Translation Invariant Quantum Walks with Discrete Symmetries

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To the loving memory of Andreas Reiners.
1968 – 2015

ABSTRACT

Quantum walks are discrete-time evolutions of single particles on lattices that transfer the concept of classical random walks to quantum theory. Topological insulators are objects that promise symmetry-protected edge-states for transportation along the edge. Together, both subjects lay the foundation to a description of new materials that may be used e.g. for quantum computation or transport.

In this thesis, we study topological phases in quantum walks. Given a representation of the discrete symmetry groups of the tenfold way, we develop a topological classification which distinguishes three symmetry indices whose values lie in the group of integers, the group of two elements, or the trivial group, depending on the symmetry type under consideration. The classification is applicable to quantum walks that are gapped at the symmetry-protected points. All symmetry indices are proven to be stable under norm-continuous perturbations, but only two of the three indices are invariant under compact non-continuous perturbations. These two indices describe the asymptotic behaviour far to the left and far to the right, respectively. The third index reflects whether a compact perturbation can be performed in arbitrarily small steps without violating the symmetries. Given two walks in the same phase (i.e. the symmetry indices coincide), we show that there is a norm-continuous path of walks in that phase which connects them. This renders the set of invariants we introduced complete.

Our theory covers translation invariant bulks as well, where we prove that the third index vanishes and the left- and right indices add up to zero. Hence these systems are fully classified by the right index alone. Joining two bulks in different phases (one left, one right), we show that eigenvalues emerge in the gap (bulk-boundary correspondence), whose eigenfunctions decay exponentially away from the boundary. Since our theory does not demand translation invariance at all, these composed systems are still described by our general classification.

Restricting to the translation invariant case, we express the symmetry index as a winding number of a loop in momentum space. Within this restricted class, we prove that our classification is complete as well.

Keywords:
quantum walks, topological phases, bulk-boundary correspondence

ZUSAMMENFASSUNG

Quantenwalks sind diskrete Zeitentwicklungen von Einteilchen-Gittersystemen, die Konzepte klassischer Random Walks in die Quantentheorie übertragen. Topologische Isolatoren versprechen Randzustände für Transport an Grenzflächen, die topologisch geschützt sind. Zusammengenommen bilden beide Themengebiete die Grundlage für eine Beschreibung vollkommen neuartiger Materialien, die z.B. für Quantum Computation oder elektrischen Transport genutzt werden könnten.

Diese Arbeit behandelt topologische Phasen in Quantenwalks. Mithilfe dreier Symmetrieindizes entwickeln wir eine Klassifikation topologischer Quantenwalks, deren Werte je nach Darstellung der Symmetriegruppe des Tenfold Way in der Gruppe der ganzen Zahlen, der Gruppe mit zwei Elementen oder der trivialen Gruppe liegen. Die Klassifikation lässt sich auf Quantenwalks mit spektraler Lücke um die topologisch geschützten Punkte anwenden. Die Robustheit gegenüber normstetigen Störungen wird für alle Symmetrieindizes gezeigt, doch nur zwei der drei Indizes sind invariant unter kompakten nichtstetigen Störungen. Diese zwei Indizes beschreiben jeweils das asymptotische Verhalten weit links und weit rechts. Der dritte Index zeigt an, ob eine kompakte Störung in beliebig kleine Schritte zerlegt werden kann ohne die Symmetrien zu verletzen. Wir zeigen, dass zwei Quantenwalks in der gleichen topologischen Phase normstetig innerhalb der Menge der Quantenwalks dieser Phase verbunden werden können. Dies beweist die Vollständigkeit der Indizes.

Es wird gezeigt, dass der dritte Index im Falle translationsinvarianter Quantenwalks verschwindet, und sich die links- und rechtsseitigen Indizes zu 0 addieren. Daher werden diese Systeme vom rechten Index allein bereits vollständig bestimmt. Wir beweisen die Volumen-Rand-Korrespondenz, welche exponentiell abfallende Eigenzustände mit Eigenwerten in der Lücke vorhersagt, wenn man Systeme in unterschiedlichen Phasen kombiniert. Diese Systeme werden ebenfalls von unserer Klassifikation beschrieben.

Ferner gelingt es im translationsinvarianten Fall den Symmetrieindex als Windungszahl über der Brillouin-Zone darzustellen. Außerdem beweisen wir die Vollständigkeit des Index in diesem Fall.

Schlüsselworte:
Quantenwalks, topologische Phasen, Volumen-Rand-Korrespondenz

PUBLICATIONS

1. C. Cedzich, F. A. Grünbaum, C. Stahl, L. Velázquez, A. H. Werner, and R. F. Werner. "Bulk-edge correspondence of one-dimensional quantum walks." In: *Journal of Physics A: Mathematical and Theoretical* 49.21 (2015). arXiv: 1502.02592

2. C. Cedzich, T. Geib, F. A. Grünbaum, C. Stahl, L. Velázquez, A. H. Werner, and R. F. Werner. "The topological classification of one-dimensional symmetric quantum walks." In: *Annales Henri Poincaré* (2017). ISSN: 1424-0661. DOI: 10.1007/s00023-017-0630-x. arXiv: 1611.04439

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1 INTRODUCTION

1.1 MOTIVATION

The omnipresence of information technology and the internet has made knowledge and information accessible to nearly everyone in the world, almost instantly and at minimal costs. Still, besides the technical organisation of such a large network to which everyone can contribute, it is a major challenge to provide a central index or search engine for the internet. Remarkably, a stochastic algorithm called *PageRank* [AT05] simulates the activities of countless people following links by using weighted classical *random walks* to create the weights that are assigned to different web pages and their keywords, creating such an index. But also in disciplines other than computer science classical random walks were applied, e.g. in finance to model stock market prices [Fam65], in biology to determine genomic distance in DNA [EST92] or in psychology to model the timing and probability of decisions [NP97].

After the introduction of a quantum analogue [ADZ93] (called *quantum walks*), its faster propagation was quickly applied e.g. in search algorithms [Gro96; AKR05]. These quantum walks might also serve as *quantum simulators*, precisely controlled devices which allow us to simulate quantum systems much like a classical computer today simulates classical systems. This quantum simulator approach was already suggested by Feynman [Fey82] to overcome the issues that arise due to the exponential scaling of classical descriptions of quantum systems.

But besides using quantum walks for applications or simulations, they are also very suitable to describe single-particle quantum mechanics or effective single-particle descriptions like free fermions. After all, they are unitary, discrete-time evolutions of single-particles on lattices or graphs and hence suitable to describe Hamiltonian systems that are periodic in time, or to provide a stroboscopic view of their dynamics. As such, they are experimentally realized in very different scenarios: neutral atoms in optical lattices [Kar+09], trapped ions [Sch+09], wave guide lattices [Per+10] and light pulses in optical fibres [Sch+10] as well as single photons in free space [Bro+10].

The flow of quantum information in a 1D-quantum walk measured by the *index* [Kit06; Gro+12] was identified as an integer valued *homotopy invariant* for quantum walks. Analysing translation invariant walks [Gro+12] showed that the index is the total winding number of the energy bands on the torus formed by quasi-energy and quasi-momentum. Since the index was well defined without demanding any additional symmetries and is a complete homotopy invariant for

quantum walks, we wanted to know what happened if we introduced symmetries which were well-known to yield *topological phases* in Hamiltonian systems. Moreover, since the index was a feature that had no counterpart in Hamiltonian systems, we wondered whether there are different indices or features that are unique to quantum walks.

After reading various publications (e.g. [Kit+10; Asb12]), we realized that there are numerous questions unanswered and a rigorous classification of topological phases in quantum walks was not yet written. The tenfold way [AZ97] promised to be a good starting point for the additional symmetries the quantum walks should satisfy, for these lead to the topological classification of Hamiltonian systems, which describes topological insulators and topological order [HK10]. The theoretical treatment almost everyone pointed to was [Kit09] which yields the expected index groups for the tenfold way in the Hamiltonian case, but does not provide results for quantum walks. Furthermore, the K-theoretic formulation of the paper lowers the accessibility considerably. This hints at why most authors simply applied the results from Hamiltonian systems to quantum walks or simply took them for granted, like the bulk-boundary correspondence predicting topologically protected states at the edge of two joined bulks that are in different topological phases.

This encouraged us to develop our own topological classification of 1D-quantum walks and the tenfold way, which is found in this thesis.

1.2 OUTLINE

This thesis is organized as follows: In Chapter 2 we collect basic mathematical and physical results and definitions, mainly to fix notation. Furthermore, it covers technical calculations regarding the involutions of the tenfold way, necessary results on the spectral theory of unitary operators and an introduction to the Fredholm index.

After introducing random walks and quantum walks, Chapter 3 provides the rigorous definition of quantum walks, an analysis of the simplifications in the translation invariant setting and a summary of the index theory without symmetries.

In Chapter 4 we introduce the abstract symmetry indices we assign to finite dimensional representations of the tenfold way. Then, using an elementary group theoretic construction, we obtain all the index groups of the tenfold way that are known from [Kit09].

Chapter 5 applies the abstract symmetry index to (infinite dimensional) quantum walks, leading to three independent indices representing the behaviour far to the left, far to the right and the interplay between homotopy and compactness of perturbations. The stability of the left and right indices under compact perturbations allows us to prove the bulk-boundary correspondence; predicting topologically protected eigenstates in the gap. Moreover, we provide a decoupling scheme that homotopically splits symmetric quantum walks into a left and a right part, which serves as a key ingredient to show the completeness of our invariants in three different scenarios.

In Chapter 6 we show that if the joined systems we need for the bulk-boundary correspondence are translation invariant on their half-chains, the eigenfunctions predicted are edge-states and thus decay exponentially. Still restricting to bulk (i.e. translation invariant) systems, we prove that the minimal locality condition we demand in our general theory is equivalent to the continuity of the band structure. This is required for winding numbers to be well-defined.

Exploring bulk systems even further, in Chapter 7 we show how our general theory simplifies in the translation invariant setting. Furthermore, we introduce a standard form for chiral symmetric systems which allows us to represent the classifying index as the winding of a curve parametrized by quasi-momentum. Then we show the completeness of the symmetry index in the restricted class of translation invariant systems.

In Chapter 8 we provide a set of examples that generates every index value predicted by our classification. Multiple other examples demonstrate the milestones of our classification and visualize the results, before we conclude with a summary and an outlook in Chapter 9.

2

QUANTUM ESSENTIALS

This chapter provides the basic definitions and notations, as well as some well-known results that are needed throughout the thesis.

Section 2.1 provides a brief overview about states and operators in quantum mechanics, before treating symmetries and their representations as operators on Hilbert spaces in Section 2.2. The specific class of symmetries and their representation theory we need later, namely involutions, are analysed separately in Section 2.3. In Section 2.4, we collect a few important definitions and theorems from functional calculus and spectral theory, before we focus on Fredholm operators and the notion of compactness in Section 2.5.

2.1 STATES AND MEASUREMENTS

In quantum mechanics, the state space of a physical system is a *Hilbert space* $\mathcal{H}$, which is a vector space that is complete with respect to the norm induced by a scalar product. We will always assume $\mathcal{H}$ to be separable, meaning it possesses a countable orthonormal basis. Its vectors are typically denoted by greek letters, e.g. $\varphi \in \mathcal{H}$. For every linear operator A on $\mathcal{H}$, its *adjoint* operator A^* is defined via $\langle \varphi, A^*\psi \rangle = \langle A\varphi, \psi \rangle$. We call an operator A *unitary*, if $AA^* = A^*A = \mathbb{1}$ and *Hermitian*, if $A = A^*$. The set of *bounded linear operators* on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$, while the set of *unitary operators* is denoted by $\mathcal{U}(\mathcal{H})$. Occasionally, we use Dirac's notation to denote a linear functional by $\langle\psi|$, and a linear function by $|\psi\rangle$. Then, $|\psi\rangle\langle\psi|$ describes a projection onto the subspace of $\mathcal{H}$ spanned by ψ.

The state of a physical system is described by a normalized, positive trace-class operator ρ, called a *density operator*. The set of density operators is denoted by

$$\mathcal{D}(\mathcal{H}) = \left\{ \rho \in \mathcal{B}(\mathcal{H}) | \rho \geq 0, \operatorname{tr} \rho = 1 \right\}. \tag{2.1}$$

A state ρ is *pure*, if it is a projection, e.g. $\exists \varphi \in \mathcal{H}$ s.t. $\rho = |\psi\rangle\langle\psi|$, else it is called a *mixed* state.

To learn something about the state of a system, one has to allow for measurements or observations. Measurements (or observables) are represented by *positive operator-valued measures* $\mathcal{P}$ (POVM), which throughout this thesis stem from a *projection-valued measurement* P (PVM for short), see Definition 2.7. The only example we need is a measurement of a particle's position represented by the *observable* of position Q, which is a self-adjoint operator. We often choose the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$, where $\ell^2(\mathbb{Z})$ represents the position, while $\mathbb{C}^d$ re-

flects the internal state (like a spin). Choosing an orthonormal basis $\{|x\rangle\}_x \in \mathbb{Z}$ for $\ell^2(\mathbb{Z})$ allows to represent $Q = \sum_{x\in\mathbb{Z}} x|x\rangle\langle x| \otimes \mathbb{1}_d$, allowing in this basis the possible measurement outcomes $x \in \mathbb{Z}$. The result of the measurement is then described by the *expectation value* $\langle Q\rangle_\rho = \mathrm{tr}(Q\rho)$. If ρ is a pure state stemming from $\psi \in \mathcal{H}$, its expectation value is given by $\langle Q\rangle_\rho = \langle \psi, Q\psi\rangle$.

Between the preparation of a state ρ and the measurement of an observable, the system might change due to some operation performed on it, which is expressed by the action of a quantum channel[1] T. There are two equivalent ways how to describe transformations in this framework: In the *Schroedinger picture*, T^* transforms the state ρ, whereas in the *Heisenberg picture*, T transforms the observable A. Both representations are equally legitimate, and they are connected via $\mathrm{tr}(T^*(\rho))A = \mathrm{tr}(\rho T(A))$.

2.2 SYMMETRIES AND REPRESENTATIONS

In this section, we a brief description of symmetries and symmetry groups in quantum mechanics is provided. In Chapter 4, we will look at a specific class of symmetry groups, given by the so called tenfold-way. A few technical results about anti-unitary operators that are needed, will be provided in this section for the sake of completeness. A detailed treatment of symmetries and representation theory is found e.g. in [Wei05; BR86; Lan17].

In the previous section we have seen that there are different ways to describe a quantum mechanical system. Depending on the choice, the definition of a symmetry has to be similarly adjusted. Broadly speaking, a symmetry describes an invariance of certain aspects of a physical system under corresponding symmetry transformations. For example Emmy Noether's famous theorem shows that the time translation symmetry of a system, i.e. the freedom to shift the time scale arbitrarily, implies the conservation of energy.

Let us continue this section by stating what we mean by a symmetry in quantum mechanics:

Definition 2.1 (Symmetry)
A map $S : \mathcal{D}(\mathcal{H}) \to \mathcal{D}(\mathcal{H})$ is called a **symmetry**, *if it is one-to-one and onto, as well as preserves convex sums, i.e. for $t \in [0,1]$ and $\rho_1, \rho_2 \in \mathcal{D}(\mathcal{H})$,*

$$S(t\rho_1 + (1-t)\rho_2) = t\,S(\rho_1) + (1-t)\,S(\rho_2). \tag{2.2}$$

This formulation is due to Kadison [Kad65] and equivalent to e.g. the formulation Wigner [Wig31; WG59] used almost 40 years earlier, where he described states as rays, i.e. equivalence classes of normalized elements of $\mathcal{H}$ that differ only by a phase. Wigner provided the important theorem that symmetries in quantum mechanics are represented by unitary or anti-unitary operators [Wig31], following his

1 completely positive, trace-preserving map

formulation with rays. For our purposes, the formulation by Kadison is more suitable:

Theorem 2.2 (Wigner / Kadison)
Every symmetry S can be represented such that $\forall \rho \in \mathcal{D}(\mathcal{H})$

$$S(\rho) = V \rho V^*, \tag{2.3}$$

where V is either unitary or anti-unitary[2] *and unique up to a phase $e^{i\alpha}$ for $\alpha \in [0, 2\pi]$.*

This theorem and the equivalence of the different descriptions of symmetries and their representations as unitary or anti-unitary operators from Wigner or Kadison (as well as those attributed to Jordan, Ludwig, von Neumann and Bohr) is proven in [Lan17]. The fact that symmetries are represented by unitary operators is not surprising, at least if one considers the mathematical structure of quantum mechanics as described in Section 2.1. Since states[3] and measurements rely on the scalar product between $\psi, \phi \in \mathcal{H}$, and unitary operators $U \in \mathcal{U}(\mathcal{H})$ leave scalar products invariant, i.e.

$$\langle U\psi, U\phi \rangle = \langle \psi, \phi \rangle, \tag{2.4}$$

a unitary representation of a symmetry appears to be the natural choice.

The seeming peculiarity of the theorem is that there are symmetries which cannot be represented by unitary operators but by anti-unitary operators; hence operators that are not even linear. But before we investigate this peculiarity further, we have to introduce anti-unitary operators properly:

Definition 2.3 (Anti-unitary operator)
An operator $A : \mathcal{H} \to \mathcal{H}$ is **anti-linear**, *if* $\forall z \in \mathbb{C}$

$$A(z\psi) = \bar{z} A\psi. \tag{2.5}$$

If furthermore,

$$\langle A\phi, A\psi \rangle = \overline{\langle \phi, \psi \rangle} = \langle \psi, \phi \rangle. \tag{2.6}$$

we call A **anti-unitary** *(or* **conjugate-unitary***).*
The adjoint A^* of an anti-unitary operator is defined as

$$\langle A^*\phi, \psi \rangle = \overline{\langle \phi, A\psi \rangle}. \tag{2.7}$$

Thus, A anti-unitary is equal to A anti-linear with $AA^* = A^*A = \mathbb{1}$.

If one follows the proof of Wigner's theorem and applies it to Hilbert spaces over $\mathbb{R}$ instead of $\mathbb{C}$, it yields only unitary transformations. This is to be expected, since every anti-unitary transformations over $\mathbb{C}$ is unitary if restricted to $\mathbb{R}$. More precisely, as Barut explains in [BR86, §13.2], this is due to the fact that the only automorphism of

2 see Definition 2.3
3 Here, we restrict ourselves to the case of a pure state $\rho = |\psi\rangle\langle\psi|$ for simplicity

the real field that preserves the absolute value is the identity, where the complex field has the complex conjugation, which is a second automorphism that preserves the absolute value. This explains why the perceived peculiarity of anti-unitary operators is not strange, but a technical consequence and (potential) difficulty in the treatment of symmetries and their representations to be aware of. In Chapter 4, we will see that most of our theory would be of little interest if there were no antiunitarily represented symmetries.

Since we know that unitary operators leave scalar products invariant, it is interesting to look at the action of an antiunitary operator on scalar products. This allows us to understand how *all* symmetry representations provided through Wigner's theorem act on scalar products. The application of an antiunitary operator

$$\langle A\psi, A\phi\rangle = \overline{\langle \psi, \phi\rangle} \tag{2.8}$$

has no effect on the real part of the scalar product, but flips the sign of the imaginary part. However, the transition probabilities between ψ and ϕ are not affected by antiunitary operators, since

$$|\langle A\psi, A\phi\rangle|^2 = |\overline{\langle \psi, \phi\rangle}|^2 = |\langle \psi, \phi\rangle|^2. \tag{2.9}$$

Note that for e.g. Wigner [Wig31] and Weinberg [Wei05], this invariance of the transition probabilities is the starting point to the definition of a symmetry, hence provides a physical motivation to the mathematical definition provided above.

Let us note that a system typically not only satisfies one single symmetry, but a whole group of symmetries, the ***symmetry group***. Since in this thesis, we analyse quantum walks, which are discrete in space and time[4], we will not describe continuous symmetry groups that usually occur in the analysis of systems in continuous space and time. Hence from now on, the symmetry group $\mathcal{S}(\mathcal{H})$ of our system is assumed to be discrete.

Wigner's theorem describes how a symmetry is ***represented*** as an operator on $\mathcal{H}$ (or equivalently $\mathcal{D}(\mathcal{H})$). The issue with terminology here is that one usually defines a representation as a map from a group to the set of *linear* operators - which would hence not include the antiunitarily represented symmetries. Many important properties of antiunitary operators are summarized in Wigner's paper [Wig60], in which he explains, how each antiunitary operator can be considered as a complex conjugation w.r.t. a fixed basis:

Given a Hilbert space $\mathcal{H}$ and a corresponding orthonormal basis $\{\varphi_k\}_{k\in\mathbb{N}}$, let K denote the antiunitary operator that yields complex conjugation in that basis, i.e.

$$K\psi = K\sum_{k\in\mathbb{N}} c_k\varphi_k = \sum_{k\in\mathbb{N}} \overline{c_k}\varphi_k. \tag{2.10}$$

4 See Chapter 3, where we define the systems under consideration in this thesis, quantum walks

Then, since K leaves the φ_k invariant, every antiunitary operator A on $\mathcal{H}$ can be written as

$$A\psi = \sum_{k\in\mathbb{N}} \overline{c_k} A\varphi_k = \sum_{k\in\mathbb{N}} \overline{c_k} AK\varphi_k. \tag{2.11}$$

But since AK is a unitary operator[5], we conclude that once there is a complex conjugation K and a corresponding basis $\{\varphi_k\}_{k\in\mathbb{N}}$, every antiunitary operator A can be written as

$$A = UK, \tag{2.12}$$

with a suitable unitary operator U.

Since every element of the symmetry group is either represented unitarily or anti-unitarily, we can split the group into a unitary and an antiunitary part. Hence there is a function $u : \mathcal{S}(\mathcal{H}) \to \{\pm 1\}$ that assigns to each element $S \in \mathcal{S}(\mathcal{H})$ its unitarity character[6] as a sign. In Chapter 4, we will introduce a *symmetry type*, where this character will be important for the case distinction. On the level of the representations V for a given S, this sign occurs in the exponent of a phase when it is commuted with V, i.e.

$$Ve^{i\alpha} = e^{i\alpha u(S)}V. \tag{2.13}$$

Given $S_1, S_2 \in \mathcal{S}(\mathcal{H})$, the group structure of $\mathcal{S}(\mathcal{H})$ forces $S_3 = S_1S_2$ to be a symmetry in this group as well. The aforementioned freedom of the phase that Wigner's theorem grants us now leads to a freedom in the definition of the corresponding representations: Since V and $e^{i\alpha}V$ both represent the same symmetry, they are equivalent representations of S. Therefore, the product of V_1, V_2 representing S_1, S_2 differs from V_3 by a phase ζ:

$$V_3 = \zeta(S_1, S_2)V_1V_2. \tag{2.14}$$

Instead of introducing the most general structure of these objects, we will introduce the explicit cases in Section 2.3. Thus, at this point we will conclude the discussion with the definition of a *symmetry representation*

Definition 2.4 (Symmetry representation)
Let $\mathcal{H}$ be a Hilbert space and $\mathcal{S}(\mathcal{H})$ be the symmetry group of the system under consideration. Then, we call a map π from $\mathcal{S}(\mathcal{H})$ to the set of unitary or antiunitary operators on $\mathcal{H}$ a **symmetry representation**, *if it is a projective group homomorphism, hence there is a ζ s.t. (2.14) holds for all $S_1, S_2 \in \mathcal{S}(\mathcal{H})$.*

Since this notion of a representation explicitly allows anti-linearity, we cannot simply use results which are proven only in the linear case. Luckily, in [WG59, §26] Wigner and Griffin treated time-inversion symmetries in detail and showed that any symmetry that inverts time

5 This follows directly from the definition: $\langle AK\phi, AK\psi\rangle = \langle K\psi, K\phi\rangle = \langle \phi, \psi\rangle$

6 This *character* is actually a character in the group sense as well - it maps from the group to the unit circle and is a group homomorphism.

can only be represented antiunitarily. As a consequence, they introduce symmetry representations that are not restricted to the unitary case. They do this by fixing one antiunitary element (e.g. the complex conjugation K in our case) and analyses the unitary parts U of every antiunitary operator $A = UK$ as unitary subrepresentations. They also introduce the notion of irreducibility in the antilinear case, which matches the known one in the linear case: a symmetry representation π is called ***reducible***, if there is a non-trivial, proper subspace of $\mathcal{H}$ which is invariant under the image of π. If this is not the case, π is called ***irreducible***.

The well known characterization of irreducibility in the form of Schur's lemma holds in the antiunitary case in a similar way:

Lemma 2.5 (Schur)
Let π be a representation of a group G by unitary or antiunitary operators. Then, π is irreducible if and only if every hermitian operator that commutes with the image $\pi(G)$ is a real multiple of the identity.

A proof of this lemma can be found in [Dim63, Theorem 2]. There, it is shown that the hermiticity and the reality, instead of a simple constant multiple of the identity, are needed due to the antiunitarity.

2.3 INVOLUTIONS

The symmetries that we analyse in Chapter 4 are ***involutions***, i.e. symmetries that square to the identity: $f(f(\rho)) = \rho$. As will be discussed there, the symmetry groups we are interested in either have one non-trivial symmetry, or two non-trivial symmetries whose product yields a third. Hence, the groups either have two or four distinct elements. In the following, we prepare the necessary case-distinctions by providing a pre-classification of the different cases that are possible, leading to a set of ten different symmetry groups, if one takes the signs of the squares of the representations into account. This set is called the *tenfold way* and was compiled first by Altland and Zirnbauer[7] in [AZ97].

First of all, let us analyse the single symmetries, i.e. the symmetry group $\mathcal{S} = \{\mathrm{id}, f\}$. Most of the following calculation is completely elementary, but a more detailed treatment of the special features of antiunitary operators can be found e.g. in [Wig60; WG59].

By Wigner's theorem (Theorem 2.2), every involution can be represented either by a unitary or antiunitary operator V:

$$f\big(f(\rho)\big) = V^2 \rho (V^*)^2 = \rho \quad \forall \rho \in \mathcal{D}(\mathcal{H}). \tag{2.15}$$

Since this equation holds for all $\rho \in \mathcal{D}(\mathcal{H})$,

$$V^2 = e^{i\alpha}\mathbb{1}, \quad \alpha \in [0, 2\pi] \tag{2.16}$$

has to be a multiple of the identity.

7 See the overview in Section 4.1 for more details regarding this classification.

In the case of a unitary V, the freedom of phase by Wigner allows us to modify $V \mapsto e^{-i\frac{\alpha}{2}}V$, which makes the phase of V^2 vanish. On the contrary, in the case of an antiunitary V, choosing a phase does not change the phase of the square, since

$$(e^{i\beta}V)(e^{i\beta}V) = e^{i\beta}e^{-i\beta}V^2 = V^2. \tag{2.17}$$

However in this case, the associativity of the multiplication forces the phase of V^2 to be real, since

$$(V^2)V = V(V^2) \Rightarrow e^{i\alpha}V = Ve^{i\alpha} = e^{-i\alpha}V, \tag{2.18}$$

hence $\alpha \in \{0, \pi\}$. Therefore three cases have to be distinguished:

1. V unitary
   As shown above, in this case we can choose the phase s.t. $V^2 = \mathbb{1}$. Functional calculus[8] guarantees V to then have only eigenvalues ± 1. Let P be the spectral projector to the eigenvalue $+1$. Then, V can be written as

   $$V = 2P - \mathbb{1}. \tag{2.19}$$

2. V antiunitary with $V^2 = \mathbb{1}$
   Here V behaves like the complex conjugation K in the sense that there is a basis which is V-invariant and where V acts by complex conjugation of the coefficients (compare (2.10)).

   Explicitly, let $P = (\mathbb{1} + V)/2$ be a projection onto $P\mathcal{H}$, a real subspace of $\mathcal{H}$ in the sense that scalar products of $\phi, \psi \in P\mathcal{H}$ are real (hence, $P\mathcal{H}$ is a real Hilbert space). Furthermore, since $PV = VP = P = P^2$, V leaves every element $\psi \in P\mathcal{H}$ invariant. $P\mathcal{H}$ is the subspace of V-real vectors, and since $(\mathbb{1} - P)i = iP$, we can recreate $\mathcal{H}$ from $P\mathcal{H}$ by choosing a V-real orthogonal basis of $P\mathcal{H}$, writing an element $\varphi \in \mathcal{H}$ in this basis (with potentially complex coefficients) and assigning the real and imaginary part of these coefficients to each sum of the complexification

   $$\mathcal{H} = P\mathcal{H} + iP\mathcal{H}. \tag{2.20}$$

   Given a complex conjugation K and its corresponding real-basis, the construction from (2.11) can be used to find the V-real basis simply by looking at the image of this K-basis under VK. In this sense, specifying an orthonormal basis and declaring it the V-real basis is the usual way to define V.

3. V antiunitary with $V^2 = -\mathbb{1}$
   Since for every $\phi \in \mathcal{H}$,

   $$\langle \phi, V\phi \rangle = \overline{\langle V\phi, V^2\phi \rangle} = -\overline{\langle V\phi, \phi \rangle} = -\langle \phi, V\phi \rangle = 0, \tag{2.21}$$

   $\mathcal{H}$ has to be even dimensional if such a V is supposed to exist. A normal form for V is constructed by starting with any vector

8 This is explained in Theorem 2.9

$\phi_1 \in \mathcal{H}$ and continuing with $\phi_1' = V\phi_1$, which is orthogonal to ϕ_1 (see (2.21)). Iterating this step with any ϕ_2 from the orthogonal complement of $\{\phi_1, \phi_1'\}$ until one has a basis for $\mathcal{H}$ leads to the simple decomposition of $V = UK$ into the complex conjugation K with corresponding real basis $\{\phi_j, \phi_j'\}_{j\in\mathbb{N}}$ and a block diagonal U to fulfil (2.21):

$$V = \bigoplus_{j\in\mathbb{N}} U_j K, \text{ where } U_j = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{2.22}$$

This finishes the analysis for single involutive symmetries.

To understand the case of a symmetry group with four elements, consider a pair of involutions f_1, f_2, whose product $f_1 f_2$ is also an involutive symmetry. The involutive property ensures commutativity (and conversely), since

$$f_2 f_1 = f_1^2 f_2 f_1 f_2^2 = f_1 (f_1 f_2)^2 f_2 = f_1 f_2. \tag{2.23}$$

Together with the identity element id, we have four elements, and since they all commute, we have an abelian group of four involutions that is isomorphic to Felix Klein's *Vierergruppe* [Kle84].

Since the identity is unitary and each element is either unitary or antiunitary, either all elements are represented unitarily, or we have exactly two antiunitary and two unitary elements. Due to the setting described in Chapter 4, we are only interested in the latter case, and hence assume f_1, f_2 to be antiunitarily represented by V_1, V_2. Since the phase of V_j^2 is real by (2.18) and antiunitarity implies that $\|V_j\| = 1$, there is $s_j \in \{+1, -1\}$ s.t. $V_j^2 = s_j \mathbb{1}$. The representation of $f_1 f_2$ by V_3 is now determined by the product

$$V_3 := \omega V_1 V_2, \tag{2.24}$$

but only up to a phase ω, due to Wigner's theorem. Now, we will show that we can always choose a phase for V_1 s.t. V_1 and V_2 commute, and then choose ω s.t. all V_j commute.

We know that $V_1 V_2$ and $V_2 V_1$ implement the same symmetry, due to (2.23). Therefore, by Wigner's theorem, they differ at most by a phase ζ^2

$$\zeta^2 V_1 V_2 = V_2 V_1 \Leftrightarrow (\zeta V_1) V_2 = V_2 (\zeta V_1). \tag{2.25}$$

Since for every antiunitary V,

$$(\zeta V)(\zeta V) = \zeta \zeta^* V^2 = V^2 \quad \forall \zeta \in \mathbb{C},\ |\zeta| = 1, \tag{2.26}$$

absorbing a phase ζ does not change the value of V_1^2. Hence we can redefine V_1 to absorb ζ and hence choose $\omega = 1$ such that

$$V_3 = V_1 V_2 = V_2 V_1, \tag{2.27}$$

which implies $V_3^2 = s_3\mathbb{1}$, where $s_3 = s_1 s_2$. Since every V_j hence squares to $\pm\mathbb{1}$, they all commute with each other, as is shown e.g. for V_1

$$V_1 V_3 = V_1^2 V_2 = (V_2 V_1) V_1 = V_3 V_1. \tag{2.28}$$

After these simplifications, two cases remain to be distinguished:

1. $s_1 = s_2$:
   V_3 is unitary with $V_3^2 = \mathbb{1}$, and hence[9] completely determined by the projector $P = (\mathbb{1} + V_3)/2$ onto the $+1$-eigenspace of V_3. Since P (and hence $(\mathbb{1} - P)$) commutes with V_1 and V_2 due to our phase convention (2.27), $P\mathcal{H}$ and $(\mathbb{1} - P)\mathcal{H}$ are both invariant under V_1 and V_2. Furthermore, if $s_1 = -1$, they both have to be even dimensional by the same reasoning as in (2.22). V_1 acts on each of these spaces as an arbitrary conjugate-unitary involution, i.e. $V_1 = V_1' \oplus V_1''$. Since any element of the Hilbert space can be written as $\phi + \psi$, where $\phi \in P\mathcal{H}$ and $\psi \in (\mathbb{1} - P)\mathcal{H}$, the action of V_1 already fixes V_2:

   $$\begin{aligned} 2V_2\phi &= 2V_2 P\phi = V_2\phi + s_2 V_1\phi \\ 2V_2\psi &= 2V_2(\mathbb{1} - P)\psi = V_2\psi - s_2 V_1\psi. \end{aligned} \tag{2.29}$$

   Hence, with respect to the decomposition into $P\mathcal{H}$ and $(\mathbb{1} - P)\mathcal{H}$, we can write V_2 as

   $$V_2 = \begin{pmatrix} s_1 V_1' & 0 \\ 0 & -s_1 V_1'' \end{pmatrix}. \tag{2.30}$$

   Since V_1' and V_1'' are now conjugate-unitary operators in $P\mathcal{H}$ and $(\mathbb{1} - P)\mathcal{H}$ with no further assumptions to satisfy, we can simply choose a basis in $(\mathbb{1} - P)\mathcal{H}$ s.t. $V_1' = V_1''$.

2. $s_1 = -s_2$:
   Without loss of generality, we choose $V_1^2 = \mathbb{1} = -V_2^2$. Due to (2.27), the unitary operator V_3 fulfils $V_3^2 = -\mathbb{1}$. Hence, its spectrum is $\{-i, i\}$, and we can write V_3 as

   $$V_3 = iP - i(\mathbb{1} - P), \tag{2.31}$$

   where P projects onto the $+i$-eigenspace. As can be seen by the following calculation, V_1 and V_2 now both exchange $P\mathcal{H}$ and $(\mathbb{1} - P)\mathcal{H}$:

   $$\begin{aligned} 2V_1 P &= V_1 + iV_2 = 2V_1 - V_1 + iV_2 V_1^2 = 2(\mathbb{1} - P)V_1 \\ 2V_2 P &= V_2 - iV_1 = 2V_2 - V_2 + iV_1(-V_2^2) = 2(\mathbb{1} - P)V_2. \end{aligned} \tag{2.32}$$

   Since V_1 is unitary, $P\mathcal{H}$ and $(\mathbb{1} - P)\mathcal{H}$ have the same dimension n. The image of any orthonormal basis $\{\phi_j\}_{j=1}^n$ of $P\mathcal{H}$ under V_1

9 This is the same argument as in (2.19), using functional calculus

is a basis $\{\psi_j\}_{j=1}^n$ of $(\mathbb{1}-P)\mathcal{H}$, and the action of V_2 again follows directly from the action of V_1:

$$\begin{aligned} 2V_2\phi &= 2V_2P\phi = V_2\phi - iV_1\phi \\ 2V_2\psi &= 2V_2(\mathbb{1}-P)\psi = V_2\psi + iV_1\psi. \end{aligned} \tag{2.33}$$

Thus, the action of all three operators V_1, V_2, V_3 is fixed:

$$\begin{aligned} V_1\phi_j &= \psi_j & V_1\psi_j &= \phi_j \\ V_2\phi_j &= -i\psi_j & V_2\psi_j &= i\phi_j \\ V_3\phi_j &= i\phi_j & V_3\psi_j &= -i\psi_j. \end{aligned} \tag{2.34}$$

This concludes the analysis of involutions that we need in Chapter 4.

At this point, let us quickly explain how this analysis produces the ten different cases of the tenfold way. If we assume that V_1 and V_2 correspond to *different* antiunitarily represented symmetries, we distinguish by presence or absence of V_j and by the value of V_j^2, if present.

Firstly, there is a single case where there is no symmetry present. Secondly, there are two different choices $V^2 = \pm 1$ for each antiunitarily represented symmetry V_1 and V_2, and one choice for the unitarily represented V_3, amounting to five choices. In the case of four involutions, we know that the sign convention always implies $s_3 = s_1 s_2$. Thus, we can choose $s_1 = \pm 1$ and get two cases s.t. $s_1 = s_2$ and two additional cases s.t. $s_1 = -s_2$. In total this yields the ten different cases of the tenfold way.

2.4 SPECTRAL THEORY

In this section, we introduce a few results from spectral theory, functional calculus and perturbation theory that we need throughout the thesis. Additionally, spectral properties of Hamiltonians and unitary evolution operators are strongly tied to concepts like localization or recurrence and often related to the asymptotic behaviour of a system. The relation between the dynamics in quantum mechanics and spectral properties is well documented in [Las96]. There, the decomposition of the spectral measures and the implied decomposition of the Hilbert space is explained in detail.

While the famous book [RS81] by Reed and Simon is always a good reference for a thorough and well written treatment of functional analysis, Teschl has a more recent introduction with even more specific applications from quantum mechanics that is worth a read [Tes09]. Another standard textbook that covers most of this section is [Rud06]. Kato's exhaustive treatment of perturbation theory [Kat76] is a very good source to check some of the proofs that were omitted in this section.

