresponding to the upper branch of the dispersion relation can be mapped to a normalized vector in $\mathbb{R}^3$ via the Bloch sphere construction. The angles φ and θ of the polar representation of this vector also show a singularity at the origin and the corners of $[-\pi,\pi)^2$. For better visualization only a subregion of momentum space is shown.

In this equation, the left hand side is a polynomial in the variables $u_j = e^{ip_j}$ and z, and each ζ_j is a polynomial in z whose coefficients are analytic functions of the u_j. In fact, these coefficients are also polynomial in the u_j, but since this yields no further insights we consider them as general analytic functions. A core result taken from [Bau85] is that the discriminant D_γ of $\gamma = \prod_j \zeta_j$ considered as polynomial in z is a non-zero analytic function in the u_j, which implies that for almost all p all of its eigenvalues are non-degenerate. As a simple consequence of the implicit function theorem we have that each eigenvalue of $W(p)$ is analytic at p if $D_\gamma(p) \neq 0$, see Section 3.4. These observations pave the way for the following proposition.

Proposition 4.5.5. *Let W be a unitary quantum walk on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ with momentum representation $W(p)$. Then:*

i) The one parameter family $W(p+\varepsilon\lambda)$ with $p\in[-\pi,\pi)^s$ and $\lambda\in\mathbb{R}^s$ can always be chosen such that all dispersion relations ω_j and eigenprojections $\mathbf{P}_j$ are analytic functions of $\varepsilon\in G$, where $G\subset\mathbb{C}$ is a sufficiently small neighborhood of the origin. In particular, if the lattice is one-dimensional, i.e. $s=1$ and $p\in[-\pi,\pi)$, the ω_j can be chosen such that all momenta are regular.

ii) Denote the p-dependent number of different eigenvalues of $W(p)$ by κ_p. For almost all momenta p we have the equality

$$\kappa_p = \max_{p\in[-\pi,\pi)^s} \kappa_p =: \kappa\,,$$

and all ω_j and $\mathbf{P}_j$ are analytic at points p where $\kappa_p=\kappa$ holds.

iii) If $\kappa_p<\kappa$ and ω_j does not cross any other branch ω_k in a neighborhood of p, then ω_j and $\mathbf{P}_j$ are analytic at p. Moreover, two different branches ω_j and ω_k cross at most on a set of Lebesgue measure zero.

Remark 4.5.6. *As a trivial consequence of Proposition 4.5.5 we get that the set of non-regular momenta is of Lebesgue measure zero and if all eigenvalues $e^{\mathrm{i}\omega_j(p)}$ are non-degenerate at p then p is regular.*

Proof of Proposition 4.5.5. The matrix elements of $W(p)$ are finite degree Fourier polynomials in the variables $p_1,\dots,p_s$. If we allow the p_j to be complex variables in an open set, it is easy to see that $W(p)$ is an analytic family in p in the sense of Section 3.4. The same is true for the one-parameter family $W(p+\varepsilon\lambda)$ with $p\in[-\pi,\pi)^s$, $\lambda\in\mathbb{R}^s$ and ε in a complex neighborhood of the origin. Statement *i)* is a simple consequence of perturbation theory for one-parameter families of normal analytic operators, see [Kat95, §1. Thm. 1.10] and Lemma 3.4.4.

In order to prove statements *ii)* and *iii)* we use results on perturbation theory of analytic operators in several variables [Bau85], see also Section 3.4. From the factorization (4.26) of the characteristic polynomial $\chi_p(z)=\det W(p)-z\mathbb{1}$ into irreducible factors ζ_j we construct $\gamma=\prod_j\zeta_j$, which we consider as polynomial in z, see also Equation (3.29). The numbers $e^{\mathrm{i}\omega_j(p)}$ are exactly the roots z of the polynomial γ. According to Lemma 3.4.2, all objects in the spectral decomposition of $W(p)$ are analytic at points where the discriminant D_γ of γ is non-zero. Since D_γ is analytic in the complex variables p_j and not identically zero it is also analytic and non-vanishing for real $p_j\in[-\pi,\pi)$. Hence, statement *ii)* is a consequence of the fact that the zero set of a non-vanishing real analytic function is a set of Lebesgue measure zero, see e.g. [Fed69] page 240, and the observation that κ_p is maximal exactly when D_γ is non-zero.

Suppose $e^{\mathrm{i}\omega_j(p)}$ is a simple root of the polynomial γ, in other words, there is a neighborhood of p such that ω_j does not cross any other dispersion relation ω_k. According to Lemma 3.4.2 there exists a neighborhood of p in which ω_j and $\mathbf{P}_j$ are analytic functions, which proves the first half of assertion *iii)*. For the remaining part of *iii)* suppose ω_j and ω_k are distinct, but cross on a subset of $[-\pi,\pi)^s$. Then $e^{\mathrm{i}\omega_j}$ and $e^{\mathrm{i}\omega_k}$ are two different roots of γ, and since the set on which these two eigenvalues coincide is a subset of the zero set of D_γ, which is a set of Lebesgue measure zero, *iii)* is proven.

□

Statement *ii)* is essentially the technical assumption Grimmett et al. used to derive the asymptotic position distribution for a particular class of quantum walks in [GJS04b], see also [GJS04a]. More precisely, the standing assumption in [GJS04b, GJS04a] is that $\kappa_p = \dim\mathcal{K}$ for almost all p, i.e. the eigenvalues of $W(p)$ are non-degenerate for almost all momenta. Theorem 4.5.5 provides a proof for the soundness of this assumption for more general quantum walks as compared to the model considered in [GJS04b, GJS04a]. Moreover, for our method to work, it is only necessary to verify statement *i)*, i.e. points where the ω_j and $\mathbf{P}_j$ are non-analytic as functions of $p\in[-\pi,\pi)^s$ are irrelevant since we can always choose them as analytic functions of ε for fixed $\lambda\in\mathbb{R}^s$. The following example concerns quantum walks with non-analytic dispersion relations and eigenprojections, see also Figure 4.3.

Interlude 3: Non-regular momenta

The following construction yields a class of quantum walks on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ where the origin $p=0$ in momentum space is a degeneracy point such that the perturbation theory is non-analytic. Let A_j be non-commuting hermitian matrices acting on $\mathcal{K}$ with integer eigenvalues. We denote by p_j the momentum variable corresponding to the j-th spatial coordinate and define operators $U_j(p)=e^{\mathrm{i}p_jA_j}$, which clearly satisfy our definition of quantum walks. Thus we may define another quantum walk through their composition $W(p)=U_s(p)\cdot\ldots\cdot U_1(p)$ and since $W(0)=\mathbb{1}$ the origin is a degeneracy point of W. To verify non-analyticity of the dispersion relations and eigenprojections we note that the derivatives $\partial_j W(0)=\mathrm{i}A_j$ will, in general, not commute. This implies that there is no analytic choice of dispersion relations ω_k and eigenprojections $\mathbf{P}_k$ near $p=0$. To verify this statement, let us expand W near the origin into a power series

$$W(\varepsilon\lambda)=\mathbb{1}+\varepsilon\mathrm{i}\sum_i\lambda_iA_i+o(\varepsilon^2). \tag{4.27}$$

As a consequence of this equation, the limit of the eigenprojections of $W(\varepsilon\lambda)$ for $\varepsilon \to 0$ must coincide with the eigenprojections of $\sum_i \lambda_i A_i$. For non-commuting A_i these eigenprojections will depend on the direction of λ, hence there is no well-defined limit for the set of eigenprojections at $p = 0$. The derivatives of the dispersion relations ω_k corresponding to the analytic choice of the spectral decomposition of $W(\varepsilon\lambda)$ can be determined from the equation

$$\begin{aligned}\frac{d}{d\varepsilon} W(\varepsilon\lambda)\Big|_{\varepsilon=0} &= \sum_k e^{\mathrm{i}\omega_k} \left(\mathrm{i}\omega'_k \mathbf{P}_k + \mathbf{P}'_k\right)\Big|_{\varepsilon=0} = \left(\sum_k \mathrm{i}\omega'_k \mathbf{P}_k + \sum_k \mathbf{P}'_k\right)\Big|_{\varepsilon=0} \\ &= \sum_k \mathrm{i}\omega'_k \mathbf{P}_k \,,\end{aligned}$$

where we used that the derivative of $\sum_k \mathbf{P}_k = \mathbb{1}_{\mathcal{K}}$ equals zero. Since

$$\frac{d}{d\varepsilon} W(\varepsilon\lambda)\Big|_{\varepsilon=0} = \mathrm{i}\sum_l \lambda_l A_l$$

we obtain the derivatives ω'_k as eigenvalues of $\sum_l \lambda_l A_l$, which typically depends on the direction of λ and makes the gradient of the dispersion relations at $p = 0$ ill-defined, cf. Figure 4.3.

The dispersion relations contain much information about W, in particular there is a close relation between the ω_j and the spectrum of W as operator on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$. According to the RAGE Theorem 3.3.6, this in turn yields statements about the propagation behavior of W. Using the spectral decomposition (4.25) and properties of the dispersion relations we next prove the following proposition.

Proposition 4.5.7. *The spectrum of a translationally invariant unitary quantum walk W consists only of pure point and absolutely continuous spectrum. More precisely, if $W(p)$ denotes the Fourier transform of W and ω_j its dispersion relations, we have the following statements:*

i) The dispersion relations ω_j are constant either everywhere or nowhere. That is, the pre-image $\omega^{-1}(\eta)$ of $\eta \in [-\pi, \pi)$ is either for all η a set of measure zero in $[-\pi, \pi)^s$ or there exists η such that $\omega^{-1}(\eta) = [-\pi, \pi)^s$.

ii) The pure point spectrum of W coincides with the values $e^{\mathrm{i}\omega_j}$ for those j for which the dispersion relations $\omega_j(p) = \omega_j$ are constant. Each eigenvalue is infinitely degenerate and an orthonormal set of eigenvectors corresponding to ω_j can be chosen such that they differ only by spatial translations.

iii) The absolutely continuous spectrum of W is given by $\sigma_{ac}(W) = \bigcup_j \Omega_j$ with

$$\Omega_j = \{e^{i\omega_j(p)} : p \in [-\pi,\pi)^s\,,\ \omega_j \textit{ non-constant}\}\,.$$

Proof. We could invoke the fact that the zero set of a real-analytic function is either its whole domain or a set of measure zero to prove statement *i)*. However, there is a faster way to verify our claim. Given W such that one of its dispersion relations satisfies $\omega_j(q) = \eta$ for q in a set of positive measure, we can modify W by adding another dimension to $\mathcal{K}$ on which W acts by multiplication with $e^{i\eta}$. In doing so, we just add another dispersion relation which takes the constant value η and which coincides with ω_j on a set of positive measure. By Proposition 4.5.5 this already implies constancy of ω_j since two eigenvalues which coincide on a set of positive measure have to coincide on the whole of $[-\pi,\pi)^s$.

Clearly, if $\omega_j(p) = \omega_j$ is constant we can construct eigenvectors of W by multiplying the p-dependent eigenvectors of $W(p)$ with arbitrary integrable functions $f(p)$. Indeed, the vector-valued functions $f(p)\psi_j(p)$ define unique vectors in $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ since the $\psi_j(p)$ are continuous in p. If we assume the $\psi_j(p)$ are chosen normalized for all p, a complete set of eigenvectors corresponding to $e^{i\omega_j}$ can be found by constructing a set of functions $\{f_x\}_{x\in\mathbb{Z}^s}$ with $|f_x(p)| = 1$ for all p such that

$$f_0 = 1 \quad , \quad \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\, \overline{f_x} f_y = 0\,, \quad x \neq y\,,$$

that is, $\{f_x\}_{x\in\mathbb{Z}^s}$ is an orthonormal basis of $\mathcal{L}^s(\mathbb{Z}^s)$. One possible choice is the set of functions $f_x = e^{ix\cdot p}$, which assures that all eigenvectors corresponding to ω_j are linked via spatial translations. If on the other hand ψ is an eigenvector of W it is clear that there must exist j such that $\omega_j(p)$ is constant.

Now suppose there exists at least one j such that $\omega_j(p)$ is non-constant. We denote by $\mathcal{H}_{pp} \subset \ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ the subspace of all eigenvectors of W. Clearly, the restriction of W to the orthogonal complement $\mathcal{H}_{pp}^{\perp}$ is characterized by the non-constant dispersion relations. First we prove that $\mathcal{H}_{pp}^{\perp} = \mathcal{H}_{ac}$, that is, there is no singularly continuous spectrum. The measures $\mu_{\phi,\phi}$ for vectors $\phi \in \mathcal{H}_{pp}^{\perp}$ are characterized by their moments

$$\langle\phi|W^n|\phi\rangle = \int\limits_{[-\pi,\pi)} e^{in\lambda}\mu_{\phi,\phi}(d\lambda) = \sum_{j\,:\,\omega_j \text{ n.c.}} \int\limits_{[-\pi,\pi)^s} d^s p\, e^{in\omega_j(p)}\langle\phi(p)|\mathbf{P}_j|\phi(p)\rangle\,,$$

where the sum is over all j such that ω_j is non-constant. Thus, $\mu_{\phi,\phi}$ is a sum of image measures of regular measures $\nu_j(d^s p) = \langle\phi(p)|\mathbf{P}_j|\phi(p)\rangle d^s p$. More precisely, $\mu_{\phi,\phi} = \sum_{j\,:\,\omega_j \text{ n.c.}} \nu_{\omega_j}$, where ν_{ω_j} denotes the image measure of ν_j under the map

$p \mapsto \omega_j(p)$, i.e. $\nu_{\omega_j}(X) = \nu_j(\omega_j^{-1}(X))$ for all measurable $X \subset [-\pi,\pi)$. Since the functions ω_j are non-constant and analytic almost everywhere, these image measures are absolutely continuous with respect to Lebesgue measure, see Theorem 2.1 in [AKSS07]. Thus $\mathcal{H}_{pp}^{\perp} = \mathcal{H}_{ac}$ and consequently $\sigma_{sc}(W) = \emptyset$. Clearly, for any j and p_0, the operator $W - e^{\mathrm{i}\omega_j(p_0)}\mathbb{1}$ cannot be inverted in $\mathcal{B}(\mathcal{H})$. The same is true for its restriction to $\mathcal{H}_{ac}$ and j such that ω_j is non-constant. Hence, for non-constant ω_j, the numbers $e^{\mathrm{i}\omega_j(p_0)}$ are elements of the absolutely continuous spectrum of W. □

Before we enter the detailed analysis of the asymptotic propagation behavior of unitary quantum walks, let us note an immediate consequence of the RAGE Theorem 3.3.6, Theorem 3.3.7 and the fact that eigenvalues of W correspond to constant dispersion relations. Let W be a unitary quantum walk on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ such that all dispersion relations are non-constant and fix a finite subset $\Lambda \subset \mathbb{Z}^s$. We denote the projection onto the subspace $\ell^2(\Lambda)\otimes\mathcal{K} \subset \ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ by P_Λ. By Proposition 4.5.7 there is no singular continuous spectrum, i.e. $\sigma_{sc}(W) = \emptyset$ and the same is true for the pure point part of the spectrum $\sigma_{pp} = \emptyset$. Thus we conclude from Theorem 3.3.7 that

$$\lim_{t\to\infty} \left\| P_\Lambda W^t \psi \right\| = 0$$

for all $\psi \in \ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$. But this means that the particle leaves the finite volume Λ up to an arbitrarily small correction if we wait long enough. Let us note this observation.

Remark 4.5.8. *Translationally invariant unitary quantum walks without constant dispersion relations exhibit propagation in the sense that the probability to find the particle in any finite subregion of the lattice tends to zero with increasing number of time steps.*

If some dispersion relations are constant, this is no longer true. Suppose the initial state ψ has non-zero overlap with an eigenvector of W, then there are finite regions of the lattice for which the probability to find the particle is bounded from below by a strictly positive constant for all times. This simple consequence of the RAGE Theorem 3.3.6 led some authors [IKK04] to coin the term "localization" for unitary quantum walks. However, this term is misleading in the sense that it is conceptually different from the kind of localization emerging in quantum systems exposed to randomly distributed impurities, known as Anderson or dynamical localization, see [Kir07] for an introduction to this topic for hamiltonian lattice systems. These ideas were applied to quantum walks with spatially-dependent random coin operators in [JM10, ASW11] and it was proven that these systems also show dynamical localization.

Asymptotic behavior

As described in Section 4.4, we need to study the perturbation theory of the eigenvalue 1 of the family of operators $\mathbf{W}_\varepsilon$ defined via $\mathbf{W}_\varepsilon(A) = W^* A e^{\mathrm{i}\varepsilon\lambda\cdot Q} W e^{-\mathrm{i}\varepsilon\lambda\cdot Q}$. Using Lemma 3.2.8 we can equivalently express this equation as

$$\mathbf{W}_\varepsilon(A)(p) = W(p)^* A(p) W(p+\lambda\varepsilon), \tag{4.28}$$

where $W(p)$ is the momentum space representation of the unitary quantum walk $\mathbf{W}$ and A is translationally invariant, i.e. $A \in \mathcal{T}_{\mathcal{K},s}$. For the moment we ignore the spatial degree of freedom and treat p as a fixed parameter. Clearly, $\mathbb{1}$ is an eigenvector of eigenvalue 1 for the operator $\mathbf{W}$, but the eigenvalue 1 is actually quite degenerate: any operator X commuting with $W(p)$ is also in this eigenspace. The eigenspace is thus at least $\dim\mathcal{K}$-dimensional, but if some of the eigenvalues of $W(p)$ are degenerate at p, the degeneracy can be even higher. According to Proposition 4.5.5 we can choose the operators $\mathbf{P}_j(p+\varepsilon\lambda)$ such that in the neighborhood of $\varepsilon = 0$ they and the corresponding eigenvalues $\omega_j(p+\varepsilon\lambda)$ depend analytically on ε. In the sequel we assume such a choice has been made in Equation (4.25).

Not surprisingly, this leads to an analytic perturbation expression for $\mathbf{W}_\varepsilon$. Indeed, let $\{P_k\}_{k=1}^d$ and $\{R_\ell\}_{\ell=1}^d$ be families of orthogonal projections in a Hilbert space $\mathcal{K}$. Then we can consider the operators $E_{k\ell}(X) = P_k X R_\ell$ on $\mathcal{B}(\mathcal{K})$. One directly verifies that each $E_{k\ell}$ is hermitian with respect to the Hilbert-Schmidt scalar product $\langle Y|X\rangle = \mathrm{tr}_{\mathcal{K}}(Y^*X)$, and the $E_{k\ell}$ themselves are a family of orthogonal projections. Now setting $P_k = \mathbf{P}_k(p)$ and $R_k = \mathbf{P}_k(p+\varepsilon\lambda)$ we find

$$\mathbf{W}_\varepsilon = \sum_{k\ell} e^{\mathrm{i}(\omega_\ell(p+\varepsilon\lambda)-\omega_k(p))} E_{k\ell}, \tag{4.29}$$

which is clearly a spectral decomposition in terms of eigenvalues and eigenprojections, which are all analytic in ε. Therefore, the expression

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = \sum_{kl} e^{\mathrm{i}t(\omega_\ell(p+\varepsilon\lambda)-\omega_k(p))} \mathbf{P}_k(p)\mathbf{P}_\ell(p+\varepsilon\lambda) \tag{4.30}$$

is correct to all orders, and as $\varepsilon \to 0$, we have $\mathbf{P}_\ell(p+\varepsilon\lambda) \to \mathbf{P}_\ell(p)$. Since $\mathbf{P}_k(p)$ and $\mathbf{P}_\ell(p)$ are orthogonal, only the terms with $k = \ell$ survive in the limit. Moreover, with ballistic scaling $\varepsilon = 1/t$ the exponent converges to the derivative of ω_ℓ, which exists even at degeneracy points, because we have chosen Equation (4.25) such that Equation (4.29) is analytic in ε. Hence

$$\lim_{t\to\infty} \mathbf{W}_{1/t}^t(\mathbb{1}) = \sum_k e^{\left(\mathrm{i}\frac{d\omega_k(p+\varepsilon\lambda)}{d\varepsilon}\right)\Big|_{\varepsilon=0}} \mathbf{P}_k\,, \tag{4.31}$$

and this convergence is uniform in p, which is equivalent to operator norm convergence of $\mathbf{W}_{1/t}^t(\mathbb{1})$ to the operator on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ defined by the right hand side of

Equation (4.31). Note, however, that the choice of projections $\mathbf{P}_k$ at a degenerate point may well depend on the direction λ, in which p is varied. Also the gradient $\nabla\omega_j$ may be ill-defined at a degenerate point, so there is no analytic choice for the dispersion relations, see Interlude 3.

From Equation (4.31) we can already compute the characteristic function of the asymptotic position distribution in ballistic scaling. Rewriting Equation (4.18) in momentum space yields the expression

$$\begin{aligned} C(\lambda) &= \lim_{t\to\infty} \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, \mathrm{tr}_{\mathcal{K}} \rho_0(p) \mathbf{W}^t_{1/t}(\mathbb{1})(p) \\ &= \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, \mathrm{tr}_{\mathcal{K}} \rho_0(p) \sum_k e^{\left(\mathrm{i}\frac{d\omega_k(p+\varepsilon\lambda)}{d\varepsilon}\right)}\Big|_{\varepsilon=0} \mathbf{P}_k \,, \end{aligned}$$

where we used that integration and asymptotic limit commute because of uniform convergence. However, since almost all momenta are regular according to Proposition 4.5.5, we can further elaborate our results. For all regular p, we can write Equation (4.31) as the exponential of the operator $i\lambda \cdot V(p)$, where V is the p-dependent vector operator with components

$$V_\alpha(p) = \sum_k \frac{\partial\, \omega_k(p)}{\partial\, p_\alpha} \mathbf{P}_k. \tag{4.32}$$

Hence, Equation (4.32) defines a vector of translationally invariant bounded operators on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, which we call the vector operator of group velocity V. Note that, for all regular p, all of its components commute with $W(p)$, since they are linear combinations of eigenprojections of $W(p)$. Obviously, each V_α is hermitian, therefore, the components of V are jointly measurable in the sense of standard quantum mechanics. In any initial state ρ_0 this gives a probability measure on velocity space. This measure is the asymptotic position distribution starting from ρ_0. The following theorem, which is a generalization of the results of Grimmett et al. [GJS04b], summarizes the results of this section.

Theorem 4.5.9. *Let* $\mathbf{W}$ *be a unitary quantum walk and denote by* $W(p)$ *its momentum representation. Let* $Q(t)$ *denote the position observable, evolved for* t *steps, i.e.* $Q(t) = (W^*)^t Q W^t$. *Then*

$$\lim_{t\to\infty} \frac{Q(t)}{t} = V$$

in the sense that for all bounded continuous functions $f : \mathbb{R}^s \to \mathbb{C}$ *going to zero at infinity we have that the weak operator limit of* $f(Q(t)/t)$, *evaluated in the functional calculus, is* $f(V)$. *This means, for any initial state* ρ_0 *the distribution of the random variable* $Q(t)/t$ *converges weakly to the distribution of* V *in* ρ_0.

For a general unitary quantum walk **W** the characteristic function corresponding to the asymptotic position distribution is thus a linear combination of functions of the form $\int dp\, e^{i\lambda\cdot v(p)}\rho_0(p)$. If we assume that the Hessian of the dispersion relation is non-singular for almost all momenta, we can use Lemma 4.3.3 to derive the following expression for the asymptotic position distribution.

Proposition 4.5.10. *Let* **W** *be a unitary quantum walk on* $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ *and assume*

$$\det\frac{\partial^2\omega_k}{\partial p_i\partial p_j}\neq 0$$

for almost all momenta p*. Then, the asymptotic position distribution is given by the density function*

$$P(x)=\frac{1}{(2\pi)^s}\sum_{k=1}^{\dim\mathcal{K}}\sum_{q\in\nabla\omega_k^{-1}(x)}\operatorname{tr}_{\mathcal{K}}\mathbf{P}_k(q)\rho_0(q)\cdot\left|\det\frac{\partial^2\omega_k}{\partial p_i\partial p_j}\right|^{-1}(q). \tag{4.33}$$

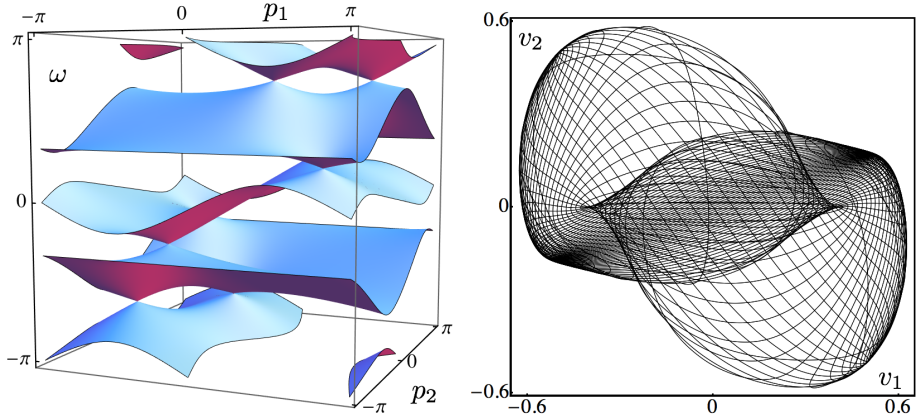
Proof. This is a straightforward consequence of Lemma 4.3.3. □

Of course, there exist situations where the Hessian is singular on a set of positive measure. A trivial example is when the group velocities are constant for all p, leading to a point measure at the value of the group velocity for the asymptotic position distribution. In higher lattice dimensions it may also happen that the dispersion relations are constant in one or several directions in momentum space leading to no transport in those directions. Although we cannot apply Proposition 4.5.10 in such cases, these are rather special examples, meaning that, for generic quantum walks, we suspect that the requirements of Proposition 4.5.10 are satisfied.

At points where the determinant of the Hessian of ω_k goes to zero we have a diverging probability density for the asymptotic position distribution. This is because if the Hessian vanishes at a point q, an infinitesimal volume $d^s p$ at q in momentum space is converted to a diverging volume $(\det\partial v_i/\partial p_j)^{-1}d^s v$ in velocity space via the transformation $p\mapsto\partial\omega_k/\partial p_i = v$. Hence, the probability weight of velocities around $v(q)$ has to diverge. Because of its apparent similarity with optical caustics, see Figure 4.4, we call points at which the Hessian of the dispersion relations vanishes caustic points.

Finite time step approximations

We have evaluated asymptotic characteristic functions by employing a perturbation series. It is therefore natural to ask, whether one cannot use the higher terms in the series to obtain better approximations to the position density for large but not infinite t. Of course, this is possible, but one has to be careful in the interpretation of the results. The main problem is that the partial sums of an expansion of the



(a) (b)

Figure 4.4.: The figure shows the dispersion relations (a) and resulting caustic (b) of one branch of the quantum walk $W(p_1,p_2)=\mathrm{diag}(e^{ip_1},e^{-ip_1},e^{ip_2},e^{-ip_2})\cdot H\otimes H\cdot C_Z$, where H denotes the Hadamard transformation and C_Z the controlled Z-gate. For symmetry reasons the other branches produce caustics which are rotated and mirrored versions of the plot shown. Closed curves in (b) correspond to the image of the map $p\mapsto\nabla\omega(p)$ applied to a discrete set of coordinate lines in momentum space $[-\pi,\pi)^2$.

characteristic function in powers of $1/t$ is *not* a characteristic function of any probability measure. Indeed, in the expansion we use we typically get combinations of λ/t, so the higher orders of the expansion will be polynomials in λ times an oscillating factor. This is clearly not integrable, so the inverse Fourier transform to get the probability density is ill-defined, and gives, at best, a rather singular distribution. However, if we only look for the expectations of sufficiently smooth functions of velocity, say $f(Q(t)/t)$, we get the integral of the characteristic function with the Fourier transform of f which decays rapidly enough to absorb all polynomial factors. Thus for a fixed smooth test function the expansion makes sense. Another way to look at this is to multiply the expanded characteristic function with a suitable cutoff-function (enforcing sufficient decay in λ) before transforming back to velocity space, resulting in a smoothed out probability density. Then "removing the cutoff" and the series expansion do not commute, and the choice of cutoff is effectively the choice of a smooth family of test functions.

We can go back directly to Equation (4.29), which is correct to all orders. That is, the characteristic function of the position distribution in ballistic scaling at time t

is

$$\begin{aligned} C_t(\lambda) &= \operatorname{tr}\rho_0 \mathbf{W}_{1/t}^t(\mathbb{1}) e^{\mathrm{i}\lambda\cdot Q/t} \qquad (4.34)\\ &= \int\limits_{[-\pi,\pi)^s} \frac{d^s p}{(2\pi)^s} \sum_{k\ell} e^{\mathrm{i}t(\omega_\ell(p+\lambda/t)-\omega_k(p))} \operatorname{tr}_{\mathcal{K}}\left(\rho_0(p+\lambda/t,p)\mathbf{P}_k(p)\mathbf{P}_\ell(p+\lambda/t)\right) \end{aligned}$$

Here, as in the previous section, $\rho_0(p_1,p_2)$ denotes the integral kernel of the initial density, and the trace is over the internal degrees of freedom. In leading order we could neglect the shift by λ/t in $\mathbf{P}_\ell$, so only terms with $k=\ell$ remain. Considering the first order term resulting from the expansion of $\mathbf{P}_\ell(p+\lambda/t)$ and $k\neq\ell$ we find an oscillatory integral with a regular integrand and rapidly oscillating exponential $e^{\mathrm{i}t(\omega_\ell(p)-\omega_k(p))}$. Assuming that this phase is not constant on sets of positive measure (as a function of p), we conclude that the integral goes to zero, so that together with the factor $1/t$ from the expansion of $\mathbf{P}_\ell$ such terms are $\mathcal{O}(t)$ and can be neglected. Of course, in higher order corrections one will have to extract the leading orders of the oscillatory integral by a stationary phase analysis.

For the expansion to first order we need the expansion of the dispersion relation to second order:

$$\omega_k(p+\lambda/t) = \omega_k(p) + \frac{\lambda}{t}\cdot v_k(p) + \frac{1}{2t^2}\omega_k''(p,\lambda) + o(t^{-3}), \qquad (4.35)$$

where ω_k'' is a quadratic from in λ containing the Hessian of the branch ω_k of the dispersion relation. This approximation eliminates one of the most prominent features of the finite t probability distributions, namely their rapid oscillations. Indeed, from inspecting such distributions it is clear that these oscillations have a frequency of order $1/t$ in ballistic scaling, i.e., they are really at the scale of the underlying lattice. This is reflected in the exact formula (4.34) by the fact that all expressions are 2π-periodic in λ/t. Therefore the Fourier transform of C_t is a sum of Dirac-distributions at the lattice points. The approximation (4.35) destroys this feature, resulting in a rather smooth function inside the allowed region of velocities. The Hessian can be determined from standard second order perturbation theory of $W(p)$. The resulting approximation of the characteristic function reads

$$\begin{aligned} C_t(\lambda) &= C_\infty(\lambda) + \frac{1}{t}\int\limits_{[-\pi,\pi)^s} \frac{d^s p}{(2\pi)^s} \sum_k e^{\mathrm{i}\lambda\cdot v_k(p)} \Bigg(\frac{\omega_k''(p)}{2} \operatorname{tr}_{\mathcal{K}}\rho_0(p)\mathbf{P}_k + \qquad (4.36)\\ &\quad + \operatorname{tr}_{\mathcal{K}}\left(\mathrm{i}(\lambda\cdot Q\rho_0)(p)\mathbf{P}_k(p) + \rho_0(p)\mathbf{P}_k(p)\lambda\cdot\nabla\mathbf{P}_k(p)\right)\Bigg) + o(t^{-2}). \end{aligned}$$

In Section 4.5.3 we compute this finite time step approximation for a particular unitary quantum walk.

4.5.2. Decoherent quantum walks

In this section we assume that $\mathbf{W}$ is a decoherent quantum walk without momentum transfer. By Theorem 4.2.2 there is a Kraus decomposition of $\mathbf{W}$ into translationally invariant Kraus operators K_j

$$\mathbf{W}(A) = \sum_j K_j^* A K_j \,, \quad [K_j, \mathcal{T}_x] = 0 \,, \forall\, x \in \mathbb{Z}^s \,. \tag{4.37}$$

In fact, we want to be slightly more general and leave the possibility for classical temporal correlations, that is, we additionally allow for an external Markov process $\mathbf{M}$ which chooses from a set of quantum walks $\mathbf{V}_\gamma$. The index γ is an element of a classical control space Γ, and each $\mathbf{V}_\gamma$ is translationally invariant, without momentum transfer, and possibly decoherent. Hence, each $\mathbf{V}_\gamma$ possesses a Kraus decomposition with translationally invariant $K_{\gamma,j}$

$$\mathbf{V}_\gamma(A) = \sum_j K_{\gamma,j}^* A K_{\gamma,j} \,, \quad [K_j, \mathcal{T}_x] = 0 \,, \forall\, x \in \mathbb{Z}^s \,. \tag{4.38}$$

For simplicity we take Γ to be finite, that is, the Markov process chooses from a finite number of quantum walks $\mathbf{V}_\gamma$. This assures that the time evolution generated from the $\mathbf{V}_\gamma$ is local again as the maximal step size of the quantum particle is bounded by the set $\mathcal{N} = \cup_\gamma \mathcal{N}_\gamma$, where $\mathcal{N}_\gamma$ denotes the neighborhood scheme of $\mathbf{V}_\gamma$. Another crucial point is that an infinite control space Γ would require infinite dimensional perturbation theory to perform the analysis of the asymptotic propagation behavior.

The space of observables on the combined system of $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ and the classical control space Γ, is given by $\mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$, where $\mathcal{L}^\infty(\Gamma)$ denotes the bounded functions on Γ. We consider the observables $A \in \mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ as measurable functions $\gamma \mapsto A(\gamma) \in \mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$. The two ingredients of each time step will then be on the one hand the γ-dependent transformation

$$(\mathbf{V}A)(\gamma) = \mathbf{V}_\gamma(A(\gamma)) = \sum_j K_{\gamma,j}^* A(\gamma) K_{\gamma,j} \,, \tag{4.39}$$

where the Kraus operators are normalized such that the sum over j with $A(\gamma) = \mathbb{1}$ gives $\mathbb{1}$. The second step is the update of the control parameters by the Markovian evolution $\mathbf{M}$, i.e.

$$(\mathbf{M}A)(\gamma) = \sum_\eta \mathbf{m}_{\gamma,\eta} A(\eta) \,, \tag{4.40}$$

with positive numbers $\mathbf{m}_{\gamma,\eta}$ such that $\sum_\eta \mathbf{m}_{\gamma,\eta} = 1$ for all $\gamma \in \Gamma$. The full evolution in the Heisenberg picture is then given by $\mathbf{W} = \mathbf{V}\mathbf{M}$ or, written out more explicitly:

$$(\mathbf{W}A)(\gamma) = \sum_\eta \mathbf{m}_{\gamma,\eta} \mathbf{V}_\gamma(A(\eta)) \tag{4.41}$$

When specifying an initial state for $\mathbf{W}$ we now also have to take care of the initialization of the classical control system. Markov processes $\mathbf{M}$ on finite state spaces Γ posses at least one stationary distribution, i.e. a probability distribution on Γ which is invariant under $\mathbf{M}$. We take such a stationary distribution $\overline{\mathbf{m}}$ as initialization for the control system Γ. One may wonder whether this is different from the situation where each $\mathbf{V}_\gamma$ is independently chosen for each time step according to the probability distribution $\overline{\mathbf{m}}$. This is indeed the case, as one can see from the simple example where the Markov process is given by a non-degenerate permutation on Γ. The invariant distribution is then given by the uniform distribution on Γ. With Markov control we obtain a classical mixture of length-$|\Gamma|$ compositions of elements $\mathbf{V}_\gamma$ and without Markov process the mixture is just over the $\mathbf{V}_\gamma$.

Strictly speaking, the time evolutions $\mathbf{W}$ generated in such a way are not covered by Definition 4.2.1 and Theorem 4.2.2. The reason being that the observable algebra $\mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ is not isomorphic to a full $\mathcal{B}(\mathcal{H})$ but only a subset of it, which leads to a different form of the Stinespring dilation, see Section 3.1. However, there is a simple way to embed this into the setting of Definition 4.2.1 by considering $\mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})\cong\oplus_{\gamma\in\Gamma}\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ as a subset of $\mathcal{B}(\mathbb{C}^{|\Gamma|})\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ and extending $\mathbf{W}$ appropriately. This entails the restriction of all observables and density operators to be block-diagonal in a certain basis, so the more natural way, which we will pursue, is to consider $\mathcal{L}^\infty(\Gamma)$ instead.

Note that the observable A which we have to evolve in order to compute the characteristic function in scaling ε is now given by $A(\gamma)=e^{\mathrm{i}\varepsilon\lambda\cdot Q}$ for all $\gamma\in\Gamma$. The set of translationally invariant operators $\mathcal{T}_{\mathcal{K},s,\Gamma}$ is now the subset of $\mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\ell^2(\mathbb{Z}^s)\otimes\mathcal{K})$ where each $A(\gamma)$ is translationally invariant in the usual sense, i.e.

$$A\in\mathcal{T}_{\mathcal{K},s,\Gamma}\quad\Leftrightarrow\quad A(\gamma)\in\mathcal{T}_{\mathcal{K},s}\;\forall\gamma\in\Gamma\,.$$

Since momentum is still a conserved quantity, the action of $\mathbf{W}$ on $\mathcal{T}_{\mathcal{K},s,\Gamma}$ is best expressed in momentum space

$$\begin{aligned}\mathbf{W}(A)(\gamma,p) &= \sum_\eta \mathbf{m}_{\gamma,\eta}\mathbf{V}_\gamma(p)(A(\eta,p)) \qquad (4.42)\\ &= \sum_\eta \mathbf{m}_{\gamma,\eta}\sum_j K^*_{\gamma,j}(p)A(\eta,p)K_{\gamma,j}(p),\end{aligned}$$

where $K_{\gamma,j}(p)$ and $\mathbf{V}_\gamma(p)$ denote the Fourier transforms of the operators $K_{\gamma,j}$ and $\mathbf{V}_\gamma$, respectively.

By Lemma 3.2.8 the action of the modified operator $\mathbf{W}_\varepsilon$ is

$$\begin{aligned}\mathbf{W}_\varepsilon(A)(\gamma,p) &= \sum_\eta \mathbf{m}_{\gamma,\eta}\mathbf{V}_{\gamma,\varepsilon}(p)(A(\eta,p)) \qquad (4.43)\\ &= \sum_\eta \mathbf{m}_{\gamma,\eta}\sum_j K^*_{\gamma,j}(p)A(\eta,p)K_{\gamma,j}(p+\varepsilon\lambda).\end{aligned}$$

From the finite range condition on the $\mathbf{V}_\gamma$ we have that the matrix elements of each $K_{\gamma,j}$ are trigonometric polynomials in $p_1,\dots,p_s$ and the degree of these polynomials is uniformly bounded by the size of $\mathcal{N}$. Therefore, $\mathbf{W}_\varepsilon$ can be expressed as a p-dependent matrix of dimension $\dim \mathcal{K}^2\cdot|\Gamma|$ with matrix elements which are analytic functions of ε. In other words, $\mathbf{W}_\varepsilon$ is an analytic family of operators in ε and for fixed p we can apply one-parameter perturbation theory as outlined in Section 3.4. In contrast to the case of unitary quantum walks, $\mathbf{W}_\varepsilon$ is in general no longer normal. Hence, we have to consider the Jordan normal form of the above operator, which reads

$$\mathbf{W}_\varepsilon(A)(p)=\sum_i\Big(\mu_i(\varepsilon)\mathbf{P}_i(\varepsilon)+\mathbf{D}_i(\varepsilon)\Big)(A(p)), \tag{4.44}$$

where $\mathbf{P}_i\mathbf{P}_j=\delta_{ij}\mathbf{P}_i$ are the eigenprojections, and $\mathbf{D}_i$ eigennilpotent operators with $\mathbf{D}_i\mathbf{P}_j=\mathbf{P}_j\mathbf{D}_i=\delta_{ij}\mathbf{D}_i$ for the eigenvalues $\mu_i(\varepsilon)$. A crucial point is to assure the analyticity of the eigenvalue branch $\mu_0(\varepsilon)$ and $\mathbf{P}_0(\varepsilon)$ corresponding to the eigenvalue 1 and eigenvector $\mathbb{1}$ of the unperturbed operator $\mathbf{W}$ in a neighborhood of $\varepsilon=0$ for almost all momenta p. The simplest situation where this is granted is when the unperturbed eigenvalue 1 is non-degenerate since possible points of non-analyticity are points where an eigenvalue splits into several branches, see Section 3.4. Our main assumption about $\mathbf{W}$ is therefore the following:

Assumption 4.1. *For almost all momenta $p\in[-\pi,\pi)^s$ the Jordan normal form* (4.44) *of $\mathbf{W}_\varepsilon$ is such that the eigenvalue $\mu_0(0)=1$ is non-degenerate and all other eigenvalues satisfy $|\mu_i(0)|<1$ for $i\neq 0$.*

To see that Assumption 4.1 is not overly restrictive we consider the following scenario.