Let us begin by defining a few of the basic objects needed, resolvent and spectrum:

Definition 2.6 (Resolvent & spectrum)
Let A be a linear operator on a Hilbert space $\mathcal{H}$. The **resolvent set** *of A is defined by*

$$\rho(A) = \{z \in \mathbb{C} | (A - z)^{-1} \in \mathcal{B}(\mathcal{H})\}. \tag{2.35}$$

Then, the function mapping the resolvent set to its defining inverses is called the **resolvent***:*

$$R_A : \rho(A) \to \mathcal{B}(\mathcal{H}),\ z \mapsto (A - z)^{-1}. \tag{2.36}$$

The complement of the resolvent set is called the **spectrum**

$$\sigma(A) = \mathbb{C} \setminus \rho(A). \tag{2.37}$$

The norm of the resolvent $R(z)$ measures the (reciprocal) distance between z and the spectrum, i.e.

$$\operatorname{dist}(z, \sigma(A)) = \|R(z)\|^{-1}. \tag{2.38}$$

In a Banach algebra with identity, the set of invertible elements is open, thus $\rho(A)$ is open and therefore the spectrum $\sigma(A)$ is closed. The other key ingredient we need in order to formulate the *spectral theorem* is a *projection-valued measure*:

Definition 2.7 (Projection-valued measure)
Let Σ denote the Borel σ-algebra of $\mathbb{R}$, $\mathcal{H}$ be a Hilbert space and (Ω, Σ) be a measurable space. A map $E : \Sigma \to \mathcal{B}(\mathcal{H})$ is called a **projection-valued measure** *(PVM) or resolution of the identity, if*

1. $E(\Omega) = \mathbb{1}$ *and* $E(\emptyset) = 0$
2. $\forall S \subset \Sigma :\ E(S) \in \mathcal{B}(\mathcal{H})$ *is an orthogonal projection* ($E^2 = E,\ E^* = E$)
3. $\forall S_1, S_2 \subset \Sigma :\ E(S_1)E(S_2) = E(S_2)E(S_1) = E(S_1 \cap S_2)$
4. *E is strongly σ-additive, i. e. if $\{S_n\}_n \subset \Sigma$, such that for $m \neq n$: $S_n \cap S_m = \emptyset$, then $E\left(\bigcup_n S_n\right)\varphi = \sum_n E(S_n)\varphi \quad \forall \varphi \in \mathcal{H}$.*

Every projection-valued measure $E(S)$ gives rise to a unique Borel measure on $\mathbb{C}$, denoted by $\mu_\varphi(S) = \langle \varphi, E(S)\varphi \rangle$. The polarization identity extends this definition to the complex Borel measure

$$\mu_{\varphi,\psi}(S) = \langle \varphi, E(S)\psi \rangle = \frac{1}{4} \sum_{k=0}^{3} i^k\, \mu_{\varphi + i^k \psi}(S). \tag{2.39}$$

The following theorem is the spectral theorem, formulated for unitary operators. The most common form is likely the formulation for self-adjoint operators, or the general one demanding only normal operators. A proof can e. g. be found in [Rud06].

Theorem 2.8 (Spectral theorem)
Let $U \in \mathcal{U}(\mathcal{H})$ be a unitary operator and $\mathbb{T}$ be the one-dimensional torus (the

one-sphere S^1 in the complex plane), parametrized by e^{it}. Then, there exists a unique projection-valued measure $E : \mathbb{T} \to \mathcal{B}(\mathcal{H})$, such that $\forall \varphi \in \mathcal{H}$

$$\langle \varphi, U\varphi \rangle = \int_{\mathbb{T}} e^{it} \langle \varphi, E(\mathrm{d}t)\varphi \rangle =: \int_{\mathbb{T}} e^{it} \, \mu_\varphi(\mathrm{d}t). \tag{2.40}$$

Hence, the projection-valued measure is a more abstract way to write down an operator in diagonal form. More precisely, to every unitary operator U there exists a measure E and a unitary V mapping $\mathcal{H}$ to $\mathcal{L}^2(\mathbb{T}, E)$ s.t. VUV^* is a multiplication operator:

$$(VUV^*\psi)(z) = u(z)\psi(z), \tag{2.41}$$

where $u : \mathbb{T} \to \mathbb{C}$. A typical example covered later is the Fourier transform $\mathcal{F}$ mapping translationally invariant operators in $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ to multiplication operators on $\mathcal{L}_2(\mathbb{T}, \mathbb{C}^d)$. Then, the task of diagonalizing this operator reduces to the task of diagonalizing a one-parameter-dependent $d \times d$-matrix.

Another useful fact about the one-to-one correspondence between spectral measures μ_φ and operators U is that one can integrate arbitrary measurable functions f with respect to μ_φ yielding a unique operator $f(U)$ in a well defined way:

Theorem 2.9 (Functional calculus)
Let $U \in \mathcal{U}(\mathcal{H})$ and E be its spectral measure. For every measurable function f there is a unique operator $f(U)$ s.t.

$$\langle \varphi, f(U)\varphi \rangle = \int_{\mathbb{T}} f(e^{it}) \langle \varphi, E(\mathrm{d}t)\varphi \rangle = \int_{\mathbb{T}} f(e^{it}) \, \mu_\varphi(\mathrm{d}t). \tag{2.42}$$

The functional calculus allows us to look at functions of operators by applying them to complex numbers and integrating w.r.t. its corresponding measure. That is, functions of operators are as easily created as functions of complex numbers.

Now, Lebesgue's decomposition theorem allows us to decompose the measure into three characteristic parts:

$$\mu_\varphi = \mu_{\mathrm{pp}} + \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}}. \tag{2.43}$$

The pure point part μ_{pp} is a linear combination of point-measures. μ_{ac} is absolutely continuous w.r.t. Lebesgue measure (there is a positive density function f s.t. $\mu_{\mathrm{ac}(\mathrm{d}t)} = f(t)\mathrm{d}t$), and μ_{sc} is supported on a null set w.r.t. Lebesgue measure and assigns zero weight to single points.

Since the three different parts are supported on disjoined sets, integrating a projection-valued measure E over each of these sets yields three mutually orthogonal projections P_{xx} that decompose the Hilbert space $\mathcal{H}$ into three orthogonal components:

$$\mathcal{H} = \mathcal{H}_{\mathrm{pp}} \oplus \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}}, \tag{2.44}$$

where each $\mathcal{H}_{xx}$ is defined as

$$\mathcal{H}_{\text{pp}} := \{\varphi \in \mathcal{H} \mid \mu_\varphi \text{ pure point}\} \tag{2.45}$$
$$\mathcal{H}_{\text{ac}} := \{\varphi \in \mathcal{H} \mid \mu_\varphi \text{ abs. cont. w.r.t. Lebesgue measure}\} \tag{2.46}$$
$$\mathcal{H}_{\text{sc}} := \{\varphi \in \mathcal{H} \mid \mu_\varphi \text{ sing. cont. w.r.t. Lebesgue measure}\}. \tag{2.47}$$

The corresponding P_{xx} then in turn imply a decomposition of the operator U

$$U = (UP_{\text{pp}}) \oplus (UP_{\text{ac}}) \oplus (UP_{\text{sc}}). \tag{2.48}$$

The spectrum of each of the restricted operators UP_{xx} coincides with the union of the support of all measures of the corresponding type. Accordingly, $\sigma_{\text{pp}}(U)$ is the set of all eigenvalues of U, hence a set of discrete points; $\sigma_{\text{ac}}(U)$ is a union of closed intervals and $\sigma_{\text{sc}}(U)$ is a Cantor set. Note that, even if this decomposition splits the Hilbert space orthogonally, the spectral decomposition is not exclusive: the different spectra may overlap, hence in general e.g.

$$\sigma_{\text{pp}}(U) \cap \sigma_{\text{ac}}(U) \neq \emptyset. \tag{2.49}$$

Nevertheless, the union of all spectral parts yields the spectrum of U.

The next theorem, named *RAGE* after Ruelle, Amrein, Georgescu and Enss[10], connects these subspaces to the propagation behaviour of U:

Theorem 2.10 (RAGE)
Let U be a unitary operator on $\mathcal{H}$ and G_n be a sequence of compact[11] operators converging strongly to the identity. Then, for $\mathcal{H}_{\text{c}} = \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$ and $\mathcal{H}_{\text{pp}}$ are characterized as follows:

$$\mathcal{H}_{\text{c}} = \left\{ \psi \in \mathcal{H};\ \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T+1} \sum_{t=0}^{T} \left\| G_n U^t \psi \right\|^2 = 0 \right\} \tag{2.50}$$

$$\mathcal{H}_{\text{pp}} = \left\{ \psi \in \mathcal{H};\ \lim_{n\to\infty} \sup_{t\geq 0} \left\| (\mathbb{1} - G_n)\, U^t \psi \right\|^2 = 0 \right\}. \tag{2.51}$$

Without going too much into the details of our systems' spatial structure[12], let us assume $\mathcal{H} = \ell^2(\mathbb{Z})$ with $|x\rangle$ labelling the standard basis. Then, an example for such a sequence $\{G_n\}_{n\in\mathbb{N}}$ is given by

$$G_n = \sum_{i=-n}^{n} |i\rangle\langle i|, \qquad \lim_{n\to\infty} G_n = \mathbb{1}. \tag{2.52}$$

Equation (2.51) now tells us that linear combinations of eigenvectors are exactly those elements $\psi \in \mathcal{H}_{\text{pp}}$ that stay in a finite section of $\mathcal{H}$, independent of the number of time steps, i.e.

$$\forall \epsilon > 0\ \exists n_0 \in \mathbb{N} :\ \sup_{t\geq 0} \left\| (\mathbb{1} - G_{n_0})\, U^t \psi_{\text{pp}} \right\|^2 < \epsilon. \tag{2.53}$$

10 For a proof, see e.g. [Las96].
11 See Definition 2.13 compact operators in the next section
12 This is detailed in Chapter 3, Quantum Walks

On the other hand, vectors $\psi_c \in \mathcal{H}_c$ leave every finite subspace, at least in the Cesaro mean as used in Theorem 2.10, which is defined as

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} G_n. \tag{2.54}$$

The RAGE-theorem thus distinguishes pure-point spectrum from continuous spectrum, but we do not know yet if there is a similar result that distinguishes absolutely-continuous spectrum from singularly-continuous spectrum. A first step in this direction is the following consequence of the Riemann-Lebesgue-Lemma (see e.g. [Wer13, §4] for a rigorous treatment of the topic in the context of recurrence):

Theorem 2.11
Let $U \in \mathcal{U}(\mathcal{H})$ be a unitary operator, $K \in \mathcal{K}(\mathcal{H})$ a compact operator (e.g. a projection of finite rank) and $\varphi \in \mathcal{H}_{ac}$. Then

$$\lim_{t\to\infty} \left\| K U^t \varphi \right\| = 0. \tag{2.55}$$

Thus we know that under the action of U, $\varphi \in \mathcal{H}_{ac}$ not only leaves every finite region in the Cesaro mean (see (2.50)), but also directly in norm. Making use of the notion of recurrence, whose proper introduction would lead a bit too far here, Theorem 1 from [Grü+13] shows the converse of Theorem 2.11 in the sense that if ψ and U are a recurrent pair, $\psi \perp \mathcal{H}_{ac}$. Altogether, these results allow us to distinguish between all three spectral components by analysing dynamical properties of unitary operators and vice versa. Note that we will introduce another decomposition of the spectrum, namely into discrete and essential spectrum, in Section 2.5.

For the rest of this section we will collect a few results on the perturbation theory of linear operators. The book of Kato [Kat76] is a good reference for a more thorough read with all the details and proofs in one place. The following results and statements are all well known and can be found e.g. in [Kat76, Chapter I, II].

An important task for many results in physics is to understand how robust the results are under small perturbations. A setting with a reasonable notion of "small perturbations" is described in the following by using norm-continuity of families of operators. This concept allows to describe homotopic operators[13] and are key ingredients in proving homotopy invariants later in this thesis.

Let $\{T_x\}$ be a family of operators on $\mathcal{B}(\mathcal{H})$ whose norm depends continuously on $x \in I \subset \mathbb{R}$. Then, we define its resolvent as

$$R_T(z, x) := (T_x - z\mathbb{1})^{-1}. \tag{2.56}$$

It (exists and) is holomorphic in z and x whenever $z \notin \sigma_{pp}(T_x)$. Furthermore, due to its holomorphy, for every x_0 there is an $\epsilon > 0$ s.t. $R_T(z, x)$ exists for every $z \in \rho(T_{x_0})$ and $x \in (x_0 - \epsilon, x_0 + \epsilon)$. Hence in this

13 A proper definition of homotopic operators in the context of our symmetries is found in Definition 5.4.

case, the domain of $R_T(z,x)$ is $\rho(T_{x_0})$, which means that the domain of the resolvent does not change under suitably small changes of x.

Let Γ be a closed curve in the resolvent set $\rho(T_{x_0})$ enclosing one isolated eigenvalue λ. Then, the existence of the resolvent $R_T(z,x)$ for $z \in \Gamma$ ensures that there are no eigenvalues of T_x on Γ. The operator

$$P(x) = -\frac{1}{2\pi i}\oint_\Gamma R_T(z,x)dz \tag{2.57}$$

is a projection and equal to the sum of the eigenprojections for all the eigenvalues of T_x lying inside Γ. Furthermore, $P(x)$ is holomorphic in x and thus

$$\dim P(x)\mathcal{H} = \dim P(x_0)\mathcal{H}. \tag{2.58}$$

This implies that the number of eigenvalues encircled by Γ does not change with the variation of x. A more detailed proof of this is found in [Kat76, II §1.4] building on the result from [Kat76, I §4.6].

Proposition 2.12 (Continuity of the eigenvalues)
Let $\{T_x\}$ be a family of operators on $\mathcal{B}(\mathcal{H})$ whose norm depends continuously on $x \in I$. Then, the eigenvalues of T_x are continuous in x.

Continuity of the eigenvalues certainly does allow for splitting of eigenvalues, e.g. a few eigenvalues $\lambda_i(x)$ branching off a highly degenerate eigenvalue $\lambda(x_0)$, but for every $\epsilon > 0$ there is a $\delta > 0$ such that $|x - x_0| < \delta$ implies $|\lambda_i(x) - \lambda(x_0)| < \epsilon$, thus the eigenvalues cannot depart arbitrarily far.

2.5 FREDHOLM THEORY

If one wants to describe perturbations or small changes of operators on infinite-dimensional Hilbert spaces, finite rank operators are a natural candidate. But in many cases throughout this thesis, we will show that it makes sense to consider the larger class of *compact* operators instead. This section provides only a brief overview of the definitions and results that we need. A more detailed review of Fredholm theory (and operator algebras in general) is e.g. given in [Bla06].

Definition 2.13 (compact operator)
An operator $K : \mathcal{H} \to \mathcal{H}$ is a **compact** *operator, if for all bounded sequences $\{\zeta_i\}$ of vectors in $\mathcal{H}$, $\{K\zeta_i\}$ has a convergent subsequence. The set of compact operators is denoted by $\mathcal{K}(\mathcal{H})$.*

$\mathcal{K}(\mathcal{H})$ is precisely the norm-closure of the set of bounded finite rank operators. The spectrum of a compact operator contains only nonzero eigenvalues of finite multiplicity which form a sequence converging to the unique accumulation point 0. By the singular value decomposition, every compact operator $K : \mathcal{H} \to \mathcal{H}$ can be written as

$$K = \sum_{i=0}^{\infty} k_i |\varphi_i\rangle\langle\psi_i|, \quad k_i \to 0 \text{ and } k_i \geq 0 \quad \forall i \in \mathbb{N}, \tag{2.59}$$

given two orthonormal bases $\{\varphi_i\}_{i\in\mathbb{N}}$ and $\{\psi_i\}_{i\in\mathbb{N}}$ and $\{k_i\}_{i\in\mathbb{N}}$. Obviously, if there is an $N \in \mathbb{N}$ s.t. $k_i = 0$ for all $i > N$, then K is of finite rank. Interestingly, there is a finer classification of compact operators, quite similar to the classification that the different ℓ^p-spaces provide in terms of absolutely convergent (ℓ^1), square-summable (ℓ^2) and bounded sequences (ℓ^∞). Phrased in terms of the singular values of compact operators (2.59), we define:

Definition 2.14 (Trace class operator)
Let $\mathcal{H}$ be a separable Hilbert space and K be a compact operator with singular value decomposition as in (2.59). K is a **trace-class operator**, *if $\|K\|_1$ is finite, which is*

$$\|K\|_1 = \operatorname{tr}|K| := \sum_{i=0}^{\infty} \langle (K^*K)^{\frac{1}{2}}\psi_i, \psi_i\rangle = \sum_{i=0}^{\infty} k_i. \tag{2.60}$$

Then, the trace of K

$$\operatorname{tr} K = \sum_{i=0}^{\infty} \langle K\psi_i, \psi_i\rangle \tag{2.61}$$

is finite and independent of the orthonormal basis chosen.

Definition 2.15 (Hilbert-Schmidt operator)
Let $\mathcal{H}$ and K be as above. The Hilbert-Schmidt norm $\|.\|_2$ is defined as

$$\|K\|_2^2 = \operatorname{tr} K^*K = \sum_{i=0}^{\infty} k_i^2. \tag{2.62}$$

Then, K is a **Hilbert-Schmidt operator**, *if $\|K\|_2$ is finite.*

Since the definitions are founded on the singular values k_i of K, the following sequence of implications is obvious[14]:

$$\text{finite rank} \Rightarrow \text{trace class} \Rightarrow \text{Hilbert-Schmidt} \Rightarrow \text{compact}. \tag{2.63}$$

The set of compact operators is a closed ideal in $\mathcal{B}(\mathcal{H})$, which means that products of bounded operators with compact operators are always compact. This allows forming the quotient Banach algebra $\mathcal{Q}(\mathcal{H}) = \mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H})$, called the Calkin algebra. Typically, we denote the corresponding natural projection by $\pi : \mathcal{B}(\mathcal{H}) \to \mathcal{Q}(\mathcal{H})$. This allows us to define Fredholm operators, which are bounded linear operators that are invertible up to a compact operator:

Definition 2.16 (Fredholm operator)
An operator $F \in \mathcal{B}(\mathcal{H})$ is a **Fredholm operator**, *if $\pi(F)$ is invertible in $\mathcal{Q}(\mathcal{H})$. The set of Fredholm operators is denoted by $\mathcal{F}(\mathcal{H})$.*

14 Actually, we defined Trace class and Hilbert-Schmidt operators in Definition 2.14 only for compact operators. This is an imprecise simplification, skipping the step of a general definition for arbitrary linear operators that leads to the lemma that implies compactness. Since this is all straight forward textbook material, we hope to be forgiven.

Atkinson's theorem shows [Bla06] that this definition is equivalent to $F \in \mathcal{B}(\mathcal{H})$ having finite dimensional kernel and a closed image of finite codimension.

Since the codimension of the image of F is equal to the dimension of the kernel of F^*, the following definition makes sense for every $F \in \mathcal{F}(\mathcal{H})$:

Definition 2.17 (Fredholm index)
The **Fredholm index** *of a Fredholm operator F is defined as*

$$\mathrm{ind}_F(F) = \dim\ker F - \dim\ker F^*, \tag{2.64}$$

therefore mapping $\mathcal{F}(\mathcal{H})$ to $\mathbb{Z}$. The set of Fredholm operators with index n is denoted by $\mathcal{F}_n(\mathcal{H})$.

The following theorem collects some important properties of the Fredholm index:

Proposition 2.18 (Properties of the Fredholm index)
Let $F, G \in \mathcal{F}(\mathcal{H})$ and $K \in \mathcal{K}(\mathcal{H})$. On $\mathcal{H} = \ell^2(\mathbb{N})$, let S denote the unilateral shift $S|x\rangle = |x+1\rangle$. Then:

1. $\mathrm{ind}_F(FG) = \mathrm{ind}_F(F) + \mathrm{ind}_F(G)$
2. $\mathrm{ind}_F(F+K) = \mathrm{ind}_F(F)$
3. $\mathrm{ind}_F(S^n) = n \quad \forall n \in \mathbb{Z}$
4. ind_F *is continuous, and therefore locally constant.*

Since the image of ind_F is a discrete set, continuity implies that you cannot leave a connected component by continuously changing F - this makes ind_F a *homotopy invariant*. That is, it does not change under norm-continuous deformations. Furthermore, every $F \in \mathcal{F}_0(\mathcal{H})$ can be connected to an invertible operator by a compact operator. Since the set of compact operators is contractible to 0, and the set of invertible operators is contractible to the identity, it follows that $\mathcal{F}_0(\mathcal{H})$ is path-connected[15]. In both cases, contractibility is easily seen with the aid of functional calculus from Theorem 2.9. In the compact case, for every K with singular value decomposition from (2.59) there is

$$K_t = \sum_{i=0}^{\infty} (k_i)^t |\varphi_i\rangle\langle\psi_i|, \tag{2.65}$$

which norm-continuously connects $K_0 = 0$ and $K_1 = K$. The case of invertible normal operators U is similar, where we define $U_t = U^t$ using functional calculus and the spectral theorem (Theorem 2.8) s.t. $U_0 = \mathbb{1}$ and $U_1 = U$. The non-normal case is a little more intricate and can be found e.g. in [Bla06].

This argument can be extended to $\mathcal{F}_n(\mathcal{H})$ for all $n \in \mathbb{N}$:

15 Path-connectedness of $\mathcal{F}_0(\mathcal{H})$ in the sense that between any two $F, G \in \mathcal{F}_0(\mathcal{H})$ there is a norm-continuous path of $F_t \in \mathcal{F}_0(\mathcal{H})$ s.t. $F_0 = F$ and $F_1 = G$.

Proposition 2.19
$\mathcal{F}_n(\mathcal{H})$ is path-connected for all $n \in \mathbb{Z}$.

Proof. Choose an isometry S such that $S_n = S^n$ with index n and $S_{-n}S_n = \mathbb{1}$ (typically, e.g. in $\ell^2(\mathbb{N})$, think of S as the unilateral shift). Then, for any $F \in \mathcal{F}_n(\mathcal{H})$, Proposition 2.18 implies that $FS_{-n} \in \mathcal{F}_0(\mathcal{H})$. Since $F = FS_{-n}S_n \in \mathcal{F}_0(\mathcal{H})S_n$, it follows that $\mathcal{F}_n(\mathcal{H}) \subseteq \mathcal{F}_0(\mathcal{H})S_n$. Conversely, Proposition 2.18 implies that $\mathcal{F}_n(\mathcal{H}) \supseteq \mathcal{F}_0(\mathcal{H})S_n$, hence $\mathcal{F}_n(\mathcal{H}) = \mathcal{F}_0(\mathcal{H})S_n$ and the path-connectedness of $\mathcal{F}_0(\mathcal{H})$ implies the path-connectedness of $\mathcal{F}_n \; \forall n \geq 0$. The result for $n \leq 0$ follows directly from taking adjoints. □

Both propositions together prove that ind_F is a *complete* homotopy invariant for $\mathcal{F}_n(\mathcal{H})$. That is, not only do continuously connected operators have the same index (homotopy invariance), but given two operators of the same index n, there is a path within $\mathcal{F}_n(\mathcal{H})$ that connects them (completeness).

Put differently, ind_F splits $\mathcal{F}(\mathcal{H})$ into a countable set of connected components $\mathcal{F}_n(\mathcal{H})$ where each connected component is uniquely labelled by an integer, hence ind_F is an isomorphism between the connected components of $\mathcal{F}_n(\mathcal{H})$ and $\mathbb{Z}$.

Having established these results about Fredholm operators, we can now introduce another decomposition of the spectrum of a bounded linear operator than the one introduced in Section 2.4.

Definition 2.20 (Essential spectrum)
Let $A \in \mathcal{B}(\mathcal{H})$ be a normal bounded linear operator on $\mathcal{H}$. Then, the **essential spectrum** *$\sigma_e(A)$ is defined as*

$$\sigma_e(A) = \{\lambda \in \mathbb{C} \mid (A - \lambda\mathbb{1}) \notin \mathcal{F}(\mathcal{H})\}, \tag{2.66}$$

while the complementing **discrete spectrum** *$\sigma_d(A)$ is*

$$\sigma_d(A) = \sigma(A) \setminus \sigma_e(A). \tag{2.67}$$

While the discrete spectrum consists of all isolated eigenvalues of finite multiplicity, the essential spectrum contains the continuous spectrum, as well as all eigenvalues of infinite multiplicity and all limit points of the set of eigenvalues.

This statement can equivalently be expressed by the dimensionality of the projection valued measure E_A [RS81]:

Theorem 2.21
Let $A \in \mathcal{B}(\mathcal{H})$ be a bounded linear operator on $\mathcal{H}$. Then, λ is in the essential spectrum of A, iff the range of $E_A(\Lambda_\epsilon)$ is infinite dimensional for all $\epsilon > 0$, where $\Lambda_\epsilon = (\lambda - \epsilon, \lambda + \epsilon)$. On the other hand, λ is in the discrete spectrum if $\lambda \in \sigma(A)$, but there is an $\epsilon > 0$, s.t. the range of $E_A(\Lambda_\epsilon)$ is finite dimensional.

In much the same way as the *essential* spectrum describes the spectrum up to compact contributions, many definitions make sense to be broadened to hold *only up to a compact part* - which we often call to

hold *essentially*. An example is given by the following definition of an *essentially unitary* operator:

Definition 2.22 (Essentially unitary)
$U \in \mathcal{B}(\mathcal{H})$ is called an **essentially unitary** *operator, if it is unitary up to a compact operator, i.e. there are $K_1, K_2 \in \mathcal{K}(\mathcal{H})$ s.t.*

$$WW^* - \mathbb{1} = K_1 \qquad\qquad W^*W - \mathbb{1} = K_2. \tag{2.68}$$

By definition, essentially unitary operators are Fredholm.

This finishes our survey of preliminaries and allows us to define the main actors in this thesis.

3 QUANTUM WALKS

After introducing some basic facts about quantum mechanics, representations and functional calculus, we want to approach the physical systems we consider in this thesis, i.e. *quantum random walks* (or *quantum walks* for short).

We present an example of a classical random walk and an overview about quantum walks in Section 3.1, before introducing the elementary building blocks to define quantum walks in Section 3.2. Then, we take a look at the implications of restricting the class of quantum walks to those that commute with lattice translations in Section 3.3. We close this chapter by providing a quick summary of the index theory for quantum walks in Section 3.4.

Note that from now on, we restrict the dynamics of quantum mechanical systems to those described by the discrete unitary time evolutions of pure states and formulate time-evolution in the Schrödinger picture: Let $\psi_0 \in \mathcal{H}$ be the initial state of the system and U be the unitary time evolution operator, e.g. a quantum walk. Then, the state of the system after t time steps is given by $\psi_t = U^t \psi_0$.

3.1 OVERVIEW

Before explaining the significance of *quantum* random walks, we want to give a brief example of a *classical* random walk. By a classical random walk, we mean a stochastic process in discrete time on a graph (e.g. a lattice), which models the trajectory of a single particle in space and time. The easiest example one can think of is the *simple random walk* in 1D, where the state space is $\mathbb{Z}$ and the *walker* starts at the position $X_0 \in \mathbb{Z}$ at the time t_0, and then moves either to the right with probability p or to the left with probability $1 - p$, decided by a coin. That is, the coin decides whether the walker is *shifted* to the left or to the right, and together, both operations denote a *time step*. This simple example is *translation invariant* in time and space[1], thus we may assume to start at $X_0 = 0$ and $t = 0$. Then, $P(X_t = x)$ denotes the probability to find the particle at position x after t time steps. It vanishes everywhere, except if $x = 2k - t$ for $k \in \{0, \dots, t\}$, where it is given as

$$P(X_t = 2k - t) = \binom{t}{k} p^k (1-p)^{t-k}. \tag{3.1}$$

1 That is, its time evolution operation does not depend on x and t, see Section 3.3 for a more precise explanation.

The characteristic Bernoulli-distribution confirms that the simple random walk is a Bernoulli process, whose distribution hence converges to the Gaussian distribution by the central limit theorem. Note that the walker never stays on the same site but always moves exactly by one site per step, thus always switches from the sublattice of even sites to the sublattice of odd sites (and vice versa) in every step. This effect denotes a sublattice symmetry, also called a *chiral* symmetry, which splits the lattice into two sublattices where the parity of x determines its *chirality*.

If we choose an unbiased coin, that is $p = \frac{1}{2}$, we see that the distribution $P(X_t = x)$ is symmetrical in x, and we get for the expectation value $E(X_t)$

$$E(X_t) = \sum_{x \in \mathbb{Z}} x \cdot P(X_t = x) = 0, \tag{3.2}$$

as we expect from an unbiased coin. Expressing X_t via the results of the individual coin tosses $Z_k \in \{-1, +1\}$, we have

$$X_t = \sum_{k=1}^{t} Z_k, \tag{3.3}$$

since we assumed to start at $X_0 = 0$. Linearity of the expectation value and independence of the coin tosses then leads to

$$E(X_t^2) = \sum_{k,j=1}^{t} E(Z_k Z_j) = \sum_{k,j=1}^{t} E(Z_k^2)\delta_{k,j} = t. \tag{3.4}$$

Thus, for the standard deviation of the position as the square root of the variance, we get

$$\sqrt{\mathrm{Var}(X_t)} = \sqrt{E(X_t^2) - E(X_t)^2} = \sqrt{t}. \tag{3.5}$$

This characteristic dependence on the square root of t is called *diffusive spreading*, as opposed to *ballistic spreading*, where

$$\sqrt{\mathrm{Var}(X_t)} \propto t. \tag{3.6}$$

Another similarly interesting property is *recurrence*, which denotes whether a walker starting at i and propagating under a random walk R is expected to return infinitely often. In our example, for $i = 0$, we have

$$\sum_{t=0}^{\infty} P(X_t = 0) = \sum_{t=0}^{\infty} \binom{t}{t/2} = \infty, \tag{3.7}$$

where the last step can be seen by applying Stirling's approximation for factorials, leading to

$$P(X_t = 0) \propto \frac{4^t}{\sqrt{t}}, \quad t \to \infty. \tag{3.8}$$

Thus we see that the simple random walk in 1D is recurrent if $p = \frac{1}{2}$ and $i = 0$ (and hence for all $i \in \mathbb{Z}$, due to translation invariance).

One of the earliest known usages of the concept of *random walks* was by Pólya in [Pól21], where he analysed the trajectory of random walkers. He prove a theorem about *simple random walks*, which in his nomenclature are d-dimensional random walks on $\mathbb{Z}^d$ that transition with equal probability $p = 1/2d$ to each of their nearest neighbours on the lattice. The theorem states, that every simple random walk on $\mathbb{Z}^d$ is recurrent if and only if $d = 1, 2$. This result is put into perspective when connecting it to recurrence in quantum walks, which was thoroughly treated in [Grü+13].

These days, in physics, mathematics and computer science, as well as in many other subjects like biology, pharmacy and engineering, there are applications of random walks. In many cases, one uses the fact, that a random walk setup is much easier to develop and much lighter on the hardware than e.g. keeping track of all combinations. Often an abstract analytical approach is simply not feasible with the tools at hand. But in order to quantitatively assess the results found, one needs general statements about the behaviour of random walks, and the simplicity of the method is often paid for by the complexity of the interpretation.

In an interesting application [DS84] Doyle and Snell apply Pólya's result about recurrence in random walks (along with a particular method attributed to Rayleigh) to finite and infinite grids of resistors and derive their electrical properties (see also [Mun07]). In another application, Engh, Sachs, and Trask show in [EST92], that random walks are a suitable tool to model genomic distance in DNA-sequences. One of the most influential applications of random walks in everyday life is most likely the *PageRank*-algorithm used by Google and eBay already since their earliest days, which treats the Internet as a connected graph of nodes (pages) and edges (hyperlinks). Broadly speaking, *PageRank* is the limit probability distribution reached in a random walk on that graph [AT05]. If the network is not the set of web pages, but e.g. content in peer-to-peer networks, Bisnik and Abouzeid showed in [BA07] that a suitably tuned random walk model can estimate the popularity of resources and approximate independent uniform sampling.

With the proposal of a quantum computer using qubits as opposed to a classical computer using bits, the notion of *quantum walks* emerged. Definitions very similar to the one we still use today was introduced by Aharonov, Davidovich, and Zagury in [ADZ93]. In their example, they showed that measuring the state of a quantum walk, and preparing it again after every time step can lead to a classical random walk. However, they already hinted at quantum effects that distinguishes quantum walks from their classical counterpart and might make quantum walks interesting for applications e.g. in modelling quantum optics.

In this thesis, we define a ***quantum walk*** W as a strictly local, unitary operator that represents the discrete time-evolution of a single particle (or *walker*) on a lattice (a complete definition is found in Section 3.2, or in [Ahl+11]). Strict locality demands, that the unitary operator imposes a spatial structure on the Hilbert space, in the sense that a particle initially localized at a single site or cell is localized in a *finite neighbourhood* of these cells after applying W.

If a random walk is supposed to be non-trivial, it needs at least two possible results for the random variable that decides the direction of propagation. For a quantum walk, the *coin-space* has to be at least of dimension 2 in order to implement non-trivial dynamics. One possible quantum analogue of the simple random walk in 1D is the following *Hadamard-Walk*:

Let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ be the Hilbert space of a single particle on the line with a two dimensional inner degree of freedom (e.g. a spin-$\frac{1}{2}$-particle), and choose a basis

$$B = \left\{ \delta_x \otimes e_j \,\middle|\, x \in \mathbb{Z},\ j \in \{+,-\} \right\}, \tag{3.9}$$

which spans $\mathcal{H}$. In Dirac's notation we write $|x, j\rangle$ to denote the linear function $\mathbb{C} \to \mathcal{H} : z \mapsto z \cdot \delta_x \otimes e_j$.

Flipping a coin in the classical random walk now corresponds to applying a coin operation C that acts on the internal degree of freedom, s.t.

$$\begin{aligned} C|x,+\rangle &= C_{++}|x,+\rangle + C_{-+}|x,-\rangle \\ C|x,-\rangle &= C_{+-}|x,+\rangle + C_{--}|x,-\rangle. \end{aligned} \tag{3.10}$$

The shifting of the state that depends on the outcome of the coin toss is then realized by a *shift* operator S s.t.

$$S|x,\pm\rangle = |x \pm 1, \pm\rangle. \tag{3.11}$$

Applying both operations consecutively then defines a *quantum walk* (operator):

$$W = SC. \tag{3.12}$$

Now, if we choose a self-adjoint coin, e.g. the eponymous *Hadamard*-coin C_H, we get the Hadamard-Walk W_H

$$W_H = SC_H, \qquad \text{where} \qquad C_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3.13}$$

Starting with the initial state

$$\psi_0 = \frac{1}{\sqrt{2}} \big(|0,+\rangle + i|0,-\rangle \big), \tag{3.14}$$

after one application of W_H, we have

$$\psi_1 = \frac{1+i}{2} |1,+\rangle + \frac{1-i}{2} |-1,-\rangle. \tag{3.15}$$

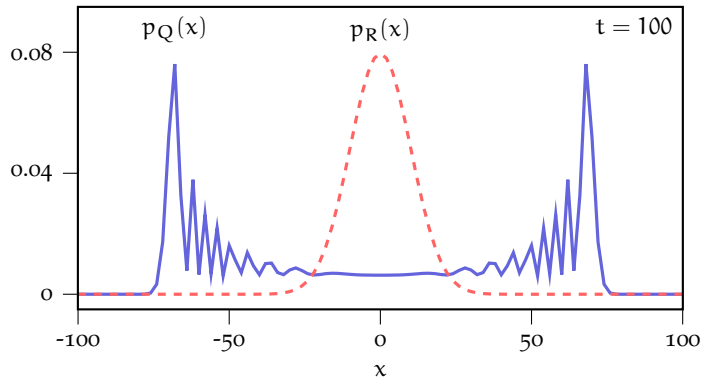


Figure 1: Probability distribution $p_Q(x)$ of the Hadamard-Quantum-Walk W_H, stemming from the squared norm of the $\mathbb{C}^2$-coefficient $\psi_t(x)$, and $p_R(x)$ stemming from the simple random walk from (3.1) with $p = 1/2$, both plotted after $t = 100$ time steps. While the classical random walk approaches a perfect Gaussian distribution in the limit, the quantum random walk has two front-runners that carry most of the probability. This indicates the ballistic propagation of the Hadamard-Walk, as opposed to the diffusive propagation of the Random Walk. Note that in both cases, the sites unreachable by chiral symmetry were skipped in connecting the points.

Thus the probability to find the particle after one time step in either $+1$ or -1 is $p = 1/2$, just as in the simple random walk. Now, we could use this quantum mechanical system to further simulate the simple random walk by measuring the position of ψ_1 and prepare a new initial state, this time localized at the measured position. Applying the walk would again lead to the same superposition of states, this time shifted by ± 1, and measuring again would generate just the same results as are known from the classical random walk. Luckily, we are not restricted to measuring and preparing anew, but can simple continue applying the walk operator until performing a measurement on an arbitrary

$$\psi_t = W_H^t \psi_0, \quad t \geq 0. \tag{3.16}$$

As Figure 1 shows, the probability distribution of a quantum walk differs greatly from its classical counterpart. It suggests the ballistic spreading that is characteristic for quantum walks, as well as the diffusive spreading, that is characteristic for classical random walks.

Grover derived a famous search algorithm in [Gro96], which allows finding a key in a database with N elements in $O(\sqrt{N})$ steps, compared to the classical counterpart, which needs $O(N)$ steps. It caused great interest in quantum walks, since it was one of the first applications where the proposed speed-up of quantum walks leads to an advantage over their classical counterpart.

In general, quantum walks that are translation invariant w.r.t. time and space, show ballistic spreading. This was proven in [Ahl+11], and is briefly discussed in the context of Fourier methods in Theorem 3.6. The general intuition, that temporal noise (that is, small changes in the walk

operator from step to step) breaks the coherence of a quantum walk, and hence reduces ballistic scaling to diffusive scaling (or even leads to localization) proves true and is thoroughly analysed in [Ahl+11; Ahl+12a; Ahl13; Wer13].

As was already stated in Theorem 2.11, Grünbaum et al. showed in [Grü+13], that on the one hand, every $\varphi \in \mathcal{H}_{\text{ac}}$, leaves every finite region eventually in norm, on the other, $\psi \perp \mathcal{H}_{\text{ac}}$ is equivalent to ψ being recurrent for W, which is defined slightly different from the classical case, namely directly via the total return probability. That is, the sum of all probabilities of returning to the state ψ after t steps *for the first time* - the so-called *first return probabilities*. Furthermore, they show that for a recurrent state ψ and walk W, every finite expected return time τ has to be a natural number, hence integer valued. This is deduced via a topological argument where τ is expressed as a winding number of the phase of a walk's corresponding Schur function.

A thorough analysis of the 1D-Hadamard-Walk with comparisons between classical random walks and quantum walks is provided by Ambainis et al. in [Amb+01]. Grimmett, Janson, and Scudo focussed on the transport properties of quantum walks from the Heisenberg picture by analysing the time-evolved position operator X_t and deriving a weak-limit theorem showing that for a certain class of translation invariant quantum walks, X_t/t converges weakly to an absolutely continuous distribution as $t \to \infty$, thus suggesting ballistic, not diffusive scaling [GJS04].

Recently, Cedzich et al. showed in [Ced+13], that the introduction of electric fields in the case of 1D-quantum walks leads to a system whose long time propagation properties, such as revivals, ballistic expansion and Anderson localization, depend very sensitively on whether the value of the electric field is rational or irrational. The corresponding experiment was performed by Genske et al. and is published in [Gen+13]. It allowed to verify the theoretical predictions within the limitations of the experiment, showing features related to Bloch oscillations and interband tunneling.

From a computational perspective, there have been improvements on search algorithms e.g. by Ambainis, Kempe, and Rivosh in [AKR05], who show how to search N items arranged on a $\sqrt{N} \times \sqrt{N}$ grid in time $O(\sqrt{N} \log N)$ using a quantum walk. A similar result was obtained by Patel and Raghunathan in [PR12] for quantum walks on fractal lattices of noninteger dimensions. Goswami and Sen analyse in [GS12] how a sudden change of the boundary conditions (by removing a detector that was placed at a specific site) changes the probability distribution of a Hadamard-Walk.

Furthermore, quantum walks have been shown to demonstrate quantum effects such as Landau-Zener tunneling [Reg+11], and Anderson localization [ASW11; Joy12]. Ahlbrecht et al. could even introduce on-

site interactions between two walkers of a quantum walk allowing the formation of molecule-like structures, as described in [Ahl+12b].

Regarding the experimental realizations, there are working simulations of quantum walks with neutral atoms in optical lattices [Kar+09], trapped ions [Sch+09], wave guide lattices [Per+10] and light pulses in optical fibres [Sch+10], as well as single photons in free space [Bro+10].

In [Kit06, C.3], Kitaev defines a quantity he calls the *flow* of a unitary operator that measures a quantum walk's mean transport of information as described later in (3.48). Then, in [Gro+12], Gross et al. provided a thorough analysis including proofs and examples of this quantity they call the *index* of a quantum walk, as well as its generalization to the class of Quantum Cellular Automatons. The topic deserves a proper introduction later in Section 3.4, where it is shown that the index is a locally computable invariant, does not change under norm-continuous deformations within the set of quantum walks, and is complete in the sense that any two quantum walks with the same index can be deformed into each other continuously, keeping a uniform bound on the size of the neighbourhood of the quantum walks along the deformation path. In Section 3.4 we extend the definition to hold for a larger class of objects called *essentially local unitary operators*, and connect the index to the Fredholm index ind_F introduced in the previous chapter.

After this brief overview let us make the definition of a quantum walk from above rigorous.

3.2 DEFINITION

Instead of providing the most general definition, we restrict ourselves to the case of s-dimensional square lattices. At each node $x \in \mathbb{Z}^s$, there is a local Hilbert space $\mathcal{H}_x \cong \mathbb{C}^{d_x}$, where $\{d_x\}_{x\in\mathbb{Z}^s} \subset \mathbb{N}$ is bounded from above by $d = \max_{x\in\mathbb{Z}^s}\{d_x\} < \infty$.

Typically, we do look at the direct sum of these local Hilbert spaces, and hence define the overall Hilbert space as

$$\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x. \tag{3.17}$$

It is tempting to avoid the varying dimension $d(x)$ by adding basis vectors at each position to equalize the $\mathcal{H}_x$'s dimensions to be d. One could then simply assume that these additional vectors are left invariant by the walk operators that implement the time evolution. But this introduces additional eigenvectors for the eigenvalue $+1$ (or whichever value one prefers), strongly interfering with assumptions regarding the spectrum (e.g. existence of gaps) we impose throughout this thesis. Therefore, we cannot *in general* remove the spatial dependence of the local Hilbert spaces' dimensions $d(x)$.

But in many situations, we demand the Hilbert space to allow for translation-invariant operators, meaning that for all $i \in \{1, \dots, s\}$ there exist unitary operators T_i s.t. $T_i \mathcal{H}_x = \mathcal{H}_{x+e_i}$, where e_i denote the unit vectors in the i-direction. This makes $\mathcal{H}$ isomorphic to $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathbb{C}^d$, and after choosing a T that represents the standard shift in the first tensor factor (gauging), we denote the chosen basis in $\ell^2(\mathbb{Z}^s)$ by $\{\delta_x\}_{x \in \mathbb{Z}^s}$, and in $\mathbb{C}^d$ by $\{\alpha_i\}$, $i \in \{1, \dots, d\}$, writing $\delta_x \otimes \alpha_i$ for the basis of $\mathcal{H}$.

We use the well-established Dirac-notation, where $|x, i\rangle : z \mapsto z \cdot \delta_x \otimes \alpha_i$ is a map from the complex numbers to the Hilbert space and $\langle x, i|$ is the corresponding linear functional $\varphi \mapsto \langle x, i|\varphi\rangle$.

There are many advantages in being given $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathbb{C}^d$ in tensor product form. For every $A \in \mathcal{B}(\mathcal{H})$ and every $x, y \in \mathbb{Z}^s$, we can look at the transition operators $\{A_{x,y}\}$ of A:

$$A_{x,y} = \langle x|A|y\rangle. \tag{3.18}$$

The transition operators $A_{x,y}$ are bounded operators on $\mathbb{C}^d$ for all $x, y \in \mathbb{Z}^s$, and every $A \in \mathcal{B}(\mathcal{H})$ can be decomposed in the following way:

$$A = \sum_{x,y \in \mathbb{Z}^s} |x\rangle\langle y| \otimes A_{x,y}. \tag{3.19}$$

Let us now define a quantum walk.

Definition 3.1 (Quantum walk)
Let $\mathcal{H} = \ell^2(\mathbb{Z}^s) \otimes \mathbb{C}^d$ be the Hilbert space as above. We call a unitary operator W a **quantum walk***, if it is strictly local, meaning there is a finite subset $\mathcal{N} \subset \mathbb{Z}^s$ of the lattice (also called a neighbourhood), such that*

$$\langle x, i|W|y, j\rangle = 0 \quad \forall\, x, y \in \mathbb{Z}^s : \; x - y \notin \mathcal{N}. \tag{3.20}$$

One can easily see, that for every $y \in \mathbb{Z}$, the condition of strict locality implies a finite number of non-vanishing transition operators $W_{x,y}$ in (3.19). Furthermore, this number is bounded for all $y \in \mathbb{Z}$ by the number of elements of a minimal $\mathcal{N} \subset \mathbb{Z}^s$ such that (3.20) holds, which we call a *minimal neighbourhood*. The diameter of this minimal neighbourhood determines the *maximal jump length* (sometimes also called *interaction length* or simply *jump length*) of the walk. It expresses the maximal distance an initially localized walker covers in a single step.

There are situations, where it makes sense to generalize this definition to also cover unitary operators obeying a less strict locality-condition, namely essential locality, leading to the definition of essentially local unitaries in Definition 3.4.

Another more constructive approach to defining quantum walks is, to introduce a set of minimal building blocks (shifts and coins), which are then combined via products to span the class of all *coined quantum walks*. The nomenclature follows the classical counterpart of random walks as mentioned in the introduction, where one tosses a coin and

then shifts the walker, depending on the outcome. More rigorously, we define:

Definition 3.2 (Shift-/Coin-operator)
An operator $S_{l,j} \in \mathcal{U}(\mathcal{H})$ is called a **minimal shift**, *if there is a basis $\{\alpha_j\}_{j\in\{1,\dots,d\}}$ s.t.*

$$S_{l,j}|x,\alpha_i\rangle = \begin{cases} |x,\alpha_i\rangle & i \neq j, \\ |x+l,\alpha_i\rangle & i = j. \end{cases} \tag{3.21}$$

A **shift operator** *is a finite product of minimal shifts, all w.r.t. the same basis.*

Complimentary, a unitary operator C on the same Hilbert space is called a **coin-operator**, *if it is diagonal in the spatial basis, e.g. $\forall x \in \mathbb{Z}^s$ there are $V_x \in \mathcal{U}(\mathbb{C}^d)$, s.t.*

$$C = \bigoplus_{x\in\mathbb{Z}^s} V_x. \tag{3.22}$$

This neatly confines the action of each building block to either only translate the sublattice labeled by α_j in one direction by l steps, or act on the local Hilbert spaces $\mathcal{H}_x$ by separate unitary operators V_x without transitioning between positions. Of course, the identity is a trivial shift and a trivial coin at the same time, therefore in the following, it is no restriction to look at alternating combinations of coins and shifts:

Definition 3.3 (Coined quantum walk)
An operator $W \in \mathcal{U}(\mathcal{H})$ is called a **coined quantum walk**, *if there is $n \in \mathcal{N}$ and for all $i \leq n$, there are coin operators C_i and shift operators S_i, all w.r.t. the same basis of $\mathcal{H}$, s.t.*

$$W = C_1 S_1 C_2 S_2 \dots C_n S_n. \tag{3.23}$$

It is an interesting question, whether all quantum walks in the sense of Definition 3.1 are coined quantum walks in a particular basis. In the special case of 1D-translation-invariant walks, this is answered affirmatively in [Vog09].

For one-dimensional quantum walks on the Hilbert space

$$\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x \tag{3.24}$$

an equivalent way of defining a quantum walk W, is by its action on half-space projections $P_{\geq x_0}$, where $P_{\geq x_0}$ is the projector onto all $\mathcal{H}_x$ for $x \geq x_0$. More precisely, given $\mathcal{H}$, a unitary operator W is a quantum walk, iff there is a finite subset $\mathcal{N} \in \mathbb{Z}$ s.t. for every $x_0 \in \mathbb{Z}$,

$$\operatorname{img}\left(P_{\geq x_0} - W^* P_{\geq x_0} W\right) \subseteq \bigoplus_{x\in\mathcal{N}} \mathcal{H}_{x_0+x}, \tag{3.25}$$

where img denotes the image of an operator. Note that the finite direct sum of finite dimensional Hilbert spaces on the right hand side ensures that the image on the left hand side is of finite dimension, which is represented in Figure 2. Now if we do not demand $P_{\geq x_0} - W^* P_{\geq x_0} W$ to

$$\left[\begin{array}{ccc:cccc} 0 & 0 & 0 & -w_{-3,0} & -w_{-3,1} & -w_{-3,2} & -w_{-3,3} \\ 0 & 0 & 0 & -w_{-2,0} & -w_{-2,1} & -w_{-2,2} & -w_{-2,3} \\ 0 & 0 & 0 & -w_{-1,0} & -w_{-1,1} & -w_{-1,2} & -w_{-1,3} \\ \hdashline w_{0,-3} & w_{0,-2} & w_{0,-1} & 0 & 0 & 0 & 0 \\ w_{1,-3} & w_{1,-2} & w_{1,-1} & 0 & 0 & 0 & 0 \\ w_{2,-3} & w_{2,-2} & w_{2,-1} & 0 & 0 & 0 & 0 \\ w_{3,-3} & w_{3,-2} & w_{3,-1} & 0 & 0 & 0 & 0 \end{array}\right]$$

Figure 2: Submatrix of $PW - WP$, with $P = P_{\geq 0}$. The dashed lines denote the cuts induced by P, while the blue shading indicates that the diagonal blocks vanish. A finite neighbourhood $\mathcal{N}$ leads to a maximal jump length L. This limits the set of non vanishing $w_{i,j}$, which necessarily fulfil $|i - j| \leq L$. Therefore, only finitely many elements in the anti-diagonal blocks do not vanish, and the overall matrix is of finite rank. This fact is not changed by multiplication with the unitary operator W^*, and therefore $P - W^*PW$ is of finite rank iff $PW - WP$ is. Note that the same argument holds for essentially local operators, where $PW - WP$ is a compact operator.

be an operator of finite rank, but allow it to be a compact operator, we arrive at the following definition:

Definition 3.4 (Essential locality, ELEU)
Let $\mathcal{H}$ be as in Definition 3.1 and U be an (essentially) unitary operator. We call U **essentially local***, if for some $x_0 \in \mathbb{Z}$, $P_{\geq x_0} - U^* P_{\geq x_0} U$ is a compact operator.*
We will sometimes use **ELEU** *as an abbreviation for* **essentially local essentially unitary (operator)**.

It might seem arbitrary to demand compactness only for some x_0. However, if $P_{\geq x_0} - U^* P_{\geq x_0} U$ is a compact operator for some $x_0 \in \mathbb{Z}$, for every $x \in \mathbb{Z}$, the difference between $P_{\geq x_0} - U^* P_{\geq x_0} U$ and $P_{\geq x} - U^* P_{\geq x} U$ is the finite rank (hence compact) operator

$$P_{\geq x_0} - P_{\geq x} - U^*(P_{\geq x_0} - P_{\geq x})U.$$

Since compact operators are closed under addition, demanding compactness for some $x_0 \in \mathbb{Z}$ leads to compactness for all $x \in \mathbb{Z}$.

In the same line of reasoning, note that for U ELEU and any $x \in \mathbb{Z}$, $P = P_{\geq x}$ decomposes U into four parts

$$U = PUP + (\mathbb{1} - P)U(\mathbb{1} - P) + PU(\mathbb{1} - P) + (\mathbb{1} - P)UP. \tag{3.26}$$

The last two summands on the right hand side are compact due to the essential locality of U, since the compactness of $UP - PU$ implies the compactness of $PU(\mathbb{1} - P)$ and $(\mathbb{1} - P)UP$.

In the following section, we will introduce translation invariant operators and use the Fourier transform to simplify the analysis of our basic objects greatly.

3.3 TRANSLATION INVARIANCE

In the previous section, we have defined quantum walks, as well as essentially local unitaries. Since we look at Hilbert spaces $\mathcal{H}$ that are isomorphic to tensor products $\ell^2(\mathbb{Z}^s) \otimes \mathbb{C}^d$, there are translation operators $\{T_i\}_{1\leq i\leq s}$ that allow to move states along the lattice directions, e.g. $T_i|x,\varphi\rangle = |x+e_i,\varphi\rangle$. In a slight abuse of notation, we will write $T_x := T_1^{x_1}\dots T_s^{x_s}$ for all $x = (x_1,\dots,x_s) \in \mathbb{Z}^s$. This allows us to define translation invariance:

Definition 3.5 (Translation invariance)
Let $\mathcal{H}$ be as in Definition 3.1 and $\{T_i\}_{1\leq i\leq s}$ be the set of minimal translation operators on this lattice. An operator $A \in \mathcal{B}(\mathcal{H})$ is called translation invariant, if it commutes with every T_i. If this is only true for some i_o, we will call A translation invariant w.r.t. the x_{i_o}-direction.

If we look at the transition operators $A_{x,y}$ in the translation invariant case, we see, that they depend only on the difference of y and x:

$$\begin{aligned}\langle\psi|A_{x,y}|\varphi\rangle_{\mathbb{C}^d} &= \langle x,\psi|A|y,\varphi\rangle_{\mathcal{H}}\\ &= \langle x,\psi|AT_y|o,\varphi\rangle_{\mathcal{H}}\\ &= \langle x-y,\psi|A|o,\varphi\rangle_{\mathcal{H}}\\ &= \langle\psi|A_{x-y,o}|\varphi\rangle_{\mathbb{C}^d}\end{aligned} \tag{3.27}$$

Applying this to (3.19), we get (after using $A_{z,o} = A_{o,-z} =: A_z$)

$$A = \sum_{x,z\in\mathbb{Z}^s} |x\rangle\langle x-z| \otimes A_z, \tag{3.28}$$

or equivalently:

$$(A\psi)(x) = \sum_{z\in\mathbb{Z}^s} A_z\psi(x-z) = \sum_{z\in\mathbb{Z}^s} A_{x-z}\psi(z). \tag{3.29}$$

For quantum walks W, their strict locality implies that only finitely many W_z are non-zero, therefore the series reduces to a finite sum.

In the following, we show that the Fourier transform

$$\begin{aligned}\mathcal{F}&: \ell^2(\mathbb{Z}^s) \to \mathcal{L}^2\left(\mathbb{T}^s, \frac{\mathrm{d}^s k}{(2\pi)^s}\right)\\ (\mathcal{F}\psi)(k) &:= \sum_{x\in\mathbb{Z}^s} e^{ik\cdot x}\psi(x) =: \widehat{\psi}(k)\\ (\mathcal{F}^*\widehat{\psi})(x) &:= \frac{1}{(2\pi)^s}\int_{\mathbb{T}^s} \mathrm{d}^s k\, e^{-ix\cdot k}\widehat{\psi}(k)\end{aligned} \tag{3.30}$$

turns the above convolution into a product (with $\mathbb{T}^s = [-\pi, \pi]^s$ denoting the s-dimensional torus):

$$\begin{aligned}(\mathcal{F}A\psi)(k) &= \sum_{x,z\in\mathbb{Z}^s} e^{ik\cdot x} A_z \psi(x-z) \\ &= \sum_{z\in\mathbb{Z}^s} A_z \sum_{x\in\mathbb{Z}^s} e^{ik\cdot(x+z)}\psi(x) \\ &= \sum_{x\in\mathbb{Z}^s} e^{ik\cdot x} A_x \widehat{\psi}(k) \\ &=: \widehat{A}(k)\widehat{\psi}(k). \end{aligned} \tag{3.31}$$

Here, we used $\mathcal{F}$ as shorthand notation for $\mathcal{F} \otimes \mathbb{1}_d$.

In the case of quantum walks W, only finitely many $d \times d$-matrices W_x do not vanish. This makes $\widehat{W}(k)$ a matrix valued Laurent polynomial[2] in the variables e^{ik_j}.

For the remaining section, let us restrict ourselves to the case of one spatial dimension $s = 1$. Then, $\widehat{W}(k)$ is a finite-dimensional, k-dependant unitary operator, that can be diagonalized due to the spectral theorem:

$$\widehat{W}(k) = \sum_{\alpha=1}^{d} e^{i\omega_\alpha(k)} Q_\alpha(k), \tag{3.32}$$

where $\omega_\alpha(k)$ are the dispersion relations or quasi energies, and $Q_\alpha(k)$ the bandprojections or eigenprojections. Note that this decomposition is unique if there are no degeneracies in $\omega_\alpha(k)$. But even when there are degeneracies, perturbation theory for one-parameter families of normal analytic operators shows [Kat76], that one can make analytical choices for the quasi energies $\omega_\alpha(k)$, as well as the eigenprojections $Q(k)$ around these degenerate points. Therefore, we always assume to have taken such a choice for all $k \in [-\pi, \pi]$.

Another useful tool derived from the diagonalization of $\widehat{W}$ is the group velocity operator (in momentum space representation):

$$\widehat{G}(k) = \sum_{\alpha=1}^{d} \frac{\partial\omega_\alpha(k)}{\partial k} Q_\alpha(k). \tag{3.33}$$

Naming this operator the group velocity operator is suitable, as the following Theorem from [Ahl+11] shows:

Theorem 3.6
Let $\widehat{W}(k)$ be a quantum walk in momentum representation, $X(t)$ the t-evolved position observable in the Heisenberg picture, s.t.

$$X(t) = (W^*)^t X W^t, \tag{3.34}$$

2 A Laurent polynomial in x is a linear combination of positive and negative powers of the variable x.

and G the group velocity operator (in position space) as defined above. Then

$$\lim_{t\to\infty} \frac{X(t)}{t} = G. \tag{3.35}$$

That is, 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 $f(X(t)/t)$ is $f(G)$.
This means, that for any initial state ρ_o, the distribution of the random variable $X(t)/t$ converges weakly to the distribution of G in ρ_o.

If we look at the standard-deviation $\sqrt{\mathrm{Var}}$ as our function f, it follows that weak convergence of $X(t)/t$ to some t-independent distribution implies that $\sqrt{\mathrm{Var}(X(t))}$ scales like t for large t, the ballistic propagation mentioned in the introduction.

As an example, let us consider T, the simple shift by one cell in $d = s = 1$:

$$\langle y, Tx\rangle = \delta_{y,x+1}. \tag{3.36}$$

Its Fourier transform is

$$\widehat{T}(k) = \sum_{x\in\mathbb{Z}} e^{ikx}\delta_{x,1} = e^{ik}, \tag{3.37}$$

and in this case, since $d = 1$, this is already the diagonalization of $\widehat{T}(k)$, with $Q(k) = 1$ and $\omega(k) = k$.

Therefore, the group velocity operator is easily found to be $\widehat{G}(k) = 1$, which by Theorem 3.6 shows that any initial state ρ_o (e.g. $\rho_o = |o\rangle\langle o|$) is, in the averaging limit and in the expectation value, moving with constant velocity of one site per time step to the right - which is exactly what we know that T does: in each step, it shifts each state to the right by one cell.

Having introduced the Fourier transform of a translation invariant operator, let us fix some notation and state a few well known results regarding the adjoint and the determinant of operators represented in momentum space. Firstly, we have to decide how we distinguish between matrix elements of the adjoint and the adjoint of a matrix-valued coefficient:

$$\left(A^*\right)_{x,y} = (A_{y,x})^* \quad \Rightarrow \quad \left(A^*\right)_{-z} = (A_z)^* =: A^*_x. \tag{3.38}$$

The consequences for $\widehat{A}(k)$ are then

$$\begin{aligned}\widehat{A^*}(k) &= \sum_{x\in\mathbb{Z}} e^{ikx}\left(A^*\right)_x = \sum_{x\in\mathbb{Z}} e^{ikx}A^*_{-x} = \sum_{x\in\mathbb{Z}} e^{-ikx}A^*_x \\ &= \left(\sum_{x\in\mathbb{Z}} e^{ikx}A_x\right)^* = \left(\widehat{A}(k)\right)^* =: \widehat{A}^*(k).\end{aligned} \tag{3.39}$$

Since we often deal with finite dimensional k-dependent matrices $\widehat{U}(k)$, we often encounter the determinant of $\widehat{U}(k)$. We know that the determinant is a polynomial, and therefore continuity and differentiability of a finite dimensional matrix valued function simply transfer to

its determinant. If we consider $\det \widehat{U}(k)$ as a differentiable function in k, it is useful to know the derivative of this function.

Lemma 3.7 (Derivative of the determinant)
Let $\widehat{U}(k)$ be an $d \times d$-matrix-valued function that is invertible and differentiable for all k, and let $\det \widehat{U}(k)$ denote its determinant, considered as a differentiable function in k. Then,

$$\frac{\mathrm{d}}{\mathrm{d}k} \det \widehat{U}(k) = \det \widehat{U}(k)\ \mathrm{tr}\left(\left(\widehat{U}(k)\right)^{-1} \frac{\mathrm{d}\widehat{U}(k)}{\mathrm{d}k} \right). \tag{3.40}$$

Proof. Since $\widehat{U}(k)$ is invertible, and det is a homomorphism for multiplication, we can write

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}k} \det \widehat{U}(k) \\
&= \lim_{h \to 0} \frac{1}{h} \left(\det \widehat{U}(k+h) - \det \widehat{U}(k) \right) \\
&= \det \widehat{U}(k) \cdot \lim_{h \to 0} \frac{\det\left(\widehat{U}^{-1}(k) \widehat{U}(k+h) \right) - 1}{h} \\
&= \det \widehat{U}(k) \cdot \lim_{h \to 0} \frac{\det\left(\mathbb{1} + h \cdot \widehat{U}^{-1}(k) \frac{\mathrm{d}}{\mathrm{d}k} \widehat{U}(k) + O(h^2) \right) - 1}{h}.
\end{aligned} \tag{3.41}$$

Due to the limit and the prefactor, as well as the fact that det is a polynomial of degree d, we can ignore terms that are $O(h^2)$. What remains is to show, that

$$\lim_{k \to 0} \frac{1}{k} \left(\det(\mathbb{1} + k \cdot V) - \det \mathbb{1} \right) = \mathrm{tr}(V). \tag{3.42}$$

In the V-eigenbasis, $\mathbb{1} + k \cdot V$ is diagonal as well. Furthermore, the determinant of a matrix is the product of its eigenvalues. Hence with $\{v_j\}$ denoting the eigenvalues of V, we have

$$\det(\mathbb{1} + k \cdot V) = \prod_{j=1}^{d} (1 + k \cdot v_j). \tag{3.43}$$

Inserting this into the limit, we see that the $\det(\mathbb{1})$ and the k-constant 1 cancel. The k linear term that remains is exactly the sum of the eigenvalues of V, which is the trace. Putting it all together, we get

$$\frac{\mathrm{d}}{\mathrm{d}k} \det \widehat{U}(k) \bigg|_{k=0} = \det \widehat{U}(0) \cdot \mathrm{tr}\left(\widehat{U}^{-1}(0)\ \frac{\mathrm{d}\widehat{U}(k)}{\mathrm{d}k} \bigg|_{k=0} \right), \tag{3.44}$$

finishing the proof. □

This concludes our section about translation invariant quantum walks. We continue with a remarkable classification of quantum walks, that gives a precise notion of the flow of quantum information of a unitary operator.

3.4 INDEX

As a foretaste of the symmetry classification in the main part of this thesis, this section introduces an index (i.e. a map from a set of operators that are supposed to be classified, to an index set, e.g. the integers), that labels the homotopy classes of 1D-quantum walks. More precisely, as was shown in [Gro+12], two quantum walks can be continuously deformed into each other if and only if they have the same index. Furthermore, along the way, the defining property of quantum walks, that is strict locality and unitarity, is not broken, e.g. there is a uniform bound on the maximal jump length on the way between the two walks, and unitarity is always kept.

General index theory

The definition of the index can be chosen to be a bit more general than absolutely necessary, in order to allow for a larger class of systems under consideration: the set of one-dimensional essentially local[3] essentially unitary[4] operators (ELEU):

Definition 3.8 (Index)
Let $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$ be the Hilbert space, $P = P_{\geq 0}$ be the half-space projection and U an ELEU. Then, the index of U is defined as:

$$\operatorname{ind}(U) := \operatorname{ind}_F(PUP). \tag{3.45}$$

Here, PUP is regarded as an operator on $\ell^2(\mathbb{N}) \otimes \mathbb{C}^d$.

Under these assumptions, it can easily be seen, that PUP is again essentially unitary (hence Fredholm), such that ind_F is well defined: since essential locality implies, that the off-diagonal blocks in a block-decomposition with respect to half-spaces induced by P and $\mathbb{1} - P$ are compact operators, dropping them neither changes the Fredholm index of U nor essential unitarity. Since the resulting operator is block-diagonal with respect to P, essential unitarity of U implies essential unitarity of the blocks on the corresponding half-spaces, finishing the argument.

Since we defined the index of U as a Fredholm index, most of its basic properties can be taken over from Fredholm theory directly (compare with Proposition 2.18):

Corollary 3.9 (Properties of the index)
Let $\mathcal{H}, P$ be as above, T be the unilateral shift as in (3.36), K a compact operator and let U, U_1, U_2 be ELEU. Then

1. $\operatorname{ind}(U) \in \mathbb{Z}$
2. $\operatorname{ind}(U_1 \oplus U_2) = \operatorname{ind}(U_1) + \operatorname{ind}(U_2) = \operatorname{ind}(U_1 U_2)$

3 see Definition 3.4
4 see Definition 2.22

3. $\operatorname{ind}(T^n) = d \cdot n \quad \forall n \in \mathbb{N}$, *esp.* $\operatorname{ind}(\mathbb{1}) = 0$
4. $\operatorname{ind}(U) = \operatorname{ind}(U + K)$
5. $\operatorname{ind}(U)$ *is a homotopy invariant*

The invariance of $\operatorname{ind}(U)$ with respect to compact additions (4.) shows, that it does not matter where we cut the line, i.e. any $P = P_{\geq a}$ $\forall a \in \mathbb{Z}$ yields the same result. (2.) tells us, how indices behave under composition and multiplication, which together with (3.) shows, that ind as a map is also onto, since a suitable combination of shifts (restricted to a subspace in the coin space if needed) and the identity generates every non-negative integer we want for ind. Furthermore, (2.) shows, that $\operatorname{ind}(U) = -\operatorname{ind}(U^*)$, and combining these two results, every integer value can be realized by a combination of shifts, identities and possibly an adjoint.

The homotopy invariance (5.) follows directly from the homotopy invariance of ind_F, since constance of the index was shown to hold along all norm-continuous paths of Fredholm operators, which is a superset to all norm-continuous paths of essentially unitary essentially local operators.

The converse of this is called the completeness of the homotopy invariant and answers the following question: Are the sets of essentially unitary essentially local operators with the same index connected? This is much harder to answer, and not as easily concluded from the completeness of the Fredholm index on the set of all Fredholm operators in Proposition 2.19. If we restrict the set of allowed operators, sets that were formerly connected might disconnect, since the connecting paths might contain now-forbidden operators.

Since quantum walks are a strict subset of the essentially local essentially unitary operators, all the above properties are valid for them as well. Surprisingly, by restricting to the class of quantum walks, a theorem from [Gro+12] proves that completeness of the index holds in this restricted class:

Theorem 3.10 (Completeness of the index)
Let W_0, W_1 be quantum walks on $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$. Then, the following are equivalent:

- $\operatorname{ind}(W_0) = \operatorname{ind}(W_1)$
- *There is a norm continuous path $[0, 1] \ni t \mapsto W_t$ of quantum walks of uniformly bounded interaction length*[5] *L connecting W_0 and W_1.*

Another result from [Gro+12] is, that the index is a *locally computable invariant*. This means, that it can be calculated from any sufficiently long slice of the walk, without further knowledge about the rest of the

5 See the comment after Definition 3.1 for the definition of the interaction length.

system[6]. For the term *locally computable invariant* to make any sense at all, it has to yield the same value everywhere - which makes it a global property that can be probed locally.

Having learned that quantum walks with different indices can not be continuously deformed into another (keeping a uniformly bounded interaction length), it is an interesting question whether the index plays a role in deciding if there is a way to locally *decouple* a quantum walk U w.r.t. the spatial structure:

Definition 3.11 (Local decoupling)
Let $\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_R$ be the Hilbert space with $\mathcal{H}_R := P\mathcal{H} = \bigoplus_{x\geq 0} \mathcal{H}_x$ and $\mathcal{H}_L := (1-P)\mathcal{H}$ and U be an essentially local operator. We call a unitary operator V a **decoupling**, *if*

$$VU = U_L \oplus U_R, \tag{3.46}$$

where U_R acts only on $\mathcal{H}_R$ and U_L only on $\mathcal{H}_L$.
An operator of the form $U' = U_L \oplus U_R$ is called a **decoupled** *operator.*
A decoupling V is called **compact**, *if $V - \mathbb{1}$ is a compact operator.*
If additionally, V differs from the identity only on finitely many $\mathcal{H}_x$, we call it a **local decoupling**. *In this case, the subspace $\mathcal{H}_V := (V-\mathbb{1})\mathcal{H}$ is of finite dimension.*

Given a local decoupling V, it is easy to construct a norm-continuous path of unitary operators $[0,1] \ni t \mapsto V_t$ with $V_0 = \mathbb{1}$ and $V_1 U = U_L \oplus U_R$, hence connecting U and the decoupled VU. This is most easily expressed in the functional calculus: as an operator that differs from the identity only on the finite dimensional $\mathcal{H}_V$, we only have to solve a finite-dimensional problem. This can be done easily by diagonalizing on $\mathcal{H}_V$ and applying $f_+(\lambda) = \lambda^t$ to the spectrum of V, thus contracting V to the identity as t goes from 1 to 0.

Since ind is a homotopy invariant, the existence of this path shows, that a walk and its decoupled version have the same index. In [Gro+12], the following theorem connects the value of the index to the existence of a decoupling:

Theorem 3.12 (Existence of a decoupling)
Let U be a quantum walk on $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$. Then, the following are equivalent:

- $\mathrm{ind}(U) = 0$
- *U admits a local decoupling*

If we simply try to extend this result to unitary, essentially local operators U, it certainly does not make sense to hope for a local decoupling

6 Typically, the index can be inferred from a slice of the walk spanning a number of cells that is at least a multiple of the maximal jump length. If one regroups the walk to a nearest neighbour-walk by collecting adjacent cells to build sufficiently large cells, a slice of length 2 suffices, see [Gro+12, Sect. 5] for details.

if the locality condition is not strict (i.e. finite jump length, U is a quantum walk). With some effort, in Section 5.5 we explicitly construct for any unitary, essentially local operator U with vanishing index a decoupling, that is connected to U. Furthermore, we generalize these results to even satisfy additional constraints of keeping a spectral gap and certain symmetry relations (*admissibility*) explained in Chapter 4.

Index theory for translation invariant operators

It is a remarkable feature of the index ind, that it is a locally computable invariant, hence can be inferred from a small number of neighbouring cells $\mathcal{H}_x$. Thus while *local computability* reduces the computation to a finite patch, the invariance implies that the value of ind is independent of where the patch lies. In this sense, the index is a translation invariant property.

In the following, we will see, that determining the index is significantly simpler if the essentially local operator is actually translation invariant. The following proposition from [Gro+12, Prop. 5] establishes this in the case of quantum walks, but the proof is similarly applicable for essentially local unitary operators as well:

Proposition 3.13 (Index: translation invariant)
Let W be a translation invariant quantum walk. Then, there is a constant $C \in \mathbb{T}$ s.t.

$$\det \widehat{W}(k) = C \cdot e^{ik \cdot \mathrm{ind}(W)}. \tag{3.47}$$

Hence calculating the determinant of the k-dependant multiplication operator in momentum space allows to read-off the index directly.

Given the group velocity in momentum space from (3.33), and using Theorem 3.6, we know that the probability distribution for the Hermitian operator G in a state ρ is equal to the asymptotic position distribution that stems from ρ in ballistic scaling (see the details in [Ahl+11]). Choosing a state where the coin-factor is unpolarized, e.g. $\rho = \sigma \otimes \mathbb{1}/d$, we find [Gro+12]:

$$\langle X(t) \rangle = \langle X(0) \rangle + \frac{t}{d} \, \mathrm{ind}(W). \tag{3.48}$$

This shows why $\mathrm{ind}(W)$ is called the flow that measures the drift of quantum information: it represents the mean velocity of the walk in units of *cells to the right per time step*.

Remarkably, in the translation invariant case, the index can also be determined by looking at the *windings* of the quasi-energy-bands $\omega_\alpha(k)$. As is shown in [Gro+12, Fig. 3], summing up the signed number of crossings of any line of constant quasi-energy for all bands together yields the same number as the sum of derivatives of all branches, which is to be the index.

The completeness of the index in the setting of arbitrary quantum walks is a strong result on its own, but it is even more conspicuous,

that restricting the class to *translation invariant* quantum walks yields a similar completeness result in this restricted class as well:

Theorem 3.14 (Completeness of the index: translation invariant)
Let W_0, W_1 be translation invariant *quantum walks on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$. Then, the following are equivalent:*

- $\mathrm{ind}(W_0) = \mathrm{ind}(W_1)$
- *There is a norm continuous path $[0,1] \ni t \mapsto W_t$ of translation invariant quantum walks of uniformly bounded interaction length L with the specified boundary values.*

This statement can be found in [Gro+12, Prop. 6]. There, proving this theorem is greatly simplified due to the result that every one-dimensional translation invariant quantum walk is a *coined quantum walk* as mentioned after Definition 3.3.

Perturbations

In the following chapter, before we introduce the strong constraints that the involutive symmetries of the tenfold-way demand, we briefly define a set of perturbations of (essentially) unitary operators that are used throughout the rest of the thesis. They give a foretaste of the kind of *perturbations* which leave the *symmetry indices* unchanged. In the following chapters, it will be of large interest whether the indices are homotopy invariants or even robust w.r.t. *local* perturbations that change only a small part of the operator in some finite neighbourhood of a cell.

For now, we define the following three types of perturbations. Note that we usually add more qualifiers to these perturbations. That is, we demand at least *admissibility* which demands that the perturbation respects the symmetry constraints. The details of this follow later, e.g. with Definition 4.2.

Definition 3.15 (Perturbations)
Let U, U' be (essentially) unitary operators on $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$. Then, U and U' are called **perturbations of** *each other, that are*

local, *if $U' - U$ is non-zero only on finitely many $\mathcal{H}_x$,*

finite rank, *if $U' - U$ is a finite rank operator,*

compact, *if $U' - U$ is a compact operator.*

A unitary operator V s.t. $U' = VU$ is called a **perturbation for** *U, that is local, finite rank or compact.*

Following the definitions of finite rank and compact operators from Section 2.5, it is obvious that *local* perturbations are contained in the set of perturbations of *finite rank*. The converse is not true, since finite rank

perturbations might be skew w.r.t. the decomposition into the $\mathcal{H}_x$, i.e. span infinitely many cells. Since compact operators are limits of finite rank operators, the set of compact operators contains the finite rank operators, but not vice versa.