Proposition 4.5.11. *Assumption 4.1 is valid if the quantum walk $\mathbf{W}$ has the following properties:*

i) For some power of the matrix $\mathbf{M}$ all entries are strictly positive.

ii) For almost all p there is a density operator $\overline{\rho}_p\in\mathcal{B}(\mathcal{K})$ with non-zero eigenvalues on $\mathcal{K}$ such that $\operatorname{tr}_\mathcal{K}\overline{\rho}_p\mathbf{V}_\gamma(A)(p)=\operatorname{tr}_\mathcal{K}\overline{\rho}_pA$ for all $\gamma\in\Gamma$ and $A\in\mathcal{B}(\mathcal{K})$.

iii) For almost all p, and some $r\in\mathbb{N}$ the set of operators $K_{\gamma_1,j_1}(p)\cdots K_{\gamma_r,j_r}(p)$ is irreducible, i.e. only multiples of $\mathbb{1}$ commute with all of them, and its linear span contains the identity.

The last condition seems difficult to check, but it is generically satisfied. In fact, the operator products usually span the whole space of matrices for relatively small r.

Proof. Since $\mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\mathcal{K})$ is finite dimensional, any simple eigenvalue is isolated, so we only have to prove that 1 is a simple eigenvalue, and the only one on the unit

circle. The transitivity assumption on the transition probabilities guarantees that there is a unique, strictly positive, invariant probability distribution $\overline{\mathbf{m}}$ on Γ. Hence, for fixed p, we have an invariant state for $\mathbf{W}(p)$, namely $\overline{\mathbf{m}} \otimes \overline{\rho}_p$, written out as

$$(\overline{\mathbf{m}} \otimes \overline{\rho}_p)(A) = \sum_\gamma \overline{\mathbf{m}}_\gamma \, \overline{\rho}_p \left(A(\gamma)\right) .$$

We first show the simplicity of 1, and since linearly independent eigenvectors of $\mathbf{W}$ will be independent eigenvectors of $\mathbf{W}^n$ we may do this for some power of $\mathbf{W}$. We choose some multiple of r, say rn, chosen sufficiently large so that all entries of the nr-step transition matrix are positive. Then condition *iii)* in the proposition is also satisfied for rn, because the identity lies in the span of the Kraus operators for $\mathbf{W}^r$. Hence, for this step we can simplify the assumptions to $\mathbf{m}_{\gamma,\eta} > 0$ for all γ, η and the irreducibility of $\{K_{\gamma,j}\}$.

The basic technique for the proof is the decomposition

$$\mathbf{W}(A^*A) - \mathbf{W}(A)^*\mathbf{W}(A) = \mathbf{V}\left(\mathbf{M}(A^*A) - \mathbf{M}(A)^*\mathbf{M}(A)\right) + \mathbf{V}(B^*B) - \mathbf{V}(B)^*\mathbf{V}(B), \qquad (4.45)$$

where $B = \mathbf{M}(A)$. Both terms are positive by the "2-positivity inequality" [Pau02] for channels. But when we evaluate for $\mathbf{W}(A) = A$ in an invariant state of $\mathbf{W}$ the left hand side becomes zero. This will provide a lot of information from the vanishing of sums of positive terms on the right. Explicitly, we obtain

$$\left(\mathbf{M}(A^*A) - \mathbf{M}(A)^*\mathbf{M}(A)\right)(\gamma) = \frac{1}{2}\sum_{\eta,\chi} \mathbf{m}_{\gamma,\eta}\mathbf{m}_{\gamma,\chi} \left(A(\eta) - A(\chi)\right)^* \left(A(\eta) - A(\chi)\right),$$

where we used that $\sum_\eta \mathbf{m}_{\gamma,\eta} = 1$ for all γ. Applying the invariant state $\overline{\mathbf{m}} \otimes \overline{\rho}_p$, and using the invariance condition for each $\mathbf{V}_\gamma$, we find

$$\sum_{\gamma,\eta,\chi} \overline{\mathbf{m}}_\gamma \mathbf{m}_{\gamma,\eta}\mathbf{m}_{\gamma,\chi} \operatorname{tr}_{\mathcal{K}} \overline{\rho}_p \left(A(\eta) - A(\chi)\right)^* \left(A(\eta) - A(\chi)\right) = 0.$$

Since the probabilities $\mathbf{m}$ and $\overline{\mathbf{m}}$ are all strictly positive, we find that each summand vanishes. Because $\overline{\rho}_p$ has no zero eigenvalue, this also implies that

$$\left(A(\eta) - A(\chi)\right)^* \left(A(\eta) - A(\chi)\right) = 0,$$

and hence $A(\eta) = A(\chi)$ for all η, χ. Hence we can set $A(\gamma) = A$ for all γ. This makes the first term in Equation (4.45) vanish for every A, and leads to $B = \mathbf{M}(A) = A$ in the second term. Moreover, from Equation (4.41) we see that $\mathbf{W}(A) = A$ just means that $\mathbf{V}_\gamma(A) = A$ for all γ.

Now consider, for each one of the operators $\mathbf{V}_\gamma$, which has Kraus operators $K_{\gamma,j}$, the expression

$$\sum_j [A, K_{\gamma,j}]^*[A, K_{\gamma,j}] = \mathbf{V}_\gamma\left(A^*A\right) - \mathbf{V}_\gamma(A)^*A - A^*\mathbf{V}_\gamma(A) + A^*A \qquad (4.46)$$

If A is invariant, this reduces to $\mathbf{V}_\gamma(A^*A)-A^*A$, which is clearly zero under the common invariant state $\overline{\rho}_p$. Hence the expectation of the positive terms on the left hand side must vanish also, and since $\overline{\rho}_p$ has no zero eigenvalues each $[A,K_{\gamma,j}]=0$ for all j and γ. By assumption this implies that A is a multiple of the identity.

It remains to be shown that there are no further eigenvalues on the unit circle. Suppose to the contrary that $\mathbf{W}(X)=\omega X\neq 0$ for some $\omega\neq 1$ with $|\omega|=1$. Then the operator $\mathbf{W}(X^*X)-\mathbf{W}(X)^*\mathbf{W}(X)=\mathbf{W}(X^*X)-X^*X$, which is positive by the 2-positivity, has vanishing expectation in the faithful invariant state, which implies that it is zero. But then X^*X is a fixed point of $\mathbf{W}$, and we have already seen that this implies that X^*X is a multiple of the identity. Since it cannot be zero, we can normalize X so that it becomes unitary. But 2-positivity also implies that if $\mathbf{W}(X^*X)-\mathbf{W}(X)^*\mathbf{W}(X)=0$ we must also have $\mathbf{W}(Y^*X)-\mathbf{W}(Y)^*\mathbf{W}(X)=0$, for all Y. Otherwise, the inequality could not be valid for linear combinations of Y and X. But then, by induction on n, we find that $\mathbf{W}(X^n)=\omega^n X^n$. In other words, all powers of ω are eigenvalues. Since the dimension of the space is finite, this means that ω must be a root of unity, say $\omega^n=1$. But then X is also an eigenvector of $\mathbf{W}^n$ with eigenvalue 1. Since our arguments for the simplicity of 1 also apply to powers of $\mathbf{W}$, this implies $X=\mathbb{1}$, and a contradiction to $\omega\neq 1$. □

Given Assumption 4.1 we have $\mathbf{D}_0=0$, and therefore

$$\mathbf{W}_\varepsilon^t(\mathbb{1})(p)=\mu_0^t(\varepsilon)\mathbf{P}_0(\varepsilon)(\mathbb{1})+\dots, \tag{4.47}$$

where the dots stand for terms with $i\neq 0$. We prove in the next section that these terms can be neglected in the asymptotic limit[3], and since $\mathbf{P}_0(\varepsilon)\mathbb{1}\to\mathbb{1}$ everything depends on the eigenvalue term $\mu_0^t(\varepsilon)$. Before we rigorously justify the applicability of non-degenerate analytic perturbation theory and subsequently enter the analysis of the different scalings ε, let us briefly discuss the general form of the results to be expected.

For ballistic scaling, i.e. $\varepsilon=1/t$ and $\mu_0(\varepsilon)=1+iv\cdot\lambda\varepsilon+o(\varepsilon^2)$, for some vector $v\in\mathbb{R}^s$, we find

$$\mu_0(\varepsilon)^t=\Big(1+\frac{iv\cdot\lambda}{t}+o(t^{-2})\Big)^t \quad\underset{t\to\infty}{\longrightarrow}\quad e^{iv\cdot\lambda}. \tag{4.48}$$

Hence, the probability distribution of Q/t converges to a point measure at a deterministic, but possibly p-dependent, velocity v.

Consider on the other hand the special case $v=0$, then the leading order contribution to μ_0 is of the form $\mu_0(\varepsilon)=1-\frac{1}{2}\varepsilon^2\lambda\cdot M\cdot\lambda+o(\varepsilon^3)$ for some matrix M. Thus, for diffusive scaling $\varepsilon=t^{-1/2}$ we have

$$\mu_0(\varepsilon)^t=\Big(1-\frac{\lambda\cdot M\cdot\lambda}{2t}+o(t^{-3/2})\Big)^t \quad\underset{t\to\infty}{\longrightarrow}\quad e^{-\frac{1}{2}\lambda\cdot M\cdot\lambda}. \tag{4.49}$$

[3]We stress that the crucial point here is the assumption $|\mu_i(0)|<1$ for $i\neq 0$.

This is the characteristic function of a Gaussian with covariance matrix M. Hence, the asymptotic distribution of $Q/\sqrt{t}$ is a mixture of p-dependent Gaussians.

Non-degenerate analytic perturbation theory

We now move on to prove that, under the premise of Assumption 4.1, the asymptotic limit of the characteristic function $C(\lambda)$ can be determined by means of analytic perturbation theory in ε. Using the momentum space representation again we can express the characteristic function as

$$C(\lambda)=\lim_{t\to\infty}\operatorname{tr}\left(\rho_0\mathbf{W}_\varepsilon^t(\mathbb{1})\right)=\lim_{t\to\infty}\frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s}d^s p\,\operatorname{tr}_{\mathcal{K}}\left(\rho_0(p)\mathbf{W}_\varepsilon^t(\mathbb{1})(p)\right). \tag{4.50}$$

The t^{th} power of the momentum representation of $\mathbf{W}_\varepsilon$ can be written in terms of the Jordan normal form (4.44) as

$$\mathbf{W}_\varepsilon^t=\sum_i\Big(\mu_i(\varepsilon)\mathbf{P}_i(\varepsilon)+\mathbf{D}_i(\varepsilon)\Big)^t=\sum_i\mathbf{P}_i(\varepsilon)\sum_{r=0}^{r_i}\binom{t}{r}\mu_i^{t-r}(\varepsilon)\mathbf{D}_i(\varepsilon)^r, \tag{4.51}$$

with r_i denoting the order of the nilpotency of $\mathbf{D}_i$. By Assumption 4.1 we have for almost all p that $r_0=0$ and $\operatorname{tr}\mathbf{P}_0=1$, which, by Lemma 3.4.2, implies that $\mathbf{P}_0(\varepsilon)$ and $\mu_0(\varepsilon)$ are analytic functions and $\mathbf{D}_0(\varepsilon)=0$ near $\varepsilon=0$ at those momenta. However, we cannot exclude that other eigenvalues of $\mathbf{W}_\varepsilon$ cross at $\varepsilon=0$, which leaves the possibility for points where some $\mathbf{P}_i$ and $\mathbf{D}_i$ are non-analytic. A basic result we use now is that, if some of these operators are non-analytic at $\varepsilon=0$, there is a number $k\in\mathbb{N}$ such that $\|\mathbf{P}_i(\varepsilon)\|=\mathcal{O}(\varepsilon^{-k})$, i.e. the singularities of $\mathbf{P}_i$ are at most algebraic, see Lemma 3.4.3. Since $\mathbf{D}_i(\varepsilon)=(\mathbf{W}_\varepsilon-\mu_i(\varepsilon))\mathbf{P}_i(\varepsilon)$ we get the same estimate for the operator norm of $\mathbf{D}_i(\varepsilon)$. Hence, for $i\neq 0$ and $\varepsilon=t^{-\alpha}$ we conclude

$$\mathbf{P}_i(t^{-\alpha})\binom{t}{r}\mu_i^{t-r}(t^{-\alpha})\mathbf{D}_i(t^{-\alpha})^r=\mu_i^t(t^{-\alpha})\mathcal{O}(t^m) \tag{4.52}$$

for some $m\in\mathbb{N}$. Consequently, the continuity of the eigenvalues together with the estimate $|\mu_i(0)|<1$ imply that the left hand side of Equation (4.52) converges exponentially to zero and

$$\mathbf{W}_{t^{-\alpha}}^t-\mu_0^t(t^{-\alpha})\mathbf{P}_0(t^{-\alpha})=\mathcal{O}(t^{-k}),\quad\forall k\in\mathbb{N}, \tag{4.53}$$

for almost all momenta p. At points p where the eigenvalue $\mu_0(\varepsilon)$ is analytic, we have a well-defined limiting behavior of $\mu_0^t(\varepsilon)$ for $\varepsilon=t^{-\alpha}$. If $\mu_0(\varepsilon)=1+\sum_{k=n}^\infty\mu_0^{(n)}\varepsilon^n$ with $\mu_0^{(n)}\neq 0$, then

$$\mu_0^t(t^{-\alpha})=\begin{cases}1 & ,\quad\alpha\cdot n>1\\ e^{\mu_0^{(n)}} & ,\quad\alpha\cdot n=1\\ \lim\limits_{t\to\infty}e^{t\mu_0^{(n)}} & ,\quad\alpha\cdot n<1\end{cases}. \tag{4.54}$$

Assuming $\varepsilon = t^{-\alpha}$ is chosen such that the limit of $\mu_0^t(\varepsilon)$ exists for almost all p it is straightforward to see that

$$C(\lambda) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \lim_{t\to\infty} \mu_0^t(\varepsilon) \cdot \mathrm{tr}_{\mathcal{K}} \rho_0(p). \tag{4.55}$$

Indeed, $\mathbf{W}_\varepsilon^t(\mathbb{1})(p) \to \mu_0^t(\varepsilon)\mathbb{1}$ for almost all p and the matrix elements of $\mathbf{W}_\varepsilon^t(\mathbb{1})(p)$ are bounded by one, since $\left\|\mathbf{W}_\varepsilon(\mathbb{1})(p)\right\|_{op} \leq 1$. Therefore, dominated convergence shows that we may exchange the order of asymptotic limit and integration in Equation (4.50), which directly yields Equation (4.55)

We have already seen that $\mu_0(\varepsilon)$ can be chosen analytic near $\varepsilon = 0$ for almost all p, hence, the p-dependent limit of $\mu_0^t(\varepsilon)$, if it exists, can be determined from the power series expansion of $\mu_0(\varepsilon)$, see Equation (4.54). Since all objects in the eigenvalue equation $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_0(\varepsilon)A_\varepsilon$ are guaranteed to be analytic, we can expand them to second order

$$\begin{aligned} \mathbf{V}_{\gamma,\varepsilon} &= \mathbf{V}_\gamma + \varepsilon \mathbf{V}'_\gamma + \frac{\varepsilon^2}{2}\mathbf{V}''_\gamma + o(\varepsilon^3) \\ \mu_0(\varepsilon) &= 1 + \varepsilon\mu' + \frac{\varepsilon^2}{2}\mu'' + o(\varepsilon^3) \\ A_\varepsilon &= \mathbb{1} + \varepsilon A' + \frac{\varepsilon^2}{2}A'' + o(\varepsilon^3). \end{aligned} \tag{4.56}$$

In the subsequent section we evaluate these equations in first and second order of ε to determine the asymptotic position distribution in ballistic and diffusive scaling.

Asymptotic position distribution via first and second order perturbation theory

The asymptotic characteristic function is determined by the first and second order correction to the eigenvalue $\mu_0(\varepsilon)$, see the limits (4.48) and (4.49), and by standard perturbation theory this can be extracted from the first and second order terms in the perturbation series of the eigenvalue equation $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_0(\varepsilon)A_\varepsilon$. Here A_ε and $\mu_0(\varepsilon)$ denote the pair of eigenvector and eigenvalue going to $\mathbb{1}$ and 1 as ε approaches zero. Since the eigenvector is only determined up to a factor we are free to choose a normalization. Our choice for this normalization is based on the following observation.

Proposition 4.5.12. *For fixed momentum p, and $\mathbf{W}$ given by Equation (4.42), there exists a state $\omega_p \in \mathcal{S}(\Gamma)\otimes\mathcal{S}(\mathcal{K})$ such that its expectation values with respect to arbitrary $A \in \mathcal{L}^\infty(\Gamma)\otimes\mathcal{B}(\mathcal{K})$ satisfy*

$$\omega_p(A) = \omega_p(\mathbf{W}(A)(p)). \tag{4.57}$$

We refer to ω_p as the invariant state for $\mathbf{W}$ at p.

Proof. For fixed momentum p, Equation (4.42) defines a completely positive map on a finite dimensional observable algebra. The assertion follows from the fact that for a given quantum channel acting on a finite dimensional system there always exists an invariant state, which may be proven using Schauder's fixed point theorem. □

Given the invariant state ω_p, which we write as $\omega_p = \sum_\gamma \overline{\mathbf{m}}_\gamma \otimes \overline{\rho}_{\gamma,p}$, where $\overline{\mathbf{m}}$ is necessarily a stationary distribution for $\mathbf{M}$, we choose A_ε such that

$$\sum_\gamma \overline{\mathbf{m}}_\gamma \operatorname{tr}_K \overline{\rho}_{\gamma,p} A_\varepsilon(\gamma,p) = 1. \tag{4.58}$$

Using Equation (4.56) we get the first order of the eigenvalue equation

$$\begin{aligned} \mathbf{W}(A')(\gamma,p) - A'(\gamma,p) &= \mu' \mathbb{1} - \sum_\eta \mathbf{m}_{\gamma,\eta}\, \mathbf{V}'_\gamma(\mathbb{1})(p) = \mu' \mathbb{1} - \mathbf{V}'_\gamma(\mathbb{1})(p) \\ &= \mu' \mathbb{1} - \sum_j K_{\gamma,j}(p)^* \left.\frac{d}{d\varepsilon} K_{\gamma,j}(p+\varepsilon\lambda)\right|_{\varepsilon=0}, \end{aligned} \tag{4.59}$$

where we evaluated the sum over η, on which $\mathbf{V}'_\gamma(\mathbb{1})(p)$ does not depend. Taking the expectation with respect to the invariant state ω_p makes the left hand side vanish, and leaves an explicit equation for μ', namely

$$\begin{aligned} \mu' &= \mathrm{i}\lambda \cdot v(p) \quad \text{with the vector} \\ v(p) &= -\mathrm{i} \sum_\gamma \overline{\mathbf{m}}_\gamma \sum_j \operatorname{tr}_K \overline{\rho}_{\gamma,p} K_{\gamma,j}(p)^* \nabla K_{\gamma,j}(p). \end{aligned} \tag{4.60}$$

This expression for $v(p)$ is real-valued. To see this we first note that the invariant state ω_p can be chosen analytic for almost all p, which follows from perturbation theory of the eigenvalue equation $\mathbf{W}_*(\omega_p) = \omega_p$. Here $\mathbf{W}_*$ denotes the Schrödinger picture representation of $\mathbf{W}$, which is again a finite dimensional analytic family of operators depending on momentum p. The gradient of the equation

$$\sum_\gamma \overline{\mathbf{m}}_\gamma \sum_j \operatorname{tr}_K \overline{\rho}_{\gamma,p} K_{\gamma,j}(p)^* K_{\gamma,j}(p) = \sum_\gamma \overline{\mathbf{m}}_\gamma \operatorname{tr}_K \overline{\rho}_{\gamma,p}$$

together with $\nabla \omega_p(\mathbb{1}) = 0$ yields

$$\sum_\gamma \overline{\mathbf{m}}_\gamma \sum_j \operatorname{tr}_K \overline{\rho}_{\gamma,p} \nabla K_{\gamma,j}(p)^* K_{\gamma,j}(p) + \sum_\gamma \overline{\mathbf{m}}_\gamma \sum_j \operatorname{tr}_K \overline{\rho}_{\gamma,p} K_{\gamma,j}(p)^* \nabla K_{\gamma,j}(p) = 0$$

which proves that $v(p)$ is real-valued.

The asymptotic characteristic function is given by the expression

$$C(\lambda) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, \mathrm{tr}_{\mathcal{K}} \rho_0(p) e^{\mathrm{i}\lambda \cdot v(p)}. \tag{4.61}$$

Two features of this formula are remarkable. Firstly, $v(p)$ is a scalar, i.e. a multiple of the identity with respect to the internal degrees of freedom from $\mathcal{K}$. Therefore, in contrast to the unitary case discussed in Section 4.5.1, the asymptotic distribution is independent of the initial state of the coin. Secondly, the transition probabilities of the control process only enter through the invariant probability distribution $\overline{\mathbf{m}}$. This means that we get the same result for a Bernoulli process, in which we take independent coins in successive steps with probability distribution $\overline{\mathbf{m}}$. The control space therefore just contributes another index to the Kraus decomposition of a one-step channel.

Next we study the asymptotic position distribution on the $\sqrt{t}$ scale. If the distribution of Q/t goes to a sharp value v the quantity of interest will be $(Q - vt)/\sqrt{t}$, and we can hope that this has a well-defined limiting distribution. Indeed for this to make sense we need that the velocity is sharply defined. Otherwise, we would just see the limiting distribution of v scaled to larger and larger variance. Therefore, we need to restrict to a setting, in which $v(p)$ is automatically constant. The interpretation of $v(p)$ is then a constant deterministic drift of the system. In the next section we will see that this assumption is indeed satisfied if the quantum channels $\mathbf{V}_\gamma$ are all unitarily implemented. In Example 2 we consider a quantum walk where the $\mathbf{V}_\gamma$ are given in terms of non-unitary Kraus operators, which results in non-constant $v(p)$, hence, leading to truly ballistic transport of a decoherent quantum walk.

When the ballistic order is completely defined by a deterministic velocity, i.e. $\mathbf{W}^t_{1/t}(\mathbb{1})(p) \to \mathrm{i}\lambda \cdot v\,\mathbb{1}$ with p-independent v, then we can subtract the ballistic motion and analyze how the probability distribution develops around it. That is, we consider the deviation operator

$$D = \frac{1}{\sqrt{t}}\big(Q - vt\big) \tag{4.62}$$

and compute the limit of the characteristic function of D, i.e.

$$\begin{aligned}\lim_{t\to\infty} C_{D,t}(\lambda) &= \lim_{t\to\infty} e^{-\mathrm{i}\lambda\cdot v\sqrt{t}} C_{Q,t}\left(\frac{\lambda}{\sqrt{t}}\right)\\ &= \lim_{t\to\infty}\frac{e^{-\mathrm{i}\lambda\cdot v\sqrt{t}}}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\sum_\gamma \overline{\mathbf{m}}_\gamma \mathrm{tr}_{\mathcal{K}}\left(\rho_0(p)\mathbf{W}^t_{1/\sqrt{t}}(\mathbb{1})(\gamma,p)\right)\\ &= \int\limits_{[-\pi,\pi)^s}\frac{d^s p}{(2\pi)^s}\mathrm{tr}_{\mathcal{K}}\big(\rho_0(p)\big)\lim_{t\to\infty} e^{-\mathrm{i}\lambda\cdot v/\sqrt{t}}\Big(1+\mathrm{i}\frac{\lambda\cdot v}{\sqrt{t}}+\frac{\mu''}{2t}+o(t^{-3/2})\Big)^t\\ &= \int\limits_{[-\pi,\pi)^s}\frac{d^s p}{(2\pi)^s}\mathrm{tr}_{\mathcal{K}}\big(\rho_0(p)\big)\, e^{\frac{1}{2}(\mu''+(\lambda\cdot v)^2)} \qquad (4.63)\end{aligned}$$

Here, at the first equality we substituted Equation (4.62), at the second introduced $\mathbf{W}_\varepsilon$ from Equation (4.43), and at the third introduced the perturbation expansion (4.56) with $\varepsilon = 1/\sqrt{t}$. At the last equality we used again the asymptotic formula $\lim_{t\to\infty}(1+x/t+\mathcal{O}(t^{-1}))^t = e(x)$, which follows immediately from the Taylor expansion of the logarithm. In the application above there is a cancelation of large phases, so the formula must be applied with care, in the form

$$\begin{aligned}e^{-\mathrm{i}a\sqrt{t}}\Big(1+\frac{\mathrm{i}a}{\sqrt{t}}+\frac{b}{t}+o(t^{-3/2})\Big)^t &= \Big(e^{-\mathrm{i}a/\sqrt{t}}\big(1+\frac{\mathrm{i}a}{\sqrt{t}}+\frac{b}{t}+o(t^{-3/2})\big)\Big)^t\\ &= \Big(1+\frac{b}{t}+\frac{a^2}{2t}+o(t^{-3/2})\Big)^t\\ &\xrightarrow[t\to\infty]{} e^{\left(b+\frac{a^2}{2}\right)}. \qquad (4.64)\end{aligned}$$

Remark 4.5.13. *Another way to handle a deterministic velocity in ballistic scaling is to consider the modified position observable $\widetilde{Q} = Q - v\,t$ and to perform the perturbation theory with the operator $e^{\mathrm{i}\varepsilon\lambda\cdot\widetilde{Q}}$ instead. It is easy to see that this yields a perturbation expansion for $\mu_0(\varepsilon)$ in which the first correction vanishes, i.e. $\mu' = 0$, cf. Remark 4.6.8. However, the approach of this section has the advantage that the formulas can also be used for non-constant velocity $v(p)$ to obtain a better approximation for a large but finite number of time steps.*

Note that, in contrast to $\mu' = i\,v\cdot\lambda$, the second order perturbation coefficient μ'' will generically depend on p. Moreover, since the perturbation is proportional to $\varepsilon\lambda$, the second order perturbation coefficient μ'' must be homogeneous quadratic in λ. Hence, according to Equation (4.63), the limiting distribution of D is a mixture of Gaussians with p-dependent covariance matrix $s(p)$ such that

$$\lambda\cdot s(p)\cdot\lambda = \sum_{jk} s_{jk}(p)\lambda_j\lambda_k = -\mu''(p) - (\lambda\cdot v)^2. \qquad (4.65)$$

In general, the covariance matrix $s(p)$ can be imaginary, see Example 2. For the moment, we fix λ, and concentrate on computing the expression (4.65) for any set of given data.

Using Equation (4.56) we expand the eigenvalue equation $\mathbf{W}_\varepsilon(A_\varepsilon)(p) = \mu_0(\varepsilon)A_\varepsilon(p)$ to first and second order in ε, and get

$$\begin{aligned} \mathbf{W}(A')(\gamma,p) - A'(\gamma,p) &= \mathrm{i}\lambda\cdot v\,\mathbb{1} - \mathbf{V}'_\gamma(\mathbb{1})(p) \qquad (4.66)\\ \mathbf{W}(A'')(\gamma,p) - A''(\gamma,p) &= \mu''\mathbb{1} + 2\mu' A'(\gamma,p) - \sum_\eta \mathbf{m}_{\gamma,\eta}\big(\mathbf{V}''_\gamma(\mathbb{1})(p) + 2\mathbf{V}'_\gamma(A'(\eta,p))\big) \end{aligned}$$

The first line is just a repetition of Equation (4.59). From the second line we extract μ'' by taking the expectation with respect to the invariant state ω_p, using also that by the convention (4.58) the second term on the right has zero expectation:

$$\mu'' = \sum_\gamma \overline{\mathbf{m}}_\gamma \,\mathrm{tr}_{\mathcal{K}}\big(\overline{\rho}_{\gamma,p}\mathbf{V}''_\gamma(\mathbb{1})(p)\big) + 2\sum_{\gamma,\eta}\overline{\mathbf{m}}_\gamma \mathbf{m}_{\gamma,\eta}\,\mathrm{tr}_{\mathcal{K}}\big(\overline{\rho}_{\gamma,p}\mathbf{V}'_\gamma(A'(\eta,p))\big) \qquad (4.67)$$

In this equation, the first order perturbation A' of the eigenvector must be extracted from Equation (4.66). Indeed, this is uniquely possible: By Assumption 4.1 the simple eigenvalue 1 of $\mathbf{W}$ is isolated, so the rank of $\mathbf{W}-\mathrm{id}$ is exactly one less than maximal. The kernel is explicitly known: $\mathbf{W}-\mathrm{id}$ annihilates precisely the multiples of the identity and maps onto the elements with vanishing expectation under ω_p. By definition of v, the right hand side hence lies in the range of $\mathbf{W}-\mathrm{id}$, so there is a unique solution A' satisfying the normalization condition (4.58). Note that since the solution is unique, and $\mathbf{V}'_\gamma$ is skew hermitian, so is A'. Moreover, since the right hand side of Equation (4.66) is linear in λ, so is A'. We stress that Equations (4.66)-(4.67) are also valid for ballistic scaling $\varepsilon = 1/t$ with non-constant $v(p)$, where they can be used for a finer analysis of the large time behavior, incorporating second order perturbation theory.

In the following we summarize the results of this section.

Theorem 4.5.14. *Let* $\mathbf{W}$ *be given by Equation* (4.41) *such that Assumption 4.1 is satisfied and denote by* ω_p *the invariant state of* $\mathbf{W}$ *at* p*. For an initial state* ρ_0*, the asymptotic limits of the position distribution are characterized by the following characteristic functions:*

i) Ballistic scaling: The weak limit of the distribution of Q/t *is determined by the characteristic function*

$$C(\lambda) = \frac{1}{(2\pi)^s}\int_{[-\pi,\pi)^s} d^s p\,\mathrm{tr}_{\mathcal{K}}\rho_0(p)e^{\mathrm{i}\lambda\cdot v(p)}$$

with $v(p)$ *according to Equation* (4.60)*.*

ii) Diffusive scaling: If $v(p) = v$ is constant, the weak limit of the distribution of $D = (Q - vt)/\sqrt{t}$ is characterized by the characteristic function

$$C(\lambda) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \operatorname{tr}_{\mathcal{K}}\left(\rho_0(p)\right) e\left(\frac{1}{2}(\lambda \cdot s(p) \cdot \lambda + (\lambda \cdot v)^2)\right)$$

with covariance matrix $s(p)$ according to Equations (4.65) *and* (4.67).

In the next section we analyze the case where each $\mathbf{V}_\gamma$ is unitarily implemented, that is, the Markov process $\mathbf{M}$ chooses from a set of unitary quantum walks. We close this section with a brief study of the situation when $\mathbf{M}$ has no memory, i.e. the classical control is a Bernoulli process.

Interlude 4: Bernoulli controlled decoherent quantum walks

We assume that the classical control process $\mathbf{M}$ has no memory, in other words, the quantum walks $\mathbf{V}_\gamma$ are chosen independently in each time step. The Markov process is then a Bernoulli process, and the probability $\mathbf{m}_{\gamma,\eta}$ to end up in η is the same from any state γ. Obviously, this probability is then also the invariant distribution, that is, we have

$$\mathbf{m}_{\gamma,\eta} = \overline{\mathbf{m}}_\eta \tag{4.68}$$

for all γ, η. As a further simplification we assume that the invariant state ω_p is of the form

$$\omega_p = \sum_\gamma \overline{\mathbf{m}}_\gamma \otimes \overline{\rho}_p\,, \tag{4.69}$$

which means there is a common invariant state $\overline{\rho}_p$ for all $\mathbf{V}_\gamma$. This simplifies the computation of the operator A' and the diffusive order μ'' considerably. We can reduce the dimension of the system of linear equations that determines μ'' by a factor $|\Gamma|$, where Γ denotes the finite state space of the classical control process $\mathbf{M}$.

Substituting Equation (4.68) into Equation (4.67) for μ'' we get

$$\mu'' = \sum_\gamma \overline{\mathbf{m}}_\gamma \operatorname{tr}\left(\overline{\rho}_p \mathbf{V}''_\gamma(\mathbb{1})(p)\right) + 2\sum_\gamma \overline{\mathbf{m}}_\gamma \operatorname{tr}\left(\overline{\rho}_p \mathbf{V}'_\gamma\left(\sum_\eta \overline{\mathbf{m}}_\eta A'(\eta, p)\right)\right). \tag{4.70}$$

So in order to determine μ'' it is not necessary to compute each individual $A'(\eta, p)$, but it suffices to know the value of the average

$$\overline{A'}(p) = \sum_\eta \overline{\mathbf{m}}_\eta A'(\eta, p). \tag{4.71}$$

Our aim is to set up an equation directly for this unknown matrix $\overline{A'}(p)$. From Equation (4.41) we find $(\mathbf{W}A')(\gamma,p)=\mathbf{V}_\gamma(\overline{A'}(p))$, which turns Equation (4.66) into a definition of $A'(\gamma,p)$ in terms of $\overline{A'}(p)$

$$A'(\gamma)=\mathbf{V}_\gamma(\overline{A'}(p))-\mathrm{i}\lambda\cdot v(p)\mathbb{1}+\mathbf{V}'_\gamma(\mathbb{1})(p). \tag{4.72}$$

The equation for $\overline{A'}(p)$ now follows by averaging:

$$\sum_\gamma \overline{\mathbf{m}}_\gamma \mathbf{V}_\gamma(\overline{A'}(p))-\overline{A'}(p)=\mathrm{i}\lambda\cdot v(p)\mathbb{1}-\sum_\gamma \overline{\mathbf{m}}_\gamma \mathbf{V}'_\gamma(\mathbb{1})(p). \tag{4.73}$$

We eliminate the control process from Equations (4.73) and (4.70) by introducing the quantum walk $\mathbf{V}=\sum_\gamma \overline{\mathbf{m}}_\gamma \mathbf{V}_\gamma$, which yields

$$\mathbf{V}\big(\overline{A'}(p)\big)-\overline{A'}(p)=\mathrm{i}\lambda\cdot v(p)\mathbb{1}-\mathbf{V}'(\mathbb{1})(p) \tag{4.74}$$

and

$$\mu''=\mathrm{tr}\left(\overline{\rho}_p\mathbf{V}''(\mathbb{1})\right)+2\,\mathrm{tr}\left(\overline{\rho}_p\mathbf{V}'(\overline{A'}(p))\right). \tag{4.75}$$

Markov controlled unitary quantum walks

A particular case where $v(p)$ is automatically constant is when all $\mathbf{V}_\gamma$ are unitarily implemented, that is, for each γ there is only one Kraus operator $K_\gamma=K_{\gamma,1}$. Those K_γ are necessarily unitary quantum walk operators.

Assumption 4.2. *The quantum walks $\mathbf{V}_\gamma$ in Equation (4.41) are unitarily implemented for all $\gamma\in\Gamma$. That is, $\mathbf{V}_\gamma(A)=K_\gamma^*AK_\gamma$ with a unitary quantum walk operator K_γ.*

Since all K_γ represent unitary quantum walks, their index $\mathrm{ind}\,K_\gamma$ is a well-defined quantity, see Definition 4.5.3. The ballistic scaling of $\mathbf{W}$ is independent of p and completely specified by the Markov process together with the index of each K_γ.

Proposition 4.5.15. *Assumption 4.1 and 4.2 together imply that the function $v(p)$, defined in Equation (4.60), and the invariant state $\omega_p=\omega$ are independent of p. Moreover,*

$$\omega = \overline{\mathbf{m}}\otimes\frac{1}{\dim\mathcal{K}}\,\mathbb{1} \quad \textit{and} \tag{4.76}$$

$$v = \sum_\gamma \overline{\mathbf{m}}_\gamma\,\frac{\mathrm{ind}\,K_\gamma}{\dim\mathcal{K}}\,. \tag{4.77}$$

Proof. Obviously, the density operator ω is an invariant state for each $\mathbf{V}_\gamma$. By definition of the index, $\det K_\gamma(p) = c e^{\mathrm{i}p\cdot \mathrm{ind}\, K_\gamma}$. Hence

$$\begin{aligned}\mathrm{i}\lambda\cdot \mathrm{ind}\, K_\gamma &= \frac{1}{\det K_\gamma(p)}\,\frac{d}{d\varepsilon}\det K_\gamma(p+\varepsilon\lambda)\Big|_{\varepsilon=0} = \frac{d}{d\varepsilon}\det\big(K_\gamma(p)^* K_\gamma(p+\varepsilon\lambda)\big)\Big|_{\varepsilon=0}\\ &= \mathrm{tr}_{\mathcal{K}}\big(K_\gamma(p)^*\frac{d}{d\varepsilon}K_\gamma(p+\varepsilon\lambda)\big) = \dim\mathcal{K}\,\mathrm{tr}_{\mathcal{K}}\overline{\rho}\mathbf{V}'_\gamma(\mathbb{1}),\end{aligned}$$

and the formula follows by dividing this equation by $\dim\mathcal{K}$ and summing with respect to $\overline{\mathbf{m}}$. □

Additionally, we may also prove that the covariance matrix $s(p)$ is positive for all momenta p if each $\mathbf{V}_\gamma$ is unitarily implemented.

Proposition 4.5.16. *Given Assumption 4.1 and 4.2, the covariance matrix $s(p)$, defined via Equation* (4.65)*, is positive for all momenta p.*

Proof. Since each K_γ is unitary, we can use this to express the derivatives of K_γ by A':

$$K'_\gamma = K_\gamma(A'(\gamma) - W(A')(\gamma) + \mathrm{i}\lambda\cdot v\,\mathbb{1}) \tag{4.78}$$

Next we determine μ'' from Equation (4.67). We can eliminate the second derivative in the first term by differentiating Equation (4.60) with respect to p, or more precisely, by setting $p = p+\varepsilon\lambda$ and differentiating with respect to ε. This gives

$$\begin{aligned}0 &= -\mathrm{i}\sum_\gamma \overline{\mathbf{m}}_\gamma \frac{d}{d\varepsilon}\mathrm{tr}_{\mathcal{K}}\big(K^*_\gamma(p+\varepsilon\lambda)K'_\gamma(p+\varepsilon\lambda)\big)\\ &= -\mathrm{i}\sum_\gamma \overline{\mathbf{m}}_\gamma \,\mathrm{tr}_{\mathcal{K}}\big(K^{*\prime}_\gamma K'_\gamma\big) - \mathrm{i}\sum_\gamma \overline{\mathbf{m}}_\gamma\,\mathrm{tr}_{\mathcal{K}}\big(\mathbf{V}''_\gamma(\mathbb{1})\big)\end{aligned} \tag{4.79}$$

and hence, using Equation (4.78) and the unitarity of K_γ:

$$\sum_\gamma \overline{\mathbf{m}}_\gamma\,\mathrm{tr}_{\mathcal{K}}\big(\mathbf{V}''_\gamma(\mathbb{1})\big) = -\sum_\gamma \overline{\mathbf{m}}_\gamma\,\mathrm{tr}_{\mathcal{K}}\big(\big|A'(\gamma) - W(A')(\gamma) + \mathrm{i}\lambda\cdot v\,\mathbb{1}\big|^2\big), \tag{4.80}$$

where, for an operator X, we use the abbreviation $|X|^2 = X^*X$. The second term in Equation (4.67) can also be simplified by eliminating the derivative in $\mathbf{V}'_\gamma(X) = K^*_\gamma X K'_\gamma$ via Equation (4.78). We obtain

$$\sum_\eta \mathbf{m}_{\gamma,\eta}\, K^*_\gamma A'(\eta)K'_\gamma = W(A')(\gamma)\big(A'(\gamma) - W(A')(\gamma) + i\lambda\cdot v\,\mathbb{1}\big).$$

Note that in Equation (4.67) we need the expectation of this expression in the invariant state ω, just as Equation (4.80) is such an expectation. Bringing together

the various terms of Equation (4.67), and using the skew hermiticity of A', $W(A)'$, and $\mathrm{i}\lambda\cdot v$, we find for Equation (4.65):

$$\begin{aligned} -\mu'' - (\lambda\cdot v)^2 &= \omega\Big(|A' - W(A') + \mathrm{i}\lambda\cdot v|^2 - 2W(A')(A' - W(A') + \mathrm{i}\lambda\cdot v)\Big) - (\lambda\cdot v)^2 \\ &= \omega\Big(W(A')^2 - (A')^2 + [A', W(A')] - 2\mathrm{i}\lambda\cdot v A'\Big) \\ &= \omega\Big(|A'|^2 - |W(A')|^2\Big). \end{aligned} \tag{4.81}$$

Since ω is invariant under W, we can also write the first term as the expectation of $W(|A'|^2)$, so that this expression is non-negative by virtue of the Cauchy-Schwarz inequality for channels [Pau02]. With A' a linear function of λ, the above expression becomes a quadratic form in λ, as claimed in Equation (4.65). □

Intuitively, one would expect that the diffusion constant becomes very large if the considered quantum walk differs only little from a unitary quantum walk with ballistic behavior. For example, if the unitary quantum walks the Markov process chooses from are close to each other in operator norm, or if the Markov process is such that it prefers one of the unitary quantum walks, we would expect reminiscences of a coherent quantum walk even for large times. Similarly, if the Markov process converges to a deterministic Markov chain, i.e. the transition matrix approaches a permutation matrix, the overall evolution up to time step t would be very similar to the average of a number of coherent quantum walks each evolved for a number of time steps proportional to t. If some of these coherent quantum walks show ballistic behavior we would again expect that the diffusion constant diverges. This effect can be seen in Example 4, where we derive an explicit formula for the variance $s(p)$ of a Markov controlled quantum walk, which diverges in the coherent limit of the considered quantum walk.