In Section 5.4, we prefer to write perturbations multiplicatively, i.e. describing perturbations *for* U instead of perturbations *of* U. Due to unitarity, the conditions from Definition 3.15 can be rephrased, with $V := U'U^*$

$$(U' - U)U^* = U'U^* - \mathbb{1} = V - \mathbb{1}. \tag{3.49}$$

For a *compact* or *finite rank* perturbation, we see that $V - \mathbb{1}$ is again a compact or finite rank operator. In the case of *local* perturbations, a similar statement is possible whenever we have a strict locality condition, i.e. U and U are quantum walks. Then, in the case of a local perturbation V for U, V differs from the identity only on finitely many sites. More precisely, given two quantum walks U, U' with maximal jump length L_1, L_2, that are *local* perturbations of each other s.t. $U - U'$ is non-zero only on $\bigoplus_{x\in C} \mathcal{H}_x$, V can only differ from the identity on $\bigoplus_{x\in C'} \mathcal{H}_x$, where

$$C' = \left\{ y \,\middle|\, \exists x \in C : |x - y| \leq \max\{L_1, L_2\} \right\}. \tag{3.50}$$

For unitary operators that are not quantum walks, even in the case of a local perturbation, a finite C' is not guaranteed. On the other hand, a V that differs from the identity on finitely many sites, clearly implies a local perturbation between U and U' independent of their locality constraints.

This finishes our treatment of perturbations, the index and the in general *non-admissible* quantum walks or essentially local unitary operators. As the following chapter shows, we will now add symmetries to the picture and develop our *topological classification of one dimensional quantum walks with discrete symmetries*.

4

SYMMETRIES AND THE INDEX OF A REPRESENTATION

In many situations in quantum mechanics we are given a system and a description of the time evolution and we try to find a suitable mathematical framework describing the features of interest. To simplify the situation, one of the first steps is to analyse which parts of the system are invariant under which operations, i.e. whether the system possesses symmetries that help in the description.

Before introducing our topological classification of essentially local unitary operators that lie in one of the symmetry classes of the *tenfold-way*, we want to provide an overview over the concept of topological phases as well as preliminary work in the field.

4.1 OVERVIEW AND PRELIMINARY WORK

Since the early days of quantum mechanics and condensed-matter physics the discovery and classification of quantum matter into different *phases* were of special interest. The Landau's approach to symmetries and phase-transitions describes how the presence or spontaneous breaking of symmetries characterizes different phases of quantum matter, indicated by a suitable order parameter.

The discovery of the quantum hall effect [KDP80; Lau81] showed that Landau theory is insufficient to describe *all* phases of quantum matter. In that scenario, describing electrons put on a two dimensional square lattice and applying a strong perpendicular magnetic field leads to Landau levels, which are quantized. Therefore, filling the Landau levels up to level N produces a gap that separates the occupied and the empty states just as in an insulator. The application of an electrical field causes the electrons to drift, leading to a *quantized Hall conductivity* in the direction orthogonal to the electric and magnetic fields, which is proportional to N, thus taking integer values (after a suitable choice of units). Today, this result is confirmed to high precision (up to 1 part in 10^9) and is e.g. used to determine the fine-structure constant [Kli05].

Describing the quantum hall effect in momentum space [Tho+82] allows one to view the Landau levels as the (constant) 2D band structure of the corresponding Hamiltonian, hence a real-valued function on the 2D-torus (the Brillouin zone). Each of these bands corresponds to an eigenfunction on the torus, which acquires a well-defined geometrical phase (the first Chern number or *Berry phase* as introduced e.g. in [Ber84], see Corollary 7.9 and (7.38)) if we follow a closed curve around the torus.

As long as the gap stays open, the sum n of all Chern numbers of occupied bands is a topological invariant, i.e. its value does not change under continuous deformations of the corresponding Hamiltonian. Since a description via quasi-momentum assumes an infinite dimensional translation invariant system, this invariant is considered a *bulk-invariant*. In [Tho+82], Thouless et al. showed that this bulk-invariant n and the number of filled Landau levels N coincide, which thus confirms the invariance of the quantized Hall conductivity under small changes of the magnetic field.

Hence, the value of the Hall conductance serves to classify a phase of the system, which is a *topological invariant*, even without breaking any symmetry. This coined the term *topological phases* differing from the Landau phases known before, as well as the term *topological insulator* instead of an ordinary insulator.

Hatsugai provided a modification of the system for rational values of the magnetic field in [Hat93b; Hat93a]. He restricts the system in one direction to a finite number of sites that is commensurate with the denominator of the magnetic field, which leads to the occurrence of edge states. After a Fourier transform with respect to the other direction, the winding of the edge states gives another topological invariant, the *edge-invariant*. Remarkably, in that paper he succeeded in showing that the value of the edge-invariant coincides with the value of the bulk-invariant. This and many similar phenomena are subsumed under the statement later coined the *bulk-boundary-correspondence* (which we analyse in Section 5.3). For more information on topological insulators in general, see the review [HK10] and references therein.

In Section 2.3 we provided a classification of the simplest kind of non-trivial symmetry groups one can think of. That is, discrete symmetry groups generated by one element which thus has to be an involution, or two distinct involutions whose product thus yields a third involution, leading to Klein's *Vierergruppe*. In his remarkable general analysis of symmetric spaces [Car26], Cartan introduced a large number of different symmetry classes. In a following publication he introduced labels for these classes e.g. AIII or BDI, which became the de-facto standard notation for symmetry classes in many fields, including topological insulators [AZ97].

The symmetries of primary interest for the theory of topological phases are (besides translational symmetry) time-reversal symmetries, particle-hole symmetries and chiral symmetries. Before defining these in Section 4.2, we give a few references. Analysing the action of *time-reversal* symmetries τ on atomic nuclei with and without taking spins into account [Dys62; Dys70], Dyson identified the classes A, AI and AII, characterized by the absence of τ, the presence of τ squaring to $+\mathbb{1}$ and the presence of τ squaring to $-\mathbb{1}$ (compare with the single antiunitarily represented symmetry in Section 2.3). Adding a unitarily represented *chiral* symmetry γ, which is present in many spin-$\frac{1}{2}$-systems, leads to

the cases AIII (compare with the single unitarily represented symmetry), BDI (compare with the four-group, where $s_1 = s_2 = +1$) and CII (compare with the four-group, where $s_1 = s_2 = -1$). An example for an explicit *particle-hole* (η) symmetric system is the superconductor described via Bogoliubov-de Gennes theory [Gen66]. If η is the only non-trivial symmetry in the symmetry-group, the symmetry classes are D or C, whose topological classification differs i.a. in the dimensionality of the system under consideration [RH02; HK10].

Altland and Zirnbauer completed this case distinction in [AZ97], providing the *tenfold-way* that lists all possible combinations of (absent or present) particle-hole symmetries, time reversal symmetries and chiral symmetries with the respective options for the squares. Using the results from Section 2.3 and restricting to 1D, we provide our own derivation of the tenfold way in Section 4.2.

Classifying quantum matter by identifying topological invariants is certainly of sufficient interest on its own. Nevertheless, there is a striking phenomenon known as the *bulk-boundary-correspondence*[1] which predicts that by joining two *bulk* systems, eigenstates localized at the edges occur. Moreover, there are topological invariants at the bulk (e.g. a Chern number derived from a band structure) and invariants at the boundary (e.g. a number of states localized at the edge, weighted with the parity of the eigenfunction w.r.t. a chiral symmetry), whose values are predicted to coincide. If the conjecture holds, these edge-states cannot simply vanish, at least as long as the bulk-invariants of the joined systems predict non trivial edge-invariants. They are supposed to be invariant of how the connection is made, which implies a stability or *protection* of the edge-states w.r.t. perturbations that do not break the symmetries.

An example of the emergence of edge states and the bulk-boundary-correspondence in a range of Hamiltonian systems is provided by [RH02] or by [HK10, II.3] and references therein. We will explicitly prove the bulk-boundary-correspondence within the range of our theory of quantum walks in Section 5.3.

In 2009, Kitaev provided a thorough analysis of the tenfold way for Hamiltonian systems using topological K-theory and Bott periodicity of the homotopy groups to classify Hamiltonian vector bundles over the Brillouin zone [Kit09]. His results are not restricted to low dimensions, but work for every spatial dimension. That is, he explains which values the topological invariants can have[2], but he does not provide a way to determine them for an explicit Hamiltonian of a certain symmetry class. Furthermore, it seems impossible to extract at least a sketch of a proof from his publication, as opposed to the very recent publication by Thiang, who provided a full framework for treating gapped

1 Sometimes, the boundary is referred to as *edge* and vice versa. We consider both terms as interchangeable.

2 More precisely, he derives the index groups $\mathbf{I}(\mathsf{S})$ as we introduce in Section 4.3.

topological insulators [Thi16], using a different K-theoretic approach than Kitaev.

To summarize, we note that in case of Hamiltonians, the classification of symmetries of the tenfold way is covered well, even though the approaches are sometimes not very well documented.

Still, it remained obscure how this theory might apply to the promising new systems explained in Chapter 3, namely quantum walks. Due to the relative recency of the concepts, there was no prior classification of topological phases for quantum walks covering more than a few examples. The approach to this problem that was taken in [Asb12; Kit+10] was to look at the classification of the Hamiltonian case from [Kit09] and generate quantum walk examples W, whose effective Hamiltonian H_{eff} is determined up to a branch cut of by the logarithm of $W = e^{iH_{\text{eff}}}$. With this approach, the authors succeeded in showing the existence of quantum walks whose effective Hamiltonians satisfied the symmetries of all cases of the tenfold way. Furthermore, they proposed topological invariants for some examples that were determined by counting gap closures along continuous paths in the examples' parameter plane.

One striking distinction from the Hamiltonian case is that in the unitary case, there are two symmetry-related gaps at ± 1, as opposed to the single gap at 0 in the Hamiltonian case. This was noted in [Jia+11] and was applied by Asbóth in [Asb12] to introduce two different invariants, corresponding to each of the gaps. Then, in [AO13], Asbóth and Obuse introduced two topological invariants for a more general class of examples, namely chiral symmetric split-step-walks[3]. They used these invariants to predict the occurrence of topologically protected edge states by *assuming* the bulk-boundary-correspondence and visualized this numerically in the following way by preparing a state at the boundary of two joined walks and looking at its time evolution. On the one hand, if it occurred that the probability to find the walker close to the boundary was bounded from below with a non-vanishing value for many steps, the initial state presumably had some overlap with an eigenstate at the edge. On the other hand, if walks of the same phase were connected, where one thus would not expect *topologically protected edge-states*, their examples suggests that no such lower bound existed, which they considered showed bulk-boundary-correspondence.

At the same time, Kitagawa published a summary of their prior work [Kit12] which suggested that their construction might extend to different examples than the Split-Step-Walk which they treat as *the* quantum walk in earlier publications. Complementing this in a more recent publication [TAD14], Tarasinski, Asbóth, and Dahlhaus suggested to consider the class of coined quantum walks and provided a way to determine two different topological invariants via a scattering-matrix they define. The scheme to determine these invariants is applicable for every coined quantum walk, and their predictions are confirmed

3 We apply our theory to this exemplary class of Split-Step-Walks in Section 8.2.

with a simulation of a Split-Step-Walk, a Four-Step-Walk and a doubled Split-Step-Walk.

Yet, none of these approaches provide a rigorous topological classification of one-dimensional quantum walks as one would hope for a topic of such broad interest. That is, a concise theory which precisely answers:

- Which assumptions do the classified objects have to satisfy?
- What are the topological invariants i and how can they be determined?
- Which perturbations leave the different i invariant?
- Is the classification provided by the i complete?
- How do we compose systems?
- Are the composed systems still described by the theory?

Clearly, one could continue this list and make it reflect exactly what a thorough theory should have in all detail. Instead, since this thesis covers large parts of such a rigorous topological classification, it appears to be more fruitful to simply start with the theory and point to the Outline in Chapter 1 or our collaborations' publications [Ced+15; Ced+17]. The collaborating team was comprised of Cedzich, Geib, Grünbaum, Stahl, Velázquez, A. H. Werner and R. F. Werner.

4.2 SYMMETRY TYPES AND CLASSES

In Section 2.2 we introduced a general notion of symmetries, symmetry groups and their representations. In the following, we provide an abstract classification of (essentially) unitary operators U (e.g. quantum walks) or Hermitian operators H (e.g. Hamiltonians) by defining what it means *to be of a certain symmetry type*. The symmetries considered are the following:

- ***particle-hole symmetry*** η, which is represented antiunitarily satisfying $\eta U = U\eta$ or $\eta H = -H\eta$,
- ***time reversal symmetry*** τ, which is represented antiunitarily satisfying $\tau U = U^*\tau$ or $\tau H = H\tau$,
- ***chiral symmetry*** γ, which is represented unitarily satisfying $\gamma U = U^*\gamma$ or $\gamma H = -H\gamma$.

Each symmetry is described by an identifying symbol[4] $S \in \{\eta, \tau, \gamma\}$, its (anti-) unitarity character, and the condition of admissibility, which is written as a commutation relation, potentially up to taking the adjoint. This last part is the necessary condition an operator U or H has to

4 which in a slight abuse of notation is also used for actual representations as an operator on a Hilbert space

fulfil in order to *satisfy* the symmetry $S \in \{\eta, \tau, \gamma\}$ if *represented* as operator on a Hilbert space. Equivalently, we call U or H ***admissible*** for S, if it satisfies S as described in its definition. Hence, while this description of a symmetry is independent of a particular representation on a Hilbert space, it already entails how the represented operators commute, given an admissible U or H. Furthermore, note that the commutation relations for U follow from those of H if one sets $U = \exp(iH)$.

Combining the results from Section 2.3, one easily verifies that each of these symmetries is an ***involution***, i.e. its action (e.g. $\rho \mapsto \eta\rho\eta^*$) squares to the identity. This allows us to finally define a symmetry type and its representation:

Definition 4.1 (Symmetry type)
Any subset $\mathcal{S}$ of symmetries $\{\eta, \tau, \gamma\}$ defined above, including the corresponding (anti-) unitarity character and admissibility conditions of S, together with the sign of S^2 for each element $S \in \mathcal{S}$, is called a **symmetry type**.

Definition 4.2 (Representation)
A **representation** *ρ of a* **symmetry type** *$\mathcal{S}$ is a collection of operators representing a symmetry type, i.e. a subset of unitary or antiunitary operators $\{\eta, \tau, \gamma\}$.*
An essentially unitary U or Hermitian operator H is called **admissible for the representation**[5] *ρ, if it fulfils the commutation relations with all operators in ρ as demanded by the respective symmetries.*

Note that the admissibility condition of essentially unitary operators U, V is in general not compatible with products. This can be seen e.g. for τ:

$$\tau UV = U^*\tau V = U^*V^*\tau = (VU)^*\tau, \tag{4.1}$$

hence in general, admissibility for U and V does not imply admissibility for UV. In contrast, if U and V commute, $UV = VU$ *is* τ-admissible.

Another important example is given by $V = f(U^*U)$, where f denotes a convergent power series with real coefficients. Then, for all k we have

$$\tau U(U^*U)^k = U^*(UU^*)^k\tau = (U(U^*U)^k)^*\tau, \tag{4.2}$$

and hence by linearity w.r.t. real coefficients, admissibility of $U\, f(U^*U)$ follows.

The definition of a symmetry type appears to allow for a large number of case distinctions for all possible subsets with all possible signs of squares. In the following, using the results from Section 2.3, we will systematically reduce the number of different inequivalent symmetry types to ten - deriving all the symmetry types of the so called ten-fold way[6].

5 In Definition 4.3, we will update this admissibility condition and demand furthermore, that U and H are *essentially gapped*.
6 Compare e.g. [AZ97], as described in the introduction to this chapter

S	A	D	C	AI	AII	AIII	BDI	CI	CII	DIII
η^2		$+\mathbb{1}$	$-\mathbb{1}$				$+\mathbb{1}$	$-\mathbb{1}$	$-\mathbb{1}$	$+\mathbb{1}$
τ^2				$+\mathbb{1}$	$-\mathbb{1}$		$+\mathbb{1}$	$+\mathbb{1}$	$-\mathbb{1}$	$-\mathbb{1}$
γ^2						$+\mathbb{1}$	$+\mathbb{1}$	$-\mathbb{1}$	$+\mathbb{1}$	$-\mathbb{1}$
$\mathbf{I}(\mathsf{S})$	0	$\mathbb{Z}_2$	0	0	0	$\mathbb{Z}$	$\mathbb{Z}$	0	$2\mathbb{Z}$	$2\mathbb{Z}_2$
si	0	$d \bmod 2$	0	0	0	$\operatorname{tr}\gamma$	$\operatorname{tr}\gamma$	0	$\operatorname{tr}\gamma$	$d \bmod 4$

Table 1: All symmetry types of the tenfold-way, determining the squares of the generators $\{\eta, \tau, \gamma\}$ and labelled by the widespread Cartan notation [Car27]. An empty cell denotes that the corresponding generator is not part of the symmetry type. Anticipating Definition 4.7 and the results from Section 4.4, $\mathbf{I}(\mathsf{S})$ denotes the range of the symmetry index si of a representation.

At this point note that whenever a symmetry type contains two of the three different symmetries considered, the third is present as well, since every composition of two of the above symmetries yields the third, fulfilling the corresponding commutation relation and having the right unitarity character. Hence under the given circumstances, the symmetry group either consists of one of the above symmetries and the identity, or all of the above symmetries and the identity. This corresponds exactly to the group of two involutions, and Klein's *Vierergruppe*[7] as introduced in Section 2.3.

Using the case-distinction from Section 2.3, we are now able to write down all symmetry types allowed in our setting. Instead of introducing another convention, we stick to the notation Cartan introduced in [Car27].

Table 1 provides an overview over every symmetry type in Cartan notation, answering which symmetries are present and whether they square to $+\mathbb{1}$ or $-\mathbb{1}$. These ten different cases are constructed as follows: There is one case with no symmetry present, called A. Then, there is AIII, the case where only one unitary symmetry (i.e. γ) is present, whose square we choose as $\mathbb{1}$. Then there are D, C, AI and AII where there is only one antiunitarily represented symmetry, two cases $\eta^2 = \pm\mathbb{1}$ and two cases $\tau^2 = \pm\mathbb{1}$. This amounts to five symmetry types with only one symmetry present. Using the convention of commuting symmetries from Section 2.3 in (2.27) (i.e. choosing the representation ρ abelian), the square of two operators determines the square of the third. This is opposing some part of the literature, where fixing $\gamma^2 = +\mathbb{1}$ is preferred, at the cost of loosing commutativity of the operators. In our case, we have $\gamma^2 = \eta^2\tau^2$ and hence fixing the squares of the antiunitary operators fixes γ^2. This yields the four remaining cases BDI, CI, CII and DIII, which are labelled as in [AZ97] (for the signs of the squares, see Table 1).

7 Restricted to the case of exactly two antiunitarily represented operators

It is an important result we see in Section 4.4, that whenever our classification predicts a non-trivial index group, there are η or γ present (or both) with at least one of them squaring to $+\mathbb{1}$. Before going into the details of the explicit construction, let us motivate what the presence of η or γ implies for the spectrum of an admissible operator.

Let U be an admissible unitary operator for a symmetry type S and let ϕ be an eigenvector of U with eigenvalue $e^{i\omega}$. Then, whenever η, τ, γ are part of the symmetry type, we have

$$\begin{aligned} U(\eta\phi) &= \eta U\ \phi = e^{-i\omega}(\eta\phi) \\ U(\tau\phi) &= \tau U^*\phi = e^{i\omega}(\tau\phi) \\ U(\gamma\phi) &= \gamma U^*\phi = e^{-i\omega}(\gamma\phi). \end{aligned} \tag{4.3}$$

Thus the admissibility condition for η and γ ensures, that the spectrum of U is symmetric w.r.t. the real axis. Indeed, as (4.3) shows, whenever $e^{i\omega} \neq \pm 1$, eigenvalues come in pairs $\{e^{i\omega}, e^{-i\omega}\}$. This distinguishes ± 1 from the rest of the spectrum. Figure 3 shows the action of the symmetry w.r.t. the real axis, as well as the special role of ± 1 by example. As we will see shortly, this invariance of the eigenspaces at ± 1 under the symmetries, as well as an absence of essential spectrum at ± 1, will be crucial for the classification. A motivation behind this is, that this setting on the one hand allows for a translation-invariant U which is gapped at ± 1, on the other allows for a U that stems from joining two gapped translation invariant systems (*bulks*), such that eigenvalues within this gap may emerge (rendering the resulting U not gapped anymore)[8]. More precisely, for both U (and H), our classification demands an ***essential gap*** at ± 1 (or 0):

Definition 4.3 (Essential gap)
Let A be a normal operator on $\mathcal{H}$. We call A **essentially gapped** *at z_0, if there is no essential spectrum at z_0, i.e. $z_0 \notin \sigma_{\text{ess}}(A)$.*
We use the same term for a unitary operator U, if it is essentially gapped *at ± 1 and for a Hermitian operator H at 0. Furthermore, we update Definition 4.2 to reflect that an* **admissible** *operator is always assumed to be essentially gapped.*

Due to the spectrum being closed, there is an $\epsilon > 0$ s.t. $z \notin \sigma_{\text{ess}}(A)$ for all $z \in \mathbb{C}, |z - z_0| < \epsilon$. That is, A has only finitely many eigenvalues in an ϵ-ball around z_0, as long as they are all of finite multiplicity. Figure 3 shows an example of a unitary and a Hermitian essentially gapped operator. A more elegant way to phrase the essential-gap condition is to use the projection π to the Calkin algebra as defined in Definition 2.16. Then, U is essentially gapped if and only if the spectrum of $\pi(U)$ does not contain ± 1. Indeed, this provides the perhaps quickest way to see, why this gap is *essential*: whenever U is perturbed by a compact

8 This notion and motivation will be made more precise e.g. in Section 5.3, where the notion of bulk and boundary are introduced and a correspondence between both is formulated.

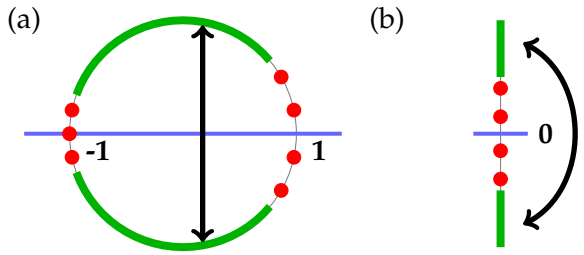


Figure 3: (a) Spectrum of an essentially gapped unitary operator U. Due to unitarity, the spectrum lies on the unit circle. While the green lines denote continuous spectrum, the red dots denote pure-point spectrum. The blue line represents the real axis, and the black arrow symbolizes the action of η, γ on the spectrum of U. The unitary operator is not gapped, since there is an eigenvalue right in the gap at -1. If this eigenvalue is only finitely degenerate, it is not part of the essential spectrum, making U *essentially gapped*.
(b) Spectrum of a gapped Hermitian operator H. Here, the real axis runs vertically with the blue line marking 0.

operator K s.t. $U' = U + K$, the essential spectrum is unaffected, since $\pi(U') = \pi(U)$. Furthermore, given an essentially gapped operator A with essential gap at z_0, the eigenspace of A at z_0 is finite dimensional by definition. Hence A, restricted to this eigenspace is a finite dimensional operator K. Removing K renders A *gapped*, thus A is *gapped at* z_0 *up to a compact operator*, which justifies calling it *essential* as announced e.g. in Section 2.5.

It is useful to note, that a translation invariant operator A on an infinite dimensional Hilbert space can only have eigenvalues of infinite degeneracy, hence $\sigma(A) = \sigma_{\text{ess}}(A)$. Therefore every essentially gapped translation invariant operator is gapped.

4.3 SYMMETRY INDEX

This section provides the last brick in the foundation we need to explain what is meant by *topological phases of quantum walks*, or how and why it makes sense that we assign numbers to admissible unitary operators and Hamiltonians.

The integral condition that allows for a topological classification in this context and that is responsible for the *topological stability* or *-protection*, is the invariance of the eigenspaces corresponding to eigenvalues in the gaps. Since we are interested in a classification that is invariant under norm-continuous perturbations that are compatible with the admissibility conditions[9], it makes sense to analyse a short example by asking: What happens in the gap of an admissible unitary operator U of symmetry type D after a small perturbation s.t. U' is still of type D?

9 The invariance of the symmetry index that labels the homotopy classes under so called gentle perturbations is thoroughly explained in Chapter 5.

The particle-hole-symmetry η forces the spectrum to be symmetric w.r.t. the real axis, hence eigenvalues moved by the perturbation have to move symmetrically in pairs. This allows the dimension of the eigenspace of one gap (e.g. at $+1$) to change only by an even number - which hints that a classification must at least distinguish between *even* or *odd* number of eigenvalues in the gap, thus corresponding at least to an index group $\mathbf{I}(\mathsf{D}) = \mathbb{Z}_2$ (Table 1 confirms that this is already the whole group).

In the following, we substantiate this argument by introducing an equivalence relation on the set of finite dimensional symmetry representations, that identifies the topologically irrelevant (trivial) representations. These are the so called ***balanced representations*** by which (as we will see later) the eigenspaces may change without changing the topological phase.

Definition 4.4 (Balanced representation)
A symmetry representation ρ is called **balanced**, *if there exists a unitary operator U (or Hermitian operator H) which is ρ-admissible and gapped.*

Indeed, balanced representations split finite dimensional Hilbert spaces (e.g. the corresponding eigenspaces of essentially gapped unitaries at ± 1) into a direct sum of spaces of equal dimension, that are mapped to each other by γ and η if they are part of the symmetry type, as the following Proposition shows[10]:

Proposition 4.5 (Balanced representations)
Let ρ be a representation on a finite dimensional Hilbert space $\mathcal{H}$. Then, the following are equivalent:

1. *ρ is balanced, i.e. there is a gapped admissible V.*
2. *There are $\mathcal{H}_+$ and $\mathcal{H}_-$ s.t. $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ that are swapped by γ and η and are invariant under τ (whenever these are part of the symmetry type), i.e.*
$$\gamma\mathcal{H}_+ = \mathcal{H}_- \qquad \eta\mathcal{H}_+ = \mathcal{H}_- \qquad \tau\mathcal{H}_+ = \mathcal{H}_+. \tag{4.4}$$
3. *There is an admissible unitary V with $V^2 = -1$.*

Proof. (1) $\Rightarrow$ (2): Since V is a unitary operator, the eigenvectors of its spectral decomposition span $\mathcal{H}$. Furthermore, since V is gapped, every eigenvalue has either positive or negative imaginary part. Hence, we can define $\mathcal{H}_+$ ($\mathcal{H}_-$) as the span of all eigenvectors of positive (negative) imaginary part, and use (4.3) to verify the relations for γ, η, τ, if they are part of the symmetry type.

(2) $\Rightarrow$ (3): Let P_+ be the projector onto $\mathcal{H}_+$ and P_- onto $\mathcal{H}_-$. Then,
$$V = iP_+ - iP_- \tag{4.5}$$
is admissible, clearly unitary, and $V^2 = -\mathbb{1}$.

(3) $\Rightarrow$ (1): By definition, since V has only eigenvalues $\pm i$. □

10 Compare e.g. (4.3) for the action of γ, η, τ on eigenvectors and the spectrum

This proposition will be especially helpful when computing the actual index groups later in this section. But before we can do this, we have to define the equivalence relation between representations ρ_1, ρ_2 of the same symmetry type. The corresponding equivalence classes will then be labelled by a map si that associates to every representation an element of an abelian group $\mathbf{I}(\mathsf{S})$, the index group.

Definition 4.6 (Equivalence modulo balanced reps.)
Let ρ_1, ρ_2 be finite dimensional *representations of a symmetry type. ρ_1 and ρ_2 are equivalent ($\rho_1 \sim \rho_2$), if there are balanced representations β_1, β_2 and a unitary operator V s.t.*

$$\rho_1 \oplus \beta_1 = V(\rho_2 \oplus \beta_2)V^*. \tag{4.6}$$

That this is actually an equivalence relation is easily shown, since reflexivity follows with $V = \mathbb{1}, \beta_1 = \beta_2$, symmetry with $V \mapsto V^*$ and transitivity follows from the following reasoning:

Given two balanced representations β_1, β_2 with corresponding gapped admissible unitary operators U_1, U_2, the direct sum $\beta_1 \oplus \beta_2$ is balanced as well, with the gapped admissible unitary $U_1 \oplus U_2$. Hence if $\rho_1 \sim \rho_2$ and $\rho_2 \sim \rho_3$ with corresponding β_1, β_2, V_{12} and $\gamma_2, \gamma_3, V_{23}$ s.t.

$$\begin{aligned} \rho_2 \oplus \gamma_2 \oplus \beta_2 &= V_{23}(\rho_3 \oplus \gamma_3)V_{23}^* \oplus \beta_2 \\ \rho_2 \oplus \beta_2 \oplus \gamma_2 &= V_{12}^*(\rho_1 \oplus \beta_1)V_{12} \oplus \gamma_2 \end{aligned} \tag{4.7}$$

there is a V s.t.

$$V^*(\rho_2 \oplus \beta_2 \oplus \gamma_2)V = \rho_2 \oplus \gamma_2 \oplus \beta_2 \tag{4.8}$$

and hence

$$\rho_3 \oplus \gamma_3 \oplus \beta_2 = V_{23}^*\big(V^*\big(V_{12}^*(\rho_1 \oplus \beta_1)V_{12} \oplus \gamma_2\big)V\big)V_{23}, \tag{4.9}$$

where the outermost V_{23} is understood as $V_{23} \oplus \mathbb{1}$.

To make the imprecise statement that si labels equivalence classes by assigning numbers rigorous, we define the symmetry index of a representation:

Definition 4.7 (Symmetry Index)
Let ρ be a finite dimensional representation of S and $\sim$ be the equivalence relation from Definition 4.6.
Then, the **symmetry index** $\mathrm{si}(\rho)$ *is defined as the equivalence class of ρ:*

$$\mathrm{si}(\rho_1) = \mathrm{si}(\rho_2) \Leftrightarrow \rho_1 \sim \rho_2. \tag{4.10}$$

The set of equivalence classes $\mathbf{I}(\mathsf{S})$ is then called the **index group** *of the symmetry type S, with group operation*

$$\mathrm{si}(\rho_1) + \mathrm{si}(\rho_2) := \mathrm{si}(\rho_1 \oplus \rho_2). \tag{4.11}$$

The sloppiness to call something a group before actually showing this, will be overcome by the following proposition:

Proposition 4.8 (Symmetry index)
There is a map si *that takes any finite dimensional representation* ρ *of* S *to an element* $\mathrm{si}(\rho) \in \mathbf{I}(\mathsf{S})$ *such that*

$$\mathrm{si}(\rho) = 0 \Leftrightarrow \rho \text{ is balanced}. \tag{4.12}$$

Furthermore, the corresponding index group $\mathbf{I}(\mathsf{S})$ *is an abelian group.*

Proof. From Definition 4.6 we know, that the relation is indeed an equivalence relation. Since the direct sum of balanced representations is balanced, the direct sum of equivalent representations yields equivalent sums, which justifies the introduction of the sum in Definition 4.7. Furthermore, a balanced representation β has trivial index, since

$$\mathrm{si}(\rho) + \mathrm{si}(\beta) = \mathrm{si}(\rho \oplus \beta) = \mathrm{si}(\rho). \tag{4.13}$$

On the other hand, any ρ' s.t. $\mathrm{si}(\rho') = 0$ is equivalent to a balanced representation ρ, and hence itself balanced by definition.

For every direct sum, there is a unitary operator V that swaps the summands, that is

$$\rho_2 \oplus \rho_1 = V\, \rho_1 \oplus \rho_2\, V^*. \tag{4.14}$$

Thus, both elements $\rho_2 \oplus \rho_1$ and $\rho_1 \oplus \rho_2$ are equivalent, making $\mathbf{I}(\mathsf{S})$ an abelian semigroup.

The last step is to explicitly construct inverses. Given $\rho = \{\eta, \gamma, \tau\}$, let ρ' be the representation created from ρ by defining

$$\eta' = \eta \qquad \tau' = -\tau \qquad \gamma' = -\gamma. \tag{4.15}$$

Since a sign does not change the admissibility conditions, ρ' is still a valid representation of S. Let V be a unitary operator on $\mathcal{H} \oplus \mathcal{H}$ s.t.

$$V(\phi_1 \oplus \phi_2) := \phi_2 \oplus (-\phi_1). \tag{4.16}$$

Then, V is unitary with eigenvalues $\pm i$ and hence gapped. Furthermore, V is admissible for $\rho \oplus \rho'$, making $\rho \oplus \rho'$ balanced. Hence, by the definition of the group action

$$\mathrm{si}(\rho) + \mathrm{si}(\rho') = 0, \tag{4.17}$$

making ρ' the inverse of ρ, finishing the proof. □

In what follows, we show that for all symmetries S of the tenfold-way, the index group $\mathbf{I}(\mathsf{S})$ is isomorphic to either the trivial group $\{0\}$, the group $\mathbb{Z}_2$ or the group $\mathbb{Z}$.

4.4 INDEX GROUPS

In this section, we will synthesize the results from this chapter, together with the abstract analysis of involutions from Section 2.3, to provide explicit formulas for si, thus allowing to identify the generators of the index group and hence the group for every symmetry type S mentioned in Table 1. Given a representation ρ, the dimension of the

Hilbert space $\mathcal{H}$ is denoted by d. We will only treat the case of unitary operators, since the Hamiltonian case follows directly from substituting $U = \exp(iH)$ and working with the corresponding admissibility conditions[11].

Symmetry types AI, AI, AII

In these cases, there is neither η nor γ present, hence the ρ-admissibility does not demand symmetry of the spectrum w.r.t. the real axis. Therefore, e.g. $U = i\mathbb{1}$ is admissible and gapped, rendering every representation balanced and thus $\mathbf{I}(\mathsf{S}) = \{0\}$.

Symmetry type D

This case corresponds to case 2 of a single antiunitarily represented symmetry $\eta^2 = +\mathbb{1}$ in Section 2.3. Therefore, any admissible unitary operator V has real entries w.r.t. the basis in which η is the complex conjugation. This makes V a real orthogonal matrix. If d is even, we can always choose V as a direct sum of 2×2-real rotation matrices[12], which has no real eigenvalues. If d is odd, this is not possible, since any odd-dimensional real-orthogonal matrix has at least one eigenvalue ± 1, in this case rendering every admissible unitary V imbalanced, yielding $\mathbf{I}(\mathsf{D}) = \mathbb{Z}_2$ with $\mathrm{si}(\rho) = d \bmod 2$.

Symmetry type C

This case corresponds to case 3 of a single antiunitarily represented symmetry $\eta^2 = -\mathbb{1}$. As shown there, in order for such an η to exist, d has to be even. But the same construction as in D shows, that in this case, there is a balanced V for all d, rendering every ρ balanced and thus $\mathbf{I}(\mathsf{C}) = \{0\}$.

Symmetry type AIII

This case corresponds to case 1 of a single unitarily represented symmetry $\gamma^2 = +\mathbb{1}$. We know, that γ can only have eigenvalues ± 1. From Proposition 4.5 we know, that a balanced representation swaps $\mathcal{H}_+$ and $\mathcal{H}_-$. Hence, to determine the balanced part of a representation, we look at the dimensions d_+, d_- of the eigenspaces $P_+\mathcal{H}$ and $P_-\mathcal{H}$ of γ. To fulfil the swapping condition, we need that $d_+ = d_-$, since then we can construct pairs of $\phi_+ \in P_+\mathcal{H}$ and $\phi_- \in P_-\mathcal{H}$ such that $\phi_+ + \phi_- \in \mathcal{H}_+$ (and hence $\phi_+ - \phi_- \in \mathcal{H}_-$). Therefore, representations not containing any balanced ones are those, where $d_+ = 0$ or $d_- = 0$. In general, given

11 As a rule of thumb, replace every $\mathbb{1}$ with 0 and $\pm i$ with ± 1 to get the corresponding relation. In [Ced+17], we cover the Hamiltonian case completely.

12 The rotation angle may not be chosen as any integer multiple of π.

a representation ρ with corresponding dimensions $d = d_+ + d_-$, one reads off

$$\mathrm{si}(\rho) = d_+ - d_- = \mathrm{tr}(\gamma). \tag{4.18}$$

Clearly, the choice of the sign is arbitrary, one could choose the opposite sign for the symmetry index. Independently of the choice, we identify the symmetry group as $\mathbf{I}(\mathsf{AIII}) = \mathbb{Z}$.

Symmetry type BDI

This case corresponds to case 1 of the *Vierergruppe*, with two antiunitarily represented symmetries, $\tau^2 = \eta^2 = +\mathbb{1}$. As in the case of AIII, $\gamma^2 = +\mathbb{1}$, and hence a balanced representation must have $\mathrm{tr}\,\gamma = 0$. Conversely, we have to show that $\mathrm{tr}\,\gamma = 0$ already implies ρ balanced. Since γ and η commute, we can choose an η-real basis $\{\phi_j^\pm\}$ in the corresponding ± 1-eigenspaces of γ. Assuming $\mathrm{tr}\,\gamma = 0$, we know that both eigenspaces have the same dimension. We define $\phi_j = \phi_j^+ + i\phi_j^-$ and $\mathcal{H}_+$ as the span of the $\{\phi_k\}$, and $\mathcal{H}_- = \gamma\mathcal{H}_+$. Since $\phi \in \mathcal{H}_+$ is mapped by γ and η to $\mathcal{H}_-$ (and vice versa), but $\tau = \gamma\eta$ leaves both spaces invariant, we conclude by Proposition 4.5 that $\mathrm{tr}\,\gamma = 0$ implies ρ balanced. Hence the index group $\mathbf{I}(\mathsf{BDI}) = \mathbb{Z}$ as in the case of AIII, and $\mathrm{si}(\rho) = \mathrm{tr}\,\gamma$ accordingly.

Symmetry type CI

This case corresponds to case 2 of the *Vierergruppe*, with two antiunitarily represented symmetries, $-\tau^2 = \eta^2 = -\mathbb{1}$. Analogous to the case C, the condition for η^2 demands an even dimensional $\mathcal{H}$. Following the convention in Section 2.3 by identifying $V_1 = \tau$, we can construct $\mathcal{H}_+$ by writing down the basis $\{\phi'_j\}$, where

$$\phi'_j = \frac{1}{\sqrt{2}}(\phi_j + \psi_j). \tag{4.19}$$

$\mathcal{H}_-$ then follows by applying $V_2 = \eta$, leading to a basis $\{\psi'_j\}$, where

$$\psi'_j = -i\eta\,\phi'_j = \frac{1}{\sqrt{2}}(\phi_j - \psi_j). \tag{4.20}$$

On these spaces, τ, η, γ act as desired by Proposition 4.5, hence in the case of CI, every representation is balanced, s.t. $\mathbf{I}(\mathsf{CI}) = \{0\}$.