Finite time step approximations

The general remarks about higher order expansions in Section 4.5.1 apply also in this case. In this section we focus on just the first (i.e., $o(1/t)$) correction to the ballistic scaling. When the ballistic velocity is independent of p, this is in fact best expressed by the diffusive scaling. However, almost all of the second order perturbation theory developed in the previous sections is independent of that assumption. Therefore, we have already done most of the work necessary to determine the first correction to ballistic scaling in the general case.

We adopt Assumption 4.1, but not necessarily constancy of $v(p)$. Let us consider the Jordan normal form (4.44) of $\mathbf{W}_\varepsilon$ for small ε. The t^{th} power of this operator, see Equation (4.51), is built from the terms

$$\Big(\mu_i(\varepsilon)\mathbf{P}_i(\varepsilon) + \mathbf{D}_i(\varepsilon)\Big)^t = \mathbf{P}_i(\varepsilon)\sum_{r=0}^{r_i}\binom{t}{r}\mu_i^{t-r}(\varepsilon)\mathbf{D}_i(\varepsilon)^r\,.$$

Here r_i is the order of nilpotency of $\mathbf{D}_i(\varepsilon)$, which is bounded by the algebraic multiplicity of $\mu_i(\varepsilon)$. When we choose the label $i=0$ for the key eigenvalue (i.e. $\mu_0(0)=1$) we have $|\mu_i|<1$ for all $i\neq 0$ by Assumption 4.1. Hence expressions such as $t^n\mu_i^{t-r}$ tend to zero faster than any power of t^{-n} ($n\in\mathbb{N}$). Using again that the poles of $\mathbf{P}_i$ and $\mathbf{D}_i$ for $i\neq 0$ can be bounded by ε^m for some $m\in\mathbb{N}$, we see that in any expansion in such powers, all terms but the one with $i=0$ can be neglected. Moreover, μ_0 is simple and therefore $r_0=0$. Thus, only the term $\mathbf{P}_0(\varepsilon)\mu_0(\varepsilon)^t$ remains. Since we were only interested in the leading order so far, it was enough to replace $\mathbf{P}_0(\varepsilon)$ by $\mathbf{P}_0(0)$. However, for a systematic expansion we also have to expand the rank one projection $\mathbf{P}_0(\varepsilon)$ in powers of ε. This will give $\mathbf{P}_0(\varepsilon)(X)(\gamma)=A_\varepsilon(\gamma)\sum_\eta \mathrm{tr}_{\mathcal{K}}(B_\varepsilon^*(\eta)X(\eta))$, where A_ε is the eigenvector of $\mathbf{W}_\varepsilon(p)$ and B_ε the corresponding eigenvector of the adjoint. Of course, eigenvectors are only defined up to a (possibly ε-dependent) factor. We have already used the convention that $\omega_p(A_\varepsilon)=1$. This fixes the factor also for B_ε, since we must have $\mathbf{P}_0(\varepsilon)^2=\mathbf{P}_0(\varepsilon)$, and hence $\sum_\gamma \mathrm{tr}_{\mathcal{K}}A_\varepsilon(\gamma)B_\varepsilon^*(\gamma)=1$. Expanding B_ε as in Equation (4.56) we get $\sum_\gamma \mathrm{tr}_{\mathcal{K}}A'(\gamma)+\mathrm{tr}_{\mathcal{K}}B'^*(\gamma)=0$, so that for an expansion to order t^{-1} we do not need B'. Then

$$\mathbf{P}_0(t^{-1})(\mathbb{1})(\gamma)=\mathbb{1}+\frac{1}{t}\left(A'(\gamma)-\sum_\eta \mathrm{tr}_{\mathcal{K}}A'(\eta)\cdot\mathbb{1}\right)+o(t^{-2}), \tag{4.82}$$

where A' is determined exactly as above. For the eigenvalue $\mu_0(t^{-1})^t=(1+\frac{\mu'}{t}+\frac{\mu''}{2t^2}+o(t^{-3}))^t$, we first expand the logarithm, which yields $e^{\mu'+\frac{1}{2t}(\mu''-(\mu')^2)}+o(t^{-2})$. With the p-dependent covariance matrix s (see Equation (4.65)) we can thus write

$$\begin{aligned}\mu_0(t^{-1})^t &= e^{\mathrm{i}\lambda\cdot v(p)-\frac{1}{2t}\lambda\cdot s(p)\cdot\lambda}+o(t^{-2}) \\ &= e^{i\lambda\cdot v(p)}\Big(1-\frac{1}{2t}\lambda\cdot s(p)\cdot\lambda\Big)+o(t^{-2}).\end{aligned} \tag{4.83}$$

From the point of view of a series expansion in inverse powers of t these two forms are equivalent. However, the first form is preferable, because it is the characteristic function of a Gaussian distribution and hence has a probabilistic interpretation. However, this has to be taken with a grain of salt: The proof of positivity of $s(p)$ given in the previous section does depend on Assumption 4.2. Indeed, we will see in Example 2 that $s(p)$ may be complex, and only represents a probability after integration of the whole expression with respect to p.

Finally, we have to expand the factor $e^{\mathrm{i}\varepsilon\lambda\cdot Q}$ in the exact formula

$$C_t(\lambda)=\frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\,\mathrm{tr}_{\mathcal{K}}e^{\mathrm{i}\varepsilon\lambda\cdot Q}\rho_0(p)\mathbf{W}_\varepsilon^t(\mathbb{1})(p) \tag{4.84}$$

for the characteristic function at time step t. This correction contains some information about the initial position distribution, although contracted by a factor $1/t$.

When $\rho_0(p_1,p_2)$ denotes the integral kernel of the initial density, the effect of the factor $e^{i\lambda\cdot Q/t}$ under the trace is to shift the first argument of ρ_0. We therefore introduce the function

$$C_0(\lambda,p)=\mathrm{tr}_{\mathcal{K}}\rho_0(p+\lambda,p), \tag{4.85}$$

where the trace is over the internal degrees of freedom. This notation is to suggest that this is some kind of characteristic function of the initial distribution. This is not literally true, since we keep the momentum variable, so at best it is a phase space distribution function. Indeed, a slightly more symmetric version $\mathrm{tr}_{\mathcal{K}}\rho_0(p+\lambda/2,p-\lambda/2)$ is the Fourier transform of the "position distribution at fixed momentum" according to the Wigner distribution function. Of course, this distribution is contracted by a factor $1/t$ in ballistic scaling. Together, we get

$$\begin{aligned} C_t(\lambda) &= \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\; e^{i\lambda\cdot v(p)-\frac{1}{2t}\lambda\cdot s(p)\cdot\lambda}\Big(C_0(\lambda/t,p)+ \\ &+ \frac{1}{t}\left(\mathrm{tr}_{\mathcal{K}}\rho_0(p+\lambda/t,p)\sum_\gamma \overline{\mathbf{m}}_\gamma A'(\gamma)-C_0(\lambda/t,p)\sum_\gamma \mathrm{tr}_{\mathcal{K}}A'(\gamma)\right)\Big)+o(t^{-2}). \end{aligned} \tag{4.86}$$

Heuristically, the interpretation of the first term is the distribution of the sum of two independent quantities for each p: a Gaussian centered at $v(p)$, with decreasing variance, plus a scaled down version of the initial position distribution. This is then averaged over momentum. The second term does not allow such a simple interpretation. We numerically compute this approximation for some examples in Section 4.5.3.

Degenerate perturbation theory

The key assumption in the preceding sections was non-degeneracy of the eigenvalue 1 of $\mathbf{W}_0$ for almost all momenta p. This enabled us to conclude that the corresponding eigenvalue-branch of $\mathbf{W}_\varepsilon$ is non-degenerate and analytic in a neighborhood of $\varepsilon=0$. If this assumption is not satisfied, that is, there is a set of positive measure such that 1 is a degenerate eigenvalue of $\mathbf{W}_0$, we immediately get the stronger statement that the eigenvalue 1 is permanently degenerate. Indeed, using similar arguments as in the proof of Lemma 4.5.5 *iii)* we may verify that the multiplicity of the eigenvalue 1 is a constant except for at most a set of measure zero on which the multiplicity of 1 is even larger. The question is now whether the degenerate eigenvalue 1 splits under the perturbation into several branches. By the same arguments it follows that the corresponding eigenvalue branch of the characteristic polynomial $\zeta_z(p,\varepsilon)=\det\mathbf{W}_\varepsilon(p)-z$ retains its multiplicity for $\varepsilon\neq 0$ or the eigenvalue splits under the perturbation for almost all p.

If the eigenvalue $\mu_0(0)=1$ does not split under the perturbation by ε it is easy to see that we are essentially in the same situation as in the non-degenerate case. By

Lemma 3.4.2 we have that the corresponding eigenprojections $\mathbf{P}_0$ and eigennilpotents $\mathbf{D}_0$ can be chosen analytic near $\varepsilon = 0$ for almost all p. Another property of the Jordan normal form, which translates almost trivially to the degenerate case, is the vanishing of the eigennilpotent $\mathbf{D}_0(0)$. To see this we fix p and suppose $\mathbf{D}_0(0) \neq 0$, which implies the existence of two operators $X, Y \in \mathcal{B}(\mathcal{K})$ such that $\mathbf{W}(X)(p) = Y + X$ and $\mathbf{W}(Y)(p) = Y$. Iterating this equality yields $\mathbf{W}^n(X)(p) = nY + X$. But for fixed momentum p the map $\mathbf{W}(p)$ is nothing else but a finite dimensional quantum channel, hence it satisfies $\left\|\mathbf{W}^n(p)\right\|_{cb} = 1$ for all n, which is in contradiction with the equality we have just derived. Since $\mathbf{D}_0(\varepsilon)$ is analytic we conclude $\mathbf{D}_0(\varepsilon) = 0$ near $\varepsilon = 0$, and we get the following analogue of Equation (4.47)

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = \mathbf{P}_0(\varepsilon)\mu_0^t(\varepsilon)(\mathbb{1}) + \dots, \tag{4.87}$$

where the dots again indicate terms which vanish in the asymptotic limit. Here the crucial assumption is again that all other eigenvalues satisfy $|\mu_i(0)| < 1$ for almost all p. However, in order to determine the corrections $\mu_0^{(n)}$ to the unperturbed eigenvalue there is a subtlety left we need to take care of. In principle, we may determine, say, the first order correction μ_0' by equating coefficients of the corresponding eigenvalue equation. But since the eigenvectors near $\varepsilon = 0$ are not unique this time we have to ensure we choose the right basis in the degenerate subspace, so in general a closer analysis is necessary to determine the kind of asymptotic behavior displayed by $\mathbf{W}$.

The situation where the degenerate eigenvalue $\mu_0(0) = 1$ splits under the perturbation into several branches $\mu_{0,k}(\varepsilon)$ is more complicated since we cannot exclude that $\mathbf{P}_{0,k}(\varepsilon)$ and $\mathbf{D}_{0,k}(\varepsilon)$ have poles at $\varepsilon = 0$. Moreover, even if we can exclude singularities at $\varepsilon = 0$, the analysis is more involved as we possibly get contributions from all branches to $\mu_{0,k}$, see Example 3.

4.5.3. Examples

In this section we apply the methods developed in the preceding sections to particular quantum walks. We start with unitary quantum walks and visualize the structural properties of their dispersion relations and group velocities, see Section 4.5.1. Subsequently, we analyze decoherent quantum walks with the aim to provide examples for several remarks made in Section 4.5.2.

Example 1: Unitary quantum walks on $\mathbb{Z}^2$

We consider a unitary quantum walk W on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^2$ according to the construction introduced in Interlude 3. Let W be defined by its momentum space representation

$$W(p_1, p_2) = e^{-\mathrm{i}p_1\sigma_1} e^{-\mathrm{i}p_2\sigma_3}, \tag{4.88}$$

where $\sigma_{1,2,3}$ denote the Pauli operators. The dispersion relations of this quantum walk are given by

$$\omega_{\pm} = \pm \arccos(\cos(p_1)\cos(p_2)),$$

and by construction there is a singular point at the origin $p_1 = 0 = p_2$, see Figure 4.3 and Figure 4.5 below. Furthermore, there is an additional singularity at the point $p_1 = -\pi = p_2$.

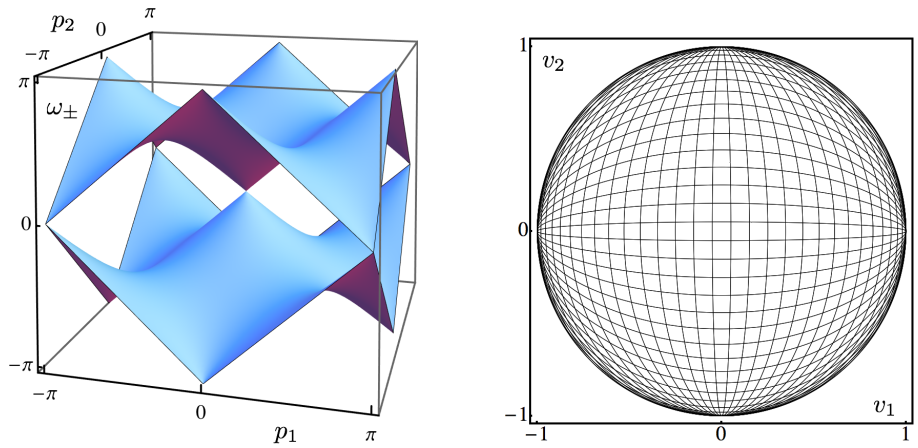


Figure 4.5.: The figure shows a plot of the dispersion relations (a) and the caustic (b) of the quantum walk according to Equation (4.88)

For the group velocities we obtain

$$v_{1,\pm}(p_1,p_2) = \frac{\pm\sin(p_1)\cos(p_2)}{\sqrt{1-\cos^2(p_1)\cos^2(p_2)}} \quad \text{and} \quad v_{2,\pm}(p_1,p_2) = \frac{\pm\cos(p_1)\sin(p_2)}{\sqrt{1-\cos^2(p_1)\cos^2(p_2)}},$$

and it is straightforward to verify that the determinant of the Hessian $\partial^2\omega_{\pm}/\partial p_i \partial p_j$ can be expressed as

$$\begin{aligned} \left|\det \frac{\partial^2 \omega_{\pm}}{\partial p_i \partial p_j}\right| &= \frac{|\sin(p_1)\sin(p_2)|}{\sqrt{1-\cos^2(p_1)\cos^2(p_2)}} \\ &= (1-v_{1,\pm}^2)(1-v_{2,\pm}^2). \end{aligned} \tag{4.89}$$

If we plot the group velocities of one branch, say $v_{j,+}$, along a discrete set of coordinate lines in momentum space, we obtain the caustic of this branch of W. Figure 4.5 shows such a plot for the coordinate lines

$$(p_1,p_2) = \left(r, -\pi + \frac{2\pi}{30}m\right) \quad \text{and} \quad (p_1,p_2) = \left(-\pi + \frac{2\pi}{30}n, r\right),$$

with $n, m = 1, 2, \ldots, 30$ and $r \in [-\pi, \pi)$. Obviously, the propagation region is a disc of diameter one. However, the set of caustic points, which are the points where the determinant of the Hessian vanishes, is not the whole boundary of this disc. In fact, Equation (4.89) equals zero iff one of the velocities equals one, hence, the only caustic points within the propagation region are $(v_1, v_2) = (\pm 1, 0)$ and $(v_1, v_2) = (0, \pm 1)$. At all other points on the boundary of this disc we have a non-singular Hessian, and the corresponding probability density is finite for any initial state.

Since the Hessian is non-singular for almost all momenta, we can use Proposition 4.5.10 to compute the asymptotic position distribution. Obviously, since the Hessian of the branches $\omega_\pm$ only differ by a sign, Equation (4.89) yields the same result for both branches. Hence, according to Equation (4.33) we obtain the probability density

$$P(v_1, v_2) = \frac{1}{(2\pi)^2 (1 - v_1^2)(1 - v_2^2)} \sum_{k=\pm} \sum_{q \in \nabla \omega_k^{-1}(v_1, v_2)} \operatorname{tr}_{\mathbb{C}^2} \mathbf{P}_k(q) \rho_0(q), \tag{4.90}$$

where $\mathbf{P}_k$ denotes the eigenprojection of $W(p_1, p_2)$ corresponding to ω_k. The coordinate lines $p_1 = 0$ and $p_2 = 0$ decompose the set $[-\pi, \pi)^s$ into four regions on which the map $(p_1, p_2) \mapsto (v_{1,\pm}, v_{2,\pm})$ is invertible. Indeed, the four functions

$$(v_1, v_2) \mapsto \left(\pm \arccos\left(\frac{v_2}{\sqrt{1 - v_1^2}} \right), \pm \arccos\left(\frac{v_1}{\sqrt{1 - v_2^2}} \right) \right)$$

invert $(p_1, p_2) \mapsto (v_{1,\pm}, v_{2,\pm})$ on the respective regions of momentum space. With these maps and the eigenprojections $\mathbf{P}_\pm$ we can now compute the asymptotic position distribution for arbitrary initial states ρ_0.

For the plots shown in Figure 4.6 we have chosen several initial states of the quantum walk to illustrate the dependence of the asymptotic position distribution. Plot (a) shows the asymptotic distribution for an initial state which is localized at the origin. Such states have a uniform momentum distribution such that all group velocities contribute to the asymptotic distribution. The momentum distribution of the initial state in (b) is confined to a rectangular region in momentum space without caustic points. Hence, the corresponding asymptotic distribution takes on a finite value at all points. In (c) and (d) we have chosen initial states with momentum distributions which are given by a Gaussian centered at a point with small and large group velocities, respectively.

Example 2: A quantum walk with imaginary covariance matrix

The following example is a simple version of a quantum walk which satisfies Assumption 4.1 but not Assumption 4.2. This means for almost all p the eigenvalue 1

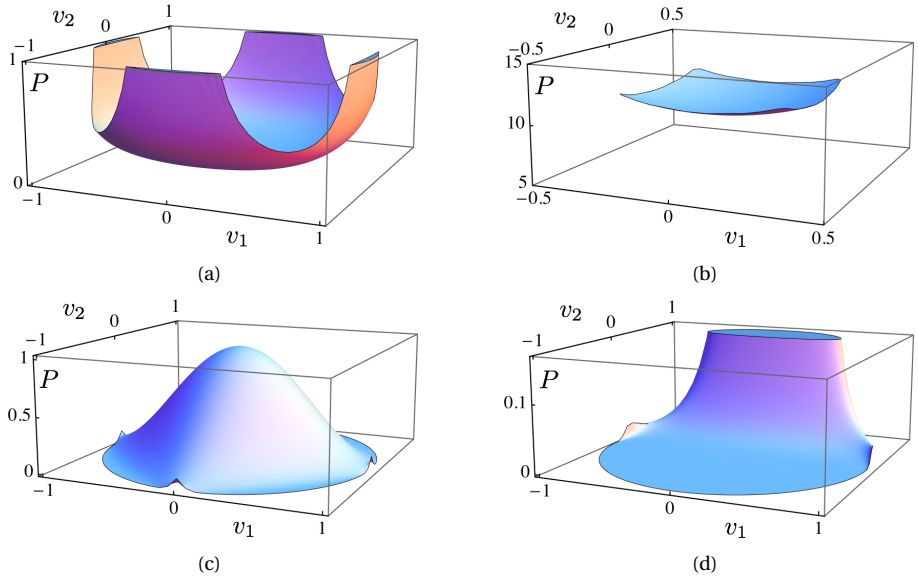


Figure 4.6.: The figure shows a plot of the asymptotic position distributions of the quantum walk defined by Equation (4.88) with different initial states.

of **W** is non-degenerate, but the Kraus operators are non-unitary. Hence, the results of the last section are applicable, and in particular Equation (4.60) determines the asymptotic behavior of the position distribution in ballistic scaling but now with a momentum dependent velocity $v(p)$.

We consider a one dimensional lattice with no internal degree of freedom. The decoherence will be of Bernoulli type, i.e. the Markov chain is actually trivial, and the Kraus operators of the quantum walk are defined by

$$(K_1\psi)_x = \frac{1}{2}(\psi_x + \psi_{x+1}) \quad , \quad (K_2\psi)_x = \frac{1}{2}(\psi_x - \psi_{x-1}). \tag{4.91}$$

These operators satisfy the normalization condition $\sum_i K_i^* K_i = \mathbb{1}$ and their Fourier transforms are given by

$$K_1(p) = \frac{1}{2}(1 + e^{ip}) \quad , \quad K_2(p) = \frac{1}{2}(1 - e^{-ip}).$$

In fact, the Kraus operators K_1 and K_2 commute, hence the behavior of this quantum walk will be ballistic [AVWW11]. Clearly, $\omega_p = 1$ is an invariant state for **W** and using Theorem 4.5.14 we see that the characteristic function of the asymptotic

position distribution is determined by the p-dependent velocity

$$v(p) = \frac{\cos(p)}{2}.$$

By decomposing momentum space into subsets $[-\pi, 0)$ and $[0, \pi)$ on which the function $v(p)$ is invertible and exploiting the point symmetry of $v(p)$ we obtain the asymptotic position distribution

$$P(x) = \frac{1}{\pi\sqrt{1-4x^2}} \left(\rho_0(v^{-1}(x)) + \rho_0(-v^{-1}(x))\right),$$

where v^{-1} denotes the inverse of v restricted to $[-\pi, 0)$. Again, we see that at the points where the derivative $\partial v/\partial p$ vanishes, i.e. at the caustic points, there are peaks in the limiting distribution. If we choose ρ_0 to be located at the origin, i.e. $\rho_0(p) = 1$, we can use Lemma 4.3.3 to get

$$P(x) = \frac{2}{\pi\sqrt{1-4x^2}}.$$

Figure 4.7 compares this asymptotic distribution with the scaled probability distributions for a finite number of time steps. In fact, it is not hard to see that the exact

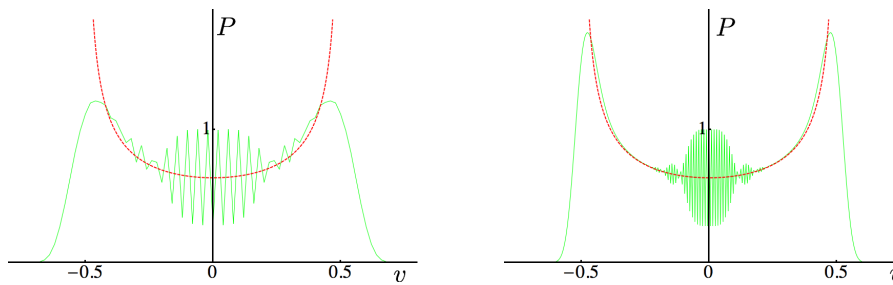


Figure 4.7.: Position distribution of the quantum walk defined by Equation (4.91) after (a) 50 and (b) 200 time steps (green/dotted lines) in ballistic scaling. The red/dashed line shows the asymptotic position distribution for comparison.

formula for the perturbed eigenvector is

$$\begin{aligned} \mu_\varepsilon &= \sum_i K_i^*(p) K_i(p + \lambda\varepsilon) \\ &= \frac{1 + \cos(\lambda\varepsilon) + \mathrm{i}(\sin(p + \lambda\varepsilon) - \sin(p))}{2} \end{aligned}$$

see [AVWW11]. Our knowledge of the exact eigenvalue μ_ε allows us to analyze the asymptotic distribution in further detail. The Taylor expansion of μ_ε to second order reads

$$\mu_\varepsilon = 1 + \varepsilon\mu' + \frac{\varepsilon^2}{2}\mu'' + o(\varepsilon^3) = 1 + \mathrm{i}\frac{\varepsilon\lambda}{2}\cos(p) - \frac{\varepsilon^2\lambda^2}{4}(\mathrm{i}\sin(p)+1) + o(\varepsilon^3).$$

Hence, the variance $s(p)$ for this example is a complex valued function

$$s(p)\lambda^2 = -\mu'' - (v\cdot\lambda)^2 = \frac{2+\mathrm{i}2\sin(p)-\cos^2(p)}{4}\lambda^2.$$

The imaginary part of this "variance" defies its interpretation as the variance of added Gaussian noise. However, the corrections to the probability distribution computed from it will be real after integration over momenta.

Using the techniques from the previous section we can determine the $1/t$ correction to the asymptotic distribution stemming from the second order of the perturbation expansion in ε. Since we have $A' = 0$ and we have chosen $\rho_0(p_1,p_2) = 1$ we obtain

$$C_t(\lambda) = \frac{1}{2\pi}\int dp\, e^{\mathrm{i}\lambda v(p)}\Big(1 - \frac{2+\mathrm{i}2\sin(p)-\cos^2(p)}{8t}\lambda^2\Big) + o(t^{-2})$$

for the characteristic function of the position distribution at time t. With $v(p) = \cos(p)/2$ the integral over p yields a sum of two Bessel functions for the first order approximation $C_1(\lambda,t)$ of $C_t(\lambda)$, i.e. $C_t(\lambda) = C_0(\lambda) + C_1(\lambda,t) + o(t^{-2})$ and

$$C_1(\lambda,t) = \frac{1}{8t}\left((8t-\lambda^2)J_0(\lambda/2) - 2\lambda J_1(\lambda/2)\right).$$

As already pointed out in Section 4.5.1, C_1 is not integrable over $\mathbb{R}$ (cf. Figure 4.8) and therefore we need to introduce a cutoff in the integration for the inverse Fourier transform of $C_t(\lambda)$. In order to smoothen the resulting probability distribution we multiplied $C_1(\lambda,t)$ with a Gaussian $g(\lambda,t) = e^{-(\lambda/t)^2}$ and computed the inverse Fourier transform numerically. This smoothening was necessary because of the rapidly oscillating behaviour of $C_1(\lambda,t)$, which can be seen in Figure 4.8, leading to a poor convergence of the numerical integration. The resulting correction to the asymptotic position distribution for 10 time steps, also shown in Figure 4.8, is in good agreement with the exact position distribution.

Example 3: Decoherent coin operator from completely positive maps

We consider quantum walks on $\ell^2(\mathbb{Z})\otimes\mathbb{C}^2$ which admit a decomposition $\mathbf{W}(A) = S^*\mathbf{C}(A)S$ into a unitary shift operator S and a decoherent coin operator $\mathbf{C}$. For the

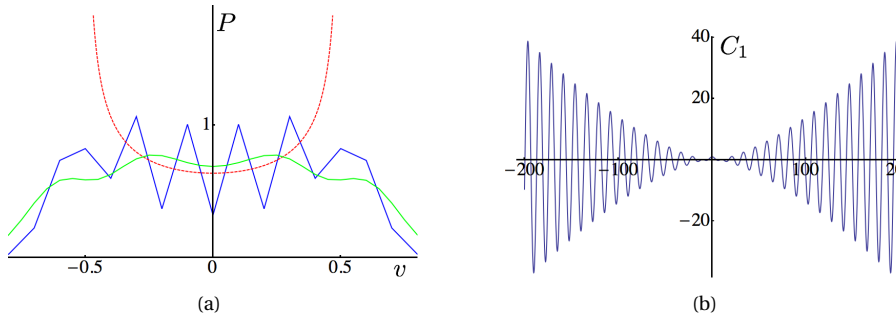


Figure 4.8.: Plot (a) shows the correction of order $1/t$ (green) to the asymptotic distribution (red-dashed) for the quantum walk defined by Equation (4.91). The exact values (connected by a blue polygon) are shown for the same value ($t = 10$) as the correction. In (b) the $1/t$ correction $C_1(\lambda, t)$ to the characteristic function $C_t(\lambda)$ is shown for $t = 10$.

shift operator we choose the standard shift defined by $S|x,\pm\rangle = |x \pm 1, \pm\rangle$, where $\pm$ labels a basis of $\mathbb{C}^2$, and for the quantum channel $\mathbf{C}$ we choose completely positive maps T on $\mathbb{C}^2$ and write $\mathbf{C} = \mathrm{id}_{\mathbb{Z}} \otimes T$.

The first example shows that the invariant state ω_p may be p-dependent if the Kraus operators of the quantum walk are non-unitary. We choose the map T as a mixture of a unitary Hadamard evolution and a reset of the particle in the $|+\rangle$-state. That is, in the Schrödinger picture the channel T_* can be written as

$$T_*(\rho) = wH \cdot \rho \cdot H + (1-w)\mathrm{tr}\,\rho \cdot |+\rangle\langle +|, \quad w \in (0,1),$$

with

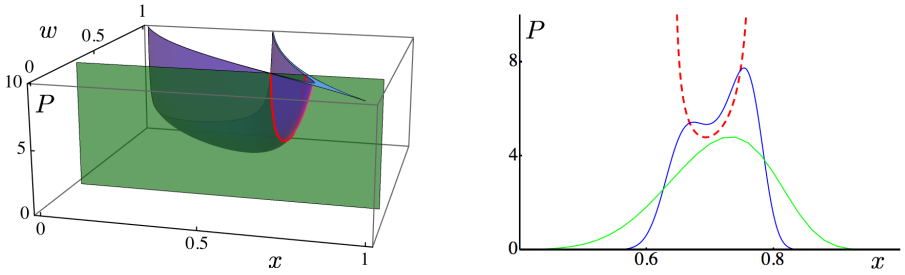
$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

In the following we choose the Pauli operators $\sigma_0 = \mathbb{1}, \sigma_1, \sigma_2$ and σ_3 as operator basis. A straightforward calculation shows that Assumption 4.1 is valid and there is a p-dependent invariant state

$$\begin{aligned} \omega_p &= \frac{1}{2}\mathbb{1} + \frac{w\sin(2p)}{2(1+w(1+w+\cos(2p)))}\sigma_2 + \\ &+ \frac{w(w+\cos(2p)}{2(1+w(1+w+\cos(2p)))}(\sigma_1 + \sigma_3) \end{aligned}$$

for $\mathbf{W}$. The identity $\mathbf{W}'(A) = \mathrm{i}\lambda\mathbf{W}(A)\cdot\sigma_3$, which follows from the expression $S(p) = e^{\mathrm{i}p\sigma_3}$, leads to $\mathbf{W}'(\mathbb{1}) = \mathrm{i}\lambda\sigma_3$. This results in the p-dependent velocity

$$v(p) = \frac{1 + w\cos(2p)}{1 + w(1 + w + \cos(2p))}.$$



(a) (b)

Figure 4.9.: Plot (a) shows the asymptotic position distribution depending on w with a plane at $w = 0.3$. In (b) a comparison of asymptotic (red-dashed) and finite time position distributions for $w = 0.3$, $t = 100$ (green) and $t = 800$ (blue) is plotted. In order to eliminate oscillations in the finite time step distributions we computed the average of two neighboring lattice sites.

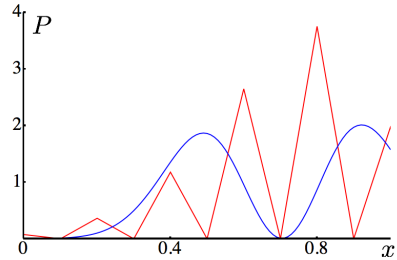
Solving this equation for $\cos(2p)$ and inserting this into the equation for $v'(p)$ leads to the asymptotic probability density

$$P(x) = \frac{1+w}{4\pi(1-x^2)\sqrt{1-\left(\frac{1-x(1+w(1+w))}{(1-x)w}\right)^2}} \sum_{q\in v^{-1}(x)} \operatorname{tr}\rho(q).$$

Figure 4.9 shows a plot of the asymptotic position distribution for initial states localized at the origin and a comparison with a finite time step distribution. In order to compute the $1/t$ correction to the asymptotic position distribution we need to determine the first correction to the eigenvector A' from which we compute the second order correction μ'' to the eigenvalue. This leads to a four-dimensional linear system of equations, which is straightforward to solve. The resulting $1/t$-correction to the characteristic function is not a well-defined characteristic function. Therefore we multiply this function again with a Gaussian $g(\lambda,t) = e^{-(\lambda/t)^2}$ to enforce sufficient decay such that the Fourier transform of this function leads to a well-defined probability density. We compute this Fourier transform numerically, Figure 4.10 shows the resulting correction to the asymptotic position distribution for $t = 10$.

Our second example illustrates a case where the degenerate eigenvalue 1 splits into several branches for almost all p. We define the map T by

$$T(\sigma_k) = \begin{cases} \sigma_k & , \quad k = 0,3 \\ r\cdot\sigma_k & , \quad k = 1,2 \end{cases} .$$



(a)

Figure 4.10.: The plot shows the $1/t$-correction to the asymptotic position distribution (blue) for $t = 10$ and initial state $\rho = |+\rangle\langle+|$. For comparison we plotted the exact position distribution (red), which is in good agreement with this $1/t$-correction.

Such channels are known as Pauli channels, see e.g. [RSW02], and complete positivity of this map is assured for $|r| \leq 1$. The matrix representation of $\mathbf{W}_\varepsilon$ reads accordingly

$$\mathbf{W}_\varepsilon = \begin{pmatrix} \cos(\varepsilon\lambda) & 0 & 0 & \mathrm{i}\sin(\varepsilon\lambda) \\ 0 & r\cos(2p+\varepsilon\lambda) & -r\sin(2p+\varepsilon\lambda) & 0 \\ 0 & r\sin(2p+\varepsilon\lambda) & r\cos(2p+\varepsilon\lambda) & 0 \\ \mathrm{i}\sin(\varepsilon\lambda) & 0 & 0 & \cos(\varepsilon\lambda) \end{pmatrix}.$$

Clearly, the matrix is reducible with respect to the two invariant subspaces spanned by σ_0, σ_3 and σ_1, σ_2, where the first space is the eigenspace of the degenerate eigenvalue $\mu_0(0) = 1$. Under the perturbation by ε the eigenvalue 1 splits into the two branches $\mu_{0,\pm}(\varepsilon) = e^{\pm \mathrm{i}\varepsilon\lambda}$ with corresponding eigenvectors $A_\pm = (\sigma_0 \pm \sigma_3)/2$. Thus, the eigenprojections $\mathbf{P}_{0,\pm}$ are defined by

$$\mathbf{P}_{0,\pm}(\varepsilon)(A) = \frac{1}{4}(\sigma_0 \pm \sigma_3)\mathrm{tr}\left((\sigma_0 \pm \sigma_3)A\right).$$

To summarize, the eigenvalue 1 splits for almost all p into two different eigenvalues, and these eigenvalues as well as the eigenprojections are analytic at $\varepsilon = 0$. If $r < 1$ the other two eigenvalues have modulus strictly smaller than 1 and we can determine the asymptotic behavior of $\mathbf{W}$ from the equation

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = e^{\mathrm{i}\varepsilon\lambda t}\mathbf{P}_{0,+}(\varepsilon)(\mathbb{1}) + e^{-\mathrm{i}\varepsilon\lambda t}\mathbf{P}_{0,-}(\varepsilon)(\mathbb{1}) + \ldots.$$

We need to compute the limiting values of $\mathbf{P}_{0,\pm}(\varepsilon)(\mathbb{1})$ for $\varepsilon \to 0$, but this is easily seen to be $\mathbf{P}_{0,\pm}(\varepsilon)(\mathbb{1}) = (\sigma_0 \pm \sigma_3)/2$. This finally yields the ballistic scaling

$$\mathbf{W}_{1/t}^t(\mathbb{1}) \underset{t\to\infty}{\longrightarrow} \cos(\lambda)\mathbb{1} + \mathrm{i}\sin(\lambda)\sigma_3$$

and accordingly the characteristic function

$$C(\lambda)=\frac{1}{2\pi}\int\limits_{[-\pi,\pi)} dp\left(e^{i\lambda}\langle+|\rho_0(p)|+\rangle+e^{-i\lambda}\langle-|\rho_0(p)|-\rangle\right).$$

The corresponding probability distribution is the linear combination of two point measures at ±1 with weights $w_\pm=\mathrm{tr}\left(\mathbb{1}_{\mathbb{Z}}\otimes|\pm\rangle\langle\pm|\rho_0\right)$.

Example 4: Coherent limit of decoherent quantum walks

The aim of this example is to shed some light on the behavior of the variance $s(p)$ for a coherent limit of a quantum walk $\mathbf{W}$. More precisely, we consider a decoherent quantum walk $\mathbf{W}$ which is a classical mixture of two coherent quantum walks $\mathbf{V}_{1,2}$ controlled by a Markov process $\mathbf{M}$ and our interest is in the behavior of $s(p)$ for various coherent limits of $\mathbf{W}$, i.e. if the Markov chain approaches a deterministic process. The unitary quantum walks, the control process chooses from, admit a decomposition into shift and coin operators. The shift operator is assumed to be the same for both walks, hence, the control process chooses only the coin operator for each time step. For the shift operator we choose again the standard shift defined by $S|x,\pm\rangle=|x\pm1,\pm\rangle$. The two coins $\mathbf{M}$ chooses from are the Hadamard coin, which, on its own, would lead to ballistic behavior, and the Pauli matrix σ_3, which trivially results in ballistic transport. Hence, the quantum channels $\mathbf{V}_{1,2}$ are unitarily implemented, that is, $\mathbf{V}_{1,2}(A)=K_{1,2}^*AK_{1,2}$ and the Kraus operators $K_{1,2}(p)$ in momentum space read

$$K_1(p)=\frac{1}{\sqrt{2}}\begin{pmatrix} e^{ip} & e^{ip}\\ e^{-ip} & -e^{-ip}\end{pmatrix}\quad,\quad K_2(p)=\begin{pmatrix} e^{ip} & 0\\ 0 & -e^{-ip}\end{pmatrix}. \tag{4.92}$$

First, we note that Assumptions 4.1 and 4.2 are satisfied, hence we may use Equation (4.77) to confirm that the velocity $v(p)$ is zero. This means in ballistic scaling the position distribution of the quantum particle converges to a point measure at the origin. We parametrize the Markov process $\mathbf{M}$ by

$$\mathbf{M}=\begin{pmatrix} 1-m_1 & m_1\\ m_2 & 1-m_2\end{pmatrix}.$$

Solving again the equation for A' and inserting this into Equation (4.67) yields the p-dependent variance

$$\begin{aligned} s(p) &= 1+\frac{3+(m_1-3)m_1}{(m_1-2)m_2}+\frac{m_2}{2m_1}-\frac{2}{(m_1-2)m_1(m_1+m_2-2)}+\frac{1}{m_1+m_2}-\\ &- \frac{(m_1+m_2-1)(m_1+m_2)}{m_1m_2(m_1+m_2-2)}\cos(2p)\end{aligned}$$

There are several coherent limits of **W** along which this variance diverges. If the Markov process **M** prefers one of the coins, that is if $m_1 \to 0$ or $m_2 \to 0$, $s(p)$ clearly diverges. Also if $m_{1,2} \to 1$ simultaneously, i.e. the Markov process **M** becomes a deterministic permutation of the classical control states, we have $s(p) \to \infty$.

4.6. Quantum walks with momentum transfer

If the momentum variable p is not conserved by **W**, it makes no longer sense to perform the asymptotic analysis separately for all p. Hence, one has to consider the infinite dimensional operator **W** instead of a family of finite dimensional matrices. However, if **W** is unitarily implemented one can reduce the analysis to finite dimensional matrices in some cases, but for decoherent **W** there is in general no hope for such an approach to work. Therefore we are led to incorporate infinite dimensional perturbation theory to obtain the asymptotic position distribution in this case. For the sake of brevity, we will mostly omit to mention that **W** is assumed to show momentum transfer throughout this section.

4.6.1. Unitary quantum walks

If the quantum walk **W** is unitarily implemented by $W \in \mathcal{B}(\ell^2(\mathbb{Z}^s) \otimes \mathcal{K})$, i.e. $\mathbf{W}(A) = W^*AW$, it is again sufficient to consider the unitary operator W instead of **W**. We already encountered a basic example of a unitary quantum walk with momentum transfer in Section 3.2. The operator $W_\varphi = e^{-\mathrm{i}\varphi\cdot Q}$, with $\varphi \in [-\pi,\pi)^s$, acts on translationally invariant operators as $(W_\varphi^* A W_\varphi)(p) = A(p+\varphi)$, see Lemma 3.2.8. A basic observation is that all unitary quantum walks with momentum transfer are related to a particular W_φ by the following proposition.

Proposition 4.6.1. *Let* **W** *be a unitary quantum walk on* $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ *with momentum transfer. Then there exists a unitary quantum walk* $\widetilde{\mathbf{W}}$ *on* $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ *without momentum transfer and* $\varphi \in [-\pi,\pi)^s$ *such that*

$$\mathbf{W}(A) = e^{-\mathrm{i}\varphi\cdot Q}\widetilde{\mathbf{W}}(A)e^{\mathrm{i}\varphi\cdot Q}$$

for all $A \in \mathcal{B}(\ell^2(\mathbb{Z}^s) \otimes \mathcal{K})$.

Proof. Using Theorem 4.2.2 we see that the dilation space $\mathcal{D}$ must be trivial, i.e. $\mathcal{D} = \mathbb{C}$ since **W** is unitarily implemented. Thus, the representation $\{U_x\}_{x\in\mathbb{Z}^s}$ is given by a set of phases $U_x = e^{\mathrm{i}\varphi_x} \in \mathbb{S}$. In fact, there even exists $\varphi \in [-\pi,\pi)^s$ such that $U_x = e^{\mathrm{i}\varphi\cdot x}$ since we have a representation of $\mathbb{Z}^s$. Clearly, the minimal isometry $\mathcal{V}$ implementing **W** is a unitary operator on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ and by Equation (4.3) we have

$$\mathcal{V}|x \otimes \phi\rangle = \sum_{y\in\mathcal{N}} e^{\mathrm{i}\varphi\cdot x}|x+y\rangle \otimes |v_y\phi\rangle\,.$$

The unitary operator $\mathcal{V}\cdot e^{-\mathrm{i}\varphi\cdot Q}$ is obviously translationally invariant and hence defines a unitary quantum walk $\widetilde{\mathbf{W}}$ without momentum transfer via $\widetilde{\mathbf{W}}(A)=e^{\mathrm{i}\varphi\cdot Q}\mathcal{V}^*A\mathcal{V}\cdot e^{-\mathrm{i}\varphi\cdot Q}$. □

By Proposition 4.6.1, unitary quantum walks with momentum transfer are exactly those operators which can be written as

$$\mathbf{W}_\varphi(A)=e^{-\mathrm{i}\varphi\cdot Q}\widetilde{\mathbf{W}}(A)e^{\mathrm{i}\varphi\cdot Q} \tag{4.93}$$

where $\widetilde{\mathbf{W}}$ is a unitary quantum walk without momentum transfer and $\varphi\in[-\pi,\pi)^s$. Thus, the unitary operator W can be written as $W=\widetilde{W}e^{\mathrm{i}\varphi\cdot Q}$ with translationally invariant $\widetilde{W}$. Such quantum walks on $\mathbb{Z}$ with $\mathcal{K}=\mathbb{C}^2$ have been studied in [WŁK+04, BB04, BNP+06] where it was found that, compared to the case without momentum transfer, i.e. $\varphi=0$, the propagation behavior is remarkably different. A crucial assumption in these references is rationality of the phase φ with respect to π. We adopt this assumption for the moment, that is, we consider vectors $\varphi\in[-\pi,\pi)^s$ such that all of its components φ_i can be written as

$$\varphi_i=\frac{n_i}{m_i}2\pi,\quad m_i,n_i\in\mathbb{N},$$

where we assume n_i and m_i to be coprime. These quantum walks generically show two contradicting propagation effects: On small to medium time scales the behavior is oscillatory in the sense that propagation measures such as the standard deviation show clear oscillations, whereas the asymptotic behavior is of ballistic nature. Figure 4.11 illustrates this for the well-known Hadamard walk with momentum transfer of $\pi/5$ and $\pi/10$. That is, the time evolution is given by the unitary $W=S\cdot(\mathbb{1}_{\mathbb{Z}}\otimes H)\cdot e^{\mathrm{i}\varphi\cdot Q}$ on $\ell^2(\mathbb{Z})\otimes\mathbb{C}^2$ with

$$S|x,\pm\rangle=|x\pm1,\pm\rangle\quad\text{and}\quad H=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}, \tag{4.94}$$

and $\varphi=\pi/5$ and $\varphi=\pi/10$. To understand the asymptotic behavior we note that the quantum walk $\widetilde{W}e^{\mathrm{i}\varphi\cdot Q}$ with rational phase φ is equivalent to a translationally invariant quantum walk defined on a super-lattice. Indeed, after grouping exactly m_i lattice sites in lattice direction i we get a new quantum walk $\widehat{\mathbf{W}}$ with enlarged internal state space of dimension $\dim\mathcal{K}\prod_i m_i$. It is straightforward to see that the matrix representation $\widehat{W}$ of the quantum walk $\widehat{\mathbf{W}}$ commutes with translations of the super-lattice. Hence, the asymptotic analysis of this quantum walk is covered by the results of Section 4.5.1. Of course, the asymptotic position distribution of $\widehat{\mathbf{W}}$ is just a rescaled version of the limiting distribution of the quantum walk $\mathbf{W}$, where the proportionality in lattice direction i is exactly m_i. Thus, we obtain the asymptotic position distribution of $\mathbf{W}$ by considering its regrouped version $\widehat{\mathbf{W}}$. Another way to

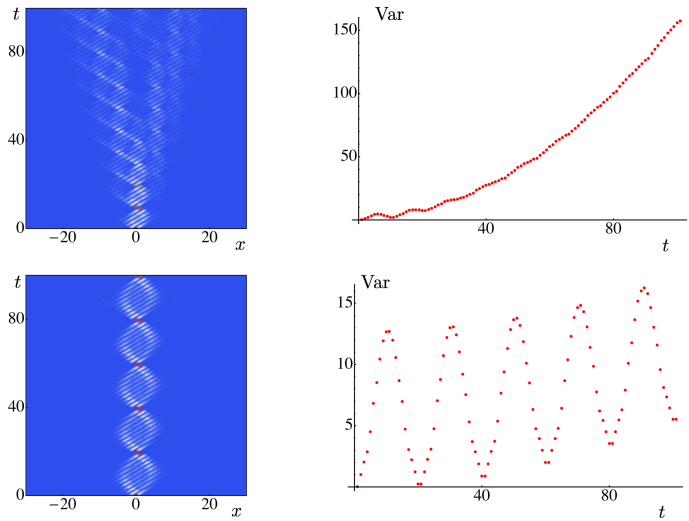


Figure 4.11.: The figure shows a density plot of the position distribution (left) and a plot of the variance (right) for the Hadamard walk $W = S\cdot(\mathbb{1}_{\mathbb{Z}}\otimes H)\cdot e^{i\varphi\cdot Q}$, see Equation (4.94), with $\varphi = \pi/5$ (upper) and $\varphi = \pi/10$ (lower). Ballistic propagation is clearly visible for $\varphi = \pi/5$, whereas the case $\varphi = \pi/10$ shows oscillatory behavior, which eventually becomes ballistic.

obtain the asymptotic distribution follows from the simple observation that W acts in momentum space as

$$(W^n\psi)(p) = \widetilde{W}(p)\cdot\widetilde{W}(p+\varphi)\ldots\widetilde{W}(p+(n-1)\varphi)\cdot\psi(p+n\varphi). \tag{4.95}$$

Let us denote the smallest common multiple of all m_i by m. By grouping exactly m time steps of $\mathbf{W}$ as a single time step of a new quantum walk $\widehat{\mathbf{W}}$ we obtain a translationally invariant quantum walk and the limiting distribution of $\widehat{\mathbf{W}}$ is rescaled by a factor of $1/m$ compared to $\mathbf{W}$.

This nicely explains the ballistic propagation of $\mathbf{W}$ in the asymptotic regime. If W has no eigenvectors there is only absolutely continuous spectrum for $\widehat{W}$ leading to ballistic propagation. However, there is still the oscillatory behavior for the short time scale regime to be explained. To this end, suppose for the moment the initial state of the particle has a narrowly peaked momentum distribution around some value p^*. It is apparent from Equation (4.95) that a single time step of the walk operator W first shifts the momentum distribution of the particle by $-\varphi$ and subsequently applies the translationally invariant quantum walk $\widetilde{W}$. In other words, the particles momentum distribution after t time steps is approximately peaked

around $p = p^* - t \cdot \varphi$ and at time t the particle is mostly affected by the group velocities of $\widetilde{W}$ at $p = p^* - t \cdot \varphi$. But since the dispersion relations are 2π-periodic functions, the particle successively feels all values of the group velocities. Hence, if the average value of the group velocities $v_i(p)$ vanishes for each branch individually, which is the case in [WŁK+04, BB04, BNP+06], we expect the particle to undergo an oscillation around its initial position, see Figure 4.11. This is because of the apparent similarity with Bloch oscillations of an electron in a periodic potential subject to a constant force. However, this physical intuition tells only half the story. The reason for ballistic behavior to set in eventually is twofold. Firstly, we neglected the p-dependent eigenprojections of $\widetilde{W}$ in our analysis. That is, the shift of the momentum distribution created by $e^{i\varphi \cdot Q}$ also induces transitions between the p-dependent eigenstates of $\widetilde{W}$. So despite the fact that the average of group velocities of a single branch v_i may vanish, there are transitions to other branches of the group velocities. The second point is that for some momenta p the average velocity over the discrete set of momenta $p - t \cdot \varphi$ may vanish while it is non-zero for other momenta.

If, on the other hand, φ is irrational for some components we cannot regroup to get a translationally invariant operator $\widehat{\mathbf{W}}$ and the propagation behavior, as well as the spectral properties of W, may differ significally from the case without momentum transfer. Indeed, let $\mathcal{T}_x$ denote a translation of the lattice by a vector $x \in \mathbb{Z}$. It follows from

$$\mathcal{T}_x^* W \mathcal{T}_x = e^{i\varphi \cdot x} W \quad \forall x \in \mathbb{Z} \tag{4.96}$$

that for $z \in \sigma(W)$ all numbers $e^{i\varphi \cdot x} z$ are also elements of the spectrum of W. In fact, this argument also applies to parts of the spectrum as pure point or continuous spectrum. As a consequence we have the following proposition.

Proposition 4.6.2. *Let $W = \widetilde{W} e^{i\varphi \cdot Q}$, with $\widetilde{W}$ translationally invariant, be a quantum walk with momentum transfer. Suppose at least one coordinate of φ is irrational with respect to π. The spectrum of W satisfies $\overline{\sigma(W)} = \mathbb{S}$ and for the parts of $\sigma(W)$ we have*

$$\sigma_{pp,sc}(W) = \emptyset \quad or \quad \overline{\sigma_{pp,sc}(W)} = \mathbb{S} \quad as\ well\ as \quad \sigma_{ac}(W) = \emptyset \quad or \quad \sigma_{ac} = \mathbb{S}. \tag{4.97}$$

Proof. The conjugation of W by any unitary operator leaves the spectrum invariant and multiplication of W by $e^{i\varphi \cdot x}$ rotates the spectrum by an angle of $\varphi \cdot x \mod 2\pi$. Hence, it follows from Equation (4.96) and the ergodicity of the phases $e^{i\varphi \cdot x}$ that the spectrum of W is dense in $\mathbb{S}$, i.e. $\overline{\sigma(W)} = \mathbb{S}$. The same argument also applies to the subparts of the spectrum, hence, pure point and singular continuous part are also dense in $\mathbb{S}$ or empty. For the absolutely continuous part we have an even stronger statement. If the absolutely continuous part is non-empty there exists an open arc of absolutely continuous spectrum in $\mathbb{S}$. By shifting this arc around via phases $e^{i\varphi \cdot x}$ we cover all of $\mathbb{S}$ with absolutely continuous spectrum. □

Based on heuristic arguments it was conjectured in [WŁK+04] that for irrational φ the particle's propagation is suppressed even in the asymptotic limit. In the following we sketch a line of arguments meant to strengthen doubts in this conclusion. Quantum walks with quasi-periodic spatial modulations of the coin operator exhibit effects which indicate singularly continuous spectrum for the evolution operator W. For instance, it was observed in [SK10] that a similar model displays Hofstadter butterfly like spectrum. Thus we conjecture that the singularly continuous spectrum of unitary quantum walks with irrational momentum transfer is in general non-empty. Assuming moreover that W has no pure point spectrum, we conclude from the RAGE theorem 3.3.6 that for any finite subset $\Lambda \subset \mathbb{Z}^s$ and $\psi \in \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$

$$\lim_{T\to\infty} \frac{1}{T+1} \sum_{t=0}^{T} \left\| P_\Lambda W^t \psi \right\| = 0, \tag{4.98}$$

where P_Λ denotes the projection onto Λ, see the discussion before Remark 4.5.8. For vectors ψ_{ac} in the absolutely continuous subspace $\mathcal{H}_{ac}$ we conclude from Theorem 3.3.7 that $\left\| P_\Lambda W^t \psi_{ac} \right\|$ goes to zero as $t \to \infty$ so the particle leaves any finite volume Λ. For vectors in the singularly continuous subspace $\psi_{sc} \in \mathcal{H}_{sc}$ we only have Equation (4.98) and the sequence $\left\| P_\Lambda W^t \psi_{sc} \right\|$ may have several limiting points one of them being zero. This means the particle leaves each finite volume almost perfectly but also returns at least partially to Λ after some time. In fact, this happens infinitely often and the times in between leaving a region and returning have to grow unboundedly to ensure Equation (4.98). In a similar context it was proven recently [GVWW12] that singularly continuous spectrum is exactly the part which leads to such transient or recurrent behavior. This is also consistent with the occurrence of oscillations for rational φ and small enough time steps as we may approximate W with irrational φ by quantum walks with rational φ to arbitrary precision such that the respective probability distributions for finite numbers of time steps differ only by an arbitrarily small amount in trance norm. Therefore we expect the behavior of the particle subject to W to be transient instead of localized as conjectured in [WŁK+04] as this conclusion would require dense pure point spectrum instead of singularly continuous spectrum for W.

4.6.2. Decoherent quantum walks

As already mentioned, the presence of momentum transfer in general defies a description of a decoherent quantum walk **W** by finite dimensional matrices depending on momentum p. Instead, we need to consider the whole operator **W** as acting on an infinite dimensional vector space. A characterization of all decoherent quantum walks **W** with momentum transfer is provided by Theorem 4.2.2 and Proposition 4.2.4, the part of **W** leading to momentum transfer is specified by the spectral measure $E(dq)$. Although this characterization is satisfying from the abstract point

of view, it is less practical for deriving the asymptotic limit of such a quantum walk **W**. Instead, we restrict ourself to quantum walks with a particular structure in this section, which we extend to a more general class of quantum walks at the end of this section.

The model we are going to study in this section has an intuitive physical interpretation. Suppose we are given a unitary quantum walk with shift and coin decomposition, that is, the unitary implementing **W** is given by $W = S \cdot (\mathbb{1}_{\mathbb{Z}^s} \otimes U)$, where $U \in \mathcal{U}(\mathcal{K})$ and

$$S = \sum_{i=1}^{\dim \mathcal{K}} \mathcal{T}_{x_i} \cdot (\mathbb{1}_{\mathbb{Z}^s} \otimes |\psi_i\rangle\langle\psi_i|), \tag{4.99}$$

with $\{\psi_i\}$ an orthonormal basis of $\mathcal{K}$ and $x_i \in \mathbb{Z}^s$, see Equations (4.20) and (3.9). A way to introduce decoherence is to assume the unitary operator U is not fixed but varies in time, which leads to a quantum walk **W** without momentum transfer as considered in Section 4.5.2. Indeed, this situation can be modeled by a probability distribution on a set of possible coin operators, i.e. we consider a probability space (Ω, Σ, ν) where the sample space Ω can be identified with $\mathcal{U}(\mathcal{K})$, that is, for each $\omega \in \Omega$ there is a unique $U_\omega \in \mathcal{U}(\mathcal{K})$. With this notation we can write the action of **W** on translationally invariant operators $A \in \mathcal{T}_{\mathcal{K},s}$ in momentum space as

$$\mathbf{W}(A)(p) = S(p)^* \int_\Omega \nu(d\omega) U_\omega^* A(p) U_\omega S(p). \tag{4.100}$$

Therefore, the quantum walk **W** admits a decomposition into translationally invariant Kraus operators, and hence exhibits no momentum transfer. This is no longer true if we assume that the operator U fluctuates in time and space. The resulting operator is of the form

$$\mathbf{W}(A) = S^* \mathbf{C}(A) S, \tag{4.101}$$

where S again denotes the unitary shift operator and **C** is a decoherent and strictly local coin operator. We think of the map **C** as being again generated by a probability space (Ω, Σ, ν), but now a U_ω is chosen for each time step and lattice site. The action of the coin operator **C** on a generic operator $A = \sum_{x,y} |x\rangle\langle y| \otimes A_{xy}$ can hence be written as

$$\begin{aligned} \mathbf{C}\left(\sum_{x,y} |x\rangle\langle y| \otimes A_{xy}\right) &= \sum_{x,y} |x\rangle\langle y| \otimes \left(\delta_{xy} \int_\Omega \nu(d\omega) U_\omega^* A_{xy} U_\omega \right. \\ &\quad \left. + (1-\delta_{xy}) \widetilde{U}^* A_{xy} \widetilde{U}\right), \quad \widetilde{U} = \int_\Omega \nu(d\omega) U_\omega . \end{aligned} \tag{4.102}$$

One crucial assumption at this point is that the randomness in the coin operator happens in an independent and identical fashion, both in time and space. This implies that **W** is indeed translationally invariant.

Before we enter the asymptotic analysis of this particular model, let us prove that this indeed is a quantum walk with momentum transfer. To this end, we translate the definition of the quantum walk into momentum space by Fourier transform. The shift operator S is represented in momentum space by conjugation with the p-dependent $\dim\mathcal{K}$-dimensional matrix

$$S(p)=\begin{pmatrix} e^{\mathrm{i}x_1\cdot p} & 0 & \cdots \\ 0 & \ddots & \\ \vdots & & e^{\mathrm{i}x_{\dim\mathcal{K}}\cdot p} \end{pmatrix}, \tag{4.103}$$

hence, the operator $\mathbf{W}$ acts on a translationally invariant bounded operator $A(p)$ in the following way:

$$\begin{aligned} \mathbf{W}(A)(p) &= S(p)^*\left(\int_\Omega \nu(d\omega)U_\omega^* A_0 U_\omega + \widetilde{U}^*(A(p)-A_0)\widetilde{U}\right)S(p) \qquad (4.104)\\ A_0 &= (2\pi)^{-s}\int_{[-\pi,\pi)^s} d^s p A(p) \end{aligned}$$

In this equation A_0 denotes the p-independent term in $A(p)$. Clearly, the shift operator S conserves momentum, but the coin operator $\mathbf{C}$ mediates momentum transfer. This can be seen from the momentum representation

$$\mathbf{C}(A)(p)=\int_\Omega \nu(d\omega)U_\omega^* A_0 U_\omega + \widetilde{U}^*(A(p)-A_0)\widetilde{U} \tag{4.105}$$

of the coin operator. If $\mathbf{C}$ were without momentum transfer we would have

$$\mathbf{W}(f(p)A)=f(p)\mathbf{W}(A)$$

for any function f and $A\in\mathcal{B}(\mathcal{K})$. This is clearly violated by Equation (4.105), hence, the model exhibits momentum transfer.

The modified operator $\mathbf{W}_\varepsilon$ acts on a translationally invariant $A\in\mathcal{T}_{\mathcal{K},s}$ via

$$\mathbf{W}_\varepsilon(A)(p)=S(p)^*\left(\int_\Omega \nu(d\omega)U_\omega^* A_0 U_\omega + \widetilde{U}^*(A(p)-A_0)\widetilde{U}\right)S(p+\varepsilon\lambda), \tag{4.106}$$

where the momentum shift of $\varepsilon\lambda$ arises from the definition of the perturbed walk operator $\mathbf{W}_\varepsilon$ and the fact that the coin operator $\mathbf{C}$ commutes with $e^{\mathrm{i}\varepsilon\lambda\cdot Q}$, together

with Lemma 3.2.8. In Section 3.2 it was proven that $\mathcal{T}_{\mathcal{K},s}$, the set of translationally invariant bounded operators on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, can be turned into a separable Hilbert space by introducing the scalar product (3.12) on $\mathcal{T}_{\mathcal{K},s}$. We denote this scalar product and its induced norm by $\langle .|.\rangle$ and $\|.\|$ as this is essentially the only scalar product used in this section, so there is no source of confusion. The basic idea is to equivalently describe $\mathbf{W}_\varepsilon$ as an operator acting on the Hilbert space $\mathcal{T}_{\mathcal{K},s}\cong\ell^2(\mathbb{Z})\otimes\mathcal{B}(\mathcal{K})$. Thus, $\mathbf{W}_\varepsilon$ can be regarded as ε-dependent family of operators on the Hilbert space $\mathcal{T}_{\mathcal{K},s}$ to which we apply perturbation theory. It is instructive to reconsider the case of a decoherent quantum walk without momentum transfer, as considered in Section 4.5.2, in this setting. So, for the moment, let $\mathbf{V}$ denote a quantum walk without momentum transfer and $\mathbf{V}_\varepsilon$ the modified operator according to Equation (4.14). The Hilbert space $\mathcal{T}_{\mathcal{K},s}\cong\ell^2(\mathbb{Z})\otimes\mathcal{B}(\mathcal{K})$ comes with a natural set of translation operators, an element $A\in\mathcal{T}_{\mathcal{K},s}$ is translated by a lattice vector $x\in\mathbb{Z}^s$ under the action of the map $\widehat{\tau}_x(A)=A\mathcal{T}_x$ with the unitary operators $\mathcal{T}_x$ defined via Equation (3.9). Absence of momentum transfer is expressed by the existence of a Kraus decomposition of $\mathbf{V}$ in terms of translationally invariant Kraus operators, therefore $\mathbf{V}_\varepsilon\circ\widehat{\tau}_x(A)=\widehat{\tau}_x\circ\mathbf{V}_\varepsilon(A)$, or $[\mathbf{V}_\varepsilon,\widehat{\tau}_x]=0$ for short. But this means we can use the Fourier transform on $\ell^2(\mathbb{Z})\otimes\mathcal{B}(\mathcal{K})$ to define a Fourier transform of $\mathbf{V}_\varepsilon$, which yields a momentum dependent finite dimensional matrix for the action of $\mathbf{V}_\varepsilon$, which brings us back to the setting of Section 4.5. However, if the quantum walk $\mathbf{W}$ exhibits momentum transfer, these considerations are no longer true. In fact, the model we consider could be seen as a perturbation of a translationally invariant operator at the origin, cf. Equation (4.102).

Similarly to the case of decoherent quantum walks without momentum transfer we have to impose some conditions on our model for the perturbation theory to be non-degenerate. Here, the crucial assumption will be that some power of $\mathbf{W}$ is contractive in the following sense.

Assumption 4.3. *Denote by $\{\mathbb{1}\}^\perp$ the orthogonal complement of $\mathbb{C}\cdot\mathbb{1}$ in $\mathcal{T}_{\mathcal{K},s}$ with respect to the scalar product* (3.12)*. There exists $n\in\mathbb{N}$ such that $\|\mathbf{W}^n(A)\|<\|A\|$ for all non-zero $A\perp\mathbb{1}$. The operator $\mathbf{W}$ is said to be strictly n-contractive.*

Of course, the contractivity of $\mathbf{W}$ or a power of it depends on the probability distribution ν of the operators U_ω. A particular case where the operator $\mathbf{W}$ is strictly 1-contractive is when the set of operators $\{U_{\omega'}^*U_\omega:\omega',\omega\in\Omega\}$ is irreducible in the following sense.

Definition 4.6.3. *A set of matrices $\{M_i:i\in I\}$, where I is an index set and each M_i acts on $\mathcal{K}$, is said to be irreducible if any invariant subspace is trivial, that is, if $\mathcal{S}$ is a subspace of $\mathcal{K}$ such that $M_i\mathcal{S}\subset\mathcal{S}$ for all $i\in I$, we have $\mathcal{S}=\{0\}$ or $\mathcal{S}=\mathcal{K}$.*

Proposition 4.6.4. *Let $\mathbf{W}$ be a quantum walk according to Equations* (4.99), (4.101) *and* (4.102)*. If the set $\{U_{\omega'}^*U_\omega:\omega,\omega'\in\Omega\}$ is irreducible on $\mathcal{K}$, then $\mathbf{W}$ is strictly* 1*-contractive on $\{\mathbb{1}\}^\perp$, that is, $\|\mathbf{W}(A)\|<\|A\|$ for all non-zero $A\perp\mathbb{1}$.*

Proof. The unitarity of the shift operator S and the definition $\mathbf{W}(A) = S^*\mathbf{C}(A)S$ imply $\|\mathbf{W}(A)\| = \|\mathbf{C}(A)\|$. We denote the first part of the coin operator in Equation (4.105) by T, that is,

$$T(A) = \int_\Omega \nu(d\omega) U_\omega^* A U_\omega \tag{4.107}$$

and hence

$$\mathbf{C}(A)(p) = T(A_0) + \widetilde{U}^*(A(p) - A_0)\widetilde{U}\,.$$

The Hilbert space $\mathcal{T}_{\mathcal{K},s}$ can be decomposed into a direct sum of two orthogonal subspaces $\mathcal{T}_0$ and $\mathcal{T}_0^\perp$ defined via

$$\begin{aligned} \mathcal{T}_0 &= \{A \in \mathcal{T}_{\mathcal{K},s} : A = A_0\} \\ \mathcal{T}_0^\perp &= \{A \in \mathcal{T}_{\mathcal{K},s} : A_0 = 0\}\,. \end{aligned} \tag{4.108}$$

Clearly, $\mathbf{C}(\mathcal{T}_0) \subset \mathcal{T}_0$ and $\mathbf{C}(\mathcal{T}_0^\perp) \subset \mathcal{T}_0^\perp$, from which it also follows that $\mathbf{W}(\mathcal{T}_0) \perp \mathbf{W}(\mathcal{T}_0^\perp)$. Consequently,

$$\|\mathbf{W}(A)\|^2 = \|T(A_0)\|^2 + \left\|\widetilde{U}^*(A(p) - A_0)\widetilde{U}\right\|^2\,,$$

and $\mathbf{W}$ is strictly contractive iff $\|T(A)\| < \|A\|$ and $\left\|\widetilde{U}^* B \widetilde{U}\right\| < \|B\|$ for all non-zero $A \in \mathcal{T}_0$, $B \in \mathcal{T}_0^\perp$ and $A \perp \mathbb{1}$.

We start with the first inequality and assume $\|T(A)\| = \|A\|$ for non-zero $A \in \mathcal{T}_0$ and $A \perp \mathbb{1}$. This means

$$\int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')\mathrm{tr}_\mathcal{K} U_{\omega'}^* A^* U_{\omega'} U_\omega^* A U_\omega = \mathrm{tr}_\mathcal{K} A^* A\,,$$

where we identified $A \in \mathcal{T}_0$ with its Fourier transform $A(p) \in \mathcal{B}(\mathcal{K})$. On the other hand, we can estimate

$$\begin{aligned} \|T(A)\|^2 &= \frac{1}{\dim\mathcal{K}} \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')\mathrm{tr}_\mathcal{K} U_{\omega'}^* A^* U_{\omega'} U_\omega^* A U_\omega \\ &\leq \frac{1}{\dim\mathcal{K}} \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')|\mathrm{tr}_\mathcal{K} U_{\omega'}^* A^* U_{\omega'} U_\omega^* A U_\omega| \\ &= \frac{1}{\dim\mathcal{K}} \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')|\mathrm{tr}_\mathcal{K} A^*(U_\omega U_{\omega'}^*)^* A U_\omega U_{\omega'}^*| \\ &\leq \frac{1}{\dim\mathcal{K}} \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')\sqrt{\mathrm{tr}_\mathcal{K} A^* A}\sqrt{\mathrm{tr}_\mathcal{K} A^* A} \\ &= \frac{1}{\dim\mathcal{K}} \mathrm{tr}_\mathcal{K} A^* A\,, \end{aligned} \tag{4.109}$$

where we used the Cauchy-Schwarz inequality and unitarity of the U_ω in the fourth step. It follows from $\|T(A)\| = \|A\|$ that this inequality is actually an equality, hence, we must have

$$|\mathrm{tr}_{\mathcal{K}} A^*(U_\omega U_{\omega'}^*)^* A U_\omega U_{\omega'}^*| = \mathrm{tr}_{\mathcal{K}} A^* A\,,$$

which, by the Cauchy-Schwarz inequality, means that A and $(U_\omega U_{\omega'}^*)^* A U_\omega U_{\omega'}^*$ must be equal up to a phase factor for arbitrary ω and ω'. Thus, $(U_\omega U_{\omega'}^*)^* A U_\omega U_{\omega'}^* = c_{\omega,\omega'} \cdot A$ with $|c_{\omega,\omega'}| = 1$ and

$$\begin{aligned} \|T(A)\|^2 &= \frac{1}{\dim \mathcal{K}} \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega')\mathrm{tr}_{\mathcal{K}} U_{\omega'}^* A^* U_{\omega'} U_\omega^* A U_\omega \\ &= \frac{1}{\dim \mathcal{K}} \mathrm{tr}_{\mathcal{K}} A^* A \int_\Omega \int_\Omega \nu(d\omega)\nu(d\omega') c_{\omega,\omega'}\,. \end{aligned}$$

The assumption $\|T(A)\| = \|A\|$ entails $c_{\omega,\omega'} = 1$ for all ω, ω'. Thus, A commutes with $U_\omega U_{\omega'}^*$ and since those are irreducible it follows that $A = a \cdot \mathbb{1}$. This contradicts the assumption $A \perp \mathbb{1}$, hence, $\|T(A)\| < \|A\|$.

For the second part we first note that

$$\left\|\widetilde{U}^* B \widetilde{U}\right\|^2 = \frac{1}{\dim \mathcal{K} (2\pi)^s} \int_{[-\pi,\pi)^s} d^s p\, \mathrm{tr}_{\mathcal{K}} \widetilde{U}^* B^*(p) \widetilde{U} \widetilde{U}^* B(p) \widetilde{U}\,,$$

where the integrand is clearly positive. Now, let X and Y be positive operators on $\mathcal{K}$, then we have

$$\mathrm{tr}_{\mathcal{K}} XY \leq \|X\|_{op} \cdot \mathrm{tr}_{\mathcal{K}} Y\,,$$

and hence, by applying this inequality to the integral above, we get

$$\begin{aligned} \mathrm{tr}_{\mathcal{K}} \widetilde{U}^* B^*(p) \widetilde{U} \widetilde{U}^* B(p) \widetilde{U} &= \mathrm{tr}_{\mathcal{K}} \widetilde{U} \widetilde{U}^* B^*(p) \widetilde{U} \widetilde{U}^* B(p) \\ &\leq \left\|\widetilde{U}\widetilde{U}^*\right\|_{op} \cdot \mathrm{tr}_{\mathcal{K}} B^*(p) \widetilde{U} \widetilde{U}^* B(p) \\ &\leq \left\|\widetilde{U}\widetilde{U}^*\right\|_{op}^2 \cdot \mathrm{tr}_{\mathcal{K}} B(p) B^*(p) \\ &\leq \left\|\widetilde{U}\right\|_{op}^4 \cdot \mathrm{tr}_{\mathcal{K}} B(p) B^*(p). \end{aligned} \tag{4.110}$$

It follows from the singular value decomposition of $\widetilde{U}$ that there exist normalized vectors $\phi, \psi \in \mathcal{K}$ such that

$$\left\|\widetilde{U}\right\|_{op} = \langle \phi | \widetilde{U} \psi \rangle = \int_\Omega \nu(d\omega) \langle \phi | U_\omega \psi \rangle\,, \tag{4.111}$$

and hence, if $\left\|\widetilde{U}\right\|_{op} = 1$, we must have $\langle \phi | U_\omega \psi \rangle = 1$ for all ω since U_ω is unitary. This implies $\langle \psi | U_{\omega'}^* U_\omega \psi \rangle = 1$, thus, ψ is an eigenvector of $U_{\omega'}^* U_\omega$ for arbitrary ω

and ω', which is forbidden since the set $\{U^*_{\omega'}U_\omega : \omega,\omega' \in \Omega\}$ is assumed to be irreducible. Consequently, $\left\|\widetilde{U}^* B \widetilde{U}\right\| < \|B\|$ for all non-zero $B \in \mathcal{T}_0^\perp$. □

In the coming sections we rigorously analyze the asymptotic behavior of quantum walks **W** according to Equations (4.99), (4.101) and (4.102). We will see that the ballistic and diffusive scaling of the position distribution in the asymptotic limit is determined by the first and second order of the power series expansion

$$\mu_\varepsilon = 1 + \varepsilon\mu' + \varepsilon^2/2\mu'' + \ldots$$

of the eigenvalue μ_ε of $\mathbf{W}_\varepsilon$ corresponding to the unperturbed eigenvalue 1 of **W**. And indeed, our analysis will show that

$$C(\lambda) = \lim_{t\to\infty} \operatorname{tr} \rho_0 \mathbf{W}_\varepsilon^t(\mathbb{1}) = \lim_{t\to\infty} \mu_\varepsilon^t . \tag{4.112}$$

Hence, in ballistic scaling, i.e. $\varepsilon = 1/t$, we obtain the asymptotic limit of the characteristic function

$$C(\lambda) = \lim_{t\to\infty} \mu_{1/t}^t = \lim_{t\to\infty} \left(1 + \frac{\mu'}{t} + \ldots\right)^t = e^{\mu'} . \tag{4.113}$$

If, however, the first order is zero, that is $\mu' = 0$, we may consider the diffusive scaling $\varepsilon = 1/\sqrt{t}$ of the position distribution and get

$$C(\lambda) = \lim_{t\to\infty} \mu_{1/\sqrt{t}}^t = \lim_{t\to\infty} \left(1 + \frac{\mu''}{2t} + \ldots\right)^t = e^{\frac{\mu''}{2}} . \tag{4.114}$$

At this point, we already encounter one of the differences to decoherent quantum walks without momentum transfer as considered in Section 4.5.2:

Remark 4.6.5. *In contrast to quantum walks without momentum transfer as considered in Section 4.5.2, where for some models a dependence on the initial state ρ_0 was observed, we see that for quantum walks with momentum transfer according to the model considered in this section the initial state ρ_0 is irrelevant for the asymptotic position distribution.*

Non-degenerate analytic perturbation theory

Our goal is to apply non-degenerate perturbation theory to the operator $\mathbf{W}_\varepsilon$. In particular, the aim is to determine the first and second order equations of the perturbation theory in ε. The correctness of the results obtained by equating coefficients of powers of ε is in fact non-trivial since $\mathbf{W}_\varepsilon$ is defined on an infinite dimensional Hilbert space $\mathcal{T}_{\mathcal{K},s}$. Hence, we first have to establish analyticity of $\mathbf{W}_\varepsilon$, the eigenvector A_ε, and the corresponding eigenvalue μ_ε, which obey $A_\varepsilon \to \mathbb{1}$ and $\mu_\varepsilon \to 1$ as $\varepsilon \to 0$. To this end we use the following adaption of Theorem 3.4.5 from Section 3.4.

Theorem 4.6.6. *Assume that the operator* $\mathbf{W}_\varepsilon$ *is bounded on* $\mathcal{T}_{\mathcal{K},s}$ *and the limit of the difference quotient*

$$\lim_{\Delta\to 0}\frac{\mathbf{W}_{\varepsilon+\Delta}-\mathbf{W}_\varepsilon}{\Delta},$$

which we then call the derivative of $\mathbf{W}_\varepsilon$ *at* ε*, exists in operator norm for all* ε *in an open subset of* $\mathbb{C}$ *containing the origin. If the eigenvalue* 1 *of the unperturbed operator* $\mathbf{W}=\mathbf{W}_0$*, corresponding to* $\mathbf{W}(\mathbb{1})=\mathbb{1}$*, is isolated and non-degenerate, then, for small enough* ε*, there exists an analytic eigenvector* A_ε *with analytic and non-degenerate eigenvalue* μ_ε *such that* $A_\varepsilon\to\mathbb{1}$ *and* $\mu_\varepsilon\to 1$ *as* $\varepsilon\to 0$*.*

Now, we are left to prove that $\mathbf{W}_\varepsilon$ is bounded, differentiable and the eigenvalue 1 of $\mathbf{W}$ is isolated and non-degenerate. The following proposition in conjunction with Theorem 4.6.6 assures the analyticity and non-degeneracy of the perturbation theory of $\mathbf{W}_\varepsilon$.

Proposition 4.6.7. *Let* $\mathbf{W}$ *be a quantum walk according to Equations* (4.99), (4.101) *and* (4.102) *such that Assumption 4.3 is satisfied for some* $n\in\mathbb{N}$*. Then we have the following conclusions:*

i) The derivative of $\mathbf{W}_\varepsilon$ *exists in operator norm for all* $\varepsilon\in\mathbb{C}$*.*

ii) The operator $\mathbf{W}_\varepsilon$ *is bounded with* $\|\mathbf{W}_\varepsilon\|_{op}\leq\max_i|e^{\mathrm{i}\varepsilon\lambda\cdot v_i}|$ *for all* $\varepsilon\in\mathbb{C}$*.*

iii) The eigenvalue 1 *of* $\mathbf{W}$ *is isolated and non-degenerate.*

Proof. To prove statement *i)* we use the shift vectors x_i in Equation (4.99) to define the diagonal matrix

$$\Lambda=\begin{pmatrix}\lambda\cdot x_1 & 0 & \dots\\ 0 & \ddots & \\ \vdots & & \lambda\cdot x_{\dim\mathcal{K}}\end{pmatrix}.$$

It is straightforward to check that the operator $\mathbf{W}'_\varepsilon$, defined via its Fourier transform

$$\mathbf{W}'_\varepsilon(A)(p)=\mathbf{W}_\varepsilon(A)(p)\cdot\mathrm{i}\Lambda,$$

is indeed the operator norm limit of the difference quotient

$$\lim_{\Delta\to 0}\frac{\mathbf{W}_{\varepsilon+\Delta}-\mathbf{W}_\varepsilon}{\Delta}.$$

By Equation (4.103) we have $S(p+\varepsilon\lambda)=S(p)\cdot S(\varepsilon\lambda)$, which implies

$$\begin{aligned}\langle\mathbf{W}_\varepsilon(A)|\mathbf{W}_\varepsilon(A)\rangle &= \langle\mathbf{W}(A)|\mathbf{W}(A)S(\varepsilon\lambda)S^*(\varepsilon\lambda)\rangle\\ &\leq \max_i|e^{\mathrm{i}\varepsilon\lambda\cdot x_i}|^2\langle\mathbf{W}(A)|\mathbf{W}(A)\rangle,\end{aligned}$$

and therefore $\|\mathbf{W}_\varepsilon\|_{op} \leq \max_i |e^{i\varepsilon\lambda\cdot x_i}| \|\mathbf{W}\|_{op}$. Now, *ii)* follows from $\|\mathbf{W}\|_{op} = 1$, which we prove next.

By writing $\mathbf{W}(A) = S^*\mathbf{C}(A)S$ and observing that S is unitary we get $\|\mathbf{W}(A)\| = \|\mathbf{C}(A)\|$, and hence $\|\mathbf{W}\|_{op} = \|\mathbf{C}\|_{op}$. In a similar manner to the proof of Proposition 4.6.4 we decompose the coin operator $\mathbf{C}(A)(p) = T(A_0) + \widetilde{U}^*(A(p) - A_0)\widetilde{U}$ into T according to Equation (4.107) and conjugation by $\widetilde{U}$. We write $\mathcal{T}_{\mathcal{K},s} = \mathcal{T}_0 \oplus \mathcal{T}_0^\perp$, with the subspace $\mathcal{T}_0$ as in Equation (4.108), and note $\mathbf{C}(\mathcal{T}_0) \subset \mathcal{T}_0$ and $\mathbf{C}(\mathcal{T}_0^\perp) \subset \mathcal{T}_0^\perp$. Hence,

$$\|\mathbf{W}\|_{op} = \|\mathbf{C}\|_{op} = \max\{\|T\|_{op}, \left\|\widetilde{U}^*.\widetilde{U}\right\|_{op}\},$$

where we consider T and $\widetilde{U}^*.\widetilde{U}$ as map on $\mathcal{T}_0$ and $\mathcal{T}_0^\perp$, respectively. First, let us note that according to Inequality (4.109) we have $\|T(A)\| \leq \|A\|$, in other words, $\|T\|_{op} \leq 1$. Moreover, since $\left\|\widetilde{U}\right\|_{op} \leq 1$ by Equation (4.111), Inequality (4.110) implies $\left\|\widetilde{U}^*.\widetilde{U}\right\| \leq 1$. This finally proves $\|\mathbf{C}\|_{op} \leq 1$ and therefore statement *ii)*.