Symmetry type CII

This case corresponds to case 1 of the *Vierergruppe*, with two antiunitarily represented symmetries, $\tau^2 = \eta^2 = -\mathbb{1}$. It is analogous to the case BDI, with the exception, that both eigenspaces of γ are now of even dimension. This is shown in Section 2.3, with $V_1 = \eta$ and $V_3 = \gamma$. The

even dimensionality leads to a doubling of the eigenvectors, thus $\operatorname{tr}\gamma$ takes values in $2\mathbb{Z}$, which is isomorphic to $\mathbb{Z}$. Hence $\mathbf{I}(\mathsf{CII}) = 2\mathbb{Z}$ with $\mathrm{si}(\rho) = \operatorname{tr}\gamma$.

Symmetry type DIII

This case corresponds to case 2 of the *Vierergruppe*, with two antiunitarily represented symmetries, $-\tau^2 = \eta^2 = +\mathbb{1}$. Hence, the difference to CI is, that τ and η switch roles, i.e. we identify $V_1 = \eta$ and $V_2 = \tau$. The existence of an antiunitary operator that squares to $-\mathbb{1}$ (here: τ) forces d to be even, similar to C. But the additional constraints that the admissibility conditions for η and γ provide, prevent that every ρ is balanced, as the following example shows:

Since d has to be even, the minimal dimension is $d = 2$. In that case, if ρ is balanced, $\mathcal{H}_\pm$ both have to be one-dimensional, since γ and η are present and have to map them onto each other. Furthermore, τ has to leave them invariant. But since $\tau^2 = -\mathbb{1}$, invariant subspaces have to be of even dimension. Hence there are no balanced representations in $d = 2$ dimensions. Furthermore, for arbitrary d, this condition, together with the even splitting into $\mathcal{H}_\pm$ due to the existence of η and γ for DIII, Proposition 4.5 shows that for ρ to be balanced, the dimension $d \bmod 4 = 0$. That this is sufficient is shown by explicitly using the bases $\{\phi_j\}_{j=1}^n$ and $\{\psi_j\}_{j=1}^n$ for the γ-eigenspaces $+1$ and -1 from (2.34):

Let $d = 2n$. We define

$$\phi'_j = \phi_{2j-1} + \psi_{2j} \quad \forall\, 1 \le j \le \frac{n}{2}. \tag{4.21}$$

Then, $\left\{\phi'_j,\ \eta\phi'_j, \tau\phi'_j, \gamma\phi'_j\right\}$ is pairwise orthogonal for all j. Furthermore,

$$\left\{\phi'_j, \tau\phi'_j\right\}_{j=1}^{n/2} \text{ and } \left\{\eta\phi'_j, \gamma\phi'_j\right\}_{j=1}^{n/2} \tag{4.22}$$

form a basis for $\mathcal{H}_+$ and $\mathcal{H}_-$. If n is even, $d \bmod 4 = 0$ and $\mathcal{H} = \mathcal{H}_+ + \mathcal{H}_-$, hence ρ is balanced. This shows, that $d \bmod 4 = 0$ is sufficient for ρ balanced. If n is odd, there is a two-dimensional subspace that is not affected by the identification of the balanced part in the construction above. Hence the symmetry index is $\mathrm{si}(\rho) = d \bmod 4$, which takes values in $\mathbf{I}(\mathsf{DIII}) = 2\mathbb{Z}_2$, considered as a subgroup of $\mathbb{Z}_4$.

Forgetting symmetries

Before we apply this classification to the systems of interest, namely quantum walks and generalizations thereof, we comment on connections *between* different symmetry groups. That is: what happens to the symmetry index (and its group) if we *forget* about (or failed to identify) a symmetry? More precisely, we want to determine the homomorphisms from $\mathbf{I}(\mathsf{S}_1)$ to $\mathbf{I}(\mathsf{S}_2)$, i.e. the maps that connect indices from the

finer symmetry class S_1 to the indices of the coarser symmetry class S_2.

As can be seen from Table 1, the symmetry types are interconnected in the sense that any symmetry type with $\sigma \in \{\eta, \tau, \gamma\}$ present can be considered as the coarser symmetry type where we just *forget* about the existence of σ. Clearly, whenever σ is the only symmetry present, dropping it leaves us with the case A, which has trivial index group. Furthermore, whenever all three symmetries are present, one can not just forget one symmetry, but two, since any pair of symmetries implies the third. Starting from CI, Proposition 4.5 clearly shows that forgetting symmetries leaves balanced representations balanced[13], rendering forgetting in that case trivial as well. This leaves us with only three cases with potentially non-trivial symmetry indices through forgetting: BDI, CII and DIII.

In all three non-trivial cases, if we forget η and γ, we are left with τ alone, that is AI or AII, which has trivial $\mathbf{I}(\mathsf{S})$. Hence the homomorphism is the zero map. If we ignore τ and either η or γ, we are left with non-trivial index groups, namely $\mathbf{I}(\mathsf{D})$ or $\mathbf{I}(\mathsf{AIII})$, and another trivial case when reducing CII to C by forgetting about τ and γ. In the last case, one could think that we can simply adjust the sign of η^2 by choosing a phase for η, which is possible now that there is only one symmetry left. But (2.17) showed, that the square of an anitunitary involution is invariant under phase-shifts. Therefore, we can not transform CII to D by forgetting and we are left with only two non-trivial index groups. The homomorphisms corresponding to the remaining cases are shown in Table 2. Since BDI contains η with $\eta^2 = +\mathbb{1}$, every representation ρ of BDI is also one of D. For BDI, $\mathrm{si}_1(\rho) = \operatorname{tr}\gamma = d_+ - d_-$ as defined in (4.18). In the case of D, $\mathrm{si}_2(\rho) = d \bmod 2$, and therefore we have

$$\mathrm{si}_2(\rho) = (d_+ - d_-) \bmod 2 = (d_+ + d_-) \bmod 2 = \mathrm{si}_1(\rho) \bmod 2. \quad (4.23)$$

Therefore, the forget homomorphism between BDI and D is

$$m : \mathbb{Z} = \mathbf{I}(\mathsf{BDI}) \to \mathbf{I}(\mathsf{D}) = \mathbb{Z}_2 : m(s) = s \bmod 2. \quad (4.24)$$

The forget homomorphism between DIII and D is easily found, since both depend only on the dimension of the representation. The fact that d is even for every ρ that represents DIII directly implies that the homomorphism $m \equiv 0$.

For DIII, forgetting about η and τ leaves us with γ as the single symmetry. As can be seen from (2.34), the $\pm i$-eigenspaces of γ are of the same dimension for every representation of DIII. Due to the unitarity of γ and the absence of further antiunitarily represented symmetries, we can map γ to $i\gamma$ without changing the admissibility condition, hence transforming the $\pm i$-eigenspaces of γ to ∓ 1-eigenspaces. Therefore, regarded as a representation of AIII, $d_+ = d_-$ and therefore $\mathrm{si}(\rho) = \operatorname{tr}\gamma = 0$.

13 Note that by switching types the admissibility conditions change, hence both notions of *balanced* differ.

	BDI	CII	DIII
AIII	id	id	0
D	mod 2	-	0

Table 2: Forget homomorphisms between non-trivial index groups. The top row denotes the starting symmetry type, while the left column denotes the symmetry type after *forgetting* about two symmetries. As an example, consider BDI, which contains an η with $\eta^2 = +\mathbb{1}$. Then, every representation of BDI is also one of D. The respective symmetry indices $\mathrm{si}(\rho)$ yield potentially different results depending on the symmetry type's perspective. In this case, the thus induced homomorphism is the quotient map $m(s) = s \bmod 2$.

The two identity maps id in Table 2 now originate from the trivial fact, that the index map is given by $\mathrm{tr}\,\gamma$ for all three symmetry types involved. It is independent of whether one forgets about η and τ or not.

This completes the discussion of the forget homomorphisms and allows us to finally proceed to classifying *quantum walks* or the more general *essentially local unitary operators*.

5

SYMMETRY INDEX FOR QUANTUM WALKS

In the previous chapter, we defined the symmetry index for finite dimensional representations of a symmetry type. At this point, it is still unclear, how this might help to classify infinite dimensional quantum walks (or Hamiltonians), where the symmetries are represented as infinite-dimensional operators. We will repeat the updated notion of admissibility shortly, which distinguishes the ± 1-eigenspaces of admissible unitary operators by noting their invariance under the action of every representation of the symmetry type.

5.1 DEFINITION AND HOMOTOPY INVARIANCE

In this section, we connect the abstract introduction of symmetry indices to quantum walks (or more abstractly - unitary operators) to show how this serves us in classifying quantum walks with symmetries. For the rest of this chapter, we will stick to the general notion of our Hilbert space $\mathcal{H}$ as a direct sum of finite dimensional $\mathcal{H}_x$, instead of limiting ourselves to $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ as defined in Section 3.2. Still, the standing assumption will be that every symmetry representation ρ, restricted to each of the $\mathcal{H}_x$, is balanced. The advantage of this is that ρ commutes with every projection $P = P_{\geq x} = P^*$ for all $x \in \mathbb{Z}$, hence carrying admissibility of U over to PUP if restricted to $P\mathcal{H}$. The definition of invariants introduced in Section 5.2 requires a notion of admissibility for essentially local essentially unitary operators (ELEU, see Definition 3.4):

Definition 5.1 (Admissibility)
Let U (or H) be an essentially unitary (or Hermitian) operator on $\mathcal{H}$ and let ρ be a representation of a symmetry type S*. Then, we call U (or H) admissible for ρ, iff it is*

1. *admissible for ρ as in Definition 4.2*
2. *essentially gapped as in Definition 4.3.*

Furthermore, whenever we have a spatial structure $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$, we assume ρ to be balanced w.r.t. each $\mathcal{H}_x$.

Essentially unitary operators are not necessarily diagonalizable, thus we restrict the following definition to strictly unitary operators. In this case, the essential gap guarantees finite dimensional ± 1-subspaces for admissible unitary operators (and finite dimensional 0-eigenspaces for admissible Hermitian operators), guaranteeing that the expression is well-defined:

Definition 5.2 (Symmetry index of an operator)
Let ρ be a symmetry representation, U an admissible unitary operator and H an admissible Hermitian operator on a Hilbert space $\mathcal{H}$.
Then, we define the **symmetry index of** U **at** $+1$ *as*

$$\mathrm{si}_+(U) = \mathrm{si}(\rho_+), \tag{5.1}$$

where ρ_+ is ρ restricted to the $+1$-eigenspace of U. $\mathrm{si}_-(U)$ is defined analogously on the -1-eigenspace of U.
The **symmetry index of** U *is defined as*

$$\mathrm{si}(U) \coloneqq \mathrm{si}_+(U) + \mathrm{si}_-(U). \tag{5.2}$$

The **symmetry index of** H *is defined as the symmetry index of ρ on the* o*-eigenspace of H*

$$\mathrm{si}(H) \coloneqq \mathrm{si}(\rho_o), \tag{5.3}$$

where ρ_o is ρ restricted to the o*-eigenspace of H.*

Whenever $\mathcal{H}$ is finite dimensional with a symmetry representation ρ, we can directly make use of the formulas for $\mathrm{si}(\rho)$ and derive explicit formulas for $\mathrm{si}_\pm(U)$ in almost all non-trivial cases.

Proposition 5.3 (si for finite d)
Let ρ be a symmetry representation of a symmetry type $\mathsf{S} \neq \mathsf{DIII}$ *on a finite dimensional Hilbert space $\mathcal{H}$ of dimension d. Then, $\mathrm{si}(\rho) = \mathrm{si}(U)$ for all ρ-admissible unitary operators U. Furthermore,*

$$\begin{aligned} \mathrm{si}_\pm(U) &= \frac{1}{2}(1 - \det(\mp U)) && \mathsf{S} = \mathsf{D}, \\ \mathrm{si}_\pm(U) &= \frac{1}{2}\operatorname{tr}\left(\gamma(\mathbb{1} \pm U)\right) && \mathsf{S} \in \left\{\mathsf{AIII}, \mathsf{BDI}, \mathsf{CII}\right\}. \end{aligned} \tag{5.4}$$

Proof. We assumed a finite dimensional $\mathcal{H}$, hence U has a finite set of eigenvalues with corresponding eigenspaces. Since the ± 1-eigenspaces are ρ-invariant, we can always decompose ρ into $\rho_+ \oplus \rho_- \oplus \rho_\mathrm{b}$, where ρ_b is defined on $\mathcal{H}_\mathrm{b}$, the eigenspace of non-real eigenvalues of U. Clearly, $\mathcal{H}_\mathrm{b}$ is invariant under both U and ρ_b, hence the restriction of U onto $\mathcal{H}_\mathrm{b}$ is a gapped admissible operator, rendering ρ_b balanced. Hence, $\mathrm{si}(\rho_\mathrm{b}) = 0$ and

$$\mathrm{si}(\rho) = \mathrm{si}(\rho_+ \oplus \rho_- \oplus \rho_\mathrm{b}) = \mathrm{si}(\rho_+ \oplus \rho_-) = \mathrm{si}(U). \tag{5.5}$$

Let us now prove the formula for D. The admissibility for U guarantees that non-real eigenvalues always occur in complex-conjugate pairs with identical multiplicity. Since all eigenvalues lie on the unit-circle, the product of these pairs is always 1. Therefore, the determinant of $\mp U$, which is the product of all eigenvalues, is just $(-1)^j$, where j is the number of ± 1-eigenvalues. Hence $\mathrm{si}_\pm(U)$ can be read off by the parity of $\det(\mp U)$, proving the first formula.

For the cases $\mathsf{AIII}, \mathsf{BDI}$ and CII note that γ swaps $\mathcal{H}_+$ and $\mathcal{H}_-$ on the balanced part of $\mathcal{H}$, i.e. $\mathcal{H}_\mathrm{b} = \mathcal{H}_+ \oplus \mathcal{H}_-$. More precisely, γ acts like the Pauli-matrix σ_1 on the eigenspaces of U belonging to non-real

eigenvalues, i.e. on $\mathcal{H}_b$. Since σ_1 is traceless, $\mathcal{H}_b$ does not contribute to $\operatorname{tr}\gamma$. Hence writing $\frac{1}{2}(\mathbb{1} \pm U)$ just isolates the eigenspaces of ± 1 while mapping the eigenspaces of ∓ 1 to zero, finishing the proof. □

Since the symmetry indices $\mathrm{si}_\pm$ crucially depend on the ± 1-eigenspaces, it is interesting to analyse their stability under alterations of the quantum walk. That is, answer which perturbations leave the symmetry indices invariant. In general, we will restrict ourselves to perturbations that do not break the symmetries and do keep the essential gap. Thus every perturbation has to be admissible for the same symmetry representation as the unperturbed walk.

The perturbations introduced in Definition 3.15 are all instantaneous in the sense that we do not ask whether this perturbation can be applied in arbitrarily small steps. Before we find a criterion that distinguishes between perturbations that are instantaneous or those that are not by introducing the *relative index* in Section 5.4, we focus on the *homotopy* of admissible essentially local unitary operators, more precisely defined as ***gentle perturbations***:

Definition 5.4 (Gentle perturbation)
Let U and U' be admissible unitary operators on $\mathcal{H}$. Then, U and U' are called **gentle** *perturbations of each other (or U and U' are* **homotopic***), iff there is a norm-continuous path $[0,1] \ni t \mapsto U_t$ connecting $U_0 = U$ with $U_1 = U'$ such that U_t is admissible for all $t \in [0,1]$.*

Sometimes, when we ask for the existence of gentle perturbations, we want additional locality conditions to be fulfilled *along the way*, meaning that U_t fulfils these for all $t \in [0,1]$. Typically these are either *compact* when demanding U_t to be compact perturbations of U, *essentially local* in the context of essentially local operators, *strictly local* in the context of quantum walks or *translation invariant* in the context of translation invariant unitary operators, or combinations of these. We mention the additional conditions when needed.

The relation to be *continuously deformable* to each other within the set of admissible unitary operators is an equivalence relation[1], and as such splits the set into equivalence classes that can be labelled by *homotopy invariants*. The following theorem states that the symmetry index is such an invariant:

Theorem 5.5 (Homotopy invariance of $\mathrm{si}_\pm$)
Let U and U' be admissible unitary operators on $\mathcal{H}$ that are homotopic. Then

$$\mathrm{si}_\pm(U) = \mathrm{si}_\pm(U'). \tag{5.6}$$

That is, $\mathrm{si}_\pm$ is invariant under gentle perturbations, hence a homotopy invariant. The same result holds for $\mathrm{si}(H)$ in the Hamiltonian case.

1 Since every homotopy is an equivalence relation

Proof. The norm-continuity of the homotopy U_t connecting U and U' reduces the proof to showing that there is a $\Delta > 0$ such that

$$\mathrm{si}_\pm(U_t) = \mathrm{si}_\pm(U_{t'}) \quad \forall\, t' \in [t-\Delta, t+\Delta]. \tag{5.7}$$

On the compact interval $[0,1]$, the minimal distance between ± 1 and the rest of the spectrum exists and does not vanish. This, combined with the continuity in norm allows us to connect these Δ-intervals from 0 to 1 and conclude that the indices are constant for all $t \in [0,1]$.

But the above statement from (5.7) is a direct consequence of the following Proposition 5.6; the slightly stronger statement that $\mathrm{si}_\pm$ is locally constant. The above argument and the proposition hold identically in the Hamiltonian case. □

Proposition 5.6 (Local constance of si)
Let U be an admissible unitary operator. Then, there is an $\epsilon > 0$ s.t. for all admissible unitary operators U',

$$\|U - U'\| < \epsilon \quad \Rightarrow \quad \mathrm{si}_\pm(U) = \mathrm{si}_\pm(U'). \tag{5.8}$$

The same result holds for $\mathrm{si}(H)$ *in the Hamiltonian case.*

Proof. It suffices to prove the theorem for $\mathrm{si}_+(U)$, since the argument for $\mathrm{si}_-(U)$ and $\mathrm{si}(H)$ is identical if one replaces the eigenvalues and eigenprojections accordingly.

Let P be the projector onto the $+1$-eigenspace of U. Since U is admissible, it is essentially gapped at ± 1. Therefore, there is a distance $\delta > 0$ between $+1$ and the rest of the spectrum of U. Furthermore, $\dim P = d$ is finite. Let $R(z)$ denote the resolvent of U at z and let Γ denote a path in $\mathbb{C}$ encircling $+1$ with radius $\delta/2$. Due to the distance δ, this circle contains only eigenvalues at $+1$, and hence by (2.57), P can be expressed as a contour integral

$$P = -\frac{1}{2\pi i} \oint_\Gamma R(z)dz. \tag{5.9}$$

Let $R'(z)$ denote the resolvent of U' at z. The second resolvent identity

$$R'(z) - R(z) = R'(z)(U' - U)R(z) \tag{5.10}$$

can be reordered to yield

$$\begin{aligned} R'(z) &= R(z)\big(\mathbb{1} - \big(U' - U\big)R(z)\big)^{-1} \\ &= R(z)\sum_{n=0}^{\infty}\big(\big(U' - U\big)R(z)\big)^n. \end{aligned} \tag{5.11}$$

From (2.38) we see that $\|R(z)\|^{-1} = \delta/2$ for all $z \in \Gamma$, therefore this is a convergent series for all $z \in \Gamma$, as long as $\|U' - U\| < \delta/2$. This serves as a preliminary candidate for our ϵ, and we assume from now on that U

and U' are more than $\delta/2$-close in norm. Then, R' is defined and on Γ bounded by

$$\begin{aligned}\|R'(z)\| &= \|R(z)\| \cdot \|1 - \|U' - U\| \cdot \|R(z)\|\|^{-1} \\ &= 2\delta^{-1} \left|1 - 2\delta^{-1}\|U' - U\|\right|^{-1}. \end{aligned} \tag{5.12}$$

The projection onto the spectrum of U' encircled by Γ is then defined in the same way as P from (5.9), leading to the following expression for the difference in norm of P and P':

$$\begin{aligned}\|P' - P\| &= \frac{1}{2\pi} \left\| \oint_\Gamma R'(z) - R(z) dz \right\| \\ &\leq \frac{1}{2\pi} |\Gamma| \max_{z\in\Gamma} \|R'(z) - R(z)\|. \end{aligned} \tag{5.13}$$

Here, $|\Gamma|$ denotes the length of Γ, which is $\pi \cdot \delta$, and the maximum is equally simple expressed via (5.11) as

$$\begin{aligned}\|R'(z) - R(z)\| &\leq \|R(z)\| \sum_{n=1}^{\infty} \left(\left\|U' - U\right\| \cdot \|R(z)\|\right)^n \\ &= \frac{\left\|U' - U\right\| \cdot \|R(z)\|^2}{1 - \left\|U' - U\right\| \cdot \|R(z)\|}. \end{aligned} \tag{5.14}$$

Using $\|R(z)\|^{-1} = \delta/2$ and putting it all together, we get

$$\|P' - P\| \leq \frac{\delta}{2} \cdot \frac{\left\|U' - U\right\| \cdot \frac{4}{\delta^2}}{1 - \left\|U' - U\right\| \cdot \frac{2}{\delta}} < \frac{\delta}{2} \quad , \tag{5.15}$$

where the last inequality only holds if we assume $\|U' - U\| < \delta/4$, which is not a restriction, but only updates our candidate for ϵ. If the norm difference of two projections is smaller than 1, they have to be of the same dimension, hence

$$\dim P = \dim P' = d. \tag{5.16}$$

We thus confirmed the general result from (2.58) that P and P' have the same dimension d. That is, as long as $\|U' - U\| < \delta/4$, no eigenvalue leaves Γ.

Up to this point, we have not yet used any symmetries. But we know from (4.3) that every symmetry maps eigenvectors to eigenvectors for either the same eigenvalue, or its complex conjugate partner. Therefore, sets of eigenvalues chosen symmetrically w.r.t. the real axis induce a subspace spanned by the corresponding eigenvectors that is invariant under the symmetries. Clearly, the subspace $P'\mathcal{H}$ belonging to the eigenvalues of U' encircled by Γ is such an invariant subspace. Denote by P'_+ the projection onto the $+1$-eigenspace of U'. Then, U' is gapped on $(P' - P'_+)\mathcal{H}$, and therefore the representations $P'\rho P'$ and $P'_+\rho P'_+$ differ only by a balanced representation, yielding[2]

$$\mathrm{si}_+(U') := \mathrm{si}_+(P'_+\rho P'_+) = \mathrm{si}_+(P'\rho P'). \tag{5.17}$$

2 Here, ":=" does not denote a new definition, but reminds us that this is exactly as defined.

For $\|U' - U\|$ sufficiently small, we have to prove

$$\mathrm{si}_+(U) := \mathrm{si}_+(P\rho P) = \mathrm{si}_+(P'\rho P'). \tag{5.18}$$

In the case of trivial symmetry types $\mathbf{I}(\mathsf{S}) = \{0\}$, this is trivially true. For type D and DIII there is nothing to do either, since we already showed that $\dim P\mathcal{H} = \dim P'\mathcal{H} = d$ as long as $\|U' - U\| < \delta/4$, and the index depends only on d. Hence, the statement is proven with $\epsilon = \delta/4$.

The remaining cases are AIII, BDI and CII, for which the symmetry index of finite dimensional ρ is given by $\mathrm{si}_+(U) = \mathrm{tr}(P\gamma P)$, where P still denotes the projection onto the $+1$-eigenspace of U. We get

$$\begin{aligned} |\Delta| &:= \left|\mathrm{si}_+(P'\rho P') - \mathrm{si}_+(P\rho P)\right| = \left|\mathrm{tr}(P'\gamma P') - \mathrm{tr}(P\gamma P)\right| \\ &\leq \left|\mathrm{tr}(P'\gamma P') - \mathrm{tr}(P\gamma P')\right| + \left|\mathrm{tr}(P\gamma P') - \mathrm{tr}(P\gamma P)\right| \\ &= \left|\mathrm{tr}\left((P' - P)\gamma P'\right)\right| + \left|\mathrm{tr}\left(P\gamma(P' - P)\right)\right|. \end{aligned} \tag{5.19}$$

Now, using the trace norm $\|.\|_1$ from Definition 2.14, we see

$$\begin{aligned} |\Delta| &\leq \|P' - P\| \left(\left\|\gamma P'\right\|_1 + \left\|P\gamma\right\|_1\right) \\ &\leq 2d \|P' - P\|, \end{aligned} \tag{5.20}$$

where in the last step, we used $\|\gamma\| = 1$ and $\mathrm{tr}\, P = \mathrm{tr}\, P' = d$. Hence as long as $\|P' - P\| < 1/2d$, the integer valued Δ fulfils $|\Delta| < 1$ and is therefore 0.

The proposition thus follows with

$$\epsilon = \frac{\delta}{2}\frac{1}{2d+1}, \tag{5.21}$$

satisfying $\|U' - U\| < \delta/4$ and (5.15), as well as $|\Delta| < 1$. □

Let U and U' be ρ-admissible unitary operators. The converse of Theorem 5.5 is called the *completeness* of the invariants. That is, U and U' are *homotopic* if and only if their indices $\mathrm{si}_\pm$ match. This result is presented in Section 5.6. *Completeness* thus implies that after fixing a scenario (here: admissible unitary operators, no locality restriction) there is no finer classification than the one provided by the invariants (here: $\mathrm{si}_\pm$).

In the following section, we will change the scenario and first coarsen it by allowing *essentially unitary* operators, and then restricting it by demanding *essential locality*. That is, we will classify ELEU.

5.2 INDICES STABLE UNDER COMPACT PERTURBATIONS

The symmetry index $\mathrm{si}_\pm(U)$ introduced in the previous section proved to be invariant under *gentle perturbations*. For this, we did not need any spatial structure of the Hilbert space at all. But since we want to provide a classification of quantum walks, it appears natural to analyse how the spatial structure might influence our theory. As was mentioned in the introduction, there is strong interest in understanding so

called *topologically protected edge states* that emerge whenever two bulk systems are joined that are *in different phases*. In this section, we introduce the symmetry indices that predict these states and prepare the introduction of the bulk-boundary correspondence that will be treated in the subsequent section.

In our one-dimensional setting, spatially joining two infinite systems leads to a situation that will be described in detail in Section 5.5, namely the systems far to the left and far to the right, which should not differ notably from the systems before the joining, and (if necessary for boundary conditions or unitarity) a transition system, which serves to connect both sides. The new symmetry indices we will introduce shortly fit nicely into this setting, since each side of a system has its own symmetry index $\overleftarrow{\mathrm{si}}$ or $\overrightarrow{\mathrm{si}}$ which will be invariant under any compact admissible perturbation (hence is independent of the explicit transition) and carries over to the joined system, depending on the side.

In the previous section, $\mathrm{si}_{\pm}(U)$ was shown to be invariant under gentle perturbations of unitary operators U. But in the unitary case, admissible compact perturbations are not necessarily gentle, as will be shown in Section 5.4. In the Hamiltonian case, this distinction is not needed at all: Let H_1 and H_2 be admissible Hamiltonians that are compact perturbations of each other. Then, since the admissibility conditions regarding the symmetries are real-linear,

$$H_t := (1-t)H_1 + tH_2 \tag{5.22}$$

is admissible for all $t \in \mathbb{R}$, as long as the essential gap remains open. But this is necessarily the case, since H_t is a compact perturbation of H_1 for all t, hence leaves the essential spectrum untouched. Thus it provides a homotopy H_1 to H_2, therefore connecting all compact admissible perturbations of H_1 gently.

This encourages us to drop unitarity for this section and use *essentially unitary operators* U as introduced in Definition 2.22. The advantage is that within this larger class, we can form convex combinations of admissible compact perturbations U_1, U_2

$$U_t := (1-t)U_1 + tU_2, \tag{5.23}$$

and hence compact perturbations become gentle. Furthermore, this makes joining two systems U_1 and U_2 especially simple, since we can just pick an $a \in \mathbb{Z}$ and define

$$U = P_{\leq a}U_1P_{\leq a} + P_{>a}U_2P_{>a}. \tag{5.24}$$

If we assume U_1 and U_2 to be unitary, as long as they are not incidentally *decoupled*[3] at a, U will not be unitary any more and thus have left the class of systems we describe. But if U_1 and U_2 are *essentially local essentially unitary operators* as defined in Definition 3.4, U will be an ELEU too, and hence still be in the same class.

3 See Definition 3.11 for the definition and Section 5.5 for more details.

We note that the admissibility condition from Definition 5.1 already covered the essentially unitary case, i.e. the symmetry relations are assumed to hold exactly, not only *essentially*. Hence, as a first step towards our new invariants, we transition from an admissible essentially unitary operator to the case of an Hermitian operator by introducing its *imaginary part*

$$\operatorname{Im} U = \frac{1}{2i}\left(U - U^*\right) = (\operatorname{Im} U)^*. \tag{5.25}$$

Note that $\operatorname{Im} U$ is self-adjoint, not merely *essentially* self-adjoint. Furthermore, if U is ρ-admissible as an essentially unitary operator, $\operatorname{Im} U$ is ρ-admissible as a Hermitian operator. The non trivial step is to recognize the essential gap at o. Looking at the image

$$\pi\left(\operatorname{Im} U\right) = \frac{1}{2i}\left(\pi(U) - \pi(U)^*\right) \tag{5.26}$$

in the Calkin algebra[4] and using Theorem 2.9 shows that $\pi\left(\operatorname{Im} U\right)$ is gapped at o, making $\operatorname{Im} U$ an essentially gapped Hamiltonian.

Definition 5.7 (Symmetry index: essentially unitary operator)
Let ρ be a representation of a symmetry type S and let U be an essentially unitary operator that is ρ-admissible. Then, we call

$$\operatorname{si}(U) := \operatorname{si}(\operatorname{Im} U), \tag{5.27}$$

the **symmetry index of an essentially unitary operator**. *The Hermiticity of* $\operatorname{Im} U$ *demands to use the definition for Hamiltonians from Definition 5.2.*

Note that for an exactly unitary operator U, this is consistent with the definition $\operatorname{si}(U) = \operatorname{si}_+(U) + \operatorname{si}_-(U)$, since they coincide. But an essentially unitary operator is not necessarily diagonalizable, hence there is no direct equivalent of $\operatorname{si}_\pm$ in this case.

Adding the spatial structure, i.e. essential locality, to the definition of our systems finally allows to introduce the new indices:

Definition 5.8 (Symmetry index: ELEU)
Let ρ be as above and let U be a ρ-admissible ELEU. Furthermore, let $P = P_{\geq 0}$ be the projection onto the non-negative half-axis.
Then, $U_L = (\mathbb{1} - P)U(\mathbb{1} - P)$ and $U_R = PUP$ are ELEU on their respective half-spaces and we define the **left-** *and the* **right symmetry index** *as*

$$\overleftarrow{\operatorname{si}}(U) := \operatorname{si}(U_L), \qquad \overrightarrow{\operatorname{si}}(U) := \operatorname{si}(U_R). \tag{5.28}$$

where the Hermiticity of $\operatorname{Im} U$ *implies to use the Hamiltonian part of Definition 5.2.*

The choice of the cut-point for the definition distinguishes o without a clear reason. This is similar to the situation of defining essential locality in Definition 3.4: any other cut-point results in a compact perturbation which does not change the symmetry indices as the following theorem shows:

4 See e.g. Section 2.5

Theorem 5.9 (Properties of si for ELEU)
Let U be ρ-admissible and ELEU. Then

1. *The indices* $\mathrm{si}(U)$, $\overleftarrow{\mathrm{si}}(U)$ *and* $\overrightarrow{\mathrm{si}}(U)$ *are invariant under gentle perturbations, as well as compact admissible perturbations.*
2. $\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U)$.
3. *The definition of* $\overleftarrow{\mathrm{si}}$ *and* $\overrightarrow{\mathrm{si}}$ *is independent of the cut-point.*
4. *Let U be translation invariant. Then,* $\mathrm{si}(U) = 0$.

Proof. 1. Let U' be an admissible gentle perturbation of U with corresponding path U_t. Then, $\operatorname{Im} U_t$, $(\mathbb{1} - P) \operatorname{Im} U_t (\mathbb{1} - P)$ and $P \operatorname{Im} U_t P$ are essentially gapped on their respective Hilbert spaces $\mathcal{H}$, $(\mathbb{1} - P)\mathcal{H}$, $P\mathcal{H}$ and depend continuously on t since a projection P, as well as Im are norm-continuous. Hence, the homotopy invariance of the index from Theorem 5.5 shows that the indices $\mathrm{si}(U)$, $\overleftarrow{\mathrm{si}}(U)$ and $\overrightarrow{\mathrm{si}}(U)$ are all constant along the path.

Let U' be a compact admissible perturbation of U. Then, similar to the Hamiltonian case in (5.22),

$$(1 - t)U + tU' = U + t(U' - U) \tag{5.29}$$

is a path transforming this compact perturbation to a gentle perturbation of U, implying the constance of the indices.

2. From (3.26) we obtain the decomposition

$$U = PUP + (\mathbb{1} - P)U(\mathbb{1} - P) + PU(\mathbb{1} - P) + (\mathbb{1} - P)UP. \tag{5.30}$$

The last two summands on the right hand side are compact and fulfil the symmetry relations, since P commutes with the symmetries and U is admissible. Therefore, $PUP + (\mathbb{1} - P)U(\mathbb{1} - P)$ is a compact admissible perturbation of U and the statement follows from

$$\begin{aligned} \mathrm{si}(U) &= \mathrm{si}(PUP \oplus (\mathbb{1} - P)U(\mathbb{1} - P)) \\ &= \mathrm{si}(PUP) + \mathrm{si}((\mathbb{1} - P)U(\mathbb{1} - P)) = \overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U). \end{aligned} \tag{5.31}$$

3. Without loss of generality, let $a > 0$ be another cut-point with corresponding $P_{\geq a}$. Then, $P_M = (\mathbb{1} - P)P_{\geq a}$ is the projection onto $\bigoplus_{x=0}^{b-1} \mathcal{H}_x$. Similar to the proof of (2.), we see that $P_M U P_M \oplus P_{\geq a} U P_{\geq a}$ is an admissible compact perturbation of PUP, s.t.

$$\overrightarrow{\mathrm{si}}(U) = \mathrm{si}(PUP) = \mathrm{si}(P_M U P_M) + \mathrm{si}(P_{\geq a} U P_{\geq a}). \tag{5.32}$$

But since P_M projects onto a finite number of complete cells, on which we assume symmetry representations to be balanced, the first summand on the right hand side vanishes. Therefore, the value of $\overrightarrow{\mathrm{si}}$ does not depend on the cut-point chosen in the definition, and since $\overleftarrow{\mathrm{si}}$ follows completely analogously, all definitions in Definition 5.8 are independent of the cut-point $a \in \mathbb{Z}$.

4. Translation invariance of U implies translation invariance of $\operatorname{Im} U$ and hence $\operatorname{Im} U$ is an admissible essentially gapped Hamiltonian that commutes with translations. Hence, we can apply the Fourier transform and find eigenvalues that are continuous functions on $\mathcal{T}$. If any of these functions vanished somewhere, 0 would be part of the essential spectrum of $\operatorname{Im} U$, contradicting admissibility. Thus, $\operatorname{Im} U$ is strictly gapped, and being ρ-admissible, is its own gapped admissible Hamiltonian that renders ρ balanced, implying $\mathrm{si}(U) = 0$. □

Having shown the homotopy invariance and invariance w.r.t. compact admissible perturbations of $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ for admissible ELEU, we now have all the tools at hand to state *bulk-boundary-correspondence* in the following section.

5.3 BULK-BOUNDARY CORRESPONDENCE

In the previous section, we introduced a pair of new invariants $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ for every admissible essentially local essentially unitary operator U. Since these are independent of the cut-point, we may compute them as far out as we please. These indices can therefore not be inferred from any finite piece of U, strikingly different from ind, the index of an essentially local operator defined in Definition 3.8, which is a *locally computable invariant*, hence can be determined from an (almost) arbitrarily small piece of the walk (at least in the strictly local case of quantum walks).

Luckily, the stability of $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ w.r.t. admissible perturbations makes it clear that they suitably classify the topological phase of different bulk systems. But in order to write down *bulk-boundary correspondence* as a rigorous statement, we have to make clear what the bulk systems are and what we mean by boundary. Our theory allows for a very general definition of bulk, e.g. potentially disordered systems where the local coins are chosen from a translation invariant distribution, or even drop strict translation-invariance and demand almost-periodicity. Since in this thesis, we emphasize the translation invariant case, we define:

Definition 5.10 (Bulk)
Let ρ be a symmetry representation and U be an ELEU. Then, we call U a **bulk**, *if it is* translation invariant *and ρ-admissible.*

Demanding translation-invariance is a restriction which has multiple consequences. Firstly, it makes every *essential* unitary U *exactly* unitary. Secondly, it reduces the essential gap condition to a strict gap condition. Thirdly,it ensures that $\mathrm{si}(U) = 0$ from Theorem 5.9. Therefore, the symmetry indices $\overrightarrow{\mathrm{si}}$, $\overleftarrow{\mathrm{si}}$ differ only by a sign and are hence determined by each other. The consequence is that a classification of bulks only depends on a *single* invariant, e.g. $\overrightarrow{\mathrm{si}}$.

With the following definition of a ***crossover***, we want to describe the joining of two systems.

Definition 5.11 (Crossover)
Let ρ be a symmetry representation of a symmetry type S and U_L and U_R be bulks that are admissible for the same ρ. We call an ELEU U a **crossover** *of U_L and U_R, if*

$$\lim_{a\to\infty} \left\| P_{\geq a}(U - U_R)P_{\geq a} \right\| = 0 = \lim_{a\to\infty} \left\| P_{<a}(U - U_L)P_{<a} \right\|. \tag{5.33}$$

In words, this means that U coincides with U_L far to the left, and with U_R far to the right.