Any eigenvector of $\mathbf{W}$ is also an eigenvector of $\mathbf{W}^n$ with eigenvalue raised to the n-th power, hence, the contractivity of $\mathbf{W}^n$ yields statement *iii)*. □

Now we are ready to approach the problem of computing the asymptotic limit of the finite time steps characteristic function in ε-scaling. As a consequence of the bound $\|\mathbf{W}_\varepsilon\|_{op} \leq 1$, which is valid for $\varepsilon \in \mathbb{R}$, we obtain the estimate

$$\begin{aligned} \left\|\mathbf{W}_\varepsilon^t(\mathbb{1}) - \mu_\varepsilon^t A_\varepsilon\right\| &= \left\|\mathbf{W}_\varepsilon^t(\mathbb{1} - A_\varepsilon)\right\| \\ &\leq \|\mathbb{1} - A_\varepsilon\|. \end{aligned} \tag{4.115}$$

Once again writing the asymptotic characteristic function in momentum space we obtain the expression

$$\begin{aligned} C(\lambda) &= \lim_{t\to\infty} \operatorname{tr} \rho_0 \mathbf{W}_\varepsilon^t(\mathbb{1}) \\ &= \lim_{t\to\infty} \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \operatorname{tr}_{\mathcal{K}} \rho_0(p) \mathbf{W}_\varepsilon^t(\mathbb{1})(p) \\ &= \lim_{t\to\infty} \langle \Xi | \mathbf{W}_\varepsilon^t(\mathbb{1}) \rangle, \end{aligned} \tag{4.116}$$

where $\Xi \in \mathcal{T}_{\mathcal{K},s}$ denotes the translationally invariant bounded operator defined by ρ_0 and Lemma 3.2.6. With the estimate (4.115) we conclude that

$$\begin{aligned} C(\lambda) &= \lim_{t\to\infty} \mu_\varepsilon^t \langle \Xi | A_\varepsilon \rangle \\ &= \lim_{t\to\infty} \mu_\varepsilon^t \langle \Xi | \mathbb{1} \rangle \\ &= \lim_{t\to\infty} \mu_\varepsilon^t. \end{aligned} \tag{4.117}$$

Asymptotic position distribution via first and second order perturbation theory

Now we have all necessary tools to compute the asymptotic position distribution of quantum walks $\mathbf{W}$ with fluctuating coin operators. The first order correction μ' can be determined from the first order relation obtained from equating coefficients in $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$, which reads

$$\mathbf{W}'(\mathbb{1}) + \mathbf{W}(A') = \mu' \mathbb{1} + A', \tag{4.118}$$

where $\mathbf{W}'$ denotes the derivative of $\mathbf{W}_\varepsilon$ at $\varepsilon = 0$. The solution to the eigenvector problem $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$ is in general not unique. A common choice for A_ε is to fix the scalar product of the perturbed eigenvector with the unperturbed eigenvector in the following way

$$\langle \mathbb{1} | A_\varepsilon \rangle = 1 \quad \Leftrightarrow \quad \langle \mathbb{1} | A^{(n)} \rangle = 0 \quad \forall\, n \in \mathbb{N},$$

where $A^{(n)}$ denotes the n-th order correction of the eigenvalue A_ε. That is, A_ε can be expressed as

$$A_\varepsilon = \sum_{n=0}^{\infty} A^{(n)} \frac{\varepsilon^n}{n!}.$$

Fixing the scalar product in this way does not impair the analyticity of A_ε, at least for small enough ε, since the scalar product of an unnormalized vector with $\mathbb{1}$ is an analytic function in ε which is non-zero for small ε.

The standard approach to determine the higher order corrections to the unperturbed eigenvalue 1 is to expand the equation $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$ into a power series in ε and then take the scalar product with the unperturbed eigenvector $\mathbb{1}$. The choice $\langle \mathbb{1} | A_\varepsilon \rangle = 1$, which is equivalent to $\langle \mathbb{1} | A^{(n)} \rangle = 0$, implies

$$\langle \mathbb{1} | \mathbf{W}(A^{(n)}) \rangle = \langle \mathbb{1} | \mathbf{C}(A^{(n)}) \rangle = \langle \mathbf{C}(\mathbb{1}) | \mathbf{C}(A^{(n)}) \rangle = 0, \quad \forall\, n > 0.$$

Consequently, some terms in the power series expansion of the eigenvector equation already vanish when taking the scalar product with $\mathbb{1}$.

By Equation (4.103) and $\mathbf{W}_\varepsilon(A)(p) = S(p)^* \mathbf{C}(A)(p) S(p + \varepsilon\lambda)$ we can express the derivative of $\mathbf{W}_\varepsilon$ at $\varepsilon = 0$ as

$$\mathbf{W}'(A)(p) = \mathbf{W}(A)(p) \cdot \mathrm{i}\Lambda, \quad \Lambda = \begin{pmatrix} x_1 \cdot \lambda & 0 & \dots \\ 0 & \ddots & \\ \vdots & & x_{\dim \mathcal{K}} \cdot \lambda \end{pmatrix},$$

which leads to the following expression for the first order correction to the eigen-

value

$$\begin{aligned}\mu' &= \langle \mathbb{1}|\mathbf{W}'(\mathbb{1})\rangle = \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\, \frac{1}{\dim \mathcal{K}} \mathrm{tr}_{\mathcal{K}} \mathbf{W}'(\mathbb{1}) \\ &= \frac{1}{\dim \mathcal{K}} \sum_k \mathrm{i}\lambda \cdot x_k = \mathrm{i}\lambda \cdot v\,,\end{aligned} \tag{4.119}$$

where v is the average of all shift vectors x_i. The vector v is closely related to the index $\mathrm{ind}\, S$ of the unitary shift operator S, see Definition 4.5.3. By definition we have

$$\mathrm{ind}\, S = \sum_k x_k \tag{4.120}$$

and consequently $v = (\dim \mathcal{K})^{-1} \mathrm{ind}\, S$. Clearly, the characteristic function in ballistic scaling is given by $C(\lambda) = e^{\mathrm{i}\lambda \cdot v}$, which is the characteristic function of a point measure at position v. This represents a constant drift of the particle in the direction of $\mathrm{ind}\, S$.

Remark 4.6.8. *If* $\mathrm{ind}\, S \neq 0$ *we may subtract the constant drift according to* $\mu' = \mathrm{i}\lambda \cdot v$ *from the position variable and consider the asymptotic distribution of* $\widetilde{Q} = Q - v \cdot t$. *The characteristic function is given by*

$$C_{t,\varepsilon}(\lambda) = \mathrm{tr}\, \rho_0 \mathbf{W}^t(e^{\mathrm{i}\varepsilon\lambda\cdot\widetilde{Q}}) = \mathrm{tr}\, \rho_0 e^{-\mathrm{i}\varepsilon t\lambda\cdot v} \mathbf{W}^t(e^{\mathrm{i}\varepsilon\lambda\cdot Q}),$$

and hence we have to consider the modified operator

$$\widetilde{\mathbf{W}}_\varepsilon(A) = e^{-\mathrm{i}\varepsilon\lambda\cdot v}\mathbf{W}(Ae^{\mathrm{i}\varepsilon\lambda\cdot Q})e^{-\mathrm{i}\varepsilon\lambda\cdot Q} = e^{-\mathrm{i}\varepsilon\lambda\cdot v}\mathbf{W}_\varepsilon(A).$$

The eigenvalue $\tilde{\mu}_\varepsilon$ *is now just given by* $\tilde{\mu}_\varepsilon = e^{-\mathrm{i}\varepsilon\lambda\cdot v}\mu_\varepsilon$, *thus*

$$\begin{aligned}\tilde{\mu}_\varepsilon &= \left(1 - \mu'\varepsilon + \frac{\mu'^2}{2}\varepsilon^2 + \ldots\right)\left(1 + \mu'\varepsilon + \frac{\mu''}{2}\varepsilon^2 + \ldots\right) \\ &= 1 + \frac{\mu'' - \mu'^2}{2}\varepsilon^2 + \ldots,\end{aligned}$$

which shows that $\tilde{\mu}' = 0$.

Hence we assume in the following that $\mu' = 0$ and look at the diffusive scaling of the position distribution. To this end we need to determine the second order of the equation $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$, which reads

$$\mathbf{W}''(\mathbb{1}) + 2\mathbf{W}'(A') + \mathbf{W}(A'') = \mu''\mathbb{1} + 2\mu' A' + A''. \tag{4.121}$$

The second order derivative of the walk operator amounts to $\mathbf{W}''(A)(p) = \mathbf{W}'(A)(p) \cdot \mathrm{i}\Lambda = -\mathbf{W}(A)(p) \cdot \Lambda^2$. Again, by taking the scalar product with the unperturbed eigenvector $\mathbb{1}$ we get

$$\begin{aligned}
\mu'' &= \langle \mathbb{1} | \mathbf{W}''(\mathbb{1}) \rangle + 2\langle \mathbb{1} | \mathbf{W}'(A') \rangle \qquad (4.122)\\
&= \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \, \frac{1}{\dim \mathcal{K}} \mathrm{tr}_{\mathcal{K}} \left(\mathbf{W}''(\mathbb{1}) + 2\mathrm{i}\mathbf{W}(A')(p) \cdot \Lambda \right) \\
&= \frac{1}{\dim \mathcal{K}} \sum_i -(\lambda \cdot x_i)^2 + \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \, \frac{2\mathrm{i}}{\dim \mathcal{K}} \mathrm{tr}_{\mathcal{K}} \left(-\mathbf{W}'(\mathbb{1}) + A'(p) \right) \cdot \Lambda \\
&= \frac{1}{\dim \mathcal{K}} \sum_i (\lambda \cdot x_i)^2 + \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \, \frac{2\mathrm{i}}{\dim \mathcal{K}} \mathrm{tr}_{\mathcal{K}} A'(p) \cdot \Lambda,
\end{aligned}$$

where we have used Equation (4.118) at the fourth step and $\mathbf{W}'(A)(p) = \mathbf{W}(A)(p) \cdot \mathrm{i}\Lambda$ in every step. Next, we use Equation (4.118) to eliminate A' in this equation. Using $\mu' = 0$ and $\mathbf{W}'(\mathbb{1})(p) = \mathrm{i}\Lambda$ we get

$$\mathbf{W}(A')(p) - A'(p) = -\mathrm{i}\Lambda$$

and from $\mu' = 0$, which is equivalent to $\mathrm{tr}_{\mathcal{K}} \Lambda = 0$, it follows that $\langle \mathbb{1} | \Lambda \rangle = 0$. Since the eigenvalue 1 of $\mathbf{W}$ is non-degenerate we can invert $\mathbf{W} - \mathrm{id}$ on $\{\mathbb{1}\}^\perp$ and apply it to $\Lambda \in \{\mathbb{1}\}^\perp$. Denoting the pseudo-inverse by $(\mathbf{W} - \mathrm{id})^{-1}$ we get the following expression for A':

$$A'(p) = -\mathrm{i}(\mathbf{W} - \mathrm{id})^{-1}(\Lambda)(p). \qquad (4.123)$$

Hence, the second order correction μ'' can be written as

$$\mu'' = \frac{1}{\dim \mathcal{K}} \sum_i (\lambda \cdot x_i)^2 + \frac{2}{\dim \mathcal{K}} \frac{1}{(2\pi)^s} \int_{[-\pi,\pi)^s} d^s p \, \mathrm{tr}_{\mathcal{K}} (\mathbf{W} - \mathrm{id})^{-1}(\Lambda)(p) \cdot \Lambda. \qquad (4.124)$$

Note that the dependence of Λ on the variable λ makes μ'' a quadratic form in λ which defines a symmetric matrix D via $\mu'' = -\lambda^T \cdot D \cdot \lambda$. It is easy to see that the position distribution corresponding to the characteristic function $C(\lambda) = e^{\frac{\mu''}{2}}$ is a Gaussian with covariance matrix D.

The following theorem summarizes the results of this section.

Theorem 4.6.9. *Let* $\mathbf{W}$ *be a quantum walk as defined in Equations* (4.99), (4.101) *and* (4.102) *such that Assumption 4.3 is satisfied, i.e.* $\mathbf{W}$ *is strictly* n*-contractive for some* $n \in \mathbb{N}$*. Then:*

i) Ballistic scaling: The random variable Q/t *converges in distribution to a point measure at* $v = \frac{1}{\dim \mathcal{K}} \mathrm{ind}\, S$.

ii) Diffusive scaling: If $v = 0$ the random variable $Q/\sqrt{t}$ converges in distribution to a Gaussian with covariance matrix D. The defining equation for D is $\mu'' = -\lambda^T \cdot D \cdot \lambda$ with μ'' from Equation (4.124)*. Explicitly, the matrix elements of D are given by the formula*

$$D_{\alpha\beta} = \frac{1}{\dim \mathcal{K}} \left(\sum_i x_{i,\alpha} x_{i,\beta} + \frac{2}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, \mathrm{tr}_{\mathcal{K}} R_{\alpha\beta}(p) \right), \quad \alpha,\beta = 1,\ldots,s, \tag{4.125}$$

where $x_{i,\alpha}$ denotes the α component of the vector x_i and $R_{\alpha\beta}(p)$ is defined via

$$R_{\alpha\beta}(p) = \frac{1}{2}\Big((\mathbf{W} - \mathrm{id})^{-1}(\Lambda_\alpha)(p) \cdot \Lambda_\beta + (\mathbf{W} - \mathrm{id})^{-1}(\Lambda_\beta)(p) \cdot \Lambda_\alpha \Big). \tag{4.126}$$

The diagonal matrices Λ_α are given by $(\Lambda_\alpha)_{ij} = \delta_{ij} x_{i,\alpha}$.

Of course, for the asymptotic position distribution in diffusive scaling to be well-defined it is necessary that the covariance matrix D is positive. This is indeed the case, which we prove now.

Proposition 4.6.10. *Given the assumptions of Theorem 4.6.9 and $v = 0$ the covariance matrix D is positive, i.e., $-\mu'' \geq 0$ for all λ.*

Proof. The proof is similar to, though simpler than, the proof of the positivity of the covariance matrix for the models considered in Section 4.5.2. According to Equation (4.122) we have

$$\begin{aligned} -\mu'' &= -\langle \mathbb{1} | \mathbf{W}''(\mathbb{1}) \rangle - 2\langle \mathbb{1} | \mathbf{W}'(A') \rangle \\ &= \langle \Lambda | \Lambda \rangle + 2\langle \mathrm{i}\Lambda | \mathbf{W}(A') \rangle \\ &= \langle A' - \mathbf{W}(A') | A' - \mathbf{W}(A') \rangle + 2\langle A' - \mathbf{W}(A') | \mathbf{W}(A') \rangle \\ &= \langle A' | A' \rangle - \langle \mathbf{W}(A') | \mathbf{W}(A') \rangle, \end{aligned}$$

where we have used $\mathbf{W}'(A)(p) = \mathbf{W}(A)(p) \cdot \mathrm{i}\Lambda$, $\mathbf{W}''(A)(p) = -\mathbf{W}(A)(p) \cdot \Lambda^2$, $\mathrm{i}\Lambda = A'(p) - \mathbf{W}(A')(p)$ and the fact that A' and $\mathbf{W}(A')$ are skew-hermitian, which follows from Equation (4.123) and the fact that $\mathbf{W}(A)^* = \mathbf{W}(A^*)$ for arbitrary A. According to Proposition 4.6.7 we have $\|\mathbf{W}\|_{op} \leq 1$, which proves $-\mu'' \geq 0$. □

For practical applications it is usually sufficient to give a good approximation to the covariance matrix D. Such an approximation can be obtained by a power series expansion of the pseudo-inverse $(\mathbf{W} - \mathrm{id})^{-1}$. Indeed, if there exists $n \in \mathbb{N}$ such that $\|\mathbf{W}^n(A)\| < \|A\|$ for all $A \perp \mathbb{1}$ we have the following convergent power series expansion for the pseudo inverse.

$$(\mathbf{W} - \mathrm{id})^{-1} = -\sum_{k \in \mathbb{N}_0} \mathbf{W}^k \quad \text{on the subspace} \quad \{\mathbb{1}\}^\perp \tag{4.127}$$

This gives us the following corollary, which can be used to approximate the numbers $R_{\alpha\beta}$ and the covariance matrix D.

Corollary 4.6.11. *Given the assumptions of Theorem 4.6.9 and $v = 0$ we have the convergent power series expression*

$$R_{\alpha\beta}(p) = -\frac{1}{2}\sum_{k\in\mathbb{N}_0}\left(\mathbf{W}^k(\Lambda_\alpha)(p)\cdot\Lambda_\beta + \mathbf{W}^k(\Lambda_\beta)(p)\cdot\Lambda_\alpha\right). \tag{4.128}$$

Proof. Let $n\in\mathbb{N}$ be the smallest number such that $\mathbf{W}^n$ is strictly n-contractive on $\{\mathbb{1}\}^\perp$. The convergence of the Neumann series for $(\mathbf{W}-\mathrm{id})^{-1}$ can be seen from

$$-\sum_{k\in\mathbb{N}_0}\mathbf{W}^k = -\sum_{l=0}^{n-1}\sum_{r=0}^{\infty}\mathbf{W}^{l+r\cdot n}.$$

The assertion follows from $\langle\mathbb{1}|\Lambda\rangle = v = 0$. □

If the operator $\widetilde{U}$, which occurs in $\mathbf{C}$, vanishes, the equations for the diffusive scaling simplify considerably. In fact, we will see in the following interlude that the first order correction A' is determined by a finite dimensional p-independent system of equations.

Interlude 5: Coin operators with zero mean

We assume that the measure ν is such that $\widetilde{U} = \int \nu(d\omega)U_\omega = 0$. Thus $\mathbf{C}(A) = \mathbf{C}(A_0) = \int \nu(d\omega)U_\omega^* A_0 U_\omega$, where we again have abbreviated $(2\pi)^{-s}\int d^s p\, A(p) = A_0$. If the operator $\mathbf{W}^n$ is strictly contractive for some $n\in\mathbb{N}$, Theorem 4.6.9 is applicable and we can look at the second order correction μ'' in order to determine the diffusive scaling of the position distribution. Without loss of generality we assume $\mu' = 0$, see Remark 4.6.8, such that the first order of the eigenvalue problem reads $\mathbf{W}(A')(p) - A'(p) = -\mathrm{i}\Lambda$. Using $\mathbf{W}(A)(p) = S^*(p)\mathbf{C}(A_0)S(p)$, we get

$$S^*(p)\mathbf{C}(A_0')S(p) - A'(p) = -\mathrm{i}\Lambda$$

and since Λ commutes with $S(p)$, this is equivalent to

$$\mathbf{C}(A_0') + \mathrm{i}\Lambda = S(p)A'(p)S^*(p).$$

Now, since the left hand side of this equation is independent of p, so is the right hand side. Hence, the matrix elements of $A'(p)$ are given by

$$\langle i|A'(p)|j\rangle = \widetilde{a}_{ij}\, e^{\mathrm{i}(v_j - v_i)\cdot p}$$

with $\widetilde{a}_{ij} \in \mathbb{C}$. Let $\widetilde{A}'$ denote the matrix with entries $\widetilde{a}_{ij}$, in other words, $A'(p) = S^*(p)\widetilde{A}'S(p)$. Then, $\widetilde{A}'$ can be determined from the p-independent equation

$$\mathbf{C}(P(\widetilde{A}')) - \widetilde{A}' = -\mathrm{i}\Lambda\,,$$

where $P(\widetilde{A}')$ is defined as

$$\langle i|P(\widetilde{A}')|j\rangle = \begin{cases} \widetilde{a}_{ij} & , \quad \text{if } v_i = v_j \\ 0 & , \quad \text{if } v_i \neq v_j \end{cases} .$$

Thus it is straightforward to determine the first order correction A', and we can use Equation (4.122) to compute the second order correction μ'' which determines the asymptotic position distribution in diffusive scaling.

Finite time step approximations

The aim of this section is to link the higher orders in the perturbation theory of $\mathbf{W}_\varepsilon$ to a finer analysis of the position distribution of the quantum walk $\mathbf{W}$ for large but finite number of time steps. Analogously to the case of quantum walks without momentum transfer, our strategy is to obtain a power series expansion of the characteristic function $C_{t,\varepsilon}(\lambda) = \mathrm{tr}\,\rho_0 \mathbf{W}_\varepsilon^t(\mathbb{1}) e^{\mathrm{i}\varepsilon\lambda\cdot Q}$ in powers of $\varepsilon = t^{-1}$. We will again focus on the first order correction to the asymptotic position distribution in ballistic scaling. To begin with, let us write the characteristic function in momentum space

$$\begin{aligned} C_t(\lambda) &= \mathrm{tr}\,(e^{\mathrm{i}\lambda\cdot Q/t}\rho_0 \mathbf{W}_{1/t}^t(\mathbb{1})) \\ &= \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p\, \mathrm{tr}_{\mathcal{K}}\, \rho_0(p+\lambda/t, p)\mathbf{W}_{1/t}^t(\mathbb{1})(p). \end{aligned}$$

The operator valued function $p \to \rho_0(p+\lambda/t, p)$ defines a bounded translationally invariant operator, more precisely, we can identify this function with the operator $\Xi_{\lambda/t}$ defined via

$$\Xi_{\lambda/t} = \sum_{x\in\mathbb{Z}^s} \mathcal{T}_x \rho_0 e^{-\mathrm{i}\lambda\cdot Q/t} \mathcal{T}_x^* \tag{4.129}$$

and $\Xi_{\lambda/t} \in \mathcal{T}_{\mathcal{K},s}$, see Lemma 3.2.6. With the help of $\Xi_{\lambda/t}$ we obtain the following expression for the characteristic function in terms of the scalar product (3.12)

$$C_t(\lambda) = \dim\mathcal{K} \cdot \langle \Xi_{\lambda/t} | \mathbf{W}_{1/t}^t(\mathbb{1})\rangle\,. \tag{4.130}$$

Our next step is to use the analyticity of $\mathbf{W}_\varepsilon$ and A_ε with respect to this scalar product to derive a power series expansion of the characteristic function C_t based on the perturbation series for $\mathbf{W}_\varepsilon^t(\mathbb{1})$ with $\varepsilon = t^{-1}$. As we are only interested in the first order approximation of C_t we need to compute the power series for $\mathbf{W}_\varepsilon^t(\mathbb{1})$ to first order:

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = \mathbf{W}_\varepsilon^t(A_\varepsilon) + \mathbf{W}_\varepsilon^t(\mathbb{1} - A_\varepsilon) = \mu_\varepsilon^t A_\varepsilon - \varepsilon \mathbf{W}_0^t(A') + o(\varepsilon^2)$$

Using Assumption 4.3 and the convention $A' \perp \mathbb{1}$ again we see that $\mathbf{W}_0^t(A') = \mathcal{O}(t^{-k})$ for all $k \in \mathbb{N}$, thus $\mathbf{W}_{1/t}^t(\mathbb{1}) = \mu_{1/t}^t(\mathbb{1} + A'/t) + o(t^{-2})$. We can expand the eigenvalue $\mu_{1/t}^t$ as in Equation (4.83), which yields $\mu_{1/t}^t = e^{\mathrm{i}\lambda\cdot v - \frac{1}{2t}\lambda\cdot D\cdot\lambda} + o(t^{-2})$ with the deterministic velocity $v = (\dim \mathcal{K})^{-1}\mathrm{ind}\, S$ and the covariance matrix D. Inserting this into the equation for the characteristic function we obtain

$$\begin{aligned} C_t(\lambda) &= e^{\mathrm{i}\lambda\cdot v - \frac{1}{2t}\lambda\cdot D\cdot\lambda} \dim \mathcal{K} \cdot \left(\langle \Xi_{\lambda/t} | \mathbb{1} \rangle + \frac{1}{t} \langle \Xi_{\lambda/t} | A' \rangle \right) + o(t^{-2}) \\ &= e^{\mathrm{i}\lambda\cdot v - \frac{1}{2t}\lambda\cdot D\cdot\lambda} \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \left(\mathrm{tr}_{\mathcal{K}} \rho_0(p + \lambda/t, p) + \right. \\ &+ \left. \frac{1}{t} \mathrm{tr}_{\mathcal{K}} \rho_0(p + \lambda/t, p) A'(p) \right) + o(t^{-2}). \end{aligned}$$

This result is similar to the one we obtained for decoherent quantum walks without momentum transfer. Again we get two terms, of which the first is the distribution of the sum of two independent random variables, a Gaussian centered at v with decreasing variance and a scaled down version of the initial position distribution. In contrast to the case without momentum transfer this is no longer averaged over momentum such that this is really the characteristic function of the sum of two independent random variables. Again, the second term involving A' allows not for such a simple interpretation.

Degenerate perturbation theory

If the eigenvalue $\mu_0(0) = 1$ is finitely-degenerate we may translate some of the statements on degenerate perturbation theory from Section 4.5.2 directly to the setting considered here. This is because, as described in Section 3.4, we can reduce this problem then to the finite dimensional eigenspace defined by μ_0, which stays finite dimensional under perturbation by ε, and a large portion of the results from finite dimensional perturbation theory apply readily. However, it is easy to devise examples[4] where the degenerate eigenspace is infinite dimensional and even if this is not the case there are several subtle points left: In order to prove the convergence $\mathbf{W}_\varepsilon^t(\mathbb{1}) \to \mu_\varepsilon^t \mathbb{1}$ we used that $\mathbf{W}_\varepsilon^t(\mathbb{1} - A_\varepsilon) \to 0$, which is a consequence of the strict

[4] Consider e.g. the case where the operator $\widetilde{U}$ defined above has an eigenvalue of modulus one.

contractivity of a power $\mathbf{W}_0^n$ on the subspace$\{\mathbb{1}\}^\perp$. Hence, this convergence may crucially depend on the choice of basis in the degenerate subspace or, even worse, it may be false. Another problem related to this point is that Corollary 4.6.11 may have no appropriate analogue and we lack for a way to efficiently approximate the asymptotic position distribution.

Generalizations

The quantum walk model introduced earlier in this section, see Equations (4.99), (4.101) and (4.102), relies strongly on a particular decomposition into a single shift and coin operator. A way to characterize quantum walks more abstractly is to define them to be discrete time evolutions on a lattice $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$, which are local and translationally invariant, see Section 4.2. This definition is clearly satisfied if several quantum walks $\mathbf{W}_i$ are concatenated and considered as a single time step $\mathbf{W}$ given by

$$\mathbf{W} = \mathbf{W}_n \circ \ldots \circ \mathbf{W}_1 \,. \tag{4.131}$$

In this section, we aim for an extension of our analysis to such a more general class of quantum walks with momentum transfer. More precisely, we assume that each $\mathbf{W}_i$ is a quantum walk according to Equation (4.101), which means it can be written as

$$\mathbf{W}_i(A) = S_i^* \mathbf{C}_i(A) S_i \,,$$

where $\mathbf{C}_i$ denotes a, possibly decoherent, coin operator and S_i is a unitary state-dependent shift operator. For this generalized model of quantum walks we have the following proposition, which also covers the extremal case where several unitary quantum walks are concatenated with one decoherent quantum walk.

Proposition 4.6.12. *Let* $\mathbf{W}$ *be a generalized quantum walk according to Equation* (4.131)*. If at least one* $\mathbf{W}_i$ *is strictly* 1*-contractive on* $\{\mathbb{1}\}^\perp$ *we can apply perturbation theory to the eigenvector equation* $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$ *to determine the asymptotic position distribution of* $\mathbf{W}$*. In particular, let* $\operatorname{ind} S_i$ *denote the index of* S_i *according to Equation* (4.120)*, the asymptotic position distribution of* $\mathbf{W}$ *in ballistic scaling is given by a point measure at* $(\dim \mathcal{K})^{-1} \sum_{i=1}^n \operatorname{ind} S_i$*.*

Proof. Clearly, $\mathbf{W}$ satisfies $\mathbf{W}(\mathbb{1}) = \mathbb{1}$ and since $\mathbf{W}$ maps $\mathbb{1}$ and $\{\mathbb{1}\}^\perp$ to orthogonal subspaces it follows that $\mathbf{W}$ is strictly 1-contractive on $\{\mathbb{1}\}^\perp$ if at least one of the $\mathbf{W}_i$ is strictly 1-contractive on $\{\mathbb{1}\}^\perp$. Hence, the non-degeneracy of the eigenvalue 1 of $\mathbf{W}$ is assured.

The proof of the analyticity of $\mathbf{W}_\varepsilon$ is similar to the case in Proposition 4.6.7, hence, $\mathbf{W}_\varepsilon$ satisfies the requirements of Theorem 4.6.6. This implies that the asymptotic behavior of $\mathbf{W}$ can be determined using our perturbation method.

The first order of the power series expansion of $\mathbf{W}_\varepsilon(A_\varepsilon) = \mu_\varepsilon A_\varepsilon$ reads

$$\mathbf{W}_n' \circ \ldots \circ \mathbf{W}_1(\mathbb{1}) + \ldots + \mathbf{W}_n \circ \ldots \circ \mathbf{W}_1'(\mathbb{1}) = \mu' \mathbb{1} + A' - \mathbf{W}(A')$$

and since $\mathbf{W}_i(\mathbb{1}) = \mathbb{1}$ and $\mathbf{W}_i'(A)(p) = \mathbf{W}_i(A)(p) \cdot \mathrm{i}\Lambda_i$, with

$$\Lambda_i = \begin{pmatrix} x_{i,1} \cdot \lambda & 0 & \dots \\ 0 & \ddots & \\ \vdots & & x_{i,\dim\mathcal{K}} \cdot \lambda \end{pmatrix},$$

this simplifies to

$$\mathrm{i}\Lambda_n + \mathrm{i}\sum_{i=1}^{n-2} \mathbf{W}_n \circ \ldots \circ \mathbf{W}_{n-i}(\Lambda_{n-i-1})(p) = \mu' \mathbb{1} + A'(p) - \mathbf{W}(A')(p).$$

The scalar product of this equation with the unperturbed eigenvector $\mathbb{1}$ yields again

$$\mu' = \frac{\mathrm{i}}{\dim\mathcal{K}} \sum_{i=1}^{n} \mathrm{tr}_{\mathcal{K}}(\Lambda_i) = \lambda \cdot \frac{\mathrm{i}}{\dim\mathcal{K}} \sum_{i=1}^{n} \mathrm{ind}\, S_i\,.$$

□

The diffusive scaling of $\mathbf{W}$ can also be determined by equating coefficients of the perturbation expansion. Of course, the equations get more involved, but the general structure of the problem is the same. For example, the second order correction μ'' to the eigenvalue μ_ε is again a quadratic form in λ with constant coefficients and the asymptotic distribution in diffusive scaling is just a Gaussian independent of the initial state ρ_0.

4.6.3. Examples

In this section we provide two examples of decoherent quantum walks with momentum transfer. The first example is a modification of the well-known Hadamard walk. In our second example we analyze the propagation behavior of the model introduced in Interlude 2.

Example 5: Hadamard Walk with Dephasing

To begin with, let us define a family of quantum walks on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ which we denote by $W_\varphi = S \cdot (\mathbb{1} \otimes H_\varphi)$ with $\varphi \in [-\pi, \pi)$, and W_0 coincides with the usual Hadamard walk. We choose a basis $|\pm\rangle$ of $\mathbb{C}^2$ and define the shift operator via $S|x, \pm\rangle = |x \pm 1, \pm\rangle$. The operator H_φ accounts for an additional random relative phase shift between the states $|+\rangle$ and $|-\rangle$

$$H_\varphi = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{\mathrm{i}\varphi} & e^{\mathrm{i}\varphi} \\ e^{-\mathrm{i}\varphi} & -e^{-\mathrm{i}\varphi} \end{pmatrix}.$$

Note that, by introducing the Pauli operators σ_1, σ_2 and σ_3, we can write $H_\varphi = e^{\mathrm{i}\varphi\sigma_3} H$ with the Hadamard matrix $H = H_0$. This phase shift is assumed to happen independently and identically in time and space, in other words, the phase φ is chosen for each lattice site and in each time step according to a fixed probability measure ν on $[-\pi, \pi)$. In Fourier space we have the following expression for the Hadamard walk with dephasing:

$$\begin{aligned} \mathbf{W}(A)(p) &= S^*(p)\mathbf{C}(A)S(p) \\ \mathbf{C}(A) &= \int \nu(d\varphi) H e^{-\mathrm{i}\varphi\sigma_3} \cdot A_0 \cdot e^{\mathrm{i}\varphi\sigma_3} H + \widetilde{H}^*(A - A_0)\widetilde{H} \end{aligned} \tag{4.132}$$

Here, $\widetilde{H}$ denotes the operator $\widetilde{H} = \int \nu(d\varphi)\, e^{\mathrm{i}\varphi\sigma_3} H$. In the following we set $r_n = |\int \nu(d\varphi) e^{\mathrm{i}\varphi n}|$ and $\theta_n = \arg \int \nu(d\varphi) e^{\mathrm{i}\varphi n}$ and note that $\mathbf{C}$ only depends on r_n and θ_n for $n = 1, 2$ and not on the actual form of the distribution $\nu(d\varphi)$, see Equations (4.133) and (4.134).

It is easy to see that

$$H^*_{\varphi'} H_\varphi = H e^{\mathrm{i}(\varphi - \varphi')\sigma_3} H = e^{\mathrm{i}(\varphi - \varphi')\sigma_1} = \begin{pmatrix} \cos(\varphi - \varphi') & \mathrm{i}\sin(\varphi - \varphi') \\ \mathrm{i}\sin(\varphi - \varphi') & \cos(\varphi - \varphi') \end{pmatrix},$$

which shows that the set of matrices $\{H^*_{\varphi'} H_\varphi\}$ is reducible. Nonetheless, we can apply Theorem 4.6.9 after we proved that $\mathbf{W}^2$ is strictly contractive on $\{\mathbb{1}\}^\perp$.

Lemma 4.6.13. *Let* $\mathbf{W}$ *be according to Equation* (4.132) *and* ν *such that* $r_1, r_2 < 1$. *Then* $\mathbf{W}^2$ *is strictly contractive on* $\{\mathbb{1}\}^\perp$.

Proof. We write the coin operator as $\mathbf{C}(A) = T(A_0) + \widetilde{H}^*(A - A_0)\widetilde{H}$ and express the dephasing in the maps T and conjugation by $\widetilde{H}$ in the basis $\{\mathbb{1}, \sigma_1, \sigma_2, \sigma_3\}$ of Pauli operators. The dephasing in T corresponds to the matrix representation

$$A \mapsto \int \nu(d\varphi) e^{-\mathrm{i}\varphi\sigma_3} \cdot A \cdot e^{\mathrm{i}\varphi\sigma_3} \quad \longrightarrow \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & r_2\cos\theta_2 & -r_2\sin\theta_2 & 0 \\ 0 & r_2\sin\theta_2 & r_2\cos\theta_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.133}$$

and the dephasing in the conjugation by $\widetilde{H}$ has matrix representation

$$A \mapsto \int \nu(d\varphi) e^{-\mathrm{i}\varphi\sigma_3} \cdot A \cdot \int \nu(d\varphi') e^{\mathrm{i}\varphi'\sigma_3} \quad \longrightarrow \quad r_1^2 \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\theta_1 & -\sin 2\theta_1 & 0 \\ 0 & \sin 2\theta_1 & \cos 2\theta_1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{4.134}$$

Clearly, if $r_1 < 1$ the conjugation by $\widetilde{H}$ is strictly contractive. If $r_2 < 1$ we have that T is strictly contractive on the subspace spanned by σ_1 and σ_2. The operator σ_3 is

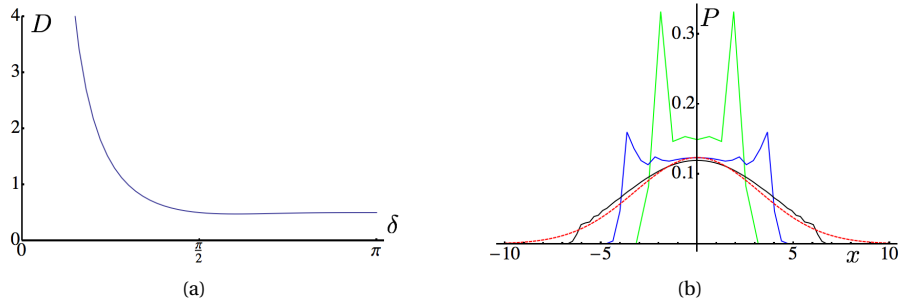


Figure 4.12.: (a) shows a plot of the diffusion constant D depending on the width δ of the interval I_δ from which the phase φ is chosen with uniform probability. For the plot shown in (b) we fixed $\delta = \pi/8$ and computed the position distribution after 10 (green), 30 (blue), and 80 (black) time steps with initial state $\rho_0 = 2^{-1}\mathbb{1}$. For better comparison with the asymptotic position distribution (red-dashed line) the average over two neighboring lattice sites was computed.

mapped to σ_1 by T, and hence, $S^*T(\sigma_3)S \in \mathcal{T}_0^\perp$, which proves $\left\|\mathbf{W}^2(A)\right\| < \|A\|$ for all $A \perp \mathbb{1}$. □

Since $\operatorname{ind} S = 0$, the ballistic scaling yields a point measure at the origin as asymptotic position distribution. For the asymptotic position distribution in diffusive scaling we need to solve the equation

$$\mathbf{W}(A')(p) - A'(p) = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix},$$

which we do by numeric approximation according to Corollary 4.6.11. For concreteness let us consider a family of measures ν_δ on $[-\pi,\pi)$, indexed by $\delta \in [0,\pi)$, and defined via

$$\nu_\delta(d\varphi) = \frac{1}{2\delta}\chi_{I_\delta}(\varphi)d\varphi\,.$$

Here, χ_{I_δ} denotes the characteristic function of the interval $I_\delta = [-\delta,\delta)$ and $d\varphi$ Lebesgue measure. The measures ν_δ represent uniform distributions of φ on I_δ and Figure 4.12 shows a plot of the diffusion constant and a comparison of the position distribution for a finite number of time steps with the asymptotic position distribution.

Example 6: An example revisited

We consider the example of a decoherent quantum walk on $\ell^2(\mathbb{Z})$ with momentum transfer constructed in Interlude 2. Its action on translationally invariant operators $A \in \mathcal{T}_{\mathcal{K},s}$ reads

$$\mathbf{W}(A)(p) = \frac{1}{2\pi} \int\limits_{[-\pi,\pi)} dq\, A(p+zq) \left(|v_{-1}(q)|^2 + |v_1(q)|^2 + 2\Re(e^{\mathrm{i}2(p-zq)} \overline{v_{-1}(q)} v_1(q)) \right)$$

and the modified operator $\mathbf{W}_\varepsilon$ acts like

$$\begin{aligned} \mathbf{W}_\varepsilon(A)(p) &= \frac{1}{2\pi} \int\limits_{[-\pi,\pi)} dq\, A(p+zq) \left(e^{-\mathrm{i}\varepsilon\lambda} |v_{-1}(q)|^2 + e^{\mathrm{i}\varepsilon\lambda} |v_1(q)|^2 \right) + \\ &+ \frac{1}{2\pi} \int\limits_{[-\pi,\pi)} dq\, A(p+zq) 2\Re(e^{\mathrm{i}\varepsilon\lambda} e^{\mathrm{i}2(p-zq)} \overline{v_{-1}(q)} v_1(q)). \end{aligned}$$

The operator $A = \mathbb{1}$ corresponds to the function $A(p) = 1$, which is easily seen to be an eigenvector of $\mathbf{W}_\varepsilon$ for all ε. Thus we can directly determine the limiting behavior of $\mathbf{W}_\varepsilon^t(\mathbb{1})$ from the equation

$$\mathbf{W}_\varepsilon^t(1)(p) = \left(e^{-\mathrm{i}\varepsilon\lambda} \frac{1}{2\pi} \int\limits_{[-\pi,\pi)} dq\, |v_{-1}(q)|^2 + e^{\mathrm{i}\varepsilon\lambda} \frac{1}{2\pi} \int\limits_{[-\pi,\pi)} dq\, |v_1(q)|^2 \right)^t,$$

or equivalently expressed in position space

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = \left(e^{-\mathrm{i}\varepsilon\lambda} \|v_{-1}\|^2 + e^{\mathrm{i}\varepsilon\lambda} \|v_1\|^2 \right)^t \cdot \mathbb{1}.$$

Since $\|v_{-1}\|^2 + \|v_1\|^2 = 1$ we set $\|v_{-1}\|^2 = r$ and get

$$\mathbf{W}_\varepsilon^t(\mathbb{1}) = (\cos(\varepsilon\lambda) + \mathrm{i}(1-2r)\sin(\varepsilon\lambda))^t \cdot \mathbb{1}.$$

Therefore we have the following formula for the perturbed eigenvalue

$$\mu_\varepsilon = \cos(\varepsilon\lambda) + \mathrm{i}(1-2r)\sin(\varepsilon\lambda) = 1 + \mathrm{i}(1-2r)\lambda\varepsilon - \lambda^2 \frac{\varepsilon^2}{2} + o(\varepsilon^3).$$

The ballistic scaling $\varepsilon = t^{-1}$ yields the limit $\lim_{t\to\infty} \mathbf{W}_{1/t}^t(\mathbb{1}) = e^{\mathrm{i}\lambda(1-2r)}\mathbb{1}$, which leads to the characteristic functions $C(\lambda) = e^{\mathrm{i}\lambda(1-2r)}$. Thus we get a point measure at position $1-2r$ in ballistic scaling. If we subtract this deterministic drift from the time evolution, i.e., consider the position operator $\widetilde{Q} = Q - (1-2r)t$, we may consider the diffusive scaling of the position distribution, which results in the characteristic function $C(\lambda) = e^{-2\lambda^2 r(1-r)}$.

4.7. Conclusion and Outlook

In the preceding sections we have studied the asymptotic behavior of translationally invariant quantum walks. Besides translation invariance, our analysis is based on the locality condition as defining feature of a quantum walk. These two requirements lead to a structure theorem for general translationally invariant quantum walks, by means of which we classified the set of all translationally invariant quantum walks into two groups. The first subset contains all quantum walks which conserve momentum and the second consists of all quantum walks which exhibit momentum transfer. Using perturbation theory, we introduced a method to compute the asymptotic position distributions of a quantum particle undergoing a translationally invariant quantum walk. For the different subclasses of quantum walks we obtained the following results:

We proved that the propagation behavior of a particle subject to a unitary quantum walk without momentum transfer is generically ballistic. It turned out that the only possibility for a unitary quantum walk to exhibit non-ballistic transport is when the unitary operator representing the time evolution has an eigenvector such that there is no propagation for this particular state.

If the quantum walk conserves momentum but interacts with the environment, that is, the time evolution is decoherent, the asymptotic scaling of the position distribution is diffusive under rather general assumptions. In order to prove this statement we used finite dimensional perturbation theory of the evolution operator. However, by means of examples we showed that decoherent quantum walks may nonetheless show ballistic transport.

The subclass of unitary quantum walks with momentum transfer includes examples where our method can be used to determine the asymptotic scaling of the position distribution. However, there are cases as well, where our procedure cannot be applied. The crucial point is whether or not the momentum transfer of the considered quantum walk is rational with respect to π. If the momentum transfer is irrational with respect to π, the propagation behavior seems to be different from ballistic or diffusive transport. Likewise, the spectral properties of the unitary operator implementing the quantum walk deviate from the picture we have for unitary quantum walk with rational momentum transfer. In particular, unitary quantum walks with irrational momentum transfer are likely to exhibit singularly continuous spectrum.

Based on a decomposition of quantum walks into shift and strictly local coin operators we introduced a model for decoherent quantum walks with momentum transfer, which can be analyzed in great detail by means of our previously introduced perturbation method. The difference to the case of decoherent quantum walks without momentum transfer is that the perturbation theory one has to perform is now infinite dimensional. The propagation behavior of these quantum

walks is again diffusive under rather general assumptions.

We conclude with a list of open questions for potential future research:

- For unitary quantum walks without momentum transfer it is still unclear if all such quantum walk can be realized as coined quantum walks. More precisely, the question is whether all quantum walks according to Remark 4.5.1 can be written in the form of Equation (4.23).
- A more technical question concerns the ε-dependent Jordan normal form of decoherent quantum walks without momentum transfer, where ε denotes the perturbation parameter. Although there are simple examples of analytic operators with singular eigenprojections and eigennilpotents, there is no example of a decoherent quantum walk showing this behavior. Of course, quantum walks have to satisfy additional requirements, as e.g. complete positivity, which may restrict the possibilities to construct such examples severely.
- The propagation behavior and spectral properties of unitary quantum walks with irrational momentum transfer are up to now unclear. Simulations seem to suggest that they differ significantly from the case with rational momentum transfer.
- Non-degeneracy of the eigenvalue 1 of the time evolution turned out to be a useful working hypothesis for decoherent quantum walks with and without momentum transfer. However, our method also applies if this assumption is not satisfied, see e.g. [APSS12, AGPS12] for a model which can easily be analyzed by means of our method despite degeneracy of the eigenvalue 1. A systematic study of this situation could potentially reveal new effects, such as the appearance of several Gaussian peaks in the asymptotic distribution as observed in [APSS12, AGPS12].
- Suppose we are given a family of decoherent quantum walks depending on a parameter in a way such that there is a coherent limit. That is, the family converges to a unitary quantum walk along an appropriate sequence of parameter values. Then we can study the behavior of the diffusion constant along this sequence, and intuitively we would expect that it diverges in the coherent limit. We observed this behavior in an example, but a general proof of this statement is missing.
- A further generalization of our model for decoherent quantum walks with momentum transfer is to allow for non-unitary Kraus operators for the coin evolution. That is, instead of a mixture of unitary coins one could consider a mixture over decoherent coin evolutions.

5. Interacting many-particle quantum walks

In experimental implementations of quantum walks, the single-particle nature of the process is not always satisfied. For example, data collection in experiments with neutral atoms in optical lattices is much more efficient if several atoms are loaded simultaneously into the lattice under the premise that the particles do not collide during the time evolution. Hence, these experiments already implement a many-particle quantum walk, but with a restricted class of initial states. Naturally, this motivates the study of the influence of particle collisions on the propagation behavior. In fact, from the experimental and theoretical point of view, single-particle quantum walks can be considered as a controllable and analytically treatable first step of a bottom-up approach to complex many-body system. In other words, our interest in quantum walks with several particles is based on the growing complexity of these systems with the number of particles and the interactions between these particles. Whilst translationally invariant and unitary single-particle quantum walks can be simulated with low computational effort, this is no longer true for general interacting many-particle quantum walks. This complexity opens the possibility for interesting applications of many-particle quantum walks as computational model or quantum simulators for other complex many-body systems.

In this chapter we consider many-particle quantum walks with interactions between the particles which only happen when several particles collide at one lattice site. Of course, any finite-range interaction can be mapped to such a contact interaction by regrouping into super-cells, hence, these interactions constitute a rather general class. Another assumption we impose on our model concerns the structure of the overall time evolution, which we take as a composition of a non-interacting part and a strictly local interaction. More precisely, the part without interaction describes the independent motion of each quantum particle according to some single-particle quantum walk, and the interaction happens when several particles, after evolving independently, reside in between these steps on one lattice site.

The remaining part of this chapter is structured as follows. We start with a short overview on the literature concerning many-particle quantum walks and mention other work related to the results of this thesis. In Section 5.2 we analyze single-particle quantum walks with point perturbations of the dynamical rule. This topic is clearly of interest in its own right, an moreover, these results are preparatory work for later sections. Subsequently, we study interacting many-particle quantum walks

in Section 5.3, which is divided into three parts. First, we comment briefly on non-interacting quantum walks of several particles, and in the second part we consider interacting quantum walks of two particles. We prove that under quite general conditions the interaction leads to a dynamically stable molecular state of the two particles. That is, the two particles form a stable compound which moves similarly to a single particle on the spatial lattice. In the last part of Section 5.3 we sketch generalizations of our model to arbitrary numbers of particles, which leads us to the notion of quantum cellular automata. Section 5.4 provides a number of examples meant to illustrate the concepts of this chapter. Finally, we conclude in Section 5.5 with a summary of our results and a list of open question.

5.1. Literature overview and related work

In the following we give a brief account of the literature concerning quantum walks of several particles and their relation to later parts of this chapter. We focus on many-particle dynamics which emerge from the independent time evolution of several particles according to translationally invariant unitary single-particle quantum walks by adding a contact interaction to the system.

5.1.1. Historical survey

The conventional terminology for the discrete time evolution of a quantum particle moving on a spatial lattice as quantum walk was accepted by a large class of authors around the beginning of this century. Before that, such dynamics was also referred to as quantum cellular automaton or quantum lattice gas for multi-particle systems, see e.g. [Mey96, Mey97b, Mey97a, Mey98, BI98a, BI98b, BB94]. In fact, most of these references clearly have the intention to study single- and multi-particle dynamics, and Meyer probably was the first to study a two-particle quantum walk with collisional interaction in [Mey96, Mey97a], see also [BI98a]. However, the focus of these studies is more on the connection of quantum walks to continuous time and space dynamics and phenomenological aspects, such as Klein's paradox or scattering at potentials, instead of asymptotic propagation behavior.

Later, explicit studies of non-interacting two-particle quantum walks were performed by Omar et al. [OPSB06] and Pathak et al. [PA07]. Since their model is equivalent to a single-particle quantum walk on a higher dimensional lattice, see Section 5.3.1 and [RSŠ+12], the propagation behavior is covered by our analysis performed in Chapter 4. Nonetheless, the aforementioned authors found some interesting propagation effects if the initial state of the quantum particles is entangled. In fact, this effect can also be viewed as a result of (anti-) symmetrization of the initial state of the particles since the time evolution treats both particles as indistin-

guishable. Afterwards, the analysis of entanglement generation in non-interacting multi-particle quantum walks was furthered by Goya et al. [GC10] and Allés et al. [AGG12].

Štefaňák et al. investigated the meeting problem for a non-interacting quantum walk of two particles in [ŠKJM06] . In a nutshell, this problem concerns the probability for the two quantum particles to meet after some number of time steps. The authors compared the asymptotic behavior of this probability with the corresponding quantity for classical random walks, and found that the quantum version decays faster with a dependence on the initial state of the quantum walk. Interestingly, it was already mentioned in the conclusion of this article that interactions of the two particles, either of infinite range or of collisional type, may lead to an increase of the meeting probability. In the subsequent article [ŠBK+11] a similar question was tackled. Instead of the meeting probability, the probability for the two particles to be found simultaneously on the positive or negative half-axis of the integer lattice was computed. The authors also introduced a collisional interacting of the two particles, and by numerical simulation it was found that this interaction indeed helps to increase the probability to find both particles on the same half-axis. In fact, from a finite time steps simulation of the joint probability distribution of the two particles presented in [ŠBK+11], one can already identify the molecular character of the two-particles, see Figure 6 in [ŠBK+11]. An explanation of this effect was provided by Ahlbrecht et al. in [AAM+12], where it was shown that such interactions in a two-particle quantum walk generically lead to a dynamically stable bound state of the two-particles. This means the particles are not just likely to be found simultaneously in a certain subregion of the lattice, but also they form a state with approximately finite relative distance, which moves as a compound on the spatial lattice. These predictions were later experimentally confirmed in [SGR+12].

5.1.2. Related work

Parts of the results presented in this chapter have been published in [AAM+12]. In particular, our analysis of interacting two-particle quantum walks in Section 5.3.2 is based on the method developed in [AAM+12]. Using this method, we identify a dynamically stable molecular state of the two-particles. A similar effect for particles tunneling continuously in time on a spatial lattice was reported in [WTL+06].

Our generalization of interacting two-particle quantum walks to an arbitrary particle number, which we construct in Section 5.3.3, is based on the concept of quantum cellular automata as introduced in [SW04]. In [Vog09] a construction scheme for quantum cellular automata simulating the single-particle dynamics of translationally invariant quantum walks was introduced. We use a similar construction to establish a connection between quantum cellular automata and interacting many-particle quantum walks.

5.2. One-particle quantum walks with point defects

As a preparatory step for later parts of this chapter we consider now local perturbations of translationally invariant unitary quantum walks. The importance of this topic, besides its interest on its own, is that two-particle quantum walks with contact interaction can be viewed as a parameter dependent family of one-particle quantum walks with such a local perturbation, see Section 5.3.2.

The precise setting we consider is as follows: Starting point is a translationally invariant unitary quantum walk W on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ in the sense of Remark 4.5.1. We modify W by multiplication with a strictly local unitary operator U_C acting non-trivially only at the origin by means of a unitary $C\in\mathcal{U}(\mathcal{K})$, i.e.

$$U_C = \sum_{0\neq x\in\mathbb{Z}^s} |x\rangle\langle x|\otimes\mathbb{1}_{\mathcal{K}} + |0\rangle\langle 0|\otimes C = \mathbb{1}_{\mathbb{Z}^s}\otimes\mathbb{1}_{\mathcal{K}} + |0\rangle\langle 0|\otimes(C-\mathbb{1}_{\mathcal{K}})\,. \tag{5.1}$$

The next definition captures the main objective of this section.

Definition 5.2.1. *Let W be a translationally invariant unitary quantum walk on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ and $C\in\mathcal{U}(\mathcal{K})$. With U_C according to Equation* (5.1) *we define the perturbation of W by C to be the operator $W_C = W\cdot U_C$.*

In Chapter 4 we analyzed the translationally invariant part W of W_C in great detail. In particular, we established a connection between the dispersion relations ω_j of W and the spectrum $\sigma(W)$, see Proposition 4.5.7. Although the pure point spectrum of W may be non-empty, we saw that the generic case is that the spectrum of W is absolutely continuous. The question we would like to answer in this sections is how the spectrum of W changes when the perturbation U_C is applied. Intuitively, we would expect that the point perturbation U_C leaves the essential part of $\sigma(W)$ unchanged, but generates finitely degenerate eigenvalues. The first part of this statement concerning stability of the essential spectrum can be proven using results from [Kat95].

Proposition 5.2.2. *Let W be a translationally invariant and unitary quantum walk on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$, and W_C the perturbation of W according to Definition 5.2.1. The spectra of W and W_C satisfy $\sigma(W)=\sigma_{ess}(W)=\sigma_{ess}(W_C)$.*

Proof. The essential spectrum of W coincides with $\sigma(W)$ since any eigenvalue of W is infinitely degenerate, see Proposition 4.5.7. The perturbation operator

$$W_C - W = W\cdot|0\rangle\langle 0|\otimes(C-\mathbb{1}_{\mathcal{K}})$$

is obviously a finite rank operator, hence, the essential spectra of W_C and W coincide [Kat95, Thm.IV.5.35]. □

To find the eigenvalues of W_C we first translate the problem into momentum space. Clearly, W_C is no longer translationally invariant, but its action can still be expressed by a simple integral kernel. The operator U_C is the sum of two terms, see Equation (5.1), of which only the second acts non-trivially by projecting onto the origin and applying the operator $C - \mathbb{1}_{\mathcal{K}}$. Since the projection onto the origin is in momentum space represented by integration over p, we can represent the action of U_C by

$$(U_C\psi)(p) = \psi(p) + \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p' \, (C - \mathbb{1}_{\mathcal{K}})\psi(p'). \tag{5.2}$$

The translationally invariant part W of W_C still acts like a multiplication operator $W(p)$ in momentum space, hence, W_C can be written as

$$(W_C\psi)(p) = W(p)\psi(p) + \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p' \, W(p)(C - \mathbb{1}_{\mathcal{K}})\psi(p'). \tag{5.3}$$

The eigenvalue equation for W_C reads $(W_C\psi)(p) = z\psi(p)$, which is equivalent to

$$\big(W(p) - z\,\mathbb{1}_{\mathcal{K}}\big)\,\psi(p) = W(p)(\mathbb{1}_{\mathcal{K}} - C)\psi_0\,, \tag{5.4}$$

where ψ_0 is the component of ψ at the origin, i.e. $\psi_0 = (2\pi)^{-s}\int_{[-\pi,\pi)^s} d^s p' \, \psi(p')$. The further analysis of this equation is much simplified if we assume the eigenvalue z to be in the spectral gap of W, which we denote by $\Gamma(W) = \mathbb{S}\backslash\sigma(W)$.

Assumption 5.1. *The solution z of Equation* (5.4) *satisfies $z \in \Gamma(W)$.*

Of course, this assumption may fail to be true, so we may not get all eigenvalues of W_C by the following analysis. Nevertheless, our method generically yields the eigenvalues in the spectral gap of W_C and corresponding eigenvectors by a strikingly simple procedure. Given Assumption 5.1 we can invert the operator on the left hand side in Equation (5.4) to obtain

$$\psi(p) = \big(W(p) - z\,\mathbb{1}_{\mathcal{K}}\big)^{-1} W(p)(\mathbb{1}_{\mathcal{K}} - C)\psi_0\,. \tag{5.5}$$

Therefore, the eigenvector ψ corresponding to z is uniquely determined by its component at the origin ψ_0 and the eigenvalue z. Integrating this equation over p leads to the consistency condition

$$\psi_0 = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, \big(W(p) - z\,\mathbb{1}_{\mathcal{K}}\big)^{-1} W(p)(\mathbb{1}_{\mathcal{K}} - C)\psi_0 \tag{5.6}$$

for z and ψ. To shorten notation we define the operator

$$R(z) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s p \, (W(p) - z\,\mathbb{1}_{\mathcal{K}})^{-1} W(p). \tag{5.7}$$

The following proposition shows that Equation (5.6) is not only a consistency condition, but equivalent to the eigenvalue equation.

Proposition 5.2.3. *Let z be a complex number satisfying Assumption 5.1. Any eigenvector ψ of W_C corresponding to z determines a solution $\varphi \neq 0$ of*

$$\varphi = R(z)(\mathbb{1}_{\mathcal{K}} - C)\varphi \tag{5.8}$$

via the relation $\varphi = (2\pi)^{-s} \int_{[-\pi,\pi)^s} d^s p\, \psi(p)$. Conversely, any solution $\varphi \neq 0$ of Equation (5.8) determines an eigenvector ψ corresponding to z via

$$\psi(p) = \left(W(p) - z\,\mathbb{1}_{\mathcal{K}}\right)^{-1} W(p)(\mathbb{1}_{\mathcal{K}} - C)\varphi\,. \tag{5.9}$$

Proof. The first half of this statement is already proven. Suppose φ is a solution of Equation (5.8). The operator $W(p)(\mathbb{1}_{\mathcal{K}} - C)$ represents a bounded operator on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$, hence, $W(p)(\mathbb{1}_{\mathcal{K}} - C)\varphi$ defines a vector in $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$. Moreover, by Assumption 5.1 the distance of z to the spectrum of W is strictly positive. Therefore $\left(W(p) - z\,\mathbb{1}_{\mathcal{K}}\right)^{-1}$ defines a bounded operator on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ as well. Consequently, Equation (5.9) defines a vector ψ in $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ by its Fourier transform $\psi(p)$. What is left to prove is that ψ is not the zero vector. Since φ is non-zero and a solution of Equation (5.8) we conclude that $(\mathbb{1}_{\mathcal{K}} - C)\varphi$ is non-zero. The assertion follows from the fact that both, $W(p)$ as well as $\left(W(p) - z\,\mathbb{1}_{\mathcal{K}}\right)^{-1}$, are invertible. □

Interestingly, it turns out that the operator $R(z)$ is invertible, and moreover $V = \mathbb{1}_{\mathcal{K}} - R(z)^{-1}$ is a unitary operator on $\mathcal{K}$, see Lemma 5.2.4 below. This means we can rewrite Equation (5.8) as

$$C\varphi = \left(\mathbb{1}_{\mathcal{K}} - R(z)^{-1}\right)\varphi = V\varphi\,, \tag{5.10}$$

and by the unitarity of V the eigenvalue condition (5.8) can be satisfied for any z in the spectral gap of W by a suitable C. In other words, for any translationally invariant unitary quantum walk such that there exists $z \in \Gamma(W)$, there is $C \in \mathcal{U}(\mathcal{K})$ such that the perturbed quantum walk $W_C = W \cdot U_C$ has an eigenvector corresponding to the eigenvalue z. In fact, for any $C \in \mathcal{U}(\mathcal{K})$ we may satisfy Equation (5.10) by multiplying C with a suitable phase factor $e^{i\eta}$ since C^*V is unitary, hence diagonalizable with unit modulus eigenvalues.

Lemma 5.2.4. *Let W be a unitary operator on a Hilbert space $\mathcal{H}$, $z \in \Gamma(W)$, and N an arbitrary projection on $\mathcal{H}$. Consider $R(z) = N(W - z\,\mathbb{1})^{-1} WN$ as an operator on $N\mathcal{H}$. Then $R(z)$ is invertible and $V = \mathbb{1} - R(z)^{-1}$ is unitary.*

Proof. The crucial step for the proof is to show the following relation

$$R(z) + R(z)^* = \mathbb{1}. \tag{5.11}$$

We can show this for the special case $N = \mathbb{1}$, and then multiply the above equation with N from both sides. Since W is unitary it has a spectral decomposition $W = \int_{[-\pi,\pi)} e^{\mathrm{i}\lambda}\, E_W(d\lambda)$, where E_W is the spectral measure corresponding to W. We can then express the operator (5.11) directly in the functional calculus:

$$\begin{aligned} R(z)+R(z)^* &= \int_{[-\pi,\pi)} \left(\frac{e^{\mathrm{i}\lambda}}{e^{\mathrm{i}\lambda}-z} + \frac{e^{-\mathrm{i}\lambda}}{e^{-\mathrm{i}\lambda}-\overline{z}} \right) E_W(d\lambda) \\ &= \int_{[-\pi,\pi)} \frac{e^{\mathrm{i}\lambda}(e^{-\mathrm{i}\lambda}-\overline{z}) + e^{-\mathrm{i}\lambda}(e^{\mathrm{i}\lambda}-z)}{|e^{\mathrm{i}\lambda}-z|^2}\, E_W(d\lambda) \\ &= \int_{[-\pi,\pi)} \frac{2-2\Re(e^{-\mathrm{i}\lambda}z)}{2-2\Re(e^{-\mathrm{i}\lambda}z)}\, E_W(d\lambda) \\ &= \mathbb{1} \end{aligned}$$

This determines the hermitian part of $R(z)$, and we can write $R(z) = \frac{1}{2}(\mathbb{1} + \mathrm{i}K)$ for some hermitian operator K on $N\mathcal{H}$.

For the next we use the functional calculus of $K = \int_{\mathbb{R}} k\, E_K(dk)$, with the spectral measure of K, which is now supported on the real axis. We note that due to the projection N, which need not commute with W, this measure cannot be easily obtained from the spectral measure E_W. Then

$$\begin{aligned} V &= \mathbb{1} - R(z)^{-1} \\ &= \int_{\mathbb{R}} \left(1 - \frac{1}{\frac{1}{2}(1+\mathrm{i}k)} \right) E_K(dk) \\ &= \int_{\mathbb{R}} \frac{-1+\mathrm{i}k}{1+\mathrm{i}k}\, E_K(dk). \end{aligned}$$

Now, since $|-1+\mathrm{i}k| = |1+\mathrm{i}k|$ the integrand has absolute value 1, and so the integral represents a unitary operator. □

Any $z \in \mathbb{S}$ in the spectral gap of W is a possible eigenvalue of W_C since we can always adjust C such that Equation (5.10) is satisfied for z and some vector φ. A similar question is, how many eigenvalues for fixed W_C exist in the spectral gap of W. Of course, the exact answer depends on the perturbation C as well as on the unitary W, but there is a general upper bound to this number depending on the number of connected components of $\Gamma(W)$.

Proposition 5.2.5. *The number of eigenvalues $z \in \Gamma(W)$ of W_C is bounded by* $\dim \mathcal{K}$ *eigenvalues per connected component of* $\Gamma(W)$ *in* $\mathbb{S}$.

Proof. We use Theorem 2.3 from [Sim07] to prove the assertion. The statement of this theorem concerns unitary operators U, V such that $U-V$ is a rank one operator. Then, if $\mathbb{S}_{a,b} = \{e^{\mathrm{i}\lambda} : a < \lambda < b\}$ is an open arc of the unit circle $\mathbb{S}$ such that $\mathbb{S}_{a,b} \cap \sigma(U) = \emptyset$, we know that the operator V has at most one eigenvalue in the closed arc $\overline{\mathbb{S}_{a,b}} = \{e^{\mathrm{i}\lambda} : a \leq \lambda \leq b\}$.

This proves the statement if $W_C - W = W \cdot |0\rangle\langle 0| \otimes (C - \mathbb{1}_{\mathcal{K}})$ is a rank one operator, i.e. $C - \mathbb{1}_{\mathcal{K}}$ is rank one. In the general case we can write W_C as a sequence of unitary rank one perturbations by using the spectral decomposition of C. Indeed, for $0 < r \leq \dim \mathcal{K}$ let

$$C_r = e^{\mathrm{i}\lambda_r} |\phi_r\rangle\langle\phi_r| + \mathbb{1}_{\mathcal{K}} - |\phi_r\rangle\langle\phi_r|,$$

with eigenvalues λ_r and eigenvectors ϕ_r of C. Clearly, the sequence $W_r = W_{r-1} \cdot U_{C_r}$, with $W_0 = W$, consists of unitary operators satisfying $W_{\dim \mathcal{K}} = W_{\mathrm{Int}}$ and $W_r - W_{r-1}$ is a rank one operator. The assertion follows from iteratively applying the above result to the sequence W_r.

□

The matrix elements of $(W(p) - z\,\mathbb{1}_{\mathcal{K}})^{-1}$ are usually infinite Fourier series instead of polynomials. Hence, the eigenvector ψ determined by Equation (5.9) is supported on the whole lattice $\mathbb{Z}^s$. We close this section with an exponential bound on the decay of the vector components of ψ.

Proposition 5.2.6. *Let z be an eigenvalue of W_C satisfying Assumption 5.1 and ψ a corresponding eigenvector. There are positive constants α and β such that the vector components ψ_x of $\psi = \sum_{x \in \mathbb{Z}^s} |x\rangle \otimes \psi_x$ satisfy*

$$\left\| \psi_x \right\| \leq \frac{\alpha}{\operatorname{dist}(z, \sigma(U))} e^{-\beta \operatorname{dist}(z,\sigma(U)) \|x\|}, \quad \forall x \in \mathbb{Z}^s. \tag{5.12}$$

Proof. This is a special case of a more general statement, see Proposition 5.3.3 □

5.3. Many-particle quantum walks

We start this section with a brief account of non-interacting many-particle quantum walks. Subsequently we study interacting two-particle quantum walks using the results of Section 5.2. In the last section we introduce a model for interacting many-particle quantum walks also allowing for infinite particle numbers.

5.3.1. Non-interacting quantum walks

Without interaction there are no additional terms beyond the single-particle dynamics to be specified. We obtain the non-interacting N-particle version of a given

single-particle quantum walk $\mathbf{W}_1$ simply by taking the tensor product of the time evolution on $\mathcal{H}_1^{\otimes N}$, where $\mathcal{H}_1$ is the system Hilbert space of a single particle. A bit more general, suppose we are given N distinguishable quantum particles moving on a lattice $\ell^2(\mathbb{Z}^s)$, each with a possibly different internal state space $\mathcal{K}_j$. The Hilbert space of the combined system of all N quantum particles is

$$\mathcal{H}_N = \bigotimes_{j=1}^{N} \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}_j \cong \ell^2(\mathbb{Z}^{sN}) \bigotimes_{j=1}^{N} \mathcal{K}_j \,, \tag{5.13}$$

thus, we may alternatively consider the quantum state of N particles on $\mathbb{Z}^s$ as quantum state of a single particle on a lattice of spatial dimension sN with internal state space given by the tensor product of the single-particle state spaces $\mathcal{K}_j$. The time evolution is then given by $\mathbf{W} = \mathbf{W}_1 \otimes \ldots \otimes \mathbf{W}_N$, where $\mathbf{W}_j$ denotes the single-particle quantum walk of the j^{th} particle. Clearly, $\mathbf{W}$ is local and translationally invariant on $\mathbb{Z}^{sN}$ if and only if each $\mathbf{W}_j$ is so on $\mathbb{Z}^s$. Thus $\mathbf{W}$ may be considered as single-particle quantum walk on $\mathbb{Z}^{sN}$.

We are mainly interested in the case where each $\mathbf{W}_j$ is a translationally invariant unitary quantum walk on $\mathbb{Z}^s$. Of course, unitarity of $\mathbf{W}$ is equivalent to unitarity of all $\mathbf{W}_j$ simultaneously, and, as we saw in Section 4.5.1, the propagation behavior of translationally invariant unitary $\mathbf{W}$ is generically ballistic. Let us denote the unitary operator implementing $\mathbf{W}$ by W, and thus $W = W_1 \otimes \ldots \otimes W_N$ with unitaries W_j corresponding to $\mathbf{W}_j$. Denoting the dispersion relations of W_j by $\omega_{\alpha_j}(p_j)$, where p_j stands for the s-dimensional momentum vector corresponding to the j^{th} particle, we obtain the dispersion relations of W by the formula $\omega_{\alpha_1,\ldots,\alpha_N}(p_1,\ldots p_N) = \omega_{\alpha_1}(p_1) + \ldots + \omega_{\alpha_N}(p_N)$. Similarly, the corresponding eigenprojections satisfy

$$\mathbf{P}_{\alpha_1,\ldots,\alpha_N}(p_1,\ldots p_N) = \mathbf{P}_{\alpha_1}(p_1) \otimes \ldots \otimes \mathbf{P}_{\alpha_N}(p_N). \tag{5.14}$$

Consequently, starting with initial state ρ_N, the asymptotic position distribution in ballistic scaling is described by the characteristic function

$$C(\lambda) = \frac{1}{(2\pi)^{sN}} \int\limits_{[-\pi,\pi)^{sN}} d^{sN}p \, \operatorname{tr}_{\mathcal{K}} \rho_N(p) \bigotimes_{j=1}^{N} \sum_{\alpha_j} e^{\mathrm{i}\lambda_j \cdot \nabla \omega_{\alpha_j}(p_j)} \mathbf{P}_{\alpha_j} \,, \tag{5.15}$$

with $p = (p_1,\ldots,p_N)$ and $\lambda = (\lambda_1,\ldots,\lambda_N)$, see Section 4.5.1. Using Equation (5.15) one verifies directly that initial states of the form $\rho_N = \sigma_1 \otimes \ldots \otimes \sigma_N$ lead to a characteristic function which is the product of N single-particle characteristic functions, hence, the corresponding probability distribution is that of N independent random variables ν_j describing the asymptotic distribution of $\mathbf{W}_j$ and σ_j.

Naturally, this is no longer true if the initial state ρ_N exhibits correlations between the different particles. For example, we may assume the N particles to be indistinguishable, in which case we have to (anti-) symmetrize initial states of the

form $\rho_N = \sigma_1 \otimes \ldots \otimes \sigma_N$ resulting in correlation effects in the position distribution of the quantum walk, see e.g. [OPSB06, PA07] for a study of such effects. However, the behavior of a translationally invariant unitary quantum walk is in general still ballistic.

5.3.2. Interacting two-particle quantum walks

In this section we consider the case where two quantum particles perform an interacting quantum walk. The overall time evolution is assumed to be unitary, and the interaction of the particles is only to happen when both occupy the same lattice site, i.e. we only consider collisional interactions. Note, however, that any interaction with strictly finite interaction length can be brought to this form by regrouping lattice sites into bigger super-cells.

To begin with, we need to specify a time evolution for the particles without interaction. We assume that each particle undergoes a translationally invariant and unitary quantum walk W_j according to Remark 4.5.1, so the overall time evolution without interaction is described by the unitary $W = W_1 \otimes W_2$ on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}_1 \otimes \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}_2$. Occasionally, we make use of the isomorphism (5.13) and consider W as single-particle quantum walk on $\ell^2(\mathbb{Z}^{2s}) \otimes \mathcal{K}_{12}$, with $\mathcal{K}_{12} = \mathcal{K}_1 \otimes \mathcal{K}_2$. Hence, the coordinates x_1 and x_2 are either considered as positions of two particles or as a set of coordinates describing together the position of a single particle. Clearly, W is translationally invariant on $\mathbb{Z}^{2s}$ and unitary, hence, it is well-described within the framework developed in Section 4.5.1.

To make the two-particle quantum walk W interacting we need to introduce a dependence on the particle coordinates. We do so by introducing a modification $W_{\text{Int}} = W \cdot U_C$ of W, where U_C is a space dependent and strictly local operator which acts trivially when the two particles occupy different lattice sites, and applies a contact interaction C otherwise. This contact interaction is assumed to be the same for all lattice sites, i.e. it is invariant with respect to joint translations of the two particles. Thus we can write U_C as

$$\begin{aligned} U_C &= \sum_{x_1 \neq x_2 \in \mathbb{Z}^s} |x_1 \otimes x_2\rangle\langle x_1 \otimes x_2| \otimes \mathbb{1}_{\mathcal{K}_{12}} + \sum_{y \in \mathbb{Z}^s} |y \otimes y\rangle\langle y \otimes y| \otimes C \qquad (5.16) \\ &= \mathbb{1}_{\mathbb{Z}^{2s}} \otimes \mathbb{1}_{\mathcal{K}_{12}} + \sum_{y \in \mathbb{Z}^s} |y \otimes y\rangle\langle y \otimes y| \otimes \left(C - \mathbb{1}_{\mathcal{K}_{12}}\right), \end{aligned}$$

with $C \in \mathcal{U}(\mathcal{K}_{12})$. We denote the projection onto the collisional points $x_1 = x_2$ in $\ell^2(\mathbb{Z}^s) \otimes \ell^2(\mathbb{Z}^s)$ by $\mathcal{P}$, such that $U_C = \mathbb{1}_{\mathbb{Z}^{2s}} \otimes \mathbb{1}_{\mathcal{K}_{12}} + \mathcal{P} \otimes \left(C - \mathbb{1}_{\mathcal{K}_{12}}\right)$ and

$$W_{\text{Int}} = (W_1 \otimes W_2)\left((\mathbb{1}_{\mathbb{Z}^{2s}} - \mathcal{P}) \otimes \mathbb{1}_{\mathcal{K}_{12}} + \mathcal{P} \otimes C\right). \qquad (5.17)$$

Similarly to the case considered in Section 5.2, the perturbation of $W = W_1 \otimes W_2$ by U_C potentially changes the spectrum of W. There we saw that a perturbation at

a single point generically leads to eigenvalues in the spectral gaps without changing the essential spectrum. So the first obvious question is how the perturbation in Equation (5.17) affects the spectrum of W. Here the answer is not as simple as in Section 5.2: The perturbation operator $W_{\mathrm{Int}} - W = W \cdot (\mathcal{P} \otimes (C - \mathbb{1}_{\mathcal{K}_{12}}))$ is far from being compact since the dimension of the subspace $\mathcal{P}\ell^2(\mathbb{Z}^{2s})$ is infinite. Thus we cannot apply the results from [Kat95] to conclude that the essential spectrum of W is stable under this perturbation. In fact, we will see later that the perturbation by U_C generically enlarges the essential spectrum without generating additional eigenvalues.

Despite the fact that the perturbed operator W_{Int} has in general no eigenvalues, the perturbation by U_C dramatically changes the propagation behavior of W. The contact interaction leads to the formation of dynamically stable molecular states of the two particles which propagate together as a compound. Before we deepen the analysis of the propagation behavior of W_{Int}, let us briefly sketch the line of arguments. Our first step is to separate the time evolution generated by W_{Int} into center of mass and relative coordinate dynamics. The focus is then on the relative motion of the particles, and unlike to the case of continuous space two-body problems we will see that the separation of the dynamics is not complete since there is a dependence of the relative motion on the total momentum p of the two particles. Further analysis for fixed p will reveal a bound state of the two particles' relative motion, which depends on p. Of course, these bound states for fixed p are non-normalizable, and because of the dependence of the corresponding eigenvalue on p there is in general no eigenvalue of the total time evolution W_{Int}. However, superpositions of these states with well-behaved distributions of the total momentum p define normalizable vectors in $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$, and the set of all such states is invariant under W_{Int}. This means that the distance of the two particles, initially in such a superposition, is upper bounded for all time steps, up to arbitrarily small corrections. Hence, we will call these states molecular states of the two particle quantum walk W_{Int}. Let us illustrate these concepts by a particular instance of an interacting two-particle quantum walk.

Interlude 6: Two-particle Hadamard walk with collisional phase interaction

We consider an interacting quantum walk of two particles on a one-dimensional spatial lattice, and the internal degree of freedom is described by $\mathbb{C}^2$, i.e. the single particle Hilbert space is $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$. The non-interacting dynamics is given by the standard shift and Hadamard coin, i.e. $W_{1,2} = S \cdot (\mathbb{1}_{\mathbb{Z}} \otimes H)$ with

$$S|x,\pm\rangle = |x \pm 1, \pm\rangle \quad \text{and} \quad H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{5.18}$$

and $|x,\pm\rangle$ the standard basis of $\ell^2(\mathbb{Z})\otimes\mathbb{C}^2$. The interaction is given by a collisional phase, that is,

$$W_{\text{Int}} = (W_1 \otimes W_2)\cdot U_g \tag{5.19}$$

with $g \in [0, 2\pi)$ and

$$U_g = \mathbb{1}_{\mathbb{Z}^2} \otimes \mathbb{1}_{\mathbb{C}^4} + \mathcal{P} \otimes \left(e^{\mathrm{i}g} - 1\right) \mathbb{1}_{\mathbb{C}^4}\,. \tag{5.20}$$

This quantum walk has a particular symmetry, it preserves (anti-) symmetrization of the two-particle initial state. Hence, we may study the problem in the fermionic or bosonic subspace of $(\ell^2(\mathbb{Z})\otimes\mathbb{C}^2)^{\otimes 2}$ independently. A finite time step simulation for the antisymmetric initial state

$$\psi = |0,0\rangle \otimes \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \tag{5.21}$$

is shown in Figure 5.1. The comparison with the non-interacting case shows the dramatic change of the propagation behavior and clearly indicates the molecular nature of the two-particle evolution. This walk can be analyzed in great detail by

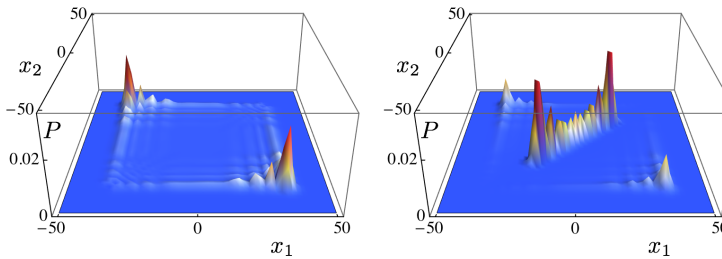


Figure 5.1.: The position distribution of two particles after $t = 50$ time steps according to Equation (5.19) with initial state (5.21) is shown. Left panel: without interaction ($g = 0$); Right panel: interaction with collision phase $g = -\pi$.

going to center of mass and relative coordinates. This separation, which we perform in the next section, leads to a quantum walk describing the relative motion of the two particles depending on the total momentum p. Using Fourier transform with respect to center of mass and relative coordinates, we can calculate the spectrum of W_{Int} by computing the p-dependent spectrum of the quantum walk in relative coordinate, see Figure 5.2. The result is an eigenvector of the relative coordinate dynamics, which depends on the total momentum p. This eigenvector is responsible for the molecular dynamics of the two particles.

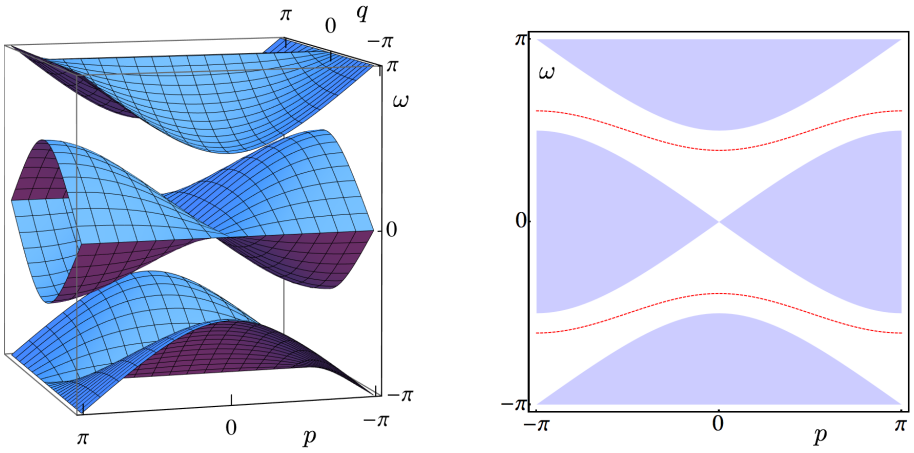


Figure 5.2.: Spectrum of the interacting quantum walk defined by Equation (5.19). Panel (a) shows the (p,q)-dependent eigenvalues of the non-interacting walk ($g=0$). The p-dependent spectrum of the interacting walk for $g=\pi$ is shown in panel (b). Blue regions indicate the continuous spectrum, the red-dashed line represents the eigenvalue in the spectral gap.