If we restrict the bulks further, e.g. to be unitary operators or quantum walks, we define a ***unitary*** or ***strictly local, unitary crossover*** respectively. Now, bulk-boundary correspondence can be stated:

Theorem 5.12 (Bulk-boundary correspondence)
Let U be a crossover of U_L and U_R. Then,

$$\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U_L) + \overrightarrow{\mathrm{si}}(U_R) = -\overrightarrow{\mathrm{si}}(U_L) + \overrightarrow{\mathrm{si}}(U_R). \tag{5.34}$$

Hence, if U_L and U_R are in different classes, $\mathrm{si}(U) = \mathrm{si}(\operatorname{Im} U) \neq 0$ and thus at least one eigenvector of $\operatorname{Im} U$ emerges at 0.
If we demand strict unitarity, at least one eigenvector of U emerges at $+1$ or -1. Furthermore, $|\mathrm{si}(U)|$ is a lower bound on the dimension of the combined ± 1-eigenspaces.

Proof. The first step is to show that $\overrightarrow{\mathrm{si}}(U) = \overrightarrow{\mathrm{si}}(U_L)$, from which $\overleftarrow{\mathrm{si}}(U) = \overleftarrow{\mathrm{si}}(U_L)$ follows analogously. Due to the invariance of $\overrightarrow{\mathrm{si}}(U)$ w.r.t. admissible compact perturbations shown in Theorem 5.9, it suffices to show that $P_{\geq a}(U - U_R)P_{\geq a}$ is compact. Then, for any $b \in \mathbb{Z}$ with $b > a$, using $P_{\geq b} + P_{<b} = \mathbb{1}$ and $P_{\geq b}P_{\geq a} = P_{\geq a}P_{\geq b} = P_{\geq b}$, we have:

$$\begin{aligned} & P_{\geq a}(U - U_R)P_{\geq a} \\ = {} & P_{<b}P_{\geq a}(U - U_R)P_{\geq a} + P_{\geq b}(U - U_R)P_{\geq a}P_{<b} + \\ & P_{<b}P_{\geq a}(U - U_R)P_{\geq b} + P_{\geq b}(U - U_R)P_{\geq b}. \end{aligned} \tag{5.35}$$

Every term that contains $P_{\geq a}P_{<b}$ or $P_{<b}P_{\geq a}$ is of finite rank, and therefore

$$K_b := P_{\geq a}(U - U_R)P_{\geq a} - P_{\geq b}(U - U_R)P_{\geq b} \tag{5.36}$$

has finite rank, too. Since limits of finite rank operators are compact[5], the limit K of K_b for $b \to \infty$ is compact, too. But since U is a crossover,

$$\lim_{b\to\infty} \left\| P_{\geq b}(U - U_R)P_{\geq b} \right\| = 0, \tag{5.37}$$

and therefore,

$$\begin{aligned} \lim_{b\to\infty} \|K_b\| &= \lim_{b\to\infty} \left\| P_{\geq b}(U - U_R)P_{\geq b} - P_{\geq a}(U - U_R)P_{\geq a} \right\| \\ &= \left\| P_{\geq a}(U - U_R)P_{\geq a} \right\|. \end{aligned} \tag{5.38}$$

5 See e.g. Definition 2.13.

Hence $P_{\geq a}(U - U_R)P_{\geq a}$ is approximated in norm by finite rank operators, and since compact operators are closed w.r.t. limits in norm, this implies $\overrightarrow{\mathrm{si}}(U) = \overrightarrow{\mathrm{si}}(U_L)$.

In the unitary case, we know that the o-eigenspace of $\operatorname{Im} U$ is precisely the direct sum of the ± 1-eigenspaces of U. For all symmetry types, $|\mathrm{si}_\pm(U)|$ is bounded by $\dim(P_{\pm 1})$, the dimension of the projection onto the ± 1-eigenspace of U, as can easily be checked using Proposition 5.3 (and in case of DIII by using Definition 5.2 directly and noting that $d \bmod 4 \leq d$). This finishes the proof. □

In the unitary case, the theorem cannot predict whether the eigenvalues emerge at $+1$ or -1. Given a crossover U, one can easily create an admissible compact perturbation U' (which necessarily is again a crossover) that creates an arbitrary number of $+1$-eigenvalues (and hence of suitable -1-eigenvalues such that the overall $\mathrm{si}(U) = \mathrm{si}_+(U) + \mathrm{si}_-(U)$ does not change). What one cannot change by admissibly and compactly changing the crossover, is the symmetry indices $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$.

The examples in Section 8.2 treat this in great detail. Furthermore, an interactive visualization that can be viewed in a browser [Sta15a], as well as in Wolfram Mathematica™ [Sta15b] was created to further investigate the phenomenon of different crossovers and changing indices. For Split-Step-Walks, this is thoroughly explained in Section 8.3.

It is at this point not clear, whether the eigenvectors belonging to the eigenvalues that emerged in the gap are decaying exponentially, or merely polynomially. We will thoroughly analyse this question for translation invariant quantum walks in Section 6.2 and prove exponential decay in Theorem 6.9. On the one hand, the scenario there is more restricted, since strict locality is imposed for the bulks, on the other, we don't even need admissibility, the result already holds for vectors fulfilling the eigenvalue equation for the gap only on one half-space.

In the following section, we will return to $\mathrm{si}_\pm$ for exactly unitary operators and use them to predict, whether an admissible compact perturbation within the set of essentially local unitary operators is gentle.

5.4 RELATIVE INDEX

In Definition 3.15 we introduced *local*, *compact* and *finite rank* perturbations for unitary operators. In (3.50), we showed how these conditions can be expressed multiplicatively. In this section, we briefly introduce a new index, the *relative index of a perturbation*, which indicates whether within the set of admissible essentially local unitary operators, a *compact* perturbation is *gentle*, or not. Clearly, this question is only of interest in the unitary case, since in the essentially unitary case, as well as in the Hamiltonian case, we already know from Theorem 5.12 that compact admissible perturbations are always gentle.

Since the admissibility condition for η is a commutation relation without an adjoint, the product of two ρ-admissible unitary operators U, V is admissible for η, but whenever τ or γ are part of ρ, products of admissible operators are not necessarily admissible any more (see (4.1)). Hence, the conditions for V such that VU is admissible, given an admissible U, are not the admissibility conditions for ρ, but those for a slightly different representation $\widetilde{\rho}$:

Lemma 5.13 (Relative representation)
Let U be an admissible essentially local unitary operator on $\mathcal{H}$ for a symmetry type S *and let V be a unitary operator. Furthermore, let*

$$\widetilde{\eta} = \eta \qquad \widetilde{\tau} = U\tau \qquad \widetilde{\gamma} = U\gamma, \tag{5.39}$$

whenever these operators are part of the symmetry type.

Then, these operators form a symmetry representation $\widetilde{\rho}$ of S*, called the* **U-relative representation**. *Moreover, $U' = VW$ is ρ-admissible iff V is $\widetilde{\rho}$-admissible. The subspace*

$$\mathcal{H}_V := (V - \mathbb{1})\mathcal{H} = (VU - U)\mathcal{H} = (V^* - \mathbb{1})\mathcal{H} \tag{5.40}$$

is invariant under $\widetilde{\eta}, \widetilde{\tau}, \widetilde{\gamma}, V, V^*$. Whenever $V - 1$ is compact, V has an essential gap at -1, and hence the -1-eigenspace $\mathcal{H}_V^- \subset \mathcal{H}_V$ is finite dimensional.

Definition 5.14 (Relative Index)
Let U, V and $\widetilde{\rho}$ be as above. Then, the symmetry index of $\widetilde{\rho}$ restricted to $\mathcal{H}_V^-$

$$\mathrm{si}(VU : U) := \widetilde{\mathrm{si}}_-(V) \tag{5.41}$$

is called the **relative index of a perturbation V for U**.

Proof of Lemma 5.13. Firstly, we have to verify that $\widetilde{\rho}$ has the same squares as ρ, that every element of $\widetilde{\rho}$ commutes, and that ρ-admissibility for VW is equivalent to $\widetilde{\rho}$-admissibility for V. The invariance of $\mathcal{H}_V$ follows directly from (5.40) and applying the admissibility conditions for $\widetilde{\rho}$ and V to the appropriate part of (5.40). All of this can be checked by a direct calculation.

The compactness of $V - \mathbb{1}$ directly implies the essential gap at -1 and hence the finite dimensionality of $\mathcal{H}_V^-$, finishing the proof and ensuring that $\mathrm{si}(VU : U)$ is well-defined. □

Since si_- is a homotopy invariant due to Theorem 5.5, $\mathrm{si}(VU : U)$ vanishes, if VU is a gentle perturbation for U. Therefore, a vanishing relative index is necessary for a compact perturbation to be gentle. We will now prove that this is actually sufficient:

Lemma 5.15
Let U be an admissible unitary operator and let V be an admissible compact *perturbation for U s.t. $U' = VU$. Then,*

$$\mathrm{si}(VU : U) = 0 \iff V \text{ is a compact gentle perturbation for } U.$$

Proof. Due to Theorem 5.5, VU and U are gentle perturbations and ($\Leftarrow$) is evident.

Conversely, suppose $\widetilde{\mathrm{si}}_-(V) = 0$. We have to create a continuous path $t \mapsto V_t$ of $\widetilde{\rho}$-admissible unitary operators on $\mathcal{H}_V$ connecting V with $\mathbb{1}$, s.t. $U_t = V_t U$ is an admissible homotopy from VU to U. Since $\widetilde{\mathrm{si}}_-(V) = 0$, there is a gapped admissible unitary V_g. The restriction of V_g to $\mathcal{H}_V$ will be called V_g^-. Using functional calculus, we can contract the eigenvalues of this finite dimensional unitary operator to 1 by applying the function $f_+(z,t) := z^t$, or to -1 by applying $f_-(z,t) := (-z)^t$. Hence by concatenating f_+ and f_- suitably, we found an admissible V_t^- on $\mathcal{H}_V^-$. On the complement of $\mathcal{H}_V^-$ in $\mathcal{H}_V$, we apply f_+ to the spectrum of V_g and compose V_t from V_t^- on $\mathcal{H}_V^-$ and the deformed V_g on the complement. This proves ($\Rightarrow$). □

An obvious disadvantage of relative indices is that they need to refer to some reference operator. As such, the previous lemma allows us to decide whether an operator is a compact perturbation of the reference, or not. But it does not tell us much about the connected components of references that are not compact perturbations of each other. Moreover, we do not know whether a compact perturbation with non-vanishing relative index is a non-compact gentle perturbation. That is, whether they can be connected by a norm-continuous path U_t of admissible operators that is not restricted to be a compact perturbation of the reference U for all t.

The following theorem rules out this possibility: by showing that the relative index can be expressed as a difference of the *absolute* indices $\mathrm{si}_\pm$. Since we know that these are invariant w.r.t. to any gentle perturbations by Theorem 5.5, we learn that a compact perturbation with non-vanishing relative index cannot be contracted.

Theorem 5.16 (Relative index from $\mathrm{si}_\pm$)
Let U be an admissible unitary operator and let V be an admissible compact *perturbation for U s.t. $U' = VU$. Then,*

$$\mathrm{si}(U' : U) = \mathrm{si}_-(U') - \mathrm{si}_-(U) = \mathrm{si}_+(U) - \mathrm{si}_+(U'). \tag{5.42}$$

The full proof of this theorem is found in [Ced+17, Thm. VI.4]. We only treat the case of a finite dimensional Hilbert space $\mathcal{H}$, excluding DIII:

Proof. Since $\mathrm{si}(U)$ is invariant under compact admissible perturbations, $\mathrm{si}(U) = \mathrm{si}(U')$ and therefore

$$\mathrm{si}_-(U) + \mathrm{si}_+(U) = \mathrm{si}(U) = \mathrm{si}_-(U') + \mathrm{si}_+(U'), \tag{5.43}$$

thus it suffices to show the first equation in (5.42).

Proving the theorem *in the finite dimensional case* is now just a matter of calculating $\widetilde{\mathrm{si}}_-(V)$ using the formulas from Proposition 5.3. In the case of D, we get (after exponentiation)

$$\begin{aligned}(-1)^{\widetilde{\mathrm{si}}_-(V)} &= \det(V) = \det(VU)\cdot\det(U^{-1})\\ &= (-1)^{\mathrm{si}_-(U')-\mathrm{si}_-(U)}.\end{aligned} \tag{5.44}$$

Since for $\mathsf{S} = \mathsf{D}$, $\mathrm{si}(U)$ takes values in $\mathbb{Z}_2$, the statement is proven.

In the case of AIII, BDI and CII, we have

$$\begin{aligned}\widetilde{\mathrm{si}}_-(V) &= \frac{1}{2}\operatorname{tr}\left(\widetilde{\gamma}(\mathbb{1}-V)\right) = \frac{1}{2}\operatorname{tr}\left(\gamma(U-U')\right)\\ &= \mathrm{si}_-(U') - \mathrm{si}_-(U),\end{aligned} \tag{5.45}$$

finishing the proof. □

This theorem, together with Lemma 5.15, is the first result in the direction of completeness of the symmetry indices $\mathrm{si}_\pm$, as described in the introduction to this chapter. More precisely, within the set of unitary admissible operators, the $\mathrm{si}_\pm$ are a homotopy invariant by Theorem 5.5. The above theorem now adds that whenever two unitaries share the same values of $\mathrm{si}_\pm$ *and are compact perturbations of each other*, their relative index vanishes and they are homotopic by Lemma 5.15. In Section 5.6 we will prove, that this restriction is superfluous.

A simple corollary is a formula that reminds of a chain rule for the relative index.

Corollary 5.17 (Chain rule of $\mathrm{si}(U':U)$)
Let U' and U'' be compact admissible perturbations of U. Then, U'' is a compact perturbation of U' and

$$\mathrm{si}(U'':U) = \mathrm{si}(U'':U') + \mathrm{si}(U':U). \tag{5.46}$$

The issue with this rule is that the perturbations $V_1 = U'U^*$ and $V_2 = U''(U')^*$ that correspond to the two relative perturbations $\mathrm{si}(U'':U')$ and $\mathrm{si}(U':U)$, are admissible for different symmetry representations of the same type, since one relative index is relative to U, and the other relative to U'. Luckily, in the case of strictly local unitary operators, i.e. quantum walks, the situation is simplified:

Lemma 5.18 (Chain rule for walks)
Let W be an admissible quantum walk and let V_1, V_2 be admissible local *perturbations for W, such that V_1 and V_2 differ from the identity only in separate regions that are further apart from each other than the jump length of W. Then,*

$$\mathrm{si}(V_2V_1W:W) = \mathrm{si}(V_2W:W) + \mathrm{si}(V_1W:W). \tag{5.47}$$

Proof. The space on which the overall perturbation V_1V_2 acts non-trivially is

$$\begin{aligned}\mathcal{H}_{V_2V_1} &= (V_2V_1-\mathbb{1})\mathcal{H} = (V_2V_1 - V_1 + V_1 - \mathbb{1})\mathcal{H}\\ &= (V_2-\mathbb{1})\mathcal{H} + (V_1-\mathbb{1})\mathcal{H} = \mathcal{H}_{V_1}\oplus\mathcal{H}_{V_2}.\end{aligned} \tag{5.48}$$

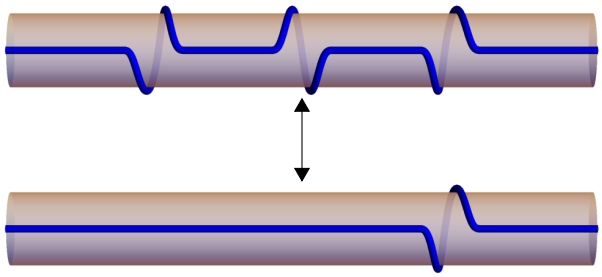


Figure 4: Schematic picture of locally contracting three perturbations to one. The tube visualizes the infinite chain, while the winding of the blue ribbon characterizes the relative index of the perturbation at the respective position. Considering each of the windings as a sufficiently separate perturbation of a quantum walk W, Lemma 5.18 tells us that we can apply the perturbations in any order. Since the relative indices as visualized are (from left to right) $+1, -1, +1$, we know by Theorem 5.16 and Lemma 5.15 that each perturbation by itself cannot be contracted admissibly, but since the relative indices for *left-center*, as well as *center-right* add up to 0, both perturbations together can be trivialized.

The last equality follows from the fact that V_1 and V_2 act sufficiently far apart. Restricting to $\mathcal{H}_{V_1}$, the representation $\widetilde{\rho}'$ that stems from $W' := V_1 W$ coincides with $\widetilde{\rho}$ that stems from W, leading to

$$\widetilde{\mathrm{si}}_-(V_1) = \widetilde{\mathrm{si}}'_-(V_1), \tag{5.49}$$

hence finishing the proof. □

Figure 4 visualizes locally contracting three perturbations to one. An important consequence of this lemma is that two spatially separated perturbations which cannot be contracted to the identity individually, might become trivial when considered as one perturbation. That is, whenever the summands on the right hand side of (5.47) are non-zero, with opposing signs.

This case will be of special interest, after we establish the gentle decoupling theorem (Theorem 5.20). Imagine a two-fold locally perturbed walk, with overall vanishing relative index. Then, decoupling the walk leads to half-space walks on either side that cannot be contracted trivially without reversing the decoupling (see Figure 5).

5.5 DECOUPLING

In Section 5.3, we discussed the consequences of joining two symmetry-admissible bulks with different $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$, namely the occurrence of topologically protected edge states at the boundary. Depending on the definition of bulks, it can be hard to satisfy the conditions of admissibility and unitarity if both are supposed to be retained after the joining. Since we assume the bulks to be translation invariant unitary operators, it suffices to describe how to join *exactly* unitary operators,

without treating essentially unitary operators. A *decoupling* in the sense of Definition 3.11 simplifies the situation considerably, since whenever unitary operators are given as direct sums w.r.t. $P\mathcal{H}$ and $(\mathbb{1}-P)\mathcal{H}$, one can freely combine left and right parts to form new unitary operators that are decoupled as well. The obvious difficulty is to do this admissibly, that is, to find a *gentle decoupling*, which not only leaves $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$ invariant, but also $\mathrm{si}_{\pm}$. In the following, we will show that this is always possible.

Independent of the explicit locality condition, or of essential or exact unitarity, we know from Theorem 3.12 that there is a necessary and sufficient criterion for the existence of a *local decoupling* for a given *quantum walk* W: $\mathrm{ind}(W) = 0$. This is the setting of [Gro+12], which is on the one hand more general than the setting in this chapter (no admissibility, i.e. no essential gap and no symmetry relations), on the other more restricted (strict unitarity, strict locality). Since the index can be defined via the Fredholm index as in Definition 3.8, it is well defined even in the most general setting of an ELEU. Hence, it makes sense to ask which role ind plays w.r.t. the question at hand: How do we determine whether an admissible essentially local unitary operator can be decoupled gently?

Corollary 3.9 shows that ind is invariant under gentle and compact perturbations (hence also invariant w.r.t. their admissibility restrictions), it adds up under products and direct sums and takes values in $\mathbb{Z}$. Thus on one hand, ind shares lots of properties with our symmetry index si. On the other, there are important differences, since e.g. in the case of quantum walks, $\mathrm{ind}(U)$ can be inferred from knowing U on any sufficiently large number of $\mathcal{H}_x$ w.r.t. its jump length[6], while e.g. $\overrightarrow{\mathrm{si}}(U)$ is completely undetermined from knowing U on any finite piece, since it does not change under compact admissible perturbations. Moreover, we note that ind is more similar to $\overrightarrow{\mathrm{si}}$ than to si, in the sense that it is a right index $\mathrm{ind}(U) = \mathrm{ind}_{\mathrm{F}}(PUP)$, where $P = P_{\geq 0}$ as usual. Since unitary operators have an empty kernel, we have that $\mathrm{ind}_{\mathrm{F}}(U) = 0$. Therefore, since for essentially local unitary operators U, the operators $PU(\mathbb{1}-P)$ and its adjoint are compact, thus they do not change the index and we have that

$$\mathrm{ind}_{\mathrm{F}}\left(U\right) = \mathrm{ind}_{\mathrm{F}}\left(PUP\right) + \mathrm{ind}_{\mathrm{F}}\left((\mathbb{1}-P)U(\mathbb{1}-P)\right) = 0. \tag{5.50}$$

Hence in our setting, the *right index* ind carries all information and we can safely ignore its counterpart on the left hand side and their sum.

If we now take admissibility into account, we see that we are in the lucky situation that admissibility implies $\mathrm{ind}(U) = 0$. This stems from two independent lines of reasoning: Firstly, we can see that for most symmetry types, the symmetry relations imply $\mathrm{ind}(U) = 0$. Secondly,

6 See the brief discussion after Theorem 3.10 about ind as a locally computable invariant, a global property of U that can be probed locally, at any position.

we show that the existence of an essential gap requires $\mathrm{ind}(U) = 0$. For symmetry types, where γ is present, we have

$$\begin{aligned}\mathrm{ind}(U) &= \mathrm{ind}_{\mathrm{F}}(\gamma^* PUP\gamma) = \mathrm{ind}_{\mathrm{F}}(P\gamma^* U\gamma P)\\ &= \mathrm{ind}_{\mathrm{F}}(PU^*P) = \mathrm{ind}(U^*) = -\mathrm{ind}(U),\end{aligned} \tag{5.51}$$

since $\mathrm{ind}_{\mathrm{F}}$ is invariant under unitary conjugation and γ is always assumed to commute with P.

If τ is present, the symmetry relation yields $PUP\tau = \tau PU^*P$. This implies that τ maps $\ker PUP$ onto $\ker PU^*P$ and therefore, their dimensions coincide. That is, $\mathrm{ind}(U) = \mathrm{ind}_{\mathrm{F}}(PUP)$ vanishes by Definition 2.17.

This argument hence covers all symmetry types except those where only η is present (or none at all). In these cases, we invoke a variant of the Brown-Douglas-Fillmore theorem [BDF73, Thm. 3.1]. It shows that in the case of non-vanishing $\mathrm{ind}(U)$, the essential spectrum of U is the full unit circle $\mathbb{T}$. But admissibility demands an essential gap, and therefore $\mathrm{ind}(U) = 0$ is necessary for U being admissible.

Theorem 5.19
Let U be an essentially local unitary operator on a separable Hilbert space $\mathcal{H}$ with $\mathrm{ind}(U) \neq 0$. Then,

$$\sigma_{\mathrm{ess}}(U) = \mathbb{T}, \tag{5.52}$$

i.e., the essential spectrum of U is the full unit circle $\mathbb{T}$.

If we add translation invariance to the assumptions of the theorem, it can be proven using the discussion after (3.48). There, it was argued that the index represents the overall winding of the quasi-energy for all bands. The setting of quantum walks from [Gro+12] can in this case even be extended to *essentially* local translation invariant unitary operators. Then, Theorem 6.1 guarantees continuity of the quasi-energy s.t. speaking of a winding at least makes sense. Since the theorem assumes that the index does not vanish, we have a non-trivial winding and hence by continuity, the full unit circle is covered with continuous spectrum. The full proof in our explicit case and without demanding translation invariance is found in [Ced+17, Prop. VII.1].

We have thus shown that for the systems under considerations, i.e. essentially local admissible unitary operators U, $\mathrm{ind}(U) = 0$ is fulfilled. In the case of quantum walks, this is a necessary and sufficient criterion for the existence of *local decouplings*, as was shown in Theorem 3.12, taken from [Gro+12]. In the case of essentially local admissible unitary operators U, we know that if $U' = VU$ is decoupled, $PU'P$ is a unitary operator on $P\mathcal{H}$, and therefore has vanishing index. With tails of arbitrary length for PUP due to essential locality (as opposed to strict locality, where the length is bounded), we cannot hope for V to be a *local* decoupling of U. But we can hope for it to be *compact* in the sense of Definition 3.11 and Lemma 5.13. Then, since ind is invariant under compact perturbations, we know that $\mathrm{ind}(U)$ has to vanish as

well. That is, vanishing index ind is a necessary condition for the existence of a compact decoupling, and since we just showed that this is fulfilled for all essentially local admissible unitary operators, we proceed by stating the main theorem of this section, the gentle decoupling theorem:

Theorem 5.20 (Gentle decoupling theorem)
Let U be an essentially local ρ-admissible unitary operator and let P be the projection to the half-line as before. If ρ is a symmetry representation of AII*, additionally assume that $P - UPU^*$ has a $+1$-eigenspace of even dimension. Then there exists an essentially local compactly gentle decoupling V for U s.t. $U' = VU$ is decoupled, i.e. $[P, U'] = 0$.*

We will only provide a sketch of the proof by describing the steps in the construction of V. The full proof can be found in [Ced+17, VII.].

Similar to the index theory in the case of quantum walks in [Gro+12], this proof relies heavily on a canonical object, the C^*-algebra generated by two projections, see e.g. [RS89]. Its connection to the index theory is studied in [ASS94]. The projections P and $Q = UPU^*$ generate the C^*-algebra of two projections, where additionally, $P - Q$ is a compact operator due to U being essentially local and unitary. The decoupling condition $[P, VU] = 0$ makes V the intertwining operator between P and Q:

$$PV = VQ. \tag{5.53}$$

Thus, we have to find a unitary V, where $V - \mathbb{1}$ is compact, that intertwines P and Q. Such a unitary V is called a *canonical decoupling*.

Similar to [Hal69; And14], decomposing $\mathcal{H}$ into the following subspaces greatly simplifies the discussion about the actions of V on $\mathcal{H}$ ($a, b \in \{0, 1\}$):

$$\mathcal{H}_{ab} = \left\{\phi \in \mathcal{H} \middle| P\phi = a\phi,\, Q\phi = b\phi\right\}, \qquad \mathcal{H}_{\perp} = \bigcap_{a,b} \mathcal{H}_{ab}^{\perp}. \tag{5.54}$$

With P and Q defined as above, e.g. $\mathcal{H}_{00}$ and $\mathcal{H}_{11}$ are associated to the regions far to the left and far to the right respectively, while it can be seen that $\mathrm{ind}(U) = 0$ demands $\mathcal{H}_{01}$ and $\mathcal{H}_{10}$ to be of the same dimension.

The canonical decoupling is then found by introducing

$$X = (\mathbb{1} - 2P)(\mathbb{1} - P - Q), \tag{5.55}$$

which correctly intertwines P and Q, and choosing the polar isometry V_{can} of X as the canonical decoupling on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_{\perp}$,

$$V_{\mathrm{can}} = \left(X^*X\right)^{-1/2} X. \tag{5.56}$$

Furthermore, $V_{\mathrm{can}} - \mathbb{1}$ is compact. Before adding the admissibility-conditions, note that any unitary V_{01} that interchanges $\mathcal{H}_{01}$ and $\mathcal{H}_{10}$ is compatible with the decoupling condition for V, since these are ex-

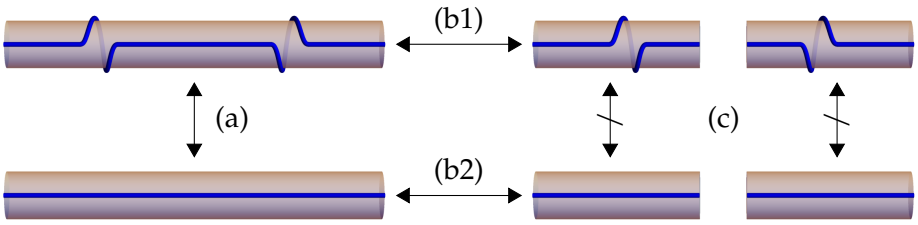


Figure 5: In the spirit of Figure 4, this figure shows consequences of the gentle decoupling theorem Theorem 5.20 and the chain rule for quantum walks Lemma 5.18: (a) By the chain rule, the admissible compact perturbations can together by contracted to the state of *no perturbation*. (b1) and (b2) are both applications of the gentle decoupling theorem, creating a crossover where the perturbations reside on each side of the cut. (c) Individually, these decoupled parts cannot be deformed to the decoupled trivial case, since the relative index does not vanish. This shows that the decoupling from the gentle decoupling theorem is not *homotopy continuous* in the sense that homotopic walks lead to homotopic half-walks after decoupling.

actly those $+1$-eigenvectors of one projection that lie in the kernel of the other projection.

Following the results from Section 5.4, the final V we construct should be an admissible compact perturbation which therefore has to be $\widetilde{\rho}$-admissible on the space $\mathcal{H}_V = \mathcal{H}_\perp \oplus \mathcal{H}_{01} \oplus \mathcal{H}_{10}$, since X and hence V acts like $\mathbb{1}$ on $\mathcal{H}_{00} \oplus \mathcal{H}_{11}$. Translating these relations to P and Q, and checking that V_{can} is admissible without eigenvalue -1 on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$, as well as showing that the representation $\widetilde{\rho}$ is balanced on $\mathcal{H}_{01} \oplus \mathcal{H}_{10}$ shows that the relative index between VU and U vanishes. For more details, see [Ced+17, Prop. VII.2].

The final step in the proof is then, to construct for every symmetry type the admissible unitary V_{01} that swaps $\mathcal{H}_{01}$ and $\mathcal{H}_{10}$, and has only eigenvalues $\pm i$. This can be checked explicitly in [Ced+17, Lem. VII.3] for every case distinction that the different types demand. Remarkably, only in the case AII this leads to an additional assumption: an even dimensional $\mathcal{H}_{01}$. To summarize:

$V = V_{\text{can}} \oplus V_{01}$ on $(\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp) \oplus (\mathcal{H}_{01} \oplus \mathcal{H}_{10})$ yields a decoupling for U via $U' = VU$, since it fulfils the intertwining relation (5.53). Furthermore, it has no eigenvalue -1 and $V - \mathbb{1}$ is compact. Hence by Lemma 5.15, we can contract it to the identity admissibly, providing for every essentially local admissible unitary U an essentially local compactly gentle perturbation U' that is a decoupling.

We can now apply the gentle decoupling theorem together with the relative index from the previous section to show that decoupling affects the homotopy, see Figure 5. The gentle decoupling theorem is a strong result that we can use to represent the different indices in a lucid way. Since we now have a uniform way to decouple admissible, essentially local unitary operators, without changing the indices $\widetilde{\text{si}}$,

$\overrightarrow{\mathrm{si}}$, $\mathrm{si}_\pm$, we can write down the following *matrix of indices for decoupled operators* $U = U_L \oplus U_R$:

$$\begin{array}{cc|c} \mathrm{si}_+(U_L) & \mathrm{si}_+(U_R) & \mathrm{si}_+(U) \\ \mathrm{si}_-(U_L) & \mathrm{si}_-(U_R) & \mathrm{si}_-(U) \\ \hline \overleftarrow{\mathrm{si}}(U) & \overrightarrow{\mathrm{si}}(U) & \mathrm{si}(U) \end{array} \tag{5.57}$$

Following Definition 5.8, we have that $\overleftarrow{\mathrm{si}}(U) = \mathrm{si}(U_L)$ and $\overrightarrow{\mathrm{si}}(U) = \mathrm{si}(U_R)$. Hence by summing rows to the right or columns to the bottom, we reproduce all the sums that we know from the respective definitions.

We learned in Theorem 5.9 that $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ are invariant under compact admissible, as well as gentle perturbations. Hence under these perturbations, $\mathrm{si}_+(U_L)$ and $\mathrm{si}_-(U_L)$ can only change by the same integer, but with opposing signs (U_R analogously). Furthermore, $\mathrm{si}_+(U)$ and $\mathrm{si}_-(U)$ are invariant under gentle perturbations by Theorem 5.5, but compact admissible perturbations can change them by $\mathrm{si}(U' : U)$ as proven in Theorem 5.16. Hence for these perturbations, $\mathrm{si}_+(U_L)$ and $\mathrm{si}_+(U_R)$ can only change by the same integer, but with opposing signs (si_- analogously). Summing up, the top-left 2×2-block in the index matrix behaves in the following way

$$\begin{pmatrix} \mathrm{si}_+(U'_L) & \mathrm{si}_+(U'_R) \\ \mathrm{si}_-(U'_L) & \mathrm{si}_-(U'_R) \end{pmatrix} = \begin{pmatrix} \mathrm{si}_+(U_L) & \mathrm{si}_+(U_R) \\ \mathrm{si}_-(U_L) & \mathrm{si}_-(U_R) \end{pmatrix} + \begin{pmatrix} -n_L & -n_R \\ n_L & n_R \end{pmatrix}$$

with $n_L, n_R \in \mathbb{Z}$ whenever U' is a compact perturbation of U, and with $n_L = -n_R$ if U' is a gentle perturbation of U. This shows that the elements of the 2×2-block are not invariant and can change, depending on the perturbation allowed. We can even create a suitable compact perturbation U' that generates any desired value of $\mathrm{si}_+(U')$ and $\mathrm{si}_-(U')$: Let U be fixed and U' be a compact admissible perturbation of U which keeps the decoupling intact, e.g. by $U' = (V_L \oplus V_R)U$. Then, $n_L = \mathrm{si}(V_L U_L : U_L)$ and $n_R = \mathrm{si}(V_R U_R : U_R)$ by Corollary 5.17. To create the desired $\mathrm{si}_\pm(U')$, we have to pick V_L and V_R suitably. Fortunately, we are not bound to do this gently. On each half-space, we have an infinite reservoir of balanced representations, and thus we have infinitely many subrepresentations where we can perturb admissibly, keeping unitarity to push the spectrum to the desired values. A demonstration of this is the change in $\mathrm{si}_\pm$ by non-gentle decouplings in Section 8.2. This matrix representation will be used in figures and examples to give a quick overview over the important indices.

Having established the gentle decoupling theorem, we can now return to the question from the beginning: is the index classification provided in the previous sections complete? The gentle decoupling theorem will turn out to be an essential milestone in proving this in the following section.

5.6 COMPLETENESS

In the previous sections, we introduced symmetry indices of different kinds and showed their invariance in broader or narrower settings. Now, if we are given an operator from a certain setting, we can determine a symmetry type, write down a symmetry representation and calculate symmetry indices. Furthermore, we know for a wide variety of perturbations whether these change the indices or not.

In this section, we tackle the reverse question: let ρ be a fixed representation of a symmetry type on a Hilbert space $\mathcal{H}$, and fix the set of admissible, essentially or strictly local, exact or essential unitary operators on $\mathcal{H}$. Is there a combination of independent invariants that decomposes this set into connected components, such that any two operators whose invariants have the same values, are in the same connected components. Put differently, is there a norm-continuous path of operators connecting the pair that fulfils the same assumptions along the way as the pair they connect?

If this question is answered in the affirmative, we call the classification ***complete***, since then the indices decompose the set of objects to be classified into sets labelled by the values of the indices that are exactly path-connected w.r.t. the transformations allowed. In other words, the map that assigns a tuple of indices to the connected components of the set of objects w.r.t. the transformations is an isomorphism.

Before we go into the details, let us first review what we already know about the index ind that is defined without symmetries. As stated in Theorem 3.10, in [Gro+12, Thm. 3.6] Gross et al. show that within the set of strictly local unitary operators, i.e. quantum walks, the index ind is a *complete homotopy invariant*. The important bit is that the conditions are satisfied *along the way*, i.e. the condition of a uniformly bounded interaction length is kept. If one allowed for e.g. essentially local unitary operators *along the way*, the result clearly would be much weaker.

Regarding *our* symmetry indices, Section 5.4 shows a partial completeness result. Fixing an admissible essentially local unitary operator U, we look at the set of compact admissible perturbations of U. Let U' denote an arbitrary element of this set. The relative index between the variable U' and the fixed U is now a homotopy invariant by Lemma 5.15. Furthermore, Theorem 5.16 teaches us that the relative index is just the difference of the absolute indices $\mathrm{si}_\pm$, and therefore we learn that the converse holds as well. That is, any pair of U_1 and U_2 with matching $\mathrm{si}(U_1 : U) = \mathrm{si}(U_2 : U)$ is homotopic within this set. Hence for this setting, there is no finer decomposition than the one provided by the relative index, i.e. the sets of operators of matching relative index are path-connected and the classification is *complete*.

After carefully analysing the perturbations that leave invariant the different indices we introduced in this Chapter, we arrive at three set-

tings that are candidates for completeness. We assume that we have fixed a representation ρ of symmetry type $\mathsf{S} \in \{\mathsf{D}, \mathsf{AIII}, \mathsf{BDI}, \mathsf{CII}, \mathsf{DIII}\}$ on a Hilbert space $\mathcal{H}$, where *admissibility* exclusively refers to. The fact that we do not allow symmetry types with trivial index group is because we cannot gain any insight from the cases where our symmetry classification is not classifying anything. A completeness theorem would then either be trivially true (C, CI) or trivially false ($\mathsf{A}, \mathsf{AI}, \mathsf{AII}$). Luckily, this section will show that in all three scenarios, the proof of completeness succeeds.

I. The set of admissible essentially local unitary operators, where we allow essentially local gentle perturbations. In this case, $\overrightarrow{\mathrm{si}}$, $\overleftarrow{\mathrm{si}}$, si_- are independent invariants, with the dependent invariant $\mathrm{si}_+ = \overleftarrow{\mathrm{si}} + \overrightarrow{\mathrm{si}} - \mathrm{si}_-$.

II. The set of admissible essentially local unitary operators, where we allow essentially local gentle perturbations and admissible compact perturbations as transformations. In this case, $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$ are independent invariants.

III. The set of admissible unitary operators without demanding a locality condition, where we allow gentle perturbations as transformations. In this case, si_+ and si_- are independent invariants.

Additionally demanding translation invariance from the set of objects or transformations requires a more specialized case distinction. For symmetry types which contain γ, this will be done in Section 7.2. The main result of this section is then the following theorem:

Theorem 5.21 (Completeness)
In each of the settings I., II., III. and for all $\mathsf{S} \in \{\mathsf{D}, \mathsf{AIII}, \mathsf{BDI}, \mathsf{CII}, \mathsf{DIII}\}$*, the respective indices are complete.*
Moreover, all values of the indices can be realized by a crossover of two translation invariant quantum walks that has a finite transition area.