Separation into center of mass and relative coordinates

If the contact interaction U_C is non-trivial, i.e. $C \neq \mathbb{1}_{\mathcal{K}_{12}}$, we break translation invariance of the time evolution. Since C is the same for every collisional point, W_{Int} is invariant under joint translations of both particles. This symmetry is the crucial property which builds a bridge to the problem studied in Section 5.2. To see this, we rephrase the time evolution W_{Int} in center of mass and relative coordinates. That is, instead of x_1 and x_2 we use the set of coordinates $x_c = (x_1+x_2)/2$ and $x_r = x_1 - x_2$. Note that these coordinates are slightly asymmetric since $x_c \in \mathbb{Z}^s/2$ whilst $x_r \in \mathbb{Z}^s$. This fact is also reflected by the corresponding momenta p and q, which are given

by $p = p_1 + p_2$ and $q = (p_1 - p_2)/2$, which follows from the simple computation

$$\begin{aligned}\psi(p_1,p_2) &= \sum_{x_1,x_2\in\mathbb{Z}^s} e^{\mathrm{i}x_1\cdot p_1} e^{\mathrm{i}x_2\cdot p_2}\psi_{x_1,x_2} \\ &= \sum_{x_c\in\frac{1}{2}\mathbb{Z}^s, x_r\in\mathbb{Z}^s} e^{\mathrm{i}x_c\cdot(p_1+p_2)} e^{\mathrm{i}x_r\cdot\frac{1}{2}(p_1-p_2)}\psi_{x_c,x_r} \\ &= \sum_{x_c\in\frac{1}{2}\mathbb{Z}^s, x_r\in\mathbb{Z}^s} e^{\mathrm{i}x_c\cdot p} e^{\mathrm{i}x_r\cdot q}\psi_{x_c,x_r} = \psi(p,q).\end{aligned} \tag{5.22}$$

Thus, $p \in [-2\pi, 2\pi)^s$ and $q \in [-\pi,\pi)^s$, but not all points in $[-2\pi,2\pi)^s \times [-\pi,\pi)^s$ are independent. Figure 5.3 visualizes how we may identify points to map this to the standard Brillouin zone, i.e. $(p,q) \in [-\pi,\pi)^{2s}$ and all points in this domain are independent. We assume in the following such an identification has been made. In these new coordinates, W_{Int} commutes with translations of x_c. This translation

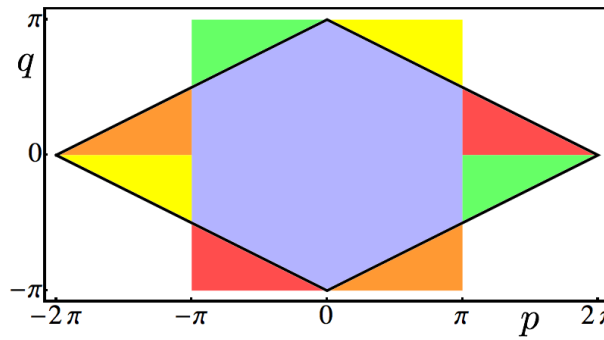


Figure 5.3.: Brillouin zone identification for $s = 1$: Starting from the Brillouin zone contained in $[-2\pi,2\pi)\times[-\pi,\pi)$ (enclosed by black rhombus), we identify points where $p \notin [-\pi,\pi)$ in the following way: Assume $p \geq \pi$, then we identify p_1 with $p_1 - 2\pi$ if $p_1 \geq p_2$, otherwise we identify p_2 and $p_2 - 2\pi$. If $p < -\pi$ we identify $p_{1,2}$ and $p_{1,2} + 2\pi$ in a similar manner. If $s > 1$ the procedure is applied to all coordinates separately.

symmetry is reflected by conservation of the corresponding total momentum p by W_{Int}, which is obvious from the formula

$$\begin{aligned}(W_{\mathrm{Int}}\psi)(p,q) &= W(p,q)\psi(p,q) + \\ &+ \frac{1}{(2\pi)^s}\int_{[-\pi,\pi)^s} d^s q\, W(p,q)(C - \mathbb{1}_{\mathcal{K}_{12}})\psi(p,q)\end{aligned} \tag{5.23}$$

with $W(p,q) = W_1(p/2+q) \otimes W_2(p/2-q)$. In this relation, we may treat p as a fixed parameter, which yields an equation of the form (5.3) for the momentum variable q. That is, we have to solve a p-parametrized family of problems of the kind considered in Section 5.2.

Naturally, our approach to separate the time evolution into center of mass and relative coordinate dynamics is motivated by the analogous strategy for two-body problems in continuous space systems. However, there is an important difference in the results:

Remark 5.3.1. *In contrast to continuous space two-body problems, the separation of the discrete space problem into center of mass and relative coordinates is not complete in the sense that there is still a dependency of the relative coordinate problem on the center of mass momentum.*

As a consequence of Gallilean invariance, the relative coordinate dynamics does not depend on total momentum if space is continuous. However, since Gallilean symmetry is broken for discrete space systems, the dependence on the total momentum p can be seen as a fingerprint of the lattice $\mathbb{Z}^s$.

Bound states for fixed total momentum

For fixed total momentum p, Equation (5.23) defines an operator $\widehat{W}_p$ on $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}_{12}$ describing the relative motion of the two particles. The position space representation of this operator reads

$$\widehat{W}_p = \left(\sum_{x_r, y_r \in \mathbb{Z}^s} |x_r\rangle\langle y_r| \otimes \sum_{x_c \in \frac{1}{2}\mathbb{Z}^s} e^{\mathrm{i} x_c \cdot p} W(x_c, x_r, y_r) \right) \cdot \left(\mathbb{1}_{\mathbb{Z}^s} \otimes \mathbb{1}_{\mathcal{K}_{12}} + |0\rangle\langle 0| \otimes (C - \mathbb{1}_{\mathcal{K}_{12}}) \right), \tag{5.24}$$

with $W(x_c, x_r, y_r)$ defined by

$$\langle \eta | W(x_c, x_r, y_r) | \gamma \rangle = \langle x_c \otimes x_r \otimes \eta | W | 0 \otimes y_r \otimes \gamma \rangle, \quad \eta, \gamma \in \mathcal{K}_{12}. \tag{5.25}$$

Note that the sum over x_c in Equation (5.24) is finite for we have

$$W(x_c, x_r, y_r) = 0 \quad \text{if} \quad (x_c, x_r - y_r) \notin \mathcal{N}, \tag{5.26}$$

where $\mathcal{N}$ denotes the neighborhood scheme of W. The corresponding momentum space representation of $\widehat{W}_p$ is given by

$$(\widehat{W}_p \psi)(q) = W(p,q)\psi(q) + \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s q \, W(p,q)(C - \mathbb{1}_{\mathcal{K}_{12}})\psi(q). \tag{5.27}$$

Clearly, for fixed p each $\widehat{W}_p$ is a unitary quantum walk with point perturbation in the sense of Definition 5.2.1, and in the following we apply the results of Section 5.2 to the family $\widehat{W}_p$. Our aim is to construct solutions of the eigenvalue equation

$$\widehat{W}_p \phi_p = z_p \phi_p \,. \tag{5.28}$$

Starting point of our analysis are the spectral gaps $\Gamma(W_p)$ of the operator W_p defined by Equation (5.24) for $C = \mathbb{1}$, i.e. W_p describes the relative motion of the non-interacting two particle quantum walk W. The spectrum of W_p is directly obtained from the Fourier transform of W. In fact, from the dispersion relations $\omega_j(p,q)$ of W, see Section 4.5.1, we obtain the dispersion relations $\omega_{j,p}(q)$ of W_p via $\omega_{j,p}(q) = \omega_j(p,q)$. Hence, by Proposition 4.5.7, we have the simple formula

$$\Gamma(W_p) = \mathbb{S} \setminus \bigcup_j \left\{ e^{\mathrm{i}\omega_j(p,q)} : q \in [-\pi,\pi)^s \right\} \tag{5.29}$$

for the spectral gaps of W_p. Assumption 5.1 translates into $z_p \in \Gamma(W_p)$, and Proposition 5.2.2 immediately shows that the essential spectrum of $\widehat{W}_p$ coincides with the spectrum of W_p. However, the eigenvalue z_p generically depends on p, which possibly leads to new components of the essential spectrum of W_{Int} as compared to W.

As in Section 5.2, we can solve the eigenvalue equation (5.28) by considering the analogous equation to (5.8). To this end, we define the operator

$$R_p(z) = \frac{1}{(2\pi)^s} \int\limits_{[-\pi,\pi)^s} d^s q \, (W(p,q) - z\,\mathbb{1}_{\mathcal{K}_{12}})^{-1} \, W(p,q). \tag{5.30}$$

Proposition 5.3.2. *For fixed $p \in [-\pi,\pi)^s$, let $z_p \in \Gamma(W_p)$ be a complex number in the spectral gap of W_p. Any eigenvector ϕ_p of $\widehat{W}_p$ corresponding to z_p determines a solution $\varphi_p \neq 0$ of*

$$\varphi_p = R_p(z_p)(\mathbb{1}_{\mathcal{K}_{12}} - C)\varphi_p \tag{5.31}$$

via the relation $\varphi_p = (2\pi)^{-s} \int_{[-\pi,\pi)^s} d^s q \, \phi_p(q)$. Conversely, any solution $\varphi_p \neq 0$ of Equation (5.31) determines an eigenvector ϕ_p corresponding to z_p via

$$\phi_p(q) = \left(W(p,q) - z_p\,\mathbb{1}_{\mathcal{K}_{12}} \right)^{-1} W(p,q)(\mathbb{1}_{\mathcal{K}_{12}} - C)\varphi_p \,. \tag{5.32}$$

Proof. This is a straightforward consequence of Proposition 5.2.3. □

Clearly, as a consequence of Lemma 5.2.4, the operator $R_p(z_p)$ is invertible for $z_p \in \Gamma(W_p)$. Thus, Equation (5.31) is equivalent to

$$C\varphi_p = (\mathbb{1}_{\mathcal{K}_{12}} - R_p(z_p)^{-1})\varphi_p \,, \tag{5.33}$$

and since the operator $(\mathbb{1}_{\mathcal{K}_{12}} - R_p(z)^{-1})$ is unitary for all $z \in \Gamma(W_p)$ we may multiply C by an appropriate phase factor to assure the existence of an eigenvalue z_p of $\widehat{W}_p$. From Proposition 5.2.5 we conclude that there are at most $\dim \mathcal{K}_{12}$ eigenvalues in each connected component of the spectral gap $\Gamma(W_p)$ in $\mathbb{S}$, cf. Figure 5.2.

Perturbation theory in p shows that the eigenvalues z_p, if they exist at a point p_0, are always defined on a sufficiently small ball around p_0. Indeed, the operator $\widehat{W}_p$ is easily seen to be bounded and analytic in a complex neighborhood of any $p \in [-\pi,\pi)^s$ in the sense of Section 3.4. Since the degeneracy of the eigenvalue z_{p_0} is at most $\dim \mathcal{K}_{12}$, we can apply the theory outlined in Section 3.4.2 to reduce the computation of z_p and corresponding eigenvectors to a finite dimensional eigenvalue problem via an analytic change of basis, see also [Bau85]. If z_{p_0} is degenerate it may split under the perturbation defining several eigenvalues $z_{j,p}$ of $\widehat{W}_p$. However, these eigenvalues are continuous, analytic for almost all p in a neighborhood G_{p_0} of p_0, and if this neighborhood is chosen sufficiently small all eigenvalues remain in the spectral gap $\Gamma(W_p)$. Since $\widehat{W}_p$ is unitary for all p we conclude that the eigenprojections corresponding to the eigenvalues $z_{j,p}$ are analytic for almost all p in G_{p_0} and cannot have poles in G_{p_0}. Hence, they define a set of normalized eigenvectors $\phi_{j,p}$ which are analytic almost everywhere in G_{p_0}. Note, however, that the behavior of eigenvectors at the boundary of G_{p_0} may very well be singular. For example, if the eigenvalue z_p approaches a value in the continuous spectrum of W_p for p moving to a point at the boundary of G_{p_0}, the estimate in Proposition 5.2.6 diverges and the corresponding eigenvector may become non-normalizable.

The typical situation is that, given an interaction operator C, there are a number of eigenvectors $\phi_{j,p}$ with eigenvalues $z_{j,p}$ in the spectral gap of W_p, which are defined for p in open subsets $A_j \subset [-\pi,\pi)^s$. The number of different $\phi_{j,p}$ at fixed p may in general depend on p, but since these are defined on open sets and there are only finitely many $\phi_{j,p}$ for any p we may chose a labeling $\alpha = 1,\dots,r < \infty$ such that the finite set of p-dependent vectors $\{\phi_{\alpha,p}\}$ covers all eigenvectors of $\widehat{W}_p$ with eigenvalues in $\Gamma(W_p)$. Here, each $\phi_{\alpha,p}$ is defined for all p in an open subset $A_\alpha \subset [-\pi,\pi)^s$. An eigenvector $\phi_{\alpha,p} \in \ell^2(\mathbb{Z}^s) \otimes \mathcal{K}_{12}$ at fixed total momentum p is clearly non-normalizable in $\ell^2(\mathbb{Z}^{2s}) \otimes \mathcal{K}_{12}$, but choosing a well-behaved momentum distribution function g on A we may construct $\psi(p) = g(p)\phi_{\alpha,p}$, which then defines a normalizable vector in $\ell^2(\mathbb{Z}^{2s}) \otimes \mathcal{K}_{12}$. More generally, we may choose well-behaved functions g_α supported on A_α and consider

$$\psi(p) = \sum_{\alpha=1}^{r} g_\alpha(p)\phi_{\alpha,p}\,, \tag{5.34}$$

which then defines a normalizable vector in $\ell^2(\mathbb{Z}^{2s}) \otimes \mathcal{K}_{12}$. For a reason, which becomes apparent momentarily, we call unit vectors of the form (5.34) molecular states of W_{Int}. Clearly, the time evolution W_{Int} maps $\psi(p)$ to another vector of the

same form, more precisely

$$(W_{\mathrm{Int}}{}^t\psi)(p)=\sum_{\alpha=1}^{r} z_{\alpha,p}^t\, g_\alpha(p)\phi_{\alpha,p}\,. \tag{5.35}$$

Next we prove that the eigenvectors $\phi_{\alpha,p}$ are exponentially localized and the decay rate is essentially determined by the distance of $z_{\alpha,p}$ to the spectrum of W_p, which clarifies the intention of our term molecular state for Equation (5.34).

Proposition 5.3.3. *Let ψ be a molecular state for W_{Int} of the form* (5.34)*. The eigenvectors $\phi_{\alpha,p}=\sum_{x\in\mathbb{Z}^s}|x\rangle\otimes\phi_{\alpha,p,x}$ at fixed total momentum p satisfy*

$$\left\|\phi_{\alpha,p,x}\right\|\leq\frac{C_1}{\mathrm{dist}(z,\sigma(W_p))}\,e^{-C_2\mathrm{dist}(z,\sigma(W_p))\|x\|}\,,\quad\forall x\in\mathbb{Z}^s\,, \tag{5.36}$$

with positive constants C_1 and C_2 which are independent of p. Moreover, if the functions $g_\alpha(p)$ are such that $z_{\alpha,p}\in\Gamma(W_p)$ for all p in the support of g_α, we have the bound

$$\mathrm{Prob}(x_1-x_2=y)\leq K_1 e^{-K_2\|y\|}\,,\quad K_1,K_2>0,\,y\in\mathbb{Z}^s \tag{5.37}$$

on the probability to obtain the result $x_r=y$ for a measurement of the particles' relative distance with constants K_1,K_2 independent of the number of time steps.

Proof. Without loss we assume the vector ψ to be of the form $\psi(p)=g(p)\phi_p$, i.e. the sum over α is trivial, and denote the eigenvalue corresponding to ϕ_p by z_p.

By Equation (5.32) we have the relation

$$\phi_p=(W_p-z_p\,\mathbb{1}_{\mathbb{Z}^s}\otimes\mathbb{1}_{\mathcal{K}_{12}})^{-1}W_p\left(\mathbb{1}_{\mathbb{Z}^s}\otimes(\mathbb{1}_{\mathcal{K}_{12}}-C)\right)\widehat{\varphi}_p$$

for some vector $\widehat{\varphi}_p\in\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ which is supported at the origin, i.e. $\widehat{\varphi}_p=|0\rangle\otimes\varphi_p$. Note that this equation is just the position space representation of Equation (5.32). Clearly, the vector $W_p(\mathbb{1}_{\mathbb{Z}^s}\otimes(\mathbb{1}_{\mathcal{K}}-C))\widehat{\varphi}_p$ is strictly localized with a bound on the region independent of p. Thus, the assertion follows if we can prove a bound of the form

$$|\langle x\otimes\eta|(W_p-z_p\,\mathbb{1}_{\mathbb{Z}^s}\otimes\mathbb{1}_{\mathcal{K}_{12}})^{-1}|y\otimes\gamma\rangle|\leq\left\|\eta\right\|\left\|\gamma\right\|\frac{C_3}{\mathrm{dist}(z,\sigma(W_p))}\,e^{-C_4\mathrm{dist}(z,\sigma(W_p))\|x-y\|}$$

with positive constants C_3 and C_4 which are independent of p. We prove such a bound in Appendix A, see Lemma A.0.1.

By the previous result we have

$$\begin{aligned}\mathrm{Prob}(x_1-x_2=y) &= \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\,|g(p)|^2\langle\phi_p|(|y\rangle\langle y|\otimes\mathbb{1}_{\mathcal{K}_{12}}|\phi_p\rangle \\ &\leq \frac{C_1^2}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\,|g(p)|^2\frac{1}{\mathrm{dist}(z_p,\sigma(W_p))^2}\,e^{-2C_2\mathrm{dist}(z_p,\sigma(W_p))\|y\|}\,.\end{aligned} \tag{5.38}$$

If the function $g(p)$ is such that $z_p \in \Gamma(W_p)$ for all p in the support of $g(p)$ we can find a strictly positive lower bound for the distance of z_p to the spectrum of $W(p)$, i.e. $\mathrm{dist}(z_p, \sigma(W_p)) \geq K$ for all $p \in \mathrm{supp}(g)$. For such functions g we get a bound

$$\mathrm{Prob}(x_1 - x_2 = y) \leq K_1 e^{-K_2 \|y\|}$$

with positive constants K_1 and K_2. □

For sufficiently well-behaved momentum distribution functions g_α, the relative distance of the two particles in a molecular state (5.34) is exponentially bounded in probability for an arbitrary number of time steps. However, if we start the quantum walk W_{Int} with an arbitrary initial state ψ, there are typically two contributions to the probability distribution of the quantum particles. The first is the contribution of the projection of ψ to the molecular states, which is characterized by

$$\psi_M(p) = \sum_{\alpha=1}^{r} \langle \phi_{\alpha,p} | \psi(p) \rangle \cdot \phi_{\alpha,p}\,, \tag{5.39}$$

where the occurring scalar products $\langle \phi_{\alpha,p} | \psi(p) \rangle$ are understood to be zero at total momenta p where the state $\phi_{\alpha,p}$ does not exist. The previous proposition shows that the relative distance of the particles described by the fraction ψ_M is typically bounded in probability by an exponential for all times. We will further analyze the dynamics of these molecular states in the next section.

The second contribution comes from the states which have no overlap with the eigenvectors of $\widehat{W_p}$ for fixed total momentum. These are states of the form (5.34), but with $\phi_{\alpha,p}$ in the continuous subspace of $\widehat{W_p}$. For these states we expect the relative distance of the two particles to grow unboundedly, since their component for fixed p is in the continuous spectrum of $\widehat{W_p}$. Therefore we call such states free states of W_{Int}.

Of course, there may be more contributions to the probability distribution. For example, if $\widehat{W_p}$ exhibits eigenvalues embedded in the continuous spectrum, or if the momentum distribution function g_α is supported on a set in which the eigenvalue $z_{\alpha,p}$ touches the continuous spectrum of W_p, both situations in which the exponential bound for the extension of the particles' relative distance according to Proposition 5.3.3 is not valid.

Dynamics of the molecular states

We saw in the last section that molecular states are invariant with respect to the time evolution W_{Int} and the relative distance of the two particles in a molecular state ψ is typically bounded by an exponential which is independent of the number of time steps. However, since the eigenvalues z_p are in general p-dependent, they are not eigenvalues of the whole operator W_{Int} and the part of the complex plane

covered by the values z_p is a subset of the continuous spectrum of W_{Int}. By the RAGE Theorem 3.3.6, this implies that the two particles, instead of being trapped in a finite region of the lattice, leave any finite volume, at least in the time averaged sense. Since ψ is assumed to be a molecular state for W_{Int} we conclude that the particles move as a compound on the lattice $\mathbb{Z}^s$. We can further analyze the motion of this compound by a method similar to the one developed in Section 4.5.1 for translationally invariant and unitary quantum walks. Since the modulus of the eigenvalues $z_{\alpha,p}$ of $\widehat{W}_p$ is one, we can write them as $z_{\alpha,p} = e^{\mathrm{i}\omega_\alpha(p)}$ with real-valued functions $\omega_\alpha(p)$. Thus Equation (5.35) takes the form

$$(W_{\text{Int}}{}^t\psi)(p) = \sum_{\alpha=1}^{r} e^{\mathrm{i}t\omega_\alpha(p)} g_\alpha(p)\phi_{\alpha,p}\,, \tag{5.40}$$

for a molecular state ψ according to Equation (5.34). This equation is very similar to the time evolution of a translationally invariant and unitary quantum walk $W(p)$ if we identify the $\phi_{\alpha,p}$ with the p-dependent eigenvectors of $W(p)$. To further amplify this similarity, we introduce the p-dependent eigenprojections $\mathbf{P}_\alpha = |\phi_{\alpha,p}\rangle\langle\phi_{\alpha,p}|$, such that the action of W_{Int} on molecular states is described by

$$W_{\text{Int}} = \sum_{\alpha=1}^{r} e^{\mathrm{i}\omega_\alpha(p)}\mathbf{P}_\alpha\,. \tag{5.41}$$

In contrast to the spectral decomposition for translationally invariant unitary quantum walks, as discussed in Section 4.5.1, the operators $\mathbf{P}_\alpha$ act on an infinite dimensional Hilbert space $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}_{12}$ and are possibly only defined on subsets $A_\alpha \subset [-\pi,\pi)^s$. Nevertheless, each $\mathbf{P}_\alpha$ is analytic at almost all p in A_α. If we now identify the center of mass coordinate $x_c = (x_1+x_2)/2$ of the two particles with the molecule's position, we have a notion of asymptotic limit for the probability distribution of the molecule's position, which is described by the observable $(Q_1+Q_2)/2$. By a similar reasoning as in Section 4.5.1, the characteristic function of this asymptotic distribution with initial state $\rho_M = |\psi_M\rangle\langle\psi_M|$ amounts to

$$\begin{aligned} C_M(\lambda) &= \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\,\mathrm{tr}\sum_{\alpha=1}^{r} e^{\left(\mathrm{i}\frac{d\omega_\alpha(p+\varepsilon\lambda)}{d\varepsilon}\right)}\Big|_{\varepsilon=0}\mathbf{P}_\alpha\rho_M(p) \\ &= \frac{1}{(2\pi)^s}\int\limits_{[-\pi,\pi)^s} d^s p\sum_{\alpha=1}^{r}|g_\alpha(p)|^2\, e^{\left(\mathrm{i}\frac{d\omega_\alpha(p+\varepsilon\lambda)}{d\varepsilon}\right)}\Big|_{\varepsilon=0}\,. \end{aligned} \tag{5.42}$$

An interesting question at this point is whether the asymptotic distribution according to this formula, as well as the finite time steps dynamics (5.40), can be interpreted as a quantum walks in its own right. In other words, we would like to answer

the question whether the effective dynamics of the molecular state of the two quantum particles is again described by a one-particle quantum walk. Of course, for this to be true the first trivial necessity is that the functions ω_α are the dispersion relations of a single-particle quantum walk V. Indeed, assume the Fourier transform $V(p)$ of V has eigenvalues $e^{\mathrm{i}\omega_\alpha(p)}$ and corresponding eigenvectors $\eta_\alpha(p)$, then Equation (5.42) describes the asymptotic position distribution of V with initial state ψ_0 defined by

$$\psi_0(p)=\sum_{\alpha=1}^{r} g_\alpha(p)\eta_\alpha(p). \tag{5.43}$$

Actually, we can multiply the eigenvectors $\eta_\alpha(p)$ by arbitrary phases $e^{\mathrm{i}f_\alpha(p)}$, with f_α real-valued, and the resulting state ψ_0 yields the same asymptotic position distribution.

The question whether Equation (5.40) can be interpreted as quantum walk of a single particle turns out to be more difficult. Suppose V is a translationally invariant unitary single-particle quantum walk on $\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ such that its dispersion relations coincide with the functions ω_α on the sets $A_\alpha\subset[-\pi,\pi)^s$. It seems to be natural to identify the eigenvectors $\eta_\alpha(p)$ of $V(p)$ with the $\phi_{\alpha,p}$, but since these eigenvectors are not unique we have to decide for a particular choice. More precisely, we may alternatively identify $e^{\mathrm{i}f_\alpha(p)}\eta_\alpha(p)$ with $\phi_{\alpha,p}$ for real-valued functions f_α. This is effectively a change of basis according to the translationally invariant unitary operator U defined via

$$U(p)=\sum_{\alpha=1}^{r} e^{\mathrm{i}f_\alpha(p)}|\eta_\alpha(p)\rangle\langle\eta_\alpha(p)|. \tag{5.44}$$

Any such choice of identification of the eigenvectors of $V(p)$ and W_{Int} gives us a notion of position for the molecular states, which, however, may be different from the center of mass coordinate. More precisely, a state $\psi\in\ell^2(\mathbb{Z}^s)\otimes\mathcal{K}$ defines a molecular state in $\ell^2(\mathbb{Z}^{2s})\otimes\mathcal{K}_{12}$ via

$$\widehat{\psi}(p)=\sum_{\alpha=1}^{r} e^{-\mathrm{i}f_\alpha(p)}\langle\eta_\alpha(p)|\psi(p)\rangle\phi_{\alpha,p}\,, \tag{5.45}$$

where the occurring scalar product is understood to be zero if the state $\phi_{\alpha,p}$ is not defined. In general, the position distribution defined by the state ψ will be different from the distribution of the center of mass coordinate according to $\widehat{\psi}$. For instance, a state ψ which is localized at the origin may be mapped to a state $\widehat{\psi}$ with center of mass distribution which is smeared out over several lattice sites. Another subtlety is that the eigenvectors $\phi_{\alpha,p}$ are possibly only defined on a subset of momentum space. Consequently, the set of possible molecular states is restricted to certain states, i.e. a molecular state with center of mass coordinate $(x_1+x_2)/2=0$ may be ill-defined.

5.3.3. Interacting many-particle quantum walks

The aim of this section is to construct a generalization of interacting two-particle quantum walks, as considered in the last section, to an arbitrary number of particles. An interaction is again only to happen if several particles collide at one lattice site, and when the particles are at different lattice sites they independently undergo translationally invariant single-particle quantum walks. The overall time evolution is assumed to be particle number conserving and unitary. In contrast to Hamiltonian systems, where the many-particle dynamics is easily obtained as a sum of all two-body interactions, the unitary time evolution of several particles is in general not uniquely determined by the one- and two-particle dynamics. For instance, consider an interacting quantum walk of two particles and add another particle to the system. In order to define the dynamics of the three particles we have to specify the interaction operator for the case when all three particles occupy the same lattice site. Naively, we could try to mimic the Hamiltonian approach by multiplying all possible two body interactions, but since these will in general not commute we have to decide for a particular ordering of this product. In fact, we could even define a quantum walk with three-body interaction, which is completely independent of the two-body interactions, e.g. no interaction if two particles collide but non-trivial interaction when all three particles meet at one lattice site.

In principle, we could use the Hilbert space introduced in Equation (5.13) to describe an interacting quantum walk of finitely many particles by a unitary operator. For this we either have to fix a number of particles, or we use a Fock space construction. However, we also want to allow for states of the system with infinitely many particles, hence, we need a suitable description of our system. In the following we make use of the concept of quantum cellular automata to construct a time evolution which generalizes interacting two-particle quantum walks to an arbitrary number of particles. We assume the particles to be indistinguishable, although we allow for several species of particles. Hence, a quantum walk of finitely many distinguishable particles can be realized by an initial state with particle number equal to one for each type of particle. Before we deepen our analysis of many-particle quantum walks we provide some background on the theory of quantum cellular automata in the next section.

Quantum cellular automata

The purpose of this section is to mostly to fix the notation and provide a basic definition of a quantum cellular automaton, which we henceforth abbreviate as QCA. For a thorough introduction to this topic we refer to [SW04, Vog09]. The physical system we consider is the composite system of infinitely many quantum systems described by Hilbert spaces $\mathcal{H}_x$, labeled by $x \in \mathbb{Z}^s$. The intuitive picture is that of a lattice $\mathbb{Z}^s$ where each cell carries a subsystem $\mathcal{H}_x$. Since the infinite tensor

product of the Hilbert spaces $\mathcal{H}_x$ has some disadvantages [Vog09], we choose another approach to describe the time evolution of the system. To begin with, we only consider translationally invariant systems, i.e. $\mathcal{H}_x = \mathcal{H}$ and we focus again on the observables rather than the states of the system, that is, we formulate the time evolution in the Heisenberg picture. Of course, we have to be a bit careful about the construction of observables on the infinite lattice, the crucial point is to restrict to observables which can be approximated by operators which are supported on finite subregions of $\mathbb{Z}^s$. This leads to the notion of the quasi-local algebra over $\mathbb{Z}^s$.

Definition 5.3.4. *Let $\mathcal{H}$ be a separable Hilbert space, $\Lambda \subset \mathbb{Z}^s$ a finite subset of $\mathbb{Z}^s$ and define*

$$\mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{B}(\mathcal{H}).$$

For $\Lambda_1 \subset \Lambda_2$ we define the embedding of $\mathcal{A}_{\Lambda_1}$ into $\mathcal{A}_{\Lambda_2}$ by tensoring with the identity on $\mathbb{1}_{\Lambda_2\setminus\Lambda_1}$. The corresponding quasi-local algebra $\mathcal{A}$ is the norm closure of the union of all $\mathcal{A}_\Lambda$ for finite $\Lambda \subset \mathbb{Z}^s$, i.e.

$$\mathcal{A} = \overline{\bigcup_\Lambda \mathcal{A}_\Lambda}.$$

A state ω of $\mathcal{A}$ is a positive and normalized linear functional, i.e. $\omega(A^*A) \geq 0$ for all $A \in \mathcal{A}$ and $\omega(\mathbb{1}) = 1$.

A QCA represents the time evolution of the quantum system described by $\mathcal{A}$ with the additional assumption of locality in the sense that propagation speed is strictly finite. On $\mathcal{A}$ there is a natural definition of operators τ_x translating the system by a lattice vector $x \in \mathbb{Z}^s$ via

$$\tau_x(\mathcal{A}_\Lambda) = \mathcal{A}_{\Lambda+x}. \tag{5.46}$$

In the following we consider QCAs which are reversible and commute with all translations τ_x.

Definition 5.3.5. *A translationally invariant and reversible quantum cellular automaton is a local $*$-automorphism $\mathbf{T} : \mathcal{A} \to \mathcal{A}$ commuting with all translations of $\mathbb{Z}^s$. That is, $\mathbf{T}$ satisfies the following conditions:*

i) $\mathbf{T}(AB) = \mathbf{T}(A)\mathbf{T}(B)$, $\mathbf{T}(A^*) = \mathbf{T}(A)^*$ *for all $A, B \in \mathcal{A}$, and $\mathbf{T}$ is invertible.*

ii) There exists a finite subset $\mathcal{N} \subset \mathbb{Z}^s$ such that for each finite subset $\Lambda \subset \mathbb{Z}^s$

$$\mathbf{T}(A_\Lambda) \subset \mathcal{A}_{\Lambda+\mathcal{N}}.$$

The set $\mathcal{N}$, which is chosen minimal, is called the neighborhood scheme of $\mathbf{T}$.

iii) $\mathbf{T} \circ \tau_x(A) = \tau_x \circ \mathbf{T}(A)$ *for all $x \in \mathbb{Z}^s$ and $A \in \mathcal{A}$.*

In this definition, invertibility is the generalization of unitarity of the time evolution. As a direct consequence of the homomorphism property and the invertibility we have that $\mathbf{T}$ is completely positive and unital. Hence, any $\mathbf{T}$ compatible with Definition 5.3.5 constitutes a quantum channel on the observable algebra $\mathcal{A}$.

Clearly, by the locality condition we have that the restriction of $\mathbf{T}$ to the lattice site at the origin is a map $\mathbf{T}_0 : \mathcal{A}_0 \to \mathcal{A}_\mathcal{N}$. Using translation invariance and the homomorphism property of $\mathbf{T}$ we get that $\mathbf{T}$ is uniquely determined by $\mathbf{T}_0$, [SW04, Vog09]. Following the terminology of [SW04, Vog09], we refer to $\mathbf{T}_0$ as the local rule for $\mathbf{T}$. If $A \in \mathcal{A}_\Lambda$, with $\Lambda \subset \mathbb{Z}^s$ finite, is a local element of the form $A = \otimes_{x\in\Lambda} A_x$ then $\mathbf{T}(A) = \prod_{x\in\Lambda} \mathbf{T}_x(A_x)$, where $\mathbf{T}_x = \tau_x \circ \mathbf{T}_0 \circ \tau_x^{-1}$ and all factors in this product commute since $\mathbf{T}$ is an automorphism. We will use this property in the following to determine $\mathbf{T}$ from a description on finitely many lattice sites.

Quantum cellular automata description for interacting quantum walks

In this section, we devise a QCA which simulates an interacting quantum walk of several particles. To this end, we further develop a construction scheme for a QCA to implement arbitrary single-particle quantum walks on a one-dimensional lattice as introduced in [Vog09]. Similarly to the case of two-particle quantum walks, we assume that the time evolution is a composition $\mathbf{T}_{\mathrm{QW}} = \mathbf{T}_{\mathrm{I}} \circ \mathbf{T}_{\mathrm{N}}$ of two building blocks, which both are particle number conserving QCAs in their own right. The QCA $\mathbf{T}_{\mathrm{N}}$ stands for the non-interacting evolution of the quantum particles, which is nothing but the independent motion of each particle according to some translationally invariant and unitary single-particle quantum walk. The second part $\mathbf{T}_{\mathrm{I}}$ mediates the collisional interaction, that is, it is a strictly local operation acting on each cell individually such that it leads to no propagation.

We take the Hilbert space $\mathcal{H}$ underlying the quasi-local algebra $\mathcal{A}$ as the linear span of vectors which represent different numbers of particles occupying the same lattice site. In order to construct $\mathcal{H}$ we assume a specific form of the non-interacting part $\mathbf{T}_{\mathrm{N}}$. Suppose there are N species of particles, which independently undergo translationally invariant unitary quantum walks if there is no interaction. We denote the unitary operator implementing the single-particle quantum walk for particle species j by W_j, and our main assumption is that these are coined quantum walks in the sense of Equation (4.23). More precisely, we assume without loss of generality that each W_j can be written as a composition of a single shift and coin operator , that is, $W_j = S_j(\mathbb{1}_{\mathbb{Z}^s} \otimes U_j)$. If W_j consists of several shift and coin operators we can write it as a composition of such simple operators, and the corresponding QCA is just the composition of several simpler QCAs. In fact, we will also compute the QCAs corresponding to the shift and coin operator separately. First we choose a basis $\{\phi_{j,k}\}$ for each internal degree of freedom $\mathcal{K}_j$ such that the shift operators S_j can be written as

$$S_j|x, \phi_{j,k}\rangle = |x + y_k, \phi_{j,k}\rangle. \tag{5.47}$$

With these states we can construct the Hilbert space $\mathcal{H}$, which defines the quasi-local algebra $\mathcal{A}$, in the following way: We introduce vectors

$$|\mathbf{n}_1,\ldots,\mathbf{n}_N\rangle = |n_1(1),\ldots,n_1(d_1)\rangle\otimes\ldots\otimes|n_N(1),\ldots,n_N(d_N)\rangle\,,\quad d_j=\dim\mathcal{K}_j\,, \tag{5.48}$$

which we interpret as a state with $n_j(k)$ particles of type j in mode $\phi_{j,k}$, and we abbreviate $\mathbf{n}_j=(n_j(1),\ldots,n_j(d_j)$. The Hilbert space $\mathcal{H}$ is defined as the closed linear span of these vectors, that is,

$$\begin{aligned}\mathcal{H} &= \overline{\operatorname{span}\left\{|n_1,\ldots,n_{d_1}\rangle\otimes\ldots\otimes|m_1,\ldots,m_{d_N}\rangle\right\}} \\ &= \bigotimes_{j=1}^{N}\ell^2(\Gamma_j)^{\otimes d_j}\,,\end{aligned} \tag{5.49}$$

where $\Gamma_j=\{0,1\}$ if species j has fermionic statistics and $\Gamma_j=\mathbb{N}_0$ if the statistics is bosonic.

Now it is straightforward to define the action of $\mathbf{T}_\mathrm{N}$ on the quasi-local algebra generated by $\mathcal{H}$. By assumption, $\mathbf{T}_\mathrm{N}$ can be written as

$$\mathbf{T}_\mathrm{N}=\left(\mathbf{T}_{S_1}\otimes\ldots\otimes\mathbf{T}_{S_N}\right)\circ\left(\mathbf{T}_{U_1}\otimes\ldots\otimes\mathbf{T}_{U_N}\right)\,, \tag{5.50}$$

where $\mathbf{T}_{S_j}$ and $\mathbf{T}_{U_j}$ are QCAs representing the shift and coin operator, respectively, acting on particle species j. Thus, it is sufficient to give a construction scheme for a single $\mathbf{T}_{S_j}$ and $\mathbf{T}_{U_j}$ to determine $\mathbf{T}_\mathrm{N}$. Consequently, we assume henceforth that there is only one particle species with non-interacting dynamics determined by $W=S(\mathbb{1}_{\mathbb{Z}^s}\otimes U)$. The single-cell Hilbert space is given by $\mathcal{H}=\ell^2(\Gamma)^{\otimes d}$ with $d=\dim\mathcal{K}$ and $\Gamma=\{0,1\}$ or $\Gamma=\mathbb{N}_0$. Since a translationally invariant QCA is uniquely determined by its local rule, we only have to specify the action of $\mathbf{T}_S$ and $\mathbf{T}_U$ on the subalgebra $\mathcal{A}_0$. In the following we use the notation $[A]_\Lambda$ for an element $A\in\mathcal{A}_\Lambda$ embedded into $\mathcal{A}$. With this notation we can identify each element $A\in\mathcal{A}_0$ with $[A]_0\in\mathcal{A}$. For determining the local rule of a QCA $\mathbf{T}$ it makes no difference whether one considers the infinite system over $\mathbb{Z}^s$, or a sufficiently large but finite subsystem with periodic boundary conditions.[1] On such a finite subset Λ of $\mathbb{Z}^s$ the QCA is unitarily implemented, that is, there is a unitary $V\in\mathcal{A}_\Lambda$ such that $\mathbf{T}(A)=V^*AV$ for all $A\in\mathcal{A}_\Lambda$. Therefore it is sufficient to have knowledge of the unitary V to determine the local rule for $\mathbf{T}$. For the shift part $\mathbf{T}_S$ of $\mathbf{T}_\mathrm{N}$, the corresponding unitary V_S acts like

$$V_S\bigotimes_{x\in\Lambda}|n_{1,x},\ldots,n_{d,x}\rangle=\bigotimes_{x\in\Lambda}|n_{1,x-v_1},\ldots,n_{d,x-v_d}\rangle\,. \tag{5.51}$$

Consequently, we obtain the local rule of the shift part as

$$\mathbf{T}_S([|n_1,\ldots,n_d\rangle\langle m_1,\ldots,m_d|]_0)=\prod_{k=1}^{d}[|n_k\rangle\langle m_k|\otimes\mathbb{1}]_{-y_k}\,, \tag{5.52}$$

[1] This is essentially the content of the so-called wrapping lemma, see [SW04, Vog09].

which is correct for both cases, fermionic and bosonic statistics.

In order to define the QCA corresponding to the coin operator $(\mathbb{1}_{\mathbb{Z}^s} \otimes U)$ we introduce the notation $\mathbb{Z}_d = \{1,\dots,d\}$, and we denote vectors in $\mathbb{Z}_d^M$ by greek letters $\alpha = (\alpha_1,\dots,\alpha_M)$ with $\alpha_j \in \mathbb{Z}_d$. Moreover, for any such α we define the vector

$$\mathbf{K}_\alpha = (K_1(\alpha),\dots,K_d(\alpha)) \quad , \quad K_j(\alpha) = |\{r : \alpha_r = j\}|, \tag{5.53}$$

that is, $\mathbf{K}_\alpha$ counts how often each mode-label k occurs in α. With this notation we can write the unitary V_U implementing $\mathbf{T}_U$ on the finite subsystem $\Lambda = \{0\}$ as

$$V_U|\mathbf{n}\rangle = \sum_{\alpha \in \mathbb{Z}_d^{|\mathbf{n}|_1}} F_\pm(\mathbf{K}_\alpha) C_\alpha^{\mathbf{n}} |\mathbf{K}_\alpha\rangle\,, \tag{5.54}$$

where $F_\pm$ are two functions which distinguish bosonic and fermionic statistics and $|\mathbf{n}|_1$ denotes the ℓ^1-norm of $\mathbf{n}$. The function F_+ for bosonic statistics is in fact identically one, i.e. $F_+(\mathbf{n}) = 1$ for all $\mathbf{n}$, and for fermionic particles we have the function F_- according to

$$F_-(\mathbf{n}) = \begin{cases} 1 & , \quad \mathbf{n} \in \{0,1\}^{|\mathbf{n}|_1} \\ 0 & , \quad \text{else} \end{cases} \quad . \tag{5.55}$$

In order to derive a formula for the coefficients $C_\alpha^{\mathbf{n}}$ we choose a sequence $\beta^{\mathbf{n}} \in \mathbb{Z}_d^{|\mathbf{n}|_1}$ such that $\mathbf{K}_{\beta^{\mathbf{n}}} = \mathbf{n}$ and define

$$C_\alpha^{\mathbf{n}} = \prod_{j=1}^{|\mathbf{n}|_1} U_{\alpha_j \beta_j^{\mathbf{n}}}\,. \tag{5.56}$$

Note that although the coefficients $C_\alpha^{\mathbf{n}}$ depend on the choice of $\beta^{\mathbf{n}}$, the action of the operator V_U defined via (5.54) is independent of this choice. To verify this statement let us abbreviate $\widehat{n} = |\mathbf{n}|_1$ and denote the set of all permutations of $\widehat{n}$ elements by $\mathcal{S}_{\widehat{n}}$. Then for any $\pi \in \mathcal{S}_{\widehat{n}}$ let $\alpha_\pi = (\alpha_{\pi(1)},\dots,\alpha_{\pi(\widehat{n})})$ denote the vector obtained by permuting the components of α according to π. The operator V_U can be expressed as

$$V_U|\mathbf{n}\rangle = \sum_{|\mathbf{k}|_1 = |\mathbf{n}|_1} F_\pm(\mathbf{k}) C_{\mathbf{k}}^{\mathbf{n}} |\mathbf{k}\rangle\,, \tag{5.57}$$

with coefficients

$$C_{\mathbf{k}}^{\mathbf{n}} = \sum_{\pi \in \mathcal{S}_{\widehat{n}}} C_{\alpha_\pi}^{\mathbf{n}} \tag{5.58}$$

which are clearly independent of the choice of $\beta^{\mathbf{n}}$.

From these formulas, we obtain the action of $\mathbf{T}_U = V_U^* . V_U$ as

$$\mathbf{T}_U([|\mathbf{n}\rangle\langle\mathbf{m}|]_0) \quad = \quad \sum_{|\mathbf{k}|_1 = |\mathbf{n}|_1} \sum_{|\mathbf{l}|_1 = |\mathbf{m}|_1} F_\pm(\mathbf{k}) F_\pm(\mathbf{l}) \overline{C_{\mathbf{n}}^{\mathbf{k}}} C_{\mathbf{m}}^{\mathbf{l}} \, [|\mathbf{k}\rangle\langle\mathbf{l}|]_0\,.$$

What remains is to define the interaction part $\mathbf{T}_{\mathrm{I}}$ of $\mathbf{T}_{\mathrm{QW}}$. Basically, the QCA $\mathbf{T}_{\mathrm{I}}$ has to satisfy two requirements: It has to be particle number conserving and strictly local in the sense that the neighborhood scheme of $\mathbf{T}_{\mathrm{I}}$ equals $\mathcal{N}_{\mathrm{I}} = \{0\}$. In fact, any QCA satisfying these two requirements yields a valid interaction for our many-particle quantum walk $\mathbf{T}_{\mathrm{QW}}$. The simplest case is an interaction phase depending on the particle numbers, which is described by a real-valued function $f(\mathbf{n}_1, \ldots, \mathbf{n}_N)$ of the particle numbers and the formula

$$\mathbf{T}_{\mathrm{I},f}([|\mathbf{n}_1, \ldots, \mathbf{n}_N\rangle\langle\mathbf{m}_1, \ldots, \mathbf{m}_N|]_0) = e^{\mathrm{i}(f(\mathbf{m}_1,\ldots,\mathbf{m}_N)-f(\mathbf{n}_1,\ldots,\mathbf{n}_N))}\,[|\mathbf{n}_1, \ldots, \mathbf{n}_N\rangle\langle\mathbf{m}_1, \ldots, \mathbf{m}_N|]_0\,. \tag{5.59}$$

In Example 9 we determine a QCA generalizing the interacting Hadamard walk considered in Interlude 6 to an arbitrary particle number with collisional interaction.

Excitations over invariant states

As an application of the formalism introduced in the previous section we study now the behavior of excitations in many-particle quantum walks. To this end we employ the Gelfand-Naimark-Segal (GNS) construction, which we briefly describe in the following. For a thorough introduction we refer to [BR02]. Given a state ω on a quasi-local algebra $\mathcal{A}$, the GNS construction yields a Hilbert space $\mathcal{H}_\omega$, a representation π of $\mathcal{A}$ on $\mathcal{H}_\omega$, and a normalized vector $\Omega \in \mathcal{H}_\omega$ such that

$$\omega(A) = \langle\Omega|\pi(A)|\Omega\rangle \quad \forall\, A \in \mathcal{A}\,. \tag{5.60}$$

Moreover, the vector Ω is cyclic with respect to the representation π, by which we mean that the set of all vectors $\pi(A)\Omega$, with $A \in \mathcal{A}$, is dense in $\mathcal{H}_\omega$. The GNS Hilbert space $\mathcal{H}_\omega$ is constructed from the algebra $\mathcal{A}$ in the following way: First one defines a sesqui-linear form on $\mathcal{A}$ via

$$(A|B) = \omega(A^*B) \tag{5.61}$$

for $A, B \in \mathcal{A}$. One can then prove that the quotient of $\mathcal{A}$ and the set $I = \{A \in \mathcal{A} : \omega(A^*A) = 0\}$ is a well-defined object. In fact, completion of this quotient yields the GNS Hilbert space, i.e. $\mathcal{H}_\omega = \overline{\mathcal{A}/I}$. We will write Ω_A for the vector in $\mathcal{H}_\omega$ associated with the equivalence class of $A \in \mathcal{A}$ in the quotient $\mathcal{A}/I$. Since the algebra $\mathcal{A}$ acts on itself via left multiplication, we obtain a representation of $\mathcal{A}$ on $\mathcal{H}_\omega$ via $\pi(A)\Omega_B = \Omega_{AB}$. The representation π takes values in the set of bounded linear operators on $\mathcal{H}_\omega$, and it is straightforward to verify that

$$\langle\Omega_A|\pi(B)|\Omega_C\rangle = \omega(A^*BC)\,. \tag{5.62}$$

Thus we obtain Equation (5.60) by setting $\Omega = \Omega_{\mathbb{1}}$.

If the state ω is invariant with respect to a QCA $\mathbf{T}$ on $\mathcal{A}$, it is straightforward to verify that $\mathbf{T}$ induces a well-defined map $\mathbf{T}_\omega$ acting on the subset $\{\pi(A) : A \in \mathcal{A}\}$ of $\mathcal{B}(\mathcal{H}_\omega)$ via $\mathbf{T}_\omega(\pi(A)) = \pi(\mathbf{T}(A))$. In fact, the map $\mathbf{T}_\omega$ is unitarily implemented [BR02].

That is, if ω satisfies $\omega(\mathbf{T}(A)) = \omega(A)$ for all $A \in \mathcal{A}$, then $\pi(\mathbf{T}(A)) = V^*\pi(A)V$ with a unitary operator $V \in \mathcal{B}(\mathcal{H}_\omega)$, and $V\Omega_{\mathbb{1}} = \Omega_{\mathbb{1}}$. Given such an invariant state and an element $A \in \mathcal{A}$, one can define an excited state over ω as the states ω_A which acts like $\omega_A(B) = \omega(A^*BA)$. Of course, for ω_A to be a state, the element A has to satisfy $\omega(A^*A) = 1$.

Of particular interest to us are excited states ω_A, where A can be identified with a change of the particle number of a single cell. For simplicity we consider only QCAs with a single species of particles, which we take as bosons, such that there is no limit on the number of particles per cell and mode. So let $\mathbf{T}$ denote a QCA according to the preceding section, i.e. $\mathbf{T}$ generalizes an interacting quantum walk to arbitrary particle numbers. We assume again that $\mathbf{T}$ is the composition of a non-interacting dynamics $\mathbf{T}_\mathrm{N}$, which represents the independent dynamics of the quantum particles according to single-particle quantum walks, and an interaction $\mathbf{T}_\mathrm{I}$. Now let ω be an invariant state for $\mathbf{T}$, and denote by $A_{x,k} \in \mathcal{A}$ the operator which increases the particle number in cell $x \in \mathbb{Z}^s$ and mode k by one, i.e.

$$A_{x,k} = \left[\mathbb{1} \otimes \sum_{n_k=0}^{\infty} |n_k+1\rangle\langle n_k| \right]_x . \tag{5.63}$$

Then, for $\mathbf{x} = (x_1, \dots x_n) \in (\mathbb{Z}^s)^n$ and $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}_d^n$, we can study the behavior of states $\omega_{\mathbf{x},\mathbf{k}}$ defined via

$$\omega_{\mathbf{x},\mathbf{k}}(B) = \omega\left(\prod_{j=1}^{n} A_{x_j,k_j}^* \, B \prod_{j=1}^{n} A_{x_j,k_j} \right) . \tag{5.64}$$

We interpret $\omega_{\mathbf{x},\mathbf{k}}$ as a state of n excitations over a background of possibly infinitely many particles as described by ω. Since ω is invariant with respect to $\mathbf{T}$, the time evolution of the expectation values of an observable $B \in \mathcal{A}$ with respect to $\omega_{\mathbf{x},\mathbf{k}}$ is described by

$$\omega_{\mathbf{x},\mathbf{k}}(\mathbf{T}(B)) = \omega\left(\mathbf{T}^{-1}\left(\prod_{j=1}^{n} A_{x_j,k_j} \right)^* B \mathbf{T}^{-1}\left(\prod_{j=1}^{n} A_{x_j,k_j} \right) \right) . \tag{5.65}$$

Using the GNS Hilbert space we can write this as

$$\omega_{\mathbf{x},\mathbf{k}}(\mathbf{T}(B)) = \langle \Omega_{\mathbf{x},\mathbf{k}} | V^*\pi(B)V | \Omega_{\mathbf{x},\mathbf{k}} \rangle , \tag{5.66}$$

with the unitary V implementing $\mathbf{T}$ and $\Omega_{\mathbf{x},\mathbf{k}} = \prod_{j=1}^{n} \pi(A_{x_j,k_j})\Omega$.

A state which is trivially invariant with respect to $\mathbf{T}$ is the vacuum state ω_0, and excitations by $A_{\mathbf{x},\mathbf{k}}$ with $\mathbf{x} = (x_1)$ and $\mathbf{x} = (x_1, x_2)$ simulate the one- and two-particle dynamics, respectively, of the QCA $\mathbf{T}$. That is, these excitations behave exactly like

an interacting quantum walk of one and two particles. For a QCA generalizing the interacting two-particle quantum walk according to Interlude 6, we construct an invariant state with infinitely many particles in Example 9. Subsequently, we study the behavior of excitations with respect to this state and find that their dynamics is described by a many-particle quantum walk again.

5.4. Examples

In the following, we study three examples, of which the first concerns quantum walks on the integer lattice with a point defect at the origin. Our second example illustrates the quantum walk of two particles with collisional interaction. The last example of this section treats the generalization of interacting quantum walks to arbitrary particle numbers by means of quantum cellular automata.

Example 7: Hadamard walk with point defects

In the first example of this section, we analyze a unitary quantum walk on $\ell^2(\mathbb{Z})\otimes\mathbb{C}^2$ with a point defect at the origin. That is, we consider an operator of the form $W_g = W\cdot U_g$, where W is a translationally invariant unitary quantum walk. We choose W to be the Hadamard walk, i.e. $W = S\cdot \mathbb{1}_{\mathbb{Z}}\otimes H$ with the Hadamard matrix H, and the shift operator S defined via $S|x,\pm\rangle = |x\pm 1,\pm\rangle$, where $|\pm\rangle$ denotes a basis of $\mathbb{C}^2$ and $x\in\mathbb{Z}$. Hence, the Fourier transform $W(p)$ of W reads

$$W(p) = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{ip} & e^{ip} \\ e^{-ip} & -e^{-ip} \end{pmatrix}.$$

The perturbation operator U_g is determined by $g\in[0,2\pi)$ and the formula

$$U_g = \mathbb{1}_{\mathbb{Z}}\otimes\mathbb{1}_{\mathbb{C}^2} + |0\rangle\langle 0|\otimes(C_g - \mathbb{1}_{\mathbb{C}^2}) \quad , \quad C_g = \begin{pmatrix} 1 & 0 \\ 0 & e^{-ig} \end{pmatrix}.$$

In order to determine the spectral gaps of W we need to compute its dispersion relations. These are given by

$$\omega_{\pm}(p) = \pm\arccos\left(\frac{\cos(p)}{\sqrt{2}}\right).$$

Hence, the spectral gaps can be identified with the intervals $I_1 = (-3\pi/4,-\pi/4)$ and $I_2 = (\pi/4,3\pi/4)$. From now on we employ Assumption 5.1, which means we assume that the eigenvalue z of W_g can be written as $z = e^{i\eta}$ with η in one of the intervals $I_{1,2}$. Next we compute the operator $R(z)$ according to Equation (5.7). To this end,

we use a change of the integration variable $u = e^{ip}$, which yields

$$R(z) = \frac{1}{2\pi i} \int_{\mathbb{S}} \frac{du}{u} (W(u) - z\,\mathbb{1})^{-1} W(u),$$

and using residual calculus we obtain

$$R(z)(\mathbb{1} - C_g) = \begin{pmatrix} 0 & \frac{1-e^{ig}}{2}\left(1 - \frac{\sqrt{2}}{\sqrt{1-\tan^{-2}(\eta)}}\right) \\ 0 & \frac{1-e^{ig}}{2}\left(1 - \frac{i\sqrt{2}}{\sqrt{\tan^2(\eta)-1}}\right) \end{pmatrix}.$$

From this equation and Proposition 5.2.3, we immediately get the eigenvalues

$$\eta_\pm(g) = \pm \arctan\left(\frac{\sqrt{1+\sin^2\left(\frac{g}{2}\right)}}{\cos\left(\frac{g}{2}\right)}\right),$$

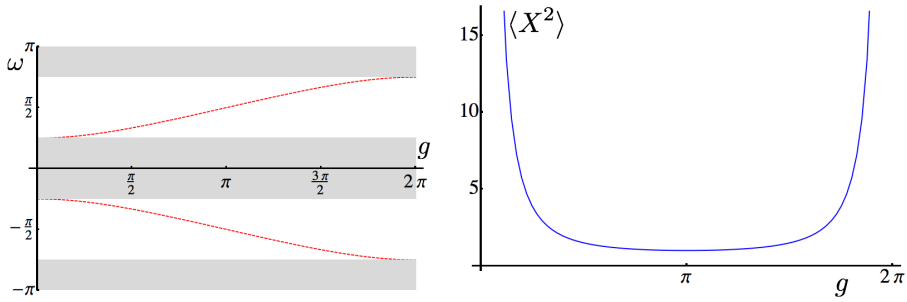
see Figure 5.4. In agreement with Proposition 5.2.5, we have less than two eigenvalues per spectral gap. In fact, $W_g - W$ is a rank-one operator, which implies that there can be at most one eigenvalue per spectral gap. The corresponding eigenvectors of W_g can be computed using Equation (5.9). According to Proposition 5.2.6, the components of these eigenvectors have to decay exponentially with the distance to the origin. However, the decay rate depends on the distance of the eigenvalue to the spectrum of W. In the limit $g \to 0$ the distance of the eigenvalues to the continuous spectrum vanishes, hence, this bound diverges. In fact, the spreading of the position distribution corresponding to one of the eigenvectors also diverges for $g \to 0$, which can be seen from a plot in Figure 5.4.

Example 8: Two-particle Hadamard walk with collisional interaction

As a second example we study the two-particle quantum walk introduced in Interlude 6, see also [AAM+12]. The time evolution of the two particles without interaction is given by the Hadamard walk on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$, i.e. $W_{1,2} = S \cdot (\mathbb{1}_\mathbb{Z} \otimes H)$ with S and H according to Equation (5.18). We consider a collisional phase as interaction operator, that is, $W_{\text{Int}} = (W_1 \otimes W_2) \cdot U_g$ with $g \in [0, 2\pi)$ and

$$U_g = \mathbb{1}_{\mathbb{Z}^2} \otimes \mathbb{1}_{\mathbb{C}^4} + \mathcal{P} \otimes \left(e^{ig} - 1\right) \mathbb{1}_{\mathbb{C}^4}.$$

Clearly, the operator W_{Int} preserves (anti-) symmetrization of the initial state, hence, it is reducible with respect to the (anti-) symmetric subspace $\mathcal{H}_\pm$ of $\mathcal{H} = \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^4$. Thus, we may perform the analysis of the propagation behavior of W_{Int} separately in



(a) (b)

Figure 5.4.: Panel (a) shows the spectrum of W_g depending on g. Gray rectangles represent the continuous spectrum of the unperturbed operator W and red-dashed lines correspond to the eigenvalues of W_g. In (b) the second moment of the position distribution corresponding to the eigenvectors is shown.

these two subspaces. In the following, we confine our analysis to the antisymmetric subspace, since this turns out to be simpler than the analysis in the symmetric subspace.

We denote the center of mass and relative momentum by p and q, respectively. As described in Section 5.3.2, we have to solve a family of p-parameterized eigenvalue problems of the kind considered in Section 5.3.1. Of course, if we restrict these eigenvalue problems to the subspace $\mathcal{H}_-$, we can still use Proposition 5.3.2 to find the eigenvalues, but now with an additional condition which the solutions of Equation (5.31) have to satisfy. More precisely, the solution φ_p of Equation (5.31) has to satisfy $\varphi_p = f(p)|\Psi_-\rangle$ with $|\Psi_-\rangle = (|+-\rangle - |-+\rangle)/\sqrt{2}$ and a scalar function f of the total momentum p. Hence, Equation (5.31) becomes a one-dimensional equation which determines the eigenvalue z_p of $\widehat{W}_p$ according to Equation (5.24). For the symmetric subspace $\mathcal{H}_+$ we would have to solve a three-dimensional equation instead. We introduce the function ω on $[-\pi,\pi)$ via $z_p = e^{i\omega(p)}$. Then we can solve Equation (5.31) using residual calculus, which yields

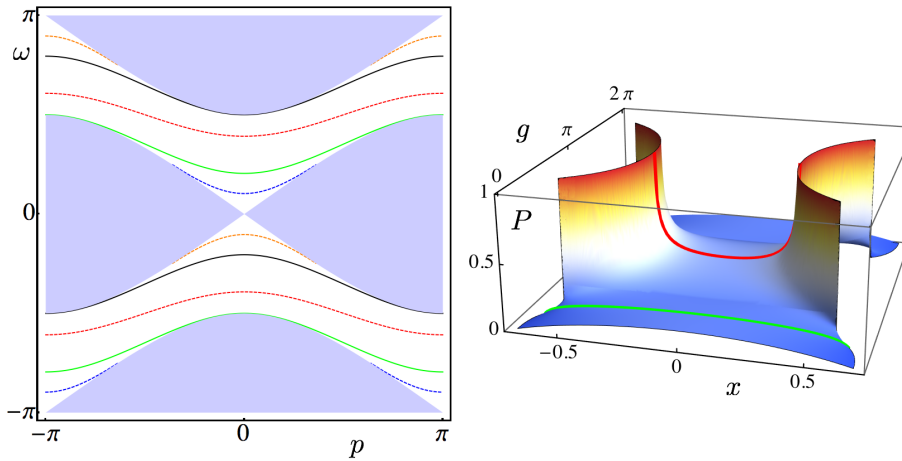
$$e^{i\omega(p)} = \frac{e^{ig}}{2e^{ig}-1}\left(\cos(p) \pm i\sqrt{\sin^2(p)+4(1-\cos(g))}\right), \tag{5.67}$$

with the condition

$$\sin(\omega(p))\sin(g-\omega(p)) > 0. \tag{5.68}$$

This condition stems from the fact that one has to choose the right pole of the matrix $(W(p,q) - z\,\mathbb{1})^{-1} W(p)$ when evaluating the complex integral for $R(z)$ in Equation (5.30). Figure 5.5 shows a plot of the function ω for some values of g. Since

the perturbation $\widehat{W}_p - W_p$ is a rank-one operator we find at most one eigenvalue per spectral gap. Interestingly, for certain values of g there are regions in momentum space where $\omega(p)$ is not defined since Inequality (5.68) is not satisfied. This has important consequences for the propagation behavior of the molecular states. For example, for $g < \pi/3$ and $g > 5\pi/3$ the inflection points of the function ω are forbidden by the condition (5.68). We observed in Section 4.5.1 that these inflection points are responsible for the characteristic peaks in the position distribution of unitary single-particle quantum walks. And indeed, the position distribution of the molecular states is rather flat for such g. This is also reflected by the asymptotic position distribution, which has no singularities for these values of g, see Figure 5.5.



(a) (b)

Figure 5.5.: Figure (a) shows the dispersion relation (5.67) of the molecular states corresponding to the interacting Hadamard walk for values g equal to $\pi/4$ (blue-dashed), $\pi/2$ (green), π (red-dashed), $3\pi/2$ (black), and $7\pi/4$ (orange-dashed). For an initial state with both particles at the same lattice site (b) shows the asymptotic position distribution depending on the collisional phase g. The red and green line highlight the cases $g = \pi/4$ and $g = \pi$, respectively.

For this particular example of an interacting two-particle quantum walk one can verify that the asymptotic position distribution of the molecular states is that of a single-particle quantum walk. In fact, it is straightforward to verify that Equation (5.67) is the dispersion relation of a standard quantum walk $W = S \cdot (\mathbb{1}_{\mathbb{Z}} \otimes C_g)$ with

S according to Equation (5.18) and

$$C_g = \frac{1}{2e^{\mathrm{i}g}-1}\begin{pmatrix} e^{\mathrm{i}g} & \sqrt{2}(e^{\mathrm{i}g}-1) \\ \sqrt{2}(e^{\mathrm{i}g}-1)e^{\mathrm{i}g} & e^{\mathrm{i}g} \end{pmatrix}. \tag{5.69}$$

Example 9: Hadamard QCA

Our aim is to construct a QCA $\mathbf{T}$ corresponding to the interacting Hadamard walk considered in Interlude 6. To begin with, let us specify the quasi-local algebra $\mathcal{A}$ corresponding to $\mathbf{T}$. We only consider a single species of particles, hence, the underlying Hilbert space is given by $\mathcal{H} = \ell^2(\Gamma)^{\otimes 2}$, with $\Gamma = \{0,1\}$ for fermions and $\Gamma = \mathbb{N}_0$ for bosons. In the following we assume the particles to be of bosonic nature, i.e. $\Gamma = \mathbb{N}_0$, and hence

$$\mathcal{H} = \overline{\mathrm{span}\{|n\rangle : n \in \mathbb{N}_0\}}. \tag{5.70}$$

The QCA $\mathbf{T} = \mathbf{T}_{\mathrm{N}} \circ \mathbf{T}_{\mathrm{I}}$ consists of a non-interacting part $\mathbf{T}_{\mathrm{N}}$ and a strictly local interaction $\mathbf{T}_{\mathrm{I}}$. The non-interacting part $\mathbf{T}_{\mathrm{N}}$ is given by a composition of a single shift and coin QCA, i.e. $\mathbf{T}_{\mathrm{N}} = \mathbf{T}_S \circ \mathbf{T}_H$, with $\mathbf{T}_S$ and $\mathbf{T}_H$ according to Equations (5.52) and (5.59), respectively. The action of $\mathbf{T}_S$ and $\mathbf{T}_H$ can be computed from Equations (5.52), (5.56), and the definitions of S and H for a single particle quantum walk according to Interlude 6

$$S|x,\pm\rangle = |x \pm 1, \pm\rangle \quad \text{and} \quad H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.71}$$

For the interaction $\mathbf{T}_{\mathrm{I}}$ we take a QCA according to Equation (5.59), but with a function f only depending on the total number of particles per cell. That is, we choose $f : \mathbb{N}_0 \to \mathbb{R}$ and define $\mathbf{T}_{\mathrm{I}}$ via

$$\mathbf{T}_{\mathrm{I}}([|\mathbf{n}\rangle\langle\mathbf{m}|]_0) = e^{\mathrm{i}(f(|\mathbf{m}|_1) - f(|\mathbf{n}|_1))}\,[|\mathbf{n}\rangle\langle\mathbf{m}|]_0\,. \tag{5.72}$$

An invariant state ω for $\mathbf{T}$ can be constructed from the following maximally entangled state two-particle state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|{+}{+}\rangle + |{-}{-}\rangle), \tag{5.73}$$

which can be expressed in occupation number basis as

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|2,0\rangle + |0,2\rangle)\,. \tag{5.74}$$

The state ω on $\mathcal{A}$ is obtained from the infinite tensor product of this state, i.e. each cell in $x \in \mathbb{Z}$ is occupied by two particles in a state defined by Equation (5.73). Strictly speaking, this infinite tensor product is not defined, but for each finite subset $\Lambda \subset \mathbb{Z}^s$ and the corresponding algebra $\mathcal{A}_\Lambda \subset \mathcal{A}$ this definition makes sense. Indeed, the restriction of the state ω to $\mathcal{A}_\Lambda$ can be identified with the pure state

$$|\Psi_\Lambda\rangle = \bigotimes_{x\in\Lambda} |\Psi\rangle\,. \tag{5.75}$$

Since any element in $\mathcal{A}$ can be approximated to arbitrary precision by elements in $\mathcal{A}_\Lambda$ with finite Λ, this infinite tensor product defines a unique state ω on $\mathcal{A}$. Obviously, ω is invariant with respect to both $\mathbf{T}_\mathrm{I}$ and $\mathbf{T}_S$. Invariance of ω with respect to $\mathbf{T}_H$ is a consequence of the $H\otimes H$ invariance of the maximally entangled state (5.73). Hence, ω is invariant with respect to each part $\mathbf{T}_S$, $\mathbf{T}_H$, and $\mathbf{T}_\mathrm{I}$ separately, and thus is trivially invariant with respect to $\mathbf{T}$.

Based on this state ω we may define excited states $\omega_{\mathbf{x},\mathbf{k}}$ according to Equation (5.64) and study their time evolution. To begin with, let us consider the effect of $\mathbf{T}_\mathrm{N} = \mathbf{T}_S \circ \mathbf{T}_H$ on such states. It is straightforward to verify that the inverse of the shift QCA $\mathbf{T}_S$ acts on $A_{x,k}$ according to Equation (5.63) like

$$\begin{aligned} \mathbf{T}_S^{-1}(A_{x,k}) &= \mathbf{T}_S^{-1}\left(\left[\mathbb{1}\otimes\sum_{n_k=0}^{\infty}|n_k+1\rangle\langle n_k|\right]_x\right) \\ &= \left[\mathbb{1}\otimes\sum_{n_k=0}^{\infty}|n_k+1\rangle\langle n_k|\right]_{x+v_k}, \end{aligned} \tag{5.76}$$

with $k=\pm$ and $v_\pm = \pm 1$. This already proves that a state $\omega_{\mathbf{x},\mathbf{k}}$ with an arbitrary number n of excitations at points specified by $\mathbf{x}$ evolves under $\mathbf{T}_S$ like a quantum walk of n particles subject to the shift dynamics S applied to each particle individually. It remains to verify that the coin QCA $\mathbf{T}_H$ leads to a quantum walk behavior of the excitations as well. To this end we use that $\mathbf{T}_H$ acts as a local transformation on each cell individually. Thus it is implemented by a unitary V_H acting on the single-cell Hilbert space $\mathcal{H} = \ell^2(\mathbb{N}_0)^{\otimes 2}$, such that we may alternatively compute the action of V_H on the pure three-particle state

$$\Psi_k = \left(\mathbb{1}\otimes\sum_{n_k=0}^{\infty}|n_k+1\rangle\langle n_k|\right)\frac{1}{\sqrt{2}}(|2,0\rangle+|0,2\rangle)\,. \tag{5.77}$$

Using $\Psi_+ = (|3,0\rangle+|1,2\rangle)/\sqrt{2}$ and $\Psi_- = (|2,1\rangle+|0,3\rangle)/\sqrt{2}$, and observing that V_H acts on this state like $H\otimes H\otimes H$ on the corresponding symmetrized state in $(\mathbb{C}^2)^{\otimes 3}$, it follows from a direct computation that $\mathbf{T}_H$ acts on each excitation like the Hadamard coin individually. Thus the excitations in $\omega_{\mathbf{x},\mathbf{k}}$ behave like particles subject to the interacting many-particle Hadamard walk when subject to $\mathbf{T}_\mathrm{N}$.

Finally, the interaction part $\mathbf{T}_\mathrm{I}$ yields a collisional phase for the excitations in $\omega_{\mathbf{x},\mathbf{k}}$. For instance, if there are exactly two excitations, they pick up an interaction phase $e^{\mathrm{i}(f(4)-f(3))}$ when they meet at the same lattice site. Thus, $\mathbf{T} = \mathbf{T}_\mathrm{N} \circ \mathbf{T}_\mathrm{I}$ acts like the interacting Hadamard walk introduced in Interlude 6 on the excitations in $\omega_{\mathbf{x},\mathbf{k}}$.

5.5. Conclusion and Outlook

In this chapter, we have studied interacting quantum walks of several particles, and we revealed a binding effect leading to the formation of a dynamically stable compound of two quantum particles undergoing an interacting quantum walk. Our analysis is based on the study of translationally invariant single-particle quantum walks with an additional point perturbation of the time evolution. We found that such perturbations generically produce an eigenvalue for the transition operator in the spectral gap. Moreover, we introduced a method to compute these eigenvalues on the corresponding eigenvectors.

By applying these results to the relative motion of two quantum particles in an interacting quantum walk, we were able to prove the existence of a bound state of the two-particle dynamics which depends on the center of mass dynamics through the total momentum of the particles. Moreover, we established an upper bound on the probability to measure the distance of the two particles which decays exponentially. These results are valid for a quite general class of interactions, hence, we demonstrated that interacting two-particle quantum walks generically exhibit a molecular binding effect despite the absence of attractive potentials.

In order to generalize the dynamics of one and two particles to an arbitrary number of particles we employed the concept of quantum cellular automata. We provided an explicit description of a quantum cellular automaton which implements the single- and two-particle dynamics of an interacting quantum walk, and opens the possibility to study the dynamics of arbitrarily many particles subject to an interacting quantum walk.

The following list contains some open questions left for future research:

- Our analysis of interacting two-particle quantum walks was based on the assumption that the eigenvalue of the relative motion transition operator lies in the spectral gap of the corresponding operator without interaction. However, there are also situations where this assumption is not satisfied. Since some crucial results, as for example the exponential bound on the probability for a measurement of the relative distance, do not generalize to this situation it is not clear whether this leads to molecular states in general.

- The formation of molecular states in interacting two-particle quantum walks is based on a complex interference effect. Thus we expect that the stability of this compound state is severely affected by decoherence.
- By means of an example we have seen that the dispersion relations of the molecular states in an interacting two-particle quantum walk can in some cases be considered as dispersion relations of a single particle quantum walk. An interesting question is whether this is always possible, that is, is there in general an effective theory for the molecular states as single-particle quantum walk.
- Further studies of interacting quantum walks with more than two particles would reveal whether simple collisional interactions can lead to the formation of molecular states of several particles.
- We introduced a notion of excitations in interacting many-particle quantum walks by means of invariant states of the corresponding quantum cellular automaton. These excitations are likely to be described by single-particle quantum walks again, hence, a study of these systems could uncover interesting effects like molecular binding of two excitations.

A. A uniform resolvent bound

In this Chapter we provide the proof of a statement we used in the preceding parts of this thesis.

In Section 5.3.2 we used an exponential bound on the matrix elements of the resolvent of a translationally invariant unitary quantum walk to derive an exponential probability-bound on the distance of two quantum particles undergoing an interacting quantum walk. Such bounds are also known a Combes-Thomas estimates, and we prove the aforementioned bound by adapting the proof of Proposition 11.1 in [HJS09] to our setting. In fact, this statement almost covers Lemma A.0.1 below, we only need a minor refinement to ensure that the bound on the matrix elements derived in [HJS09] is uniform with respect to a parameter-dependence of the operator.

The objective of the following lemma is a translationally invariant unitary quantum walk W according to Remark 4.5.1. We partition the position variable $(x,y) \in \mathbb{Z}^s$ into two subsets of coordinates $x_1 \in \mathbb{Z}^k$ and $x_2 \in \mathbb{Z}^\ell$, with $k+\ell = s$, and denote the corresponding momenta by $p_1 \in [-\pi,\pi)^k$ and $p_2 \in [-\pi,\pi)^\ell$. Hence, we can write W as

$$W = \sum_{x_1,y_1 \in \mathbb{Z}^k} \sum_{x_2,y_2 \in \mathbb{Z}^\ell} |x_1 \otimes x_2\rangle\langle y_1 \otimes y_2| \otimes W(x_1,y_1,x_2,y_2) \tag{A.1}$$

with $W(x_1,y_1,x_2,y_2) \in \mathcal{B}(\mathcal{K})$. Finally, we construct the operator

$$W_{p_1} = \sum_{x_2,y_2 \in \mathbb{Z}^\ell} |x_2\rangle\langle y_2| \otimes \sum_{x_1 \in \mathbb{Z}^k} e^{\mathrm{i}p_1 \cdot x_1} W(x_1,0,x_2,y_2), \tag{A.2}$$

where the sum over x_1 is finite since $W(x_1,0,x_2,y_2) = 0$ if $(x_1, x_2 - y_2) \notin \mathcal{N}$ with the neighborhood scheme $\mathcal{N}$ of W. For all $p_1 \in [-\pi,\pi)^k$ the operator W_{p_1} can be interpreted as translationally invariant unitary quantum walk on $\ell^2(\mathbb{Z}^\ell) \otimes \mathcal{K}$, and we have the following statement for the resolvent of this operator:

Lemma A.0.1. *Let W be a translationally invariant unitary quantum walk on the Hilbert space $\ell^2(\mathbb{Z}^s) \otimes \mathcal{K}$ and W_{p_1} according to Equation* (A.2)*. There exists a positive constant C, which is independent of $p_1 \in [-\pi,\pi)^k$, such that for any z in the resolvent set of W_{p_1} and $\phi_{x_2}, \psi_{y_2} \in \mathcal{K}$*

$$|\langle x_2 \otimes \phi_{x_2}| \left(W_{p_1} - z\,\mathbb{1}\right)^{-1} |y_2 \otimes \psi_{y_2}\rangle \leq \frac{2 \cdot \left\|\phi_{x_2}\right\| \left\|\psi_{y_2}\right\|}{\operatorname{dist}(z,\sigma(W_{p_1}))} e^{-C \cdot \operatorname{dist}(z,\sigma(W_{p_1}))\|x_2 - y_2\|}. \tag{A.3}$$

Proof. Let $\varepsilon \in \mathbb{R}^\ell$ and denote the Fourier transform of W by $W(p_1, p_2)$. Then we define the operator $W_{p_1}(\varepsilon)$ on $\ell^2(\mathbb{Z}^\ell) \otimes \mathcal{K}$ via its Fourier transform

$$W_{p_1}(\varepsilon)(p_2) = W(p_1, p_2 - \mathrm{i}\varepsilon). \tag{A.4}$$

This shows that $W_{p_1}(\varepsilon)$ is bounded for all ε since the matrix elements of $W(p_1, p_2)$ are Fourier polynomials in p_1 and p_2 and

$$\left\| W_{p_1}(\varepsilon) \right\|_{op} = \max_{p_2 \in [-\pi,\pi)^\ell} \left\| W_{p_1}(\varepsilon)(p_2) \right\|_{op} . \tag{A.5}$$

The idea of the proof is to bound the matrix elements of W_{p_1} by an estimate on the matrix elements of $W_{p_1}(\varepsilon)$. We choose ε from a ball $\mathcal{B}_r(r)$ of radius r centered at the origin in $\mathbb{R}^\ell$, which yields the following line of inequalities

$$\begin{aligned} \left\| W_{p_1}(\varepsilon) - W_{p_1} \right\|_{op} &= \max_{p_2 \in [-\pi,\pi)^\ell} \left\| W_{p_1}(\varepsilon)(p_2) - W(p_1, p_2) \right\|_{op} \\ &\leq \max_{p_2 \in [-\pi,\pi)^\ell} \left\| W_{p_1}(\varepsilon)(p_2) - W(p_1, p_2) \right\|_{HS} \\ &\leq \dim \mathcal{K} \cdot |\mathcal{N}| \cdot \max_{v \in \mathcal{N}} e^{|v \cdot \varepsilon|} \\ &\leq C_r |\varepsilon|_\infty , \end{aligned} \tag{A.6}$$

with the maximum norm $|.|_\infty$ on $\mathbb{Z}^\ell$. The constant C_r depends on the radius r of $\mathcal{B}_r(0)$, $\mathcal{K}$, and $\mathcal{N}$, but is independent of p_1. This inequality assures that both operators are arbitrarily close in operator norm if ε is chosen small enough. For two bounded linear operators A, B, and z in the resolvent set of A and B we have the resolvent identity

$$(A - z\,\mathbb{1})^{-1} - (B - z\,\mathbb{1})^{-1} = (A - z\,\mathbb{1})^{-1}(A - B)(B - z\,\mathbb{1})^{-1} . \tag{A.7}$$

If we choose ε small enough to ensure

$$\left\| (W_{p_1}(\varepsilon) - W_{p_1})(W_{p_1} - z\,\mathbb{1})^{-1} \right\|_{op} < \frac{1}{2} \tag{A.8}$$

we obtain the formulas

$$(W_{p_1}(\varepsilon) - z\,\mathbb{1})^{-1} = (W_{p_1} - z\,\mathbb{1})^{-1} \left(\mathbb{1} + (W_{p_1}(\varepsilon) - W_{p_1})(W_{p_1} - z\,\mathbb{1})^{-1} \right)^{-1} , \tag{A.9}$$

and

$$\left\| (W_{p_1}(\varepsilon) - z\,\mathbb{1})^{-1} \right\|_{op} \leq 2 \left\| (W_{p_1} - z\,\mathbb{1})^{-1} \right\|_{op} . \tag{A.10}$$

In order to assure Inequality (A.8) we choose ε such that

$$\frac{C_r |\varepsilon|_\infty}{\mathrm{dist}(z, \sigma(W_{p_1}))} < \frac{1}{2} . \tag{A.11}$$

Now, let z be in the resolvent set of W_{p_1} and denote by Q the position operator on $\ell^2(\mathbb{Z}^\ell)\otimes\mathcal{K}$. For any vector $\phi\in\ell^2(\mathbb{Z}^\ell)\otimes\mathcal{K}$ such that $e^{\varepsilon\cdot Q}\phi$ and $e^{-\varepsilon\cdot Q}\phi$ exist as normalizable vector, we may write $W_{p_1}(\varepsilon)\phi = e^{\varepsilon\cdot Q}W_{p_1}e^{-\varepsilon\cdot Q}\phi$. Hence, the matrix elements of the resolvent obey

$$\langle x_2\otimes\phi_{x_2}|(W_{p_1}(\varepsilon)-z\mathbb{1})^{-1}|y_2\otimes\psi_{y_2}\rangle = \langle x_2\otimes\phi_{x_2}|e^{\varepsilon\cdot x_2}(W_{p_1}-z\mathbb{1})^{-1}e^{-\varepsilon\cdot y_2}|y_2\otimes\psi_{y_2}\rangle\,, \tag{A.12}$$

which directly yields

$$\begin{aligned}\langle x_2\otimes\phi_{x_2}|(W_{p_1}-z\mathbb{1})^{-1}|y_2\otimes\psi_{y_2}\rangle &\leq e^{\varepsilon\cdot(y_2-x_2)}\left\|\phi_{x_2}\right\|\left\|\psi_{y_2}\right\|\left\|(W_{p_1}(\varepsilon)-z\mathbb{1})^{-1}\right\|_{op}\\ &\leq \frac{2e^{\varepsilon\cdot(y_2-x_2)}\left\|\phi_{x_2}\right\|\left\|\psi_{y_2}\right\|}{\mathrm{dist}(z,\sigma(W_{p_1}))}\,.\end{aligned} \tag{A.13}$$

By choosing the components of ε of equal modulus and with appropriate sign, we end up with the bound

$$\langle x_2\otimes\phi_{x_2}|(W_{p_1}-z\mathbb{1})^{-1}|y_2\otimes\psi_{y_2}\rangle \leq \frac{2e^{-|\varepsilon|_\infty|y_2-x_2|_\infty}\left\|\phi_{x_2}\right\|\left\|\psi_{y_2}\right\|}{\mathrm{dist}(z,\sigma(W_{p_1}))}\,. \tag{A.14}$$

The claimed bound, with $C=(\sqrt{\ell}4C_r)^{-1}$, follows if we choose ε such that $|\varepsilon|_\infty = \mathrm{dist}(z,\sigma(W_{p_1}))/4C_r$ since $\|x\|\leq\sqrt{\ell}|x|_\infty$ for all $x\in\mathbb{Z}^\ell$. □

B. List of Publications

1. A. Ahlbrecht, L. S. Georgiev, and R. F. Werner, Implementation of Clifford gates in the Ising-anyon topological quantum computer, *Physical Review A* **79** 032311, 2009

2. A. Ahlbrecht, H. Vogts, A. H. Werner, and R. F. Werner, Asymptotic evolution of quantum walks with random coin, *Journal of Mathematical Physics* **52** 042201, 2011

3. A. Ahlbrecht, V. B. Scholz, and A. H. Werner, Disordered quantum walks in one lattice dimension, *Journal of Mathematical Physics* **52** 102201, 2011

4. A. Ahlbrecht, A. Alberti, D. Meschede, V. B. Scholz, A. H. Werner, and R. F. Werner, Molecular binding in interacting quantum walks, *New Journal of Physics* **14** 073050, 2012

5. A. Ahlbrecht, C. Cedzich, R. Matjeschk, V. B. Scholz, A. H. Werner, and R. F. Werner, Asymptotic behavior of quantum walks with spatio-temporal coin fluctuations, *Quantum Information Processing* **11** 1219–1249, 2012

6. A. Ahlbrecht, F. Richter and R. F. Werner, How long can it take for a quantum channel to forget everything?, *International Journal of Quantum Information* **10** 1250057, 2012

7. R. Matjeschk, A. Ahlbrecht, M. Enderlein, Ch. Cedzich, A. H. Werner, M. Keyl, T. Schaetz, and R. F. Werner, Quantum walks with non-orthogonal position states, *arXiv:1206.0220*, accepted for publication in Physical Review Letters

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