Instead of providing the complete proof in all detail, we will provide a sketch where we emphasize important steps. The full proof is found in [Ced+17, VIII.].

We know that any decoupled operator is essentially local by definition, and the gentle decoupling theorem (Theorem 5.20) guarantees a gentle decoupling for all objects from setting I and II only using gentle transformations, hence keeping the indices as they are. This leads to two unitary half-walks on each side of the decoupling that fall into setting III.

More precisely, by Theorem 5.20, we can decouple every operator from I and II gently without changing any of the indices $\overleftarrow{\mathrm{si}}$, $\overrightarrow{\mathrm{si}}$ and si_-. Therefore, we can gently deform every operator in I and II to a decoupled one. Let $U = U_L \oplus U_R$ and $U' = U'_L \oplus U'_R$ represent the gently decoupled operators with matching indices as demanded

by the setting. Since the theorem guarantees the decoupling is done compactly, we furthermore know that essential locality does not suffer: U_L, U_R, U'_L, U'_R are all still essentially local ρ-admissible operators on their respective half-spaces. But since U and U' are unitary operators on $\mathcal{H}$ and given as a direct sum, the left and right parts of U and U' are also unitary on their corresponding half-spaces. The difficulty is now to make $\mathrm{si}_\pm(U'_L) = \mathrm{si}_\pm(U_L)$, since that is the only missing condition for the half-space operators to belong to setting III. From the example in (5.57) we know that we can find compact perturbations V_L, V_R confined to the corresponding half-space, s.t. any value for n_L and n_R is possible. In setting II, this is sufficient, since it allows compact admissible perturbations. Hence setting II is transformed to setting III. In setting I, U and U' are only equivalent if the overall perturbation V is gentle. By Lemma 5.15 this is exactly the case if

$$\mathrm{si}(U' : U) = \mathrm{si}(U'_L : U_L) + \mathrm{si}(U'_R : U_R) = 0. \tag{5.58}$$

Hence given two operators U and U' from setting I or II, whose indices relevant to the setting coincide, we can bring both into a decoupled form, such that $\mathrm{si}_\pm(U_L) = \mathrm{si}_\pm(U'_L)$ (U_R analogously). Since every decoupled operator is essentially local, any decoupled gentle perturbation of decoupled operators is essentially local. Therefore, the locality constraint vanishes and setting III remains, i.e. the commutation relations with ρ and the essential gap. Thus, in the first step, we reduced the settings I and II to III by applying the gentle decoupling theorem.

In the second step, we use continuous functional calculus to admissibly transform the spectrum of the unitary operators from setting III to be contained in $\{+1, -1, +i, -i\}$ without leaving the setting. That is, these unitary operators fulfil $U^4 = \mathbb{1}$, have infinite dimensional $\pm i$-eigenspaces and finite dimensional ± 1-eigenspaces that contain no balanced subrepresentations. These strongly simplified unitary operators are then easily described by a few algebraic rules.

In the third step, we argue that the system of symmetries together with the transformed unitary U is completely characterized up to unitary equivalence by $\mathrm{si}_\pm(U)$. This means that two unitary operators U and U' that are ρ-admissible with $\mathrm{si}_\pm(U) = \mathrm{si}_\pm(U')$ are connected via $U' = ZUZ^*$, with Z being a symmetry commuting operator due to the admissibility of U and U'.

The final step shows that any symmetry-commuting unitary operator Z on an infinite dimensional Hilbert space can be contracted to the identity with a suitable Z_t. This contraction provides the gentle perturbation between U and U' by conjugation, i.e. $U_t = Z_t U Z_t^*$, and therefore finishes the proof.

As mentioned above, the full proof can be found in [Ced+17, VIII.]. We will revisit many of the techniques used when proving completeness for translation invariant essentially local unitary operators that are admissible for a chiral symmetry in Section 7.3.

Summing up this chapter, we have provided a *complete* homotopy characterization of essentially gapped one dimensional essentially local unitary operators that satisfy the discrete symmetries of the tenfold way. As opposed to many other authors, we did not rely on translation invariance to simplify the setting, but provided a theory that does not fail to describe the non-translation invariant systems of interest, which are crossovers between two systems in different phases.

With these results, we can now proceed to the typical setting of *bulk* systems, namely translation invariant unitary operators.

6

LOCALITY AND TRANSLATION INVARIANCE

In this chapter, we connect locality-properties of translation invariant operators to the smoothness of their band structure and decay properties of their eigenfunctions. We lay the necessary foundation for later chapters where we derive general formulas for the symmetry indices in the special case of translation invariant unitary operators.

6.1 ESSENTIAL LOCALITY AND CONTINUITY OF BAND STRUCTURE

It is well known, that the Fourier transform translates local properties of W (e.g. the strength of the decay of $W(x)$) to global properties of $\widehat{W}$ (e.g. smoothness or differentiability / continuity). Remarkably, this section will show, that the most general locality condition that suits our index theory, namely essential locality, already implies the minimal necessary condition for e.g. winding numbers to make sense: continuity of the band structure.

6.1.1 *Equivalence Theorem*

Let us begin by stating the main result of this section, the equivalence theorem:

Theorem 6.1
Let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ and $A \in \mathcal{B}(\mathcal{H})$ be a translation invariant operator. Denote by $P = P_{\geq 0}$ the projection onto the non-negative half-space. Then, the following are equivalent:

1. *A is essentially local, i.e., $[P, A]$ is compact.*
2. *A can be approximated in norm by strictly local operators $(A'_n)_{n\in\mathbb{N}}$.*
3. *A can be approximated in norm by translation invariant operators $(A'_n)_{n\in\mathbb{N}}$ s.t. the map $k \mapsto \widehat{A}'_n(k)$ is smooth.*
4. *$k \mapsto \widehat{A}(k)$ is a continuous function with periodic boundary conditions.*

Furthermore, if A is unitary and admissible for all symmetries of the ten-fold-way, A'_n in (3) can be chosen to be unitary and admissible.

In order to prove this theorem, we need a few results from the theory of Fourier series and a description in terms of Hankel matrices, both provided below. For a detailed look into these topics, we recommend to the interested reader the publications [DM72], [Har58], [BDF73], [Sto48] and references therein.

The first definition will cover the Hankel operator.

Definition 6.2 (Hankel operator)
Let $P\mathcal{H}$ be the non-negative half-space and H a linear operator on $P\mathcal{H}$. We call H a Hankel operator, if there is a sequence $(h_l)_{l\in\mathbb{N}}$ and a basis $\{\varphi_i\}_{i\in\mathbb{N}}$ of $P\mathcal{H}$ s.t.

$$\langle \phi_i, H\phi_j\rangle = h_{i+j}. \tag{6.1}$$

The matrix $H_{i,j}$ corresponding to H is called the Hankel matrix. It is a matrix which is constant along its anti-diagonals.

The following example of a Hankel matrix was first used by Hilbert[1] in [Hil94], and has gained a lot of attention from 1950-1960 in a generalized form (see e.g. [Ros58]).

Example 6.3 (Generalized Hilbert matrix)
Let t be a real number that is not a positive integer. Then, $(h_l)_{l\in\mathbb{N}}$ with $h_l = (l+1-t)^{-1}$ defines a Hankel operator that is called a generalized Hilbert matrix.

As [Ros58, Thm. 5] shows, the generalized Hilbert matrix is a bounded self-adjoint operator, that has non-vanishing continuous spectrum for all t allowed in its definition.

Another class of operators we need are ***Toeplitz operators***. They are basically Hankel operators with a changed sign in its definition:

Definition 6.4 (Toeplitz operator)
Let $P\mathcal{H}$ be the non-negative half-space and H a linear operator on $P\mathcal{H}$. We call T a Toeplitz operator, if there is a sequence $(t_l)_{l\in\mathbb{N}}$ and a basis $\{\varphi_i\}_{i\in\mathbb{N}}$ of $P\mathcal{H}$ s.t.

$$\langle \phi_i, T\phi_j\rangle = t_{i-j}. \tag{6.2}$$

The matrix $T_{i,j}$ corresponding to T is called the Toeplitz matrix. It is a matrix which is constant along its diagonals.

Hence another way to phrase the definition is, that Toeplitz operators are half-space compressions of translation invariant operators[2]. Given a Toeplitz operator T with sequence t, we call the Fourier transform $\widehat{t}$ the *symbol* of the Toeplitz operator.

The connection between Hankel operators and Toeplitz operators is best seen with the help of a flipping operator

$$S\colon P\mathcal{H} \to (\mathbb{1}-P)\mathcal{H} : (S\psi)(x) = \psi(-1-x) \quad \forall x \geq 0. \tag{6.3}$$

Then, S maps any $\psi \in P\mathcal{H}$ to $(\mathbb{1}-P)\mathcal{H}$, and $S^{-1} = S^*$ thus maps from $(\mathbb{1}-P)\mathcal{H}$ to $P\mathcal{H}$. Figure 6 shows that $(\mathbb{1}-P)W(\mathbb{1}-P)$ and PWP are Toeplitz matrices representing Toeplitz operators on $P\mathcal{H}$ and $(\mathbb{1}-P)\mathcal{H}$ respectively. Furthermore, one recognizes that the anti-diagonal blocks

1 Confusingly, the historical Hilbert matrix ($t = 2$) was specifically excluded in the definition of the generalized Hilbert matrix later on, since it's properties are quite different from those of the general Hilbert matrix ($t \in \mathbb{Z}$ not a positive integer).

2 See the conventions for translation invariance in (3.29).

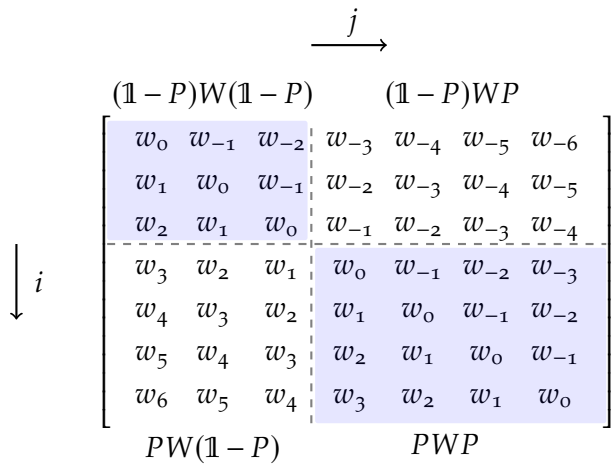


Figure 6: Finite part of the translation invariant operator $W_{i,j} = w_{i-j}$ in matrix representation. The dashed lines represent the cut positions w.r.t. P. It cuts the matrix into four blocks. The diagonal blocks shaded blue are Toeplitz matrices indicating the Toeplitz operators in the infinite dimensional case, while the anti-diagonal blocks are Hankel matrices after either flipping the sign of i or j as performed by S. Note the constant diagonals of the Toeplitz matrix, as well as the constant anti-diagonals in the Hankel matrix if one considers the sign-flip.

$(\mathbb{1} - P)WP$ and $PW(\mathbb{1} - P)$ are Hankel operators, at least after flipping the sign to identify it as an operator on $P\mathcal{H}$. We will check algebraically that $(\mathbb{1} - P)WP$ is a Hankel operator after applying S^*. For all $i, j \geq 0$ we have:

$$\langle \phi_i, S^*(\mathbb{1} - P)WP\phi_j \rangle = \langle \phi_{-i-1}, W\phi_j \rangle = w_{-(i+j)-1}, \tag{6.4}$$

which depends only on the sum of the indices, and is hence a Hankel operator, relabelled after a shift by 1. What we have thus learned is, that the off-diagonal blocks of translation invariant operators are Hankel operators. Furthermore, the definition of essential locality demands that both blocks are compact each for themselves if and only if W is essentially local. Since we are interested in essentially local translation invariant operators, this example is an important step towards proving Theorem 6.1. There, we combine it with the following Theorem from Hartman [Har58] which connects the compactness of Hankel operators to the existence of a continuous Fourier transform. It is written in matrix-valued form, as found e.g. in [Pel03, Thm. 4.2].

Theorem 6.5 (Hartman)
Let $\mathcal{H}_0$ be a finite dimensional Hilbert space, $\mathcal{B}(\mathcal{H}_0)$ the set of bounded operators on $\mathcal{H}_0$, and let $\{\Omega_j\}_{j\in\mathbb{N}}$ be a sequence in $\mathcal{B}(\mathcal{H}_0)$. Then, the block Hankel matrix $\{\Omega_{j+l}\}_{j,l\in\mathbb{N}}$ determines a compact operator on $\ell^2(\mathbb{N}) \otimes \mathcal{H}_0$ if

and only if there exists a continuous function $\widehat{\Psi} : [-\pi, \pi] \to \mathcal{L}_2(\mathcal{B}(\mathcal{H}_0))$ *such that*

$$\widehat{\Psi}(k) = \sum_{j \geq 0} \Omega_j e^{ikj} + \sum_{j<0} \Psi_j e^{ikj}. \tag{6.5}$$

This theorem covers the most important part of the proof. Still, in order to derive the useful formulas in the later chapters, we need suitable approximations of the operators under investigation. One step is provided by a classical result of Fejér [Fej04], more suitably formulated and proven in [DM72, 1.4, Thm. 3]. For our purposes, we have to extend the result to matrix valued function $\widehat{A}(k)$, which is done by replacing the absolute value with the operator norm in $\mathbb{C}^d$ in the proof just cited.

Theorem 6.6 (Fejér)
Let $\widehat{A} \in \mathcal{L}_2(\mathbb{T}, \mathbb{C}^d)$ *be a continuous function with periodic boundary conditions and corresponding Fourier transform A. Moreover, given the* $\{A_x\}$ *as in* (3.29)*, let*

$$\widehat{S}_n(k) = \sum_{x=-n}^{n} A_x e^{ikx} \tag{6.6}$$

be the Fejér kernels of A. Then, the arithmetic means

$$\widehat{A}'_n = \frac{1}{n}(\widehat{S}_0 + \widehat{S}_1 + \ldots + \widehat{S}_{n-1}) \tag{6.7}$$

converge uniformly to $\widehat{A}$*.*

The corollary follows immediately

Corollary 6.7
A can be approximated in norm by strictly local operators.

Proof. The strict locality of S_j can be seen most conveniently by

$$(S_j\psi)(x) = \frac{1}{2\pi} \sum_{y=-j}^{j} \int_{-\pi}^{\pi} \mathrm{d}k\, e^{-ik(x-y)} A_y \widehat{\psi}(k) = \sum_{y=-j}^{j} A_y \psi(x-y), \tag{6.8}$$

since a finitely supported ψ is mapped to a finitely supported $S_j\psi$. A'_n is a finite sum of strictly local operators, hence itself strictly local.

The uniform convergence of $A'_n \to A$ in norm is now a direct consequence of $\widehat{A}'_n \to \widehat{A}$ in norm by the Plancherel identity [DM72, 1.4, Thm. 1], which follows directly from the unitarity of the Fourier transform, i.e.

$$\sup_{k \in \mathbb{T}} \|\widehat{A}'_n(k) - \widehat{A}(k)\| = \|\widehat{A}'_n - \widehat{A}\| = \|A'_n - A\| \leq \epsilon_n \to 0. \tag{6.9}$$

□

Having gathered these results, we can now combine them to prove the equivalence of essential locality and continuity of the band structures:

Proof of Theorem 6.1. (1) $\Rightarrow$ (4): The essential locality of A states that the off-diagonal blocks $A_{+-} = PA(\mathbb{1} - P)$ and $A_{-+} = (\mathbb{1} - P)AP$ are compact operators. Since A is translation invariant, after applying S from Definition 6.4, A'_{+-} and A'_{-+} are compact Hankel operators with corresponding sequence $(A_l)_{l\geq 0}$ and $(A_{-l-1})_{l\geq 0}$ respectively. Then, Hartman's theorem (Theorem 6.5) implies, that there are continuous $\widehat{\Psi}_{+-}, \widehat{\Psi}_{-+}$ (with periodic boundary conditions) s.t.

$$\begin{aligned}\widehat{\Psi}_{+-}(k) &= \sum_{j\geq 0} A_j e^{ikj} + \sum_{j<0} \phi_j e^{ikj} \\ \widehat{\Psi}_{-+}(k) &= \sum_{j\geq 0} A_{-j-1} e^{ikj} + \sum_{j<0} \psi_j e^{ikj}.\end{aligned} \tag{6.10}$$

Projecting to the half-space $P\mathcal{H}$ is continuous in norm since the multiplication of bounded operators is continuous. Furthermore, relabelling $\widehat{\Psi}_{-+}$ to again be supported only on $(\mathbb{1} - P)\mathcal{H}$ by flipping with f does not break continuity. Therefore, the composition

$$\widehat{A}(k) = \left(P\widehat{\Psi}'_{+-}\right)(k) + f\left(P\widehat{\Psi}_{-+}\right)(k) = \sum_{j\in\mathbb{Z}} A_j e^{ikj} \tag{6.11}$$

is continuous as well, proving the statement.

(4) $\Rightarrow$ (2): In essence, this is the Stone-Weierstraß Theorem [Sto48], which states that every continuous function can be approximated w.r.t. the sup-norm with arbitrary precision using a suitable trigonometric polynomial. Cor. 6.7 proves this explicitly by using the arithmetic means of the Fejér-kernels $\widehat{A}'_n$.

(2) $\Rightarrow$ (1): The commutator $[P, A]$ can be written as

$$\begin{aligned}[P, A] &= PA - AP = PA - PAP - AP + PAP \\ &= PA(\mathbb{1} - P) - (\mathbb{1} - P)AP.\end{aligned} \tag{6.12}$$

Since limits of finite rank operators are compact, in order to show the compactness of $[P, A]$, we first suppose that A is strictly local. Then, due to the finite neighbourhood, strict locality implies that A maps only a finite number of sites from $P\mathcal{H}$ to $(\mathbb{1} - P)\mathcal{H}$ (and vice versa). Hence, $[P, A]$ is a finite rank operator. Therefore, if A is assumed to be the norm-limit of strictly local operators, $[P, A]$ is not necessarily finite rank any more, but as the norm-limit of finite rank operators at least compact - which proves the statement.

(2) $\Rightarrow$ (3) $\Rightarrow$ (4): We will first prove this without unitarity and admissibility. Starting from (2), we have already proven that this implies (4) via (1). Therefore, we may construct the same sequence of translation invariant, strictly local operators converging to A as in (4) $\Rightarrow$ (2),

$$\widehat{A}'_n = \frac{1}{n}(\widehat{S}_0 + \widehat{S}_1 + \ldots + \widehat{S}_{n-1}), \tag{6.13}$$

with the Fejér-kernels $\widehat{S}_n$ (as defined above) stemming from $\widehat{A}$ via (4). Since we already know that A'_n is translation invariant, to prove (3), it remains to show that the $\widehat{A}'_n$ are infinitely differentiable. But by

definition, the $\widehat{A'_n}$ are Laurent-polynomials in e^{ik} with constant, matrix-valued coefficients and therefore infinitely differentiable. This proves (4) and hence finishes the proof.

In the case of a unitary and admissible A, we cannot simply use the averaged Fejér-kernels A'_n directly, because they are in general not unitary. Nevertheless, we can use them to build a new sequence that is unitary and admissible.

Since A is admissible for the symmetry, by definition, it fulfils the commutation relations with $\sigma \in \{\eta, \tau, \gamma\}$, depending on the symmetry type. Given $\widehat{A}(k) = \sum_{x\in\mathbb{Z}} A_x e^{ikx}$, (7.3) and (3.39) together show that admissibility for $\widehat{A}(k)$ reduces to an admissibility condition for each A_x w.r.t. the single-site-symmetries σ from (7.3), which thus implies that every (finite or infinite) sum with symmetric summation indices and real-linear coefficients of $A_x e^{ikx}$ (e.g. the Fejér-kernels S_n and their averages A'_n) is again admissible. Therefore, the A'_n are all admissible, and thus their Fourier transforms $\widehat{A'_n}(k)$ as well.

In the next step, we have to restore unitarity, since in general, A'_n is not unitary. Using the $\widehat{A'_n}(k)$ we already analysed, we explicitly construct a unitary admissible sequence U_n fulfilling all the desired properties.

Let us begin by noting, that since $\|A'_n - A\| \geq \epsilon_n$, and A unitary,

$$\begin{aligned}\|{A'_n}^* A'_n - \mathbb{1}\| &= \|({A'_n}^* - A^*)(A'_n - A) + 2\mathbb{1} - {A'_n}^* A - A^* A'_n\| \\ &\leq \|{A'_n}^* - A^*\|\|A'_n - A\| + \|A^*A - {A'_n}^* A\| \\ &\quad + \|A^*A - A^* A'_n\| \\ &\leq \epsilon_n^2 + 2\epsilon_n. \end{aligned} \tag{6.14}$$

Therefore, the spectrum of $A'^*_n A'_n$ gets arbitrarily close to 1, hence there is an $n_0 \in \mathbb{N}$ such that for all $n \geq n_0$, the kernel of $A'^*_n A'_n$ is empty. The same estimate holds for $\widehat{A'_n}(k)$, since

$$\sup_{k\in[-\pi,\pi]} \|\widehat{A'_n}(k) - \widehat{A}(k)\| = \|A'_n - A'\| \geq \epsilon_n. \tag{6.15}$$

Then, the inverse square root

$$\widehat{M}_n(k) := \left(\widehat{A'_n}(k)^* \widehat{A'_n}(k)\right)^{-\frac{1}{2}} \tag{6.16}$$

exists, and is infinitely differentiable as it stems from applying a convergent power series (using functional calculus) to the polynomial $\widehat{A'_n}(k)^* \widehat{A'_n}(k)$. Now, we define

$$\widehat{U}_n(k) := A'_n(k)\widehat{M}_n(k). \tag{6.17}$$

By construction, $\widehat{U}_n(k)$ is unitary for all $n \in \mathbb{N}$ and infinitely differentiable as the product of two infinitely differentiable operators. Additionally, since A'_n is ρ-admissible and M_n is a power series in $(A'_n)^* A'_n$, U_n is admissible for all $n \in \mathbb{N}$ by (4.2). This finishes the proof of (2) $\Rightarrow$ (3) in the unitary and admissible case. Then, (3) $\Rightarrow$ (4) follows as before by stating that $\widehat{A}(k)$ is the norm-limit of the continuous func-

tions $\widehat{U}_n(k)$, hence continuous by itself. This completes the proof of Theorem 6.1.

□

For the rest of this section, we provide a few applications that shine light on this sections' theorem about the interplay between essential locality and the continuity of the band structure.

6.1.2 *Interlude: exponentials*

Given an operator A, the property of $[P, A]$ being compact, i.e. A being essentially local, is the same as stating that $[\pi(P), \pi(A)] = 0$, with π being the natural projection onto the Calkin algebra as in Definition 2.16. Therefore, commutation of A with P in the Calkin algebra is equivalent to A being essentially local. Therefore, every analytic function of an essentially local operator is essentially local, due to the linearity of the commutator.

This shows a favourable connection between Hamiltonians H and their time-evolution-operators $W = \exp(iHt)$: if H is essentially local, so is W. Additionally, if H is translation invariant, by Theorem 6.1, essential locality already implies continuity of $\widehat{H}(k)$, which then implies the continuity of $\exp(i\widehat{H}(k)t)$.

On the opposite, strict locality is not preserved by exponentiation, which can easily be seen by the strictly local bilateral one-site shift $\widehat{T}(k) = e^{ik}$ that gets mapped to

$$\exp(i\widehat{T}(k)t) = \sum_{j\in\mathbb{N}} \frac{(it)^j}{j!} e^{ikj}. \tag{6.18}$$

Since all positive integer powers of the shift e^{ik} occur, the whole positive half-axis is left as the image of $[P, \exp(i\widehat{T}(k)t)]$, which is not finite, hence contradicting strict locality. Still, as the limit of a sequence of strictly local, translation invariant operators, $\exp(i\widehat{T}(k)t)$ is still essentially local.

6.1.3 *Application: contracting the shift*

We know from Cor. 3.9 that the index ind is a homotopy invariant for essentially local essential unitaries. Furthermore, in the case of strictly local unitary operators, i.e. quantum walks, we know by Theorem 3.10 that this invariant is even complete, i.e. a matching index of two walks implies the existence of a norm-continuous path of quantum walks of the same index connecting both walks.

In what follows, we try to connect the identity $\mathbb{1}$ and the bilateral shift T on $\ell^2(\mathbb{Z})$ continuously. Obviously, any attempt to do so has to fail by the above reasoning, since

$$\operatorname{ind}(\mathbb{1}) = 0 \neq 1 = \operatorname{ind}(T). \tag{6.19}$$

Still, it is a useful example which shows *how badly* essential locality fails on deformation paths, even if one tries to connect the simplest examples of strictly local unitaries.

Let us define our deformation from $\widehat{W}_0 = \mathbb{1}$ to $\widehat{W}_1(k) = \widehat{T}(k)$ as

$$\widehat{W}_t(k) = (\widehat{T}(k))^t = e^{itk}. \tag{6.20}$$

Obviously, this is a norm-continuous interpolation between $\widehat{W}_0$ and $\widehat{W}_1$ for all $k \in [-\pi, \pi]$. But as a function of k, $\widehat{W}_t(k)$ is not continuous, since for $t \neq \{0, 1\}$, $\widehat{W}_t$ jumps from $\exp(-it\pi)$ to $\exp(it\pi)$ as k crosses from π to $-\pi$, which is a dependence on the arbitrary choice of the cut point of the Brillouin zone. This violates the constraint of periodic boundary conditions. Hence by Theorem 6.1, $\widehat{W}_t$ cannot be essentially local for any $t \in (-\pi, \pi)$.

Since we work with an explicit example, we could skip the theorem, and use a direct approach: analyse spectral properties of $\widehat{W}_t$ and contradict the compactness of $PW_t(\mathbb{1} - P)$. In order to do so, let us look at the action of $\widehat{W}_t$ in position space by applying the inverse Fourier transform:

$$\begin{aligned}(W_t\psi)(x) &= \left(\mathcal{F}^*\widehat{W}_t\mathcal{F}\psi\right)(x)\\ &= \frac{1}{2\pi}\sum_{y\in\mathbb{Z}}\int_{-\pi}^{\pi} \mathrm{d}k\, e^{-i(x-t-y)k}\psi(y)\\ &= \frac{\sin(\pi t)}{\pi}\sum_{y\in\mathbb{Z}}\frac{(-1)^{y-x}}{t+y-x}\psi(y)\\ &= \sum_{y\in\mathbb{Z}} W_t(x-y)\psi(y).\end{aligned} \tag{6.21}$$

Since we want to know whether $PW_t(\mathbb{1} - P)$ is compact, we could look at the image of $PW_t(\mathbb{1} - P)$ directly. But it proves to be considerably easier to introduce a flipping operator $S : P\mathcal{H} \to (\mathbb{1} - P)\mathcal{H}$, which performs the same flipping operation as defined in (6.3), i.e. $(S\psi)(x) = \psi(-1 - x)$. Then, any $\psi \in P\mathcal{H}$ is mapped by S to $(\mathbb{1} - P)\mathcal{H}$, leading to

$$\begin{aligned}(W_t(\mathbb{1} - P)S\psi)(x) &= \sum_{y<0} W_t(x-y)\psi(-1-y)\\ &= \sum_{z\geq 0} W_t(1+z+x)\psi(z)\\ &= \frac{\sin(\pi t)}{\pi}\sum_{z\geq 0}\frac{(-1)^{z+x}}{1+z+x-t}\psi(z).\end{aligned} \tag{6.22}$$

The missing projection P in $PW_t(\mathbb{1} - P)$ makes the above expression vanish if $x < 0$. Since we are interested in the case $t \in (0, 1)$, the prefactor is constant, non-vanishing, hence does not contribute to whether $PW_t(\mathbb{1} - P)$ is compact or not. Furthermore, the factor $(-1)^{z+x}$ can be seen as stemming from a conjugation with $-\mathbb{1}$, which is hence a unitary conjugation and therefore leaves the spectrum invariant.

The remaining operator is a generalized Hilbert matrix, which is known to have continuous spectrum for all t under consideration (see e.g. Example 6.3). Since the spectrum of a compact operator contains only non-zero eigenvalues of finite multiplicity which form a sequence converging to the unique accumulation point 0, its' spectrum is only pure-point. Therefore, $PW_t(\mathbb{1} - P)$ cannot be compact, and thus W_t is not essentially local for any $0 < t < 1$.

6.1.4 *Application: decay properties of walk matrix elements*

The spatial structure of the Hilbert space under consideration is important e.g. to analyse exponential decay of the eigenvectors ψ of quantum walks with a gap, as will be done in Section 6.2. Instead of looking at the eigenfunctions, we will analyse the decay of the matrix elements $\langle y|U|x\rangle$ in operator norm and show that polynomial decay stronger than the (diverging) *harmonic series* is sufficient to prove essential locality of U unitary (and not necessarily translation invariant).

Let U be a unitary operator whose matrix elements $U_{x,y}$ as defined in (3.18) decay polynomial w.r.t. the distance, i.e.

$$\|U_{x,y}\| \leq c|y - x|^{-\alpha} \quad \forall x \neq y. \tag{6.23}$$

The norm on the left-hand side denotes the standard operator norm, which in this case, coincides with the matrix norm for complex $d \times d$-matrices. Strictly local unitary operators W (quantum walks) obviously do belong to this class of polynomially decaying operators, since in that case, there is an $L \in \mathbb{N}$ s.t.

$$W_{x,y} = 0 \quad \forall |y - x| > L, \tag{6.24}$$

and we could simply choose a sufficiently large c, given L and the dimension d of the local Hilbert spaces, to fulfil the inequality for every α. As opposed to most of this chapter, note that for now, we do not restrict ourselves to translation invariant operators.

From (2.63) we know that Hilbert-Schmidt operators are compact. Therefore, if the Hilbert-Schmidt norm of $PU(1 - P)$ and $(1 - P)UP$ are each finite,

$$[P, U] = PU(1 - P) + (1 - P)UP \tag{6.25}$$

is compact and hence U is essentially local.

Hence, for $PU(1 - P)$, we find[3]

$$\|PU(1 - P)\|_2^2 = \operatorname{tr}\left((\mathbb{1} - P)U^*PU\right) = \sum_{y<0} \operatorname{tr}\left(\langle y|U^*PU|y\rangle\right), \tag{6.26}$$

where we used the cyclicity of the trace to get rid of one application of $\mathbb{1} - P$, since $(\mathbb{1} - P)^2 = \mathbb{1} - P$. On the right hand side, we note that the trace tr now refers to the trace on the coin space, hence simply the

3 The case $(1 - P)UP$ is completely analogous

trace on $\mathbb{C}^d$. Writing it in terms of matrix elements $U_{x,y}$ as in (3.18), we get

$$\|PU(1-P)\|_2^2 = \sum_{y<0} \operatorname{tr}\left(\sum_{x\geq 0} U_{x,y}^* U_{x,y}\right) = \sum_{x\geq 0>y} \operatorname{tr}\left(U_{x,y}^* U_{x,y}\right). \tag{6.27}$$

The right hand side is now a sum over Hilbert-Schmidt norms $\|U_{x,y}\|_2^2$. Each summand in the trace contributes at most $\|U_{x,y}\|^2$, where $\|U_{x,y}\|$ denotes the standard matrix norm for the complex $d \times d$-matrix $U_{x,y}$. Hence, we showed that $\|U_{x,y}\|_2^2 \leq d\|U_{x,y}\|^2$ and using the polynomial decay of U, we have

$$\|PU(1-P)\|_2^2 \leq d \sum_{x\geq 0>y} \|U_{x,y}\|^2 \leq cd \sum_{x\geq 0>y} |y-x|^{-2\alpha}. \tag{6.28}$$

After substituting $z = y - x$, we determine $n(z)$ as the number of identical terms $|z|^{-2\alpha}$ in this double sum

$$n(z) := \left|\{(x,y) \,\middle|\, y - x = z \wedge x \geq 0 \wedge y < 0\}\right| = |z|, \tag{6.29}$$

where $|S|$ denotes the cardinality of the set S. This leads to the final estimate in this application:

$$\|PU(1-P)\|_2^2 \leq cd \sum_{z>0} |z| \cdot |z|^{-2\alpha} = cd \sum_{n=1}^{\infty} n^{1-2\alpha}. \tag{6.30}$$

The series on the right hand side converges[4] iff $1 - 2\alpha < -1$, hence $\alpha > 1$. Therefore, any decay of the matrix-elements $U_{x,y}$ that is stronger than harmonic decay leads to finite Hilbert-Schmidt norm and hence compactness of $[P, U]$ due to (2.63). Thus, if (6.23) holds for $\alpha > 1$, U is essentially local.

In the following, we show that this criterion is optimal, by analysing the example from the previous application (6.21), the contraction of the shift, e.g. for $t = \frac{1}{2}$:

$$W(x,y) := W_t(x-y) = \frac{(-1)^{y-x}}{\frac{1}{2} + y - x}, \tag{6.31}$$

which easily fulfils (6.23) with $\alpha = 1$ and $c = 2$, i.e.

$$\|W(x,y)\| = \frac{2}{|1 + 2(y-x)|} \leq 2|y-x|^{-1} \quad \forall x, y \in \mathbb{Z},\ x \neq y. \tag{6.32}$$

Since we know, that the contracted shift is not essentially local for any $t \in (0,1)$, we learn, that the sufficient condition $\alpha > 1$ we just deduced is actually optimal: polynomial decay of matrix elements with $\alpha > 1$ implies essential locality, but there are unitary operators with matrix elements that decay with $\alpha = 1$ (e.g. the contracted shift), that are not essentially local.

4 Obviously, if the exponent is -1, we recognize the harmonic series, which diverges. Any exponent $a < -1$ leads to convergence, with the value of the series given by $\zeta(-a)$, where ζ is the Riemann zeta function.

If instead of polynomial decay, in (6.28) we demand translation invariance (hence not demanding any decay properties), we get

$$\|PU(1-P)\|_2^2 \leq d \sum_{x>0} |x| \cdot \|U_x\|^2. \tag{6.33}$$

By the same reasoning as above, this expression converges, if the series $\{U_x\}_{x>0}$ is absolutely convergent, i.e. $\sum_{x>0} \|U_x\| < \infty$. But this condition, combined with the similar condition one gets from $\|(1-P)UP\|_2^2$, which demands $\{U_x\}_{x\leq 0}$ to be absolutely convergent, is just stating that U is absolutely summable over $\mathbb{Z}$. This is exactly the case if U_x decays as in (6.23) with $\alpha > 1$ and a suitable $c > 0$:

$$\|U_x\| \leq c|x|^{-\alpha}. \tag{6.34}$$

What we have thus learned is, that polynomial decay as in (6.23) with $\alpha > 1$, i.e. decay stronger than the harmonic series, is sufficient for essential locality of U. In the translation invariant case, we know from this sections' main theorem (Theorem 6.1), that essential locality furthermore implies the continuity of $\widehat{U}$.

With the help of the following Lemma[5], the result from this special case can also be shown directly:

Lemma 6.8
Let $\{U_x\}_{x\in\mathbb{Z}}$ be absolutely summable over $\mathbb{Z}$, i.e.

$$\sum_{x\in\mathbb{Z}} \|U_x\| < \infty. \tag{6.35}$$

Then, $\widehat{U}_n(k)$ converges uniformly to a continuous limit function $\widehat{U}(k)$ as $n \to \infty$, where

$$\widehat{U}_n(k) = \sum_{x=-n}^{n} U_x e^{ikx}. \tag{6.36}$$

Proof. The absolute convergence of $\widehat{U}_n(k)$ implies the existence of $\widehat{U}(k)$ for all $k \in \mathbb{T}$. The convergence is uniform, since (as $n \to \infty$)

$$\left\|\widehat{U}(k) - \widehat{U}_n(k)\right\| = \left\| \sum_{|x|>n} U_x e^{ikx} \right\| \leq \sum_{|x|>n} \|U_x\| \to 0, \tag{6.37}$$

and therefore, by the uniform convergence theorem, a uniformly converging sequence of continuous function has a continuous limit. □

Finishing this application about decay properties of matrix elements and their implications, we look at the decay properties of eigenfunctions at a boundary created by an eigenvalue in a gap - a situation we already know briefly from the bulk-boundary-correspondence in Section 5.3.

5 This Lemma can be considered a suitable reformulation of the Riemann-Lebesgue-Lemma.

6.2 EXPONENTIAL DECAY OF BOUNDARY EIGENFUNCTIONS

Before we return to the setting and corresponding restrictions the symmetries impose as described in Chapter 4, we want to prove an important statement that is often assumed, but to our knowledge never proven in this context. This sections' main result is Theorem 6.9, which shows that given $z \in \mathbb{C}$ lying in a spectral gap of a translation invariant quantum walk, any function that fulfils the corresponding eigenvalue equation with z on a half-line decays at least exponentially:

Theorem 6.9 (Exponential decay at the boundary)
Let W be a translation invariant quantum walk with spectral gap at 1, minimal neighbourhood[6] $\mathcal{N}$ and let

$$\widetilde{W}(\lambda) := \sum_{z \in \mathcal{N}} W_z \lambda^{-z}, \tag{6.38}$$

be the λ-weighted sum of the Fourier coefficients W_z s.t. $\widetilde{W}(e^{-ik}) = \widehat{W}(k)$. Furthermore, let $\phi \in \mathcal{H}$ satisfy

$$(W\phi)(x) = \phi(x) \quad \forall x \geq 0. \tag{6.39}$$

Then, there are vectors $\phi_{\lambda,i} \in \mathbb{C}^d$ s.t., for $x \geq 0$,

$$\phi(x) = \sum_{\lambda \in M} \lambda^x \sum_{i=0}^{r_\lambda} x^i \cdot \phi_{\lambda,i}, \tag{6.40}$$

where M is the set of solutions of $\det(\widetilde{W}(\lambda) - \mathbb{1}) = 0$ with $0 < |\lambda| < 1$ and for each λ, r_λ is the algebraic multiplicity of the zero λ.

Note that to improve readability and without loss of generality, we chose the positive half-line and $z = 1$ to state the theorem.

Before we get to the proof, let us connect the result to the bulk-boundary-correspondence from Section 5.3. There, we learned[7] that whenever we join two admissible quantum walks with differing indices, an eigenvalue emerges in the gap as demanded by the conditions of admissibility. Thus after succeeding to prove this section's main result, we learn that the eigenfunction corresponding to the emerged eigenvalue in the gap has to decay exponentially[8]. A visualization of the exponential decay is shown in Section 8.2, as well as in the dynamic web-application [Sta15a], explained in Section 8.3.

In the following, let W, W' be translation invariant quantum walks with interaction lengths L, L' and spectral gaps[9] at 1. We join W, W' such that the resulting walk W'' is a crossover[10] between W' and W,

6 See Definition 3.1.
7 reducing the statement to the case of quantum walks to seamlessly connect to this section's setting
8 There might be some potentially different behaviour close to the cut point that depends on the interaction lengths of the walks on both sides of the cut, i.e. the details how the cut is made.
9 That is, there is an $\epsilon > 0$ s.t. $\forall \omega \in \mathbb{C}$, $\|\omega - 1\| < \epsilon : \omega \notin \sigma(W)$
10 See Section 5.3.

i.e. there is an $a \in \mathbb{Z}$, s.t. $(W''\psi)(x) = (W'\psi)(x)$ for all $x < -2a$, and $(W''\psi)(x) = (W\psi)(x)$ for all $x \geq 0$. Instead of choosing a symmetrical transition area, we shifted it by a to the left, to let the bulk system begin at $x = 0$. This makes the (already complicated) indices a lot better to read.

If now, e.g. due to bulk-boundary-correspondence, there is a new eigenvalue 1 for W'', i.e. an eigenvalue in the gap, the corresponding eigenfunction ϕ necessarily has to fulfil the eigenvalue equation for W on the right-hand-side of the crossover-region,

$$((W - \mathbb{1})\phi)(x) = 0 \quad \forall x > 0, \tag{6.41}$$

because there, W and W'' match. This is a $\mathbb{C}^d$-valued linear recursion relation of finite order. Usually, it *cannot* be solved by trying to invert (6.41) directly, because the non-vanishing, matrix-valued coefficients W_x in this linear system of equations are not invertible (except in the trivial case of only one non-vanishing W_x). But it has high potential to be solved by fixing a suitable (finite) selection of components $\phi(x), \phi(x+1), \ldots, \phi(x+r)$ and iteratively applying the corresponding transfer matrix T to determine all the other components[11].

If the two joined walks are decoupled as described in Section 5.5, we can write them as a direct sum of two half-space walks. Then, we can solve each side of the boundary independently, since we can decompose every eigenfunction into a left-eigenfunction and a right-eigenfunction. In this case, the transfer matrix approach is particularly promising, since a selection of components starting from the cut point needs to be propagated by the transfer matrix only in one direction.

Still, even a decoupled walk is no guarantee for the transfer matrix approach to work. If we look at a walk, which in a suitable basis $\{|\alpha_1\rangle, \ldots, |\alpha_d\rangle\}$ for $\mathbb{C}^d$ leaves one $|\alpha_i\rangle$ invariant, translation invariance implies

$$W|x, \alpha_i\rangle = |x, \alpha_i\rangle \quad \forall x \in \mathbb{Z}, \tag{6.42}$$

and thus any coefficient of $|x, \alpha_i\rangle$ is ignored by the transfer matrix equations. But this in turn forbids any prediction of decay that holds for all coefficients, at least as long as these $|x, \alpha_i\rangle$ contribute to the wanted eigenvector.

Luckily, the case of an invariant $|\alpha_i\rangle$ is excluded by our second constraint, namely the spectral gap of W at 1: assume there is an $|\alpha_i\rangle$ invariant under W. Then, we can define

$$|\phi'\rangle = \frac{1}{\pi} \sum_{x \in \mathbb{Z}} \frac{1}{x + \frac{1}{2}} |x, \alpha_i\rangle, \tag{6.43}$$

which is a normalized eigenvector to W (on the whole line!) corresponding to eigenvalue 1. This violates the gap condition and therefore indicates that walks of these kind were excluded from our setting by the constraints given in the beginning.

11 See e.g. [Wer13, §5.6] for an example of a transfer matrix in a quantum walk scenario.

To prepare the proof of the theorem, let us analyse what a *purely* exponential ansatz for ϕ within the given setting would yield:

Firstly, ϕ has to fulfil the eigenvalue-equation (6.41) for W on the right half-line. Secondly, ϕ has to decay exponentially, i.e. there is a $0 < |\lambda| < 1$ and $\phi_0 \in \mathbb{C}^d$ s.t.

$$\phi(x) = \lambda^x \phi_0 \quad \forall x \geq 0. \tag{6.44}$$

Thirdly, since W is translation-invariant, (3.29) holds

$$(W\psi)(x) = \sum_{z\in\mathbb{Z}} W_{x-z}\psi(z). \tag{6.45}$$

Using the exponential ansatz, the eigenvalue equation

$$(W\phi)(x) = \phi(x) \tag{6.46}$$

becomes

$$\sum_{z\in\mathbb{Z}} W_{x-z}\, \lambda^{-(x-z)}\phi_0 = \phi_0. \tag{6.47}$$

Since W is a quantum walk, there are only finitely many W_z non-vanishing. Let $\mathcal{N} \subset \mathbb{Z}$ denote the minimal finite neighbourhood and introduce

$$\widetilde{W}(\lambda) = \sum_{z\in\mathcal{N}} W_z \lambda^{-z}, \tag{6.48}$$

to write the eigenvalue equation as

$$\widetilde{W}(\lambda)\phi_0 = \phi_0. \tag{6.49}$$

From (3.31) we know, that the Fourier transform $\widehat{W}$ of a translation invariant quantum walk is

$$\widehat{W}(k) = \sum_{x\in\mathcal{N}} W_x e^{ik\cdot x}. \tag{6.50}$$

Furthermore, due to the finite neighbourhood $\mathcal{N}$, $\widehat{W}$ is a Laurent-polynomial in the variable e^{ik}, and hence easily continued analytically from the unit circle to the (punctured) unit disc by replacing the variable with λ restricted as above. Obviously, this is the same as extending the domain of $\widetilde{W}$ from the (punctured) and open unit disc to the (punctured) closed unit disc by noting that

$$\widehat{W}(k) = \widetilde{W}(e^{-ik}). \tag{6.51}$$

We conclude this motivation by observing that for an exponentially decaying solution ϕ as in (6.44) to exist, the corresponding λ has to fulfil

$$\det\left(\widetilde{W}(\lambda) - \mathbb{1}\right) = 0 \tag{6.52}$$

with $0 < |\lambda| < 1$. The finiteness of $\mathcal{N}$ guarantees this to be an algebraic equation for λ, but at this point the main question is still not answered: Given a translation invariant quantum walk W with spectral gap at 1

and a vector ϕ fulfilling the eigenvalue equation for eigenvalue 1 on a half-line, does this necessarily imply that ϕ decays exponentially? Finally proving this sections' theorem answers this in the affirmative:

Proof. The main idea of the proof is to use the steps sketched in the motivation and turn an integration around the unit circle into a sum of residues from the interior of the unit disc by using the Residue Theorem, hence transitioning from $\widehat{W}$ to $\widetilde{W}$.

Since we know that ϕ fulfils the eigenvalue equation on the positive half-space, it is clear that $\psi := (W - \mathbb{1})\phi$ vanishes for $x \geq 0$. Furthermore,

$$\widetilde{\psi}(\lambda) = \sum_{x<0} \psi(x)\lambda^{-x} \tag{6.53}$$

is absolutely convergent and analytic for $|\lambda| < 1$: it is written as a series in x with only positive powers of λ, whose coefficients stem from a bounded function ψ. Therefore, the geometric series of $|\lambda|$, combined with the finite constant $\|\psi\|_\infty$ is a majorant to $\widetilde{\psi}(\lambda)$. Similar to $\widehat{W}$ and $\widetilde{W}$, the boundary value

$$\widetilde{\psi}(e^{-ik}) = \widehat{\psi}(k) \tag{6.54}$$

is the Fourier transform of ψ. With this at hand, we can compute $\phi(x)$.

Let $\chi \in \mathbb{C}^d$ be an arbitrary vector, which is extended to $\delta_x \otimes \chi \in \mathcal{H}$ to represent χ at x and 0 everywhere else. Furthermore, let $x \geq 0$ be any arbitrary position on the positive half-space. Then,

$$\langle \chi | \phi(x) \rangle = \langle \delta_x \otimes \chi | \phi \rangle = \left\langle \delta_x \otimes \chi \,\middle|\, (W - \mathbb{1})^{-1}\psi \right\rangle, \tag{6.55}$$

where in the last step we used that $W - \mathbb{1}$ is invertible, since W is gapped at 1. Applying the Fourier transform to the scalar product leads to

$$\langle \chi | \phi(x) \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}k\, e^{-ikx} \left\langle \chi \,\middle|\, \left(\widehat{W}(k) - \mathbb{1}\right)^{-1} \widehat{\psi}(k) \right\rangle, \tag{6.56}$$

where we used the functional calculus from Theorem 2.9 to transition from $\widehat{W}(k)$ to $(\widehat{W}(k) - \mathbb{1})^{-1}$. Substituting $u = e^{-ik}$, we arrive at a contour integration around the unit circle C

$$\langle \chi | \phi(x) \rangle = \frac{i}{2\pi} \oint_C \mathrm{d}u\, \frac{1}{u} \cdot u^x \left\langle \chi \,\middle|\, \left(\widetilde{W}(u) - \mathbb{1}\right)^{-1} \widetilde{\psi}(u) \right\rangle, \tag{6.57}$$

where we used the fact that at the boundaries, $\widetilde{W}$ and $\widehat{W}$ coincide (and $\widetilde{\psi}$, $\widehat{\psi}$ respectively). We want to apply the Residue Theorem, hence we have to find the singularities of the integrand. Commuting the scalar u^{-1} to the right creates $u^{-1}\widetilde{\psi}(u)$, which is a power series in u that is analytic on the unit disc, thus has no singularities that might contribute residues to the integral. The same argument holds for u^x for all x under consideration.

By (6.48), $\widetilde{W}(u)$ is a Laurent-polynomial in u with $\mathbb{C}^d$-valued coefficients and highest order $n \in \mathbb{N}$. Therefore, $\widetilde{W}(u) - \mathbb{1}$ is a Laurent-polynomial as well with the same highest order n.

Let us assume[12], that $\widetilde{W}(\lambda) - \mathbb{1}$ is invertible for all $|\lambda| < 1$. Then, $\left(\widetilde{W}(\lambda) - \mathbb{1}\right)^{-1}$ exists on the whole unit disc and hence does not contribute singularities to the integral. Then, as a product of analytic functions, the integrand in (6.57) is analytic as well, and so by Cauchy's integral theorem, the integral vanishes. This means, that $\phi(x) = 0$ for all $x \geq 0$, which proves the trivial case of ϕ not being localized on the right at all[13].

In the non-trivial case, let us assume that $\widetilde{W}(\lambda) - \mathbb{1}$ is not invertible for all λ in the unit disk, i.e. there are λ such that $\widetilde{W}(\lambda) - \mathbb{1}$ is a singular operator. These λ are exactly those solutions of

$$\det\left(\widetilde{W}(\lambda) - \mathbb{1}\right) = 0, \tag{6.58}$$

that lie in the unit disk. Let us denote this set of solutions M and let r_λ count the algebraic multiplicity of the zero $\lambda \in M$. Note that r_λ is bounded by $n \cdot d$, since each element of the $d \times d$-matrix $\widetilde{W}(\lambda) - \mathbb{1}$ is a Laurent polynomial of order at most n, hence the highest possible order of each summand in the determinant is $n \cdot d$.

The Residue Theorem allows us to write (6.57) as

$$\langle \chi | \phi(x) \rangle = \frac{1}{2\pi i} \oint_C \mathrm{d}u \, f(u) = \sum_{\lambda \in M} \mathrm{Res}(f, \lambda), \tag{6.59}$$

where

$$f(u) := -u^x \sum_{y \geq 0} u^y \left\langle \chi \middle| \left(\widetilde{W}(u) - \mathbb{1}\right)^{-1} \psi(-y-1) \right\rangle. \tag{6.60}$$

By definition of r_λ, the order of the pole λ of $\left(\widetilde{W}(u) - \mathbb{1}\right)^{-1}$ is r_λ. Since all other factors in $f(u)$ are analytic functions, the order r'_λ of the pole of f at λ is at most r_λ, and for each λ, there is $h_\lambda(u)$ s.t.

$$f(u) = \frac{h_\lambda(u)}{(u-\lambda)^{r'_\lambda}} \quad , \tag{6.61}$$

where h is holomorphic and $h(\lambda) \neq 0$. By Cauchy's differentiation formula, we can then write the Residue as

$$\mathrm{Res}(f, \lambda) = \frac{1}{(r'_\lambda - 1)!} \left[\frac{\mathrm{d}^{r'_\lambda - 1} h_\lambda(u)}{\mathrm{d}u^{r'_\lambda - 1}} \right]_{u=\lambda}. \tag{6.62}$$

It is important to note, that the only x-dependency is rooted in the first factor of f. Therefore, looking at the equation above, there will be a common factor λ^x that remains unchanged, but whose derivatives create a polynomial in x of degree at most $r'_\lambda - 1$. All other factors of f

12 Note that we use the variable λ instead of u to indicate, that we are now solving for the decay coefficient in the unit disk.

13 Due to the specific setting we have in mind, namely a suitable cutting and joining of W and W', a ϕ vanishing on the right is of no interest to us, since it is no candidate for an eigenvector on the right half chain. Still, it is needed to complete the proof of the theorem in this trivial case

contribute an expression depending on λ and ψ, which is independent of x. Hence we can write

$$\phi(x) = \sum_{\lambda \in M} \lambda^x \sum_{i=0}^{r'_\lambda - 1} x^i \cdot \phi_{\lambda,i}, \tag{6.63}$$

proving the theorem. □

This finishes the chapter about the interplay between translation invariance, locality and decay properties. Adding to the applications already mentioned, Chapter 8 motivates most of this chapters' results with detailed examples.

7

SYMMETRY INDEX AND TRANSLATION INVARIANCE

After analysing translation invariant essentially local operators without explicitly demanding symmetries, let us now return to the setting of Chapter 4. As was already suggested in the definition of *bulks* in Definition 5.10, a natural assumption for a bulk system in the theory of topological phases is translation invariance. This provides a significant simplification for almost everything we do, since Fourier methods from Section 3.3, as well as some of the results derived in the previous chapter, allow us to transition to a description in terms of vector bundles over the Brillouin zone.

In Section 7.1, we apply the setting from Chapter 4 to the translation invariant systems. There, we show that we can *flatten* every ρ-admissible translation invariant essentially local unitary operator while keeping all topological properties. Then, Section 7.2 shows exemplary for all symmetry types that include a chiral symmetry γ which squares to $+\mathbb{1}$, that the so called *bulk-invariants* known from the literature can be directly derived from our classification. In Section 7.3, we discuss how translation invariance influences the result from Section 5.6 that showed *completeness* of the symmetry indices in the non-translation invariant setting.

7.1 THE TRANSLATION INVARIANT TEN-FOLD WAY

At a first glance, restricting our classification to the translation invariant case sounds straight forward. We know how translation invariant essentially local operators are defined (Definition 3.5), hence we can determine for every classified operator whether it is translation invariant or not and apply our classification as before. But clearly, there is a decision to be made: given a Hilbert space $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$, we have picked a cell structure. This cell structure is also reflected by the symmetry representation ρ, which we assume to be balanced w.r.t. the $\mathcal{H}_x = \mathbb{C}^d$. Regarding the homotopies, if we allowed this cell structure to change *along the way*, e.g. by *regrouping* neighbouring cells as if putting up domino tiles, or by *adding trivial systems*, we would weaken the equivalence relation by allowing more transformations, leading to a potentially coarser classification.

Therefore we will for the moment *not* allow these changes, but demand the cell structure to be rigid, leading to a potentially *finer* classification of translation invariant operators. Whenever we want to em-

phasize, that we do *not* fix the cell structure, we call the cell structure *flexible*.

The objects to be classified are admissible essentially local (essentially) unitary translation invariant operators, which we call *bulks*, following Definition 5.10. After Fourier transformation, the Hilbert space becomes $\mathcal{H} = \mathcal{L}^2(\mathbb{T}, \mathrm{d}k) \otimes \mathbb{C}^d$ and can be read as the space of $\mathbb{C}^d$-valued square integrable functions $\widehat{\psi}(k)$ on the quasi-momentum space. The Fourier transform of a bulk U then acts by multiplying $\widehat{\psi}(k)$ from the left with $\widehat{U}(k)$, a unitary operator on $\mathbb{C}^d$. While for quantum walks, each entry of $\widehat{U}(k)$ is a Laurent-polynomial in $\exp(ik)$, we have just shown in Theorem 6.1, that essential locality translates exactly to the minimal assumption necessary for e.g. windings to make sense: continuity of $k \mapsto \widehat{U}(k)$ on $\mathbb{T}$, i.e. continuity on the circle, emphasizing the periodic boundary conditions. The fact that every eigenvalue of a translation invariant walk on $\mathcal{H}$ is infinitely degenerate, transforms the essential gap condition to a strict gap condition, hence ± 1 are not in the spectrum of any $\widehat{U}(k)$.

In the next step, we have to determine how the symmetry relations change in the translation invariant setting. One has to be careful, because for A anti-unitary, an A-real basis in position space leads to a flip in the argument, since the Fourier basis element commutes with A up to a sign flip in the exponent $A\exp(ik) = \exp(-ik)A$. We assume, that the symmetry representation is translation invariant as well, that is, $\sigma \in \{\eta, \tau, \gamma\}$ is not only block diagonal w.r.t. the cell structure as already assumed in the definition, but it acts as the same d-dimensional unitary or anti-unitary operator σ_1 in each of the cells:

$$\sigma = \bigoplus_{x\in\mathbb{Z}} \sigma_1 \quad \Rightarrow \quad \widehat{\sigma}(k) = \sigma_1. \tag{7.1}$$

This i.a. prevents making U translation invariant in an artificial way by shifting spatial dependence to ρ.

In the unitary case (i.e. $\sigma = \gamma$), the Fourier transform of γ is hence the multiplication operator γ_1 that commutes with $\widehat{U}$ up to a star, as in position space.

In the anti-unitary case (i.e. $\sigma \in \{\eta, \tau\}$), the sign flip from above occurs as well, and we have[1]

$$\begin{aligned}
\big(\mathcal{F}\sigma U\sigma^*\psi\big)(k) &= \sum_{x,z\in\mathbb{Z}} \sigma_1 U_z \sigma_1^* \psi_{x-z} \\
&= \sum_{x,z\in\mathbb{Z}} \sigma_1 e^{-ikz} U_z \sigma_1^* e^{ik(x-z)} \psi_{x-z} \\
&= \sigma_1 \Big(\sum_{z\in\mathbb{Z}} e^{-ikz} U_z \Big) \sigma_1^* \sum_{y\in\mathbb{Z}} e^{iky} \psi_y \\
&= \sigma_1 \widehat{U}(-k) \sigma_1^* \widehat{\psi}(k).
\end{aligned} \tag{7.2}$$

1 See (3.29) and (3.31) for the definitions of translation invariant operators used.

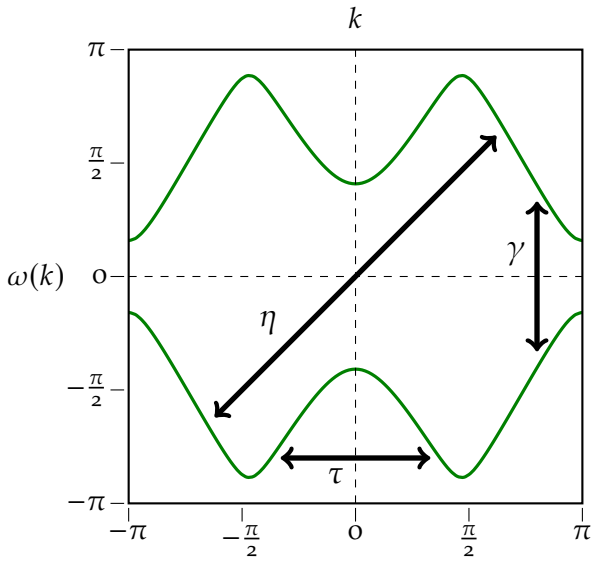


Figure 7: Action of the represented symmetries η, τ and γ on the spectrum $\omega(k)$ of $\widehat{U}(k)$, using (7.5). While γ is an axial symmetry w.r.t. vanishing quasi-energy, i.e. $\omega(k) = -\omega(k)$, τ is an axial symmetry w.r.t. vanishing momentum, i.e. $\omega(k) = \omega(-k)$. Their concatenation η is hence a point-symmetry w.r.t. the origin. This emphasizes why one cannot expect *symmetry protection of the gaps* from a symmetry type that has neither γ nor η but only τ.

This allows us to write down the symmetry conditions in momentum space (see Section 4.2). Note that from now on, we drop the index 1 indicating the action on a single cell, since it will be clear from the context whether σ or σ_1 was meant.

$$\eta\widehat{U}(k) = \widehat{U}(-k)\eta, \quad \tau\widehat{U}(k) = \widehat{U}(-k)^*\tau, \quad \gamma\widehat{U}(k) = \widehat{U}(k)^*\gamma. \tag{7.3}$$

The computation (7.2) translates directly to the Hamiltonian case as well. Let H be a translation invariant Hamiltonian, that is

$$\widehat{H}(k) = \sum_{x\in\mathbb{Z}} e^{ikx} H_x, \tag{7.4}$$

where H_x=H_x^*, and the H_x fulfil the same admissibility conditions w.r.t. the single-cell symmetries as H w.r.t. the symmetries on $\mathcal{H}$ from Section 4.2. Thus, we have

$$\begin{aligned}
\tau\widehat{H}(k) &= \tau \sum_{x\in\mathbb{Z}} e^{ikx} H_x = \sum_{x\in\mathbb{Z}} e^{-ikx} H_x \tau = \widehat{H}(-k)\tau \\
\gamma\widehat{H}(k) &= \gamma \sum_{x\in\mathbb{Z}} e^{ikx} H_x = -\sum_{x\in\mathbb{Z}} e^{ikx} H_x \gamma = -\widehat{H}(k)\gamma \\
\eta\widehat{H}(k) &= \gamma\tau^*\widehat{H}(k) = -\widehat{H}(-k)\eta.
\end{aligned} \tag{7.5}$$

This is noteworthy, since it shows how η, γ and τ act on the spectrum $\omega(k)$ of $\widehat{U}(k)$, see Figure 7.

As e.g. the RAGE-theorem (Theorem 2.10) or the index ind in the translation invariant case (3.13) shows, there are many properties of

quantum walks or bulks that directly depend on the eigenvalues of $\widehat{U}(k)$ as a function of k or on the presence / absence of specific parts of the spectrum. However, for the topological classification, spectral information - besides the gap condition and the symmetry w.r.t. the real axis - are completely irrelevant. As the following lemma shows, for every bulk, we find a homotopic one that has *flat bands*. That is, it squares to $-\mathbb{1}$ and the homotopy invariants have the same values. Moreover, the object that determines the index values is the band projection corresponding to the whole upper half-plane alone - not even the splitting into individual bands matters:

Lemma 7.1 (Flattening bands)
Let U be a bulk for a symmetry representation ρ with $\widehat{U}(k)$ diagonalized as in (3.32):

$$\widehat{U}(k) = \sum_{\alpha=1}^{d} e^{i\omega_\alpha(k)} Q_\alpha(k). \tag{7.6}$$

Furthermore, let $A = \{\alpha \mid \omega_\alpha(k) \in (0, \pi)\}$ s.t.

$$Q(k) = \sum_{\alpha \in A} Q_\alpha(k) \tag{7.7}$$

denotes the band projection for the upper half-plane. Then, within the set of bulks, there is a gentle perturbation U_t s.t. $U_0 = U$ and

$$\widehat{U}_\flat(k) := \widehat{U}_1(k) = iQ(k) - i\big(\mathbb{1} - Q(k)\big) = 2iQ(k) - i\mathbb{1}, \tag{7.8}$$

which is hence called U in **flat-band form**.
The symmetry conditions for $\widehat{U}_\flat(k)$ can then be phrased in terms of $Q(k)$:

$$\begin{aligned} \eta Q(k) \eta^* &= \mathbb{1} - Q(-k) \\ \tau Q(k) \tau^* &= Q(-k) \\ \gamma Q(k) \gamma^* &= \mathbb{1} - Q(k). \end{aligned} \tag{7.9}$$

Proof. The splitting in this way is well-defined, since U is gapped. Therefore, there is an $\epsilon > 0$ s.t. $\mathbb{T}_\epsilon$, the unit-circle without an open disc of radius ϵ around each of $+1$ and -1, contains $\sigma(U)$. Since the continuous functional calculus preserves essential locality, contracting the spectrum of $\widehat{U}(k)$ to $\pm i$ does not violate gentleness.

Let $f : [0,1] \times \mathbb{T}_\epsilon \to \mathbb{T}_\epsilon$, written as $f_t(z) := f(t,z)$, be a suitable continuous function, s.t. $f_0(z) = z$ and $f_1(z) = \operatorname{sign}\big(\operatorname{Im} z\big) i$. Besides the gap, the admissibility constraint is fulfilled if f_t has only real coefficients, or more precisely $f_t(\overline{z}) = \overline{f_t(z)}$.

Then, we define $U_t = f_t(U)$ in the continuous functional calculus, which yields in momentum space

$$\widehat{U}_t(k) = f_t\big(\widehat{U}(k)\big) = \sum_{\alpha=1}^{d} f_t\big(e^{i\omega_\alpha(k)}\big) Q_\alpha(k). \tag{7.10}$$

The symmetry conditions for $Q(k)$ now follow directly by applying (7.3) to the definition of $\widehat{U}_\flat(k)$. □

We have thus shown, that the topological classification of $\widehat{U}(k)$ depends crucially on the band projection $Q(k)$ as a function of k, not on the spectrum, or the individual band projections $Q_\alpha(k)$. Described in terms of differential geometry, we are classifying the Hermitian vector bundle $Q(k)$ over the unit circle $\mathbb{T}$ with fiber $Q(k)\mathbb{C}^d$. This view is supported e.g. by [Kit09], where the classification of symmetric Hamiltonians in terms of K-Theory leads to the same index groups $\mathbf{I}(\mathsf{S})$ that we have derived.

Denote by $\mathbf{I}_{\mathrm{ti}}(\mathsf{S})$ the symmetry groups that [Kit09] deduced with his classification of vector bundles using K-Theory. Compared to our results $\mathbf{I}(\mathsf{S})$, one sees that the resulting groups are isomorphic for each symmetry type S. In the following, let us analyse the connection between both groups more thoroughly:

Every bulk U by definition is suitable for classification through our theory. Hence, there is an index $\vec{\mathrm{si}}(U) \in \mathbf{I}(\mathsf{S})$ that is stable under gentle perturbations within the general setting, thus it is also stable under every gentle perturbation within the restricted translation invariant setting. In short, there is a map $j : \mathbf{I}_{\mathrm{ti}}(\mathsf{S}) \to \mathbf{I}(\mathsf{S})$.

By definition, addition in $\mathbf{I}_{\mathrm{ti}}(\mathsf{S})$ and $\mathbf{I}(\mathsf{S})$ is defined via direct sums, hence j is a homomorphism for addition. To show that j is surjective, we have to provide for each S a *translation invariant* example s.t. $\vec{\mathrm{si}}(U)$ spans $\mathbf{I}(\mathsf{S})$. This is done in Section 8.1. Regarding injectivity, despite the completeness of our classification (see Section 5.6), it could be that two translation invariant bulks with the same set of indices can only be connected to each other by breaking translation invariance *along the way*. Then, these would correspond to different elements in $\mathbf{I}_{\mathrm{ti}}(\mathsf{S})$ which would render j not one-to-one. We will analyse this later in Section 7.3 and show that for some symmetry types, there are additional invariants to consider, at least in the setting of *rigid cell structures*.

In the introduction to this section, we have briefly discussed the (possible) dependence of the classification on the cell structure. In the general theory, the dimension of the local Hilbert spaces $\mathcal{H}_x$ does not matter. Thus, the classification does not change if we combine neighbouring cells arbitrarily and declare the resulting cell structure as the new one[2]. In this chapter, we demand translation invariance w.r.t. a rigid cell structure. This is a tight restriction to the setting, which i.a. fixes the dimension of every $\mathcal{H}_x$ to be the same for all x. Thus, a reorganization of the cells in the way just described is clearly forbidden.

One kind of *regrouping* that is often used in the context of the index ind of a quantum walk [Gro+12] is the *flattening* of the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ onto $\mathcal{H}' = \ell^2(\mathbb{Z})$ by mapping $\delta_x \otimes \alpha_i$ to $\delta_{d\cdot x+i}$, effectively dropping the cell structure completely. Since shifts by one cell

2 More precisely, we assume that we have fixed a representation ρ of the symmetry type before we make these changes. Else, the condition of balanced cells is weakened by combining cells, which would make a difference.

on $\mathcal{H}$ become shifts by d cells on $\mathcal{H}'$, the scale of position has to be adjusted by a factor d. But besides this scaling factor, the index ind and e.g. jump lengths of quantum walks do not change under this mapping.

In the other direction, since quantum walks possess a finite jump length L, it makes sense to consider so called *nearest neighbour quantum walks*, which are walks where the underlying Hilbert space is mapped to one, where at least L neighbouring cells are put together and considered as one. This procedure brings every quantum walk into a standard form with a (potentially much) larger coin space such that it acts only on directly adjacent cells.

In our current setting of bulks with rigid cell structure, there is (in general) no finite maximal jump length L, and hence such a regrouping does not make sense. But as we will see later when considering completeness of the symmetry indices in this setting, the minimal version of this regrouping, regrouping direct neighbours in pairs of two, already changes the classification. Therefore, let us explicitly write down the effect of regrouping neighbouring cells in the sense that we consider $\mathcal{H}'_x = \mathcal{H}_{2x} \oplus \mathcal{H}_{2x+1}$ as our new cell[3]. Most importantly, this changes the notion of translation invariance: translations on the new cell structure correspond to translations by an *even* number of sites on the old cell structure. More precisely, if we allow for regrouping once, and then demand only translation invariance in the regrouped setting along the way, formerly disconnected regions might connect. That is, two bulks U and U' might not be translation invariant gentle perturbations of each other if we demand translation invariance in the rigid setting, but their regrouped versions U_r and U'_r might be in the new setting. Therefore, regrouping once *along the way* bridges the regions of U and U' within this coarser class.

Definition 7.2 (Regrouping)
Let U be a bulk on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ with Fourier transform $\widehat{U}(k)$. Then, we define the **regrouped** *bulks $\widehat{U}_r$ on $\mathcal{H}_r = \mathcal{L}^2(\mathbb{T}) \otimes \mathbb{C}^{2d} \cong \ell^2(\mathbb{Z}) \otimes \mathbb{C}^{2d}$ as*

$$\widehat{U}_r(k) := H(k/2) \begin{pmatrix} \widehat{U}(k/2) & 0 \\ 0 & \widehat{U}(k/2 + \pi) \end{pmatrix} H(k/2)^*, \tag{7.11}$$

where

$$H(k) := \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ e^{-ik}\mathbb{1} & -e^{-ik}\mathbb{1} \end{pmatrix}. \tag{7.12}$$

3 As an analogy, regard $\mathcal{H}_{2x}$ and $\mathcal{H}_{2x+1}$ as one domino tile within the infinite chain of domino tiles that is $\mathcal{H}$. Now, if we put up all these domino tiles, the standing tiles became the new basic cells, and we performed the *regrouping* just described.

Let us quickly show that this definition represents exactly what we described before. In position space, $\psi \in \mathcal{H}$ is mapped to $\psi_r \in \ell^2(\mathbb{Z}) \otimes \mathbb{C}^{2d}$, which has an even part ψ_e, and an odd part ψ_o, s.t.

$$\psi_r(x) = \begin{pmatrix} \psi_e(x) \\ \psi_o(x) \end{pmatrix} = \begin{pmatrix} \psi(2x) \\ \psi(2x+1) \end{pmatrix}. \tag{7.13}$$

The action of U_r on ψ_r as a convolution in position space is then completely determined by the action of U on ψ. Therefore let

$$(U_r\psi_r)(x) := \sum_{z\in\mathbb{Z}} U^r_{x-z}\psi_r(z) = \sum_{z\in\mathbb{Z}} U^r_{x-z} \begin{pmatrix} \psi(2z) \\ \psi(2z+1) \end{pmatrix}. \tag{7.14}$$

Using (3.29), we can read off

$$\begin{aligned} \big(U\psi\big)(2x) &= \sum_{z\in\mathbb{Z}} U_{2x-z}\psi(z) \\ \big(U\psi\big)(2x+1) &= \sum_{z\in\mathbb{Z}} U_{2x+1-z}\psi(z). \end{aligned} \tag{7.15}$$

Equating this with (7.13) and splitting the sum into even and odd contributions, the following convolution kernel results

$$U^r_x = \begin{pmatrix} U_{2x} & U_{2x-1} \\ U_{2x+1} & U_{2x} \end{pmatrix}. \tag{7.16}$$

Applying the Fourier transform to the coefficients then yields

$$\begin{aligned} &\sum_{x\in\mathbb{Z}} e^{ikx} U_{2x+s} \\ &= e^{-i\frac{k}{2}\cdot s} \sum_{x\in\mathbb{Z}} e^{i\frac{k}{2}(2x+s)} U_{2x+s} \\ &= e^{-i\frac{k}{2}\cdot s} \begin{cases} \widehat{U}_e(k/2) & s \text{ even}, \\ \widehat{U}_o(k/2) & s \text{ odd}. \end{cases} \end{aligned} \tag{7.17}$$

Here, $\widehat{U}_e$ and $\widehat{U}_o$ are the restrictions of $\widehat{U}$ to even and odd coefficients, respectively. Since $-1 = e^{i\pi} = e^{i\pi y}$ for y odd, and $1 = e^{i\pi y}$ for y even, we have

$$\begin{aligned} \widehat{U}\big(k/2 + \pi\big) = \widehat{U}_e\big(k/2 + \pi\big) + \widehat{U}_o\big(k/2 + \pi\big) &= \widehat{U}_e\big(k/2\big) - \widehat{U}_o\big(k/2\big) \\ \widehat{U}\big(k/2\big) = \widehat{U}_e\big(k/2\big) + \widehat{U}_o\big(k/2\big). \end{aligned} \tag{7.18}$$

Putting it all together, we get

$$\begin{aligned} \widehat{U}_r(k) &= \begin{pmatrix} \widehat{U}_e(k/2) & e^{ik/2}\widehat{U}_o(k/2) \\ e^{-ik/2}\widehat{U}_o(k/2) & \widehat{U}_e(k/2) \end{pmatrix} \\ &= H(k/2) \begin{pmatrix} \widehat{U}(k/2) & 0 \\ 0 & \widehat{U}(k/2+\pi) \end{pmatrix} H(k/2)^*, \end{aligned} \tag{7.19}$$

which is the form from Definition 7.2.

In the next section, we will introduce a standard form for bulks for the non-trivial symmetry types where a chiral symmetry is present that squares to $\mathbb{1}$: AIII, BDI and CII.

7.2 WINDING FORMULA FOR CHIRAL SYMMETRIES

In Section 3.4, we learned that the index of an essentially local unitary operator $\mathrm{ind}(U)$ can be determined by computing the kernel of the compression of U and U^* to $P\mathcal{H}$. Alternatively, in the case of a *translation invariant* essentially local unitary operator, after computing the Fourier transform of U, it suffices to read-off the index from the exponent of $\det \widehat{U}(k)$. Moreover, given the eigenvalues $\omega_\alpha(k)$, the index agrees with the sum of their winding numbers, providing another way of computing $\mathrm{ind}(U)$, as well as a topological interpretation. A side effect is, that in the translation invariant case, it allows us to determine the index $\mathrm{ind}(U)$ much simpler than following the standard procedure.

In the general case of an essentially local admissible unitary operator U, determining e.g. the symmetry index $\vec{\mathrm{si}}(U)$ amounts to computing $\mathrm{si}(\mathrm{Im}(PUP))$, which involves determining the kernel of $\mathrm{Im}(PUP)$ and then applying the correct formula from Proposition 5.3 restricted to this subspace.

Since in the definition of bulks, we emphasize translation invariant operators, it is advantageous to find ways to determine symmetry indices in a more practical way. Luckily, there is an approach we call the *chiral reduction*, that yields a simple formula for $\vec{\mathrm{si}}$ for every symmetry type that fulfils[4] $\gamma^2 = +\mathbb{1}$. Note that we will work within the general picture as long as possible and introduce translation invariance as late as possible. The main result of this section is the explicit translation invariant formula for $\vec{\mathrm{si}}$ in the case of non-trivial chiral symmetry:

Theorem 7.3 (Chiral index formula: TI)
Let ρ be a representation of one of the symmetry types AIII, BDI *or* CII *and let U be a bulk in chiral block form (Definition 7.4) with $\widehat{B}(k)$ as in (7.31). Then,*

$$\vec{\mathrm{si}}(U) = \mathrm{wind}(k \mapsto \det \widehat{B}(k)). \tag{7.20}$$

Furthermore, if $\widehat{U}(k)$ is continuously differentiable, we have

$$\vec{\mathrm{si}}(U) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \ \mathrm{tr}\left(\widehat{B}^*(k) \frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k}\right). \tag{7.21}$$

A visualization of the winding of the curve $\det \widehat{B}(k)$ is given in Section 8.3. The interactive *Split-Step-Explorer* shows the winding, as well as the quasi-energies and corresponding edge-states together with a brief explanation on the corresponding webpage [Sta15a].

4 Actually, most of the arguments also work for the single symmetry type, where there is a chiral symmetry, which squares to -1, i.e. DIII. But since the resulting formulas and their proofs deviate considerably, we will not cover this case, but refer to [Ced+18a] for the treatment of DIII.

In order to prove this theorem, we have to introduce the foreshadowed *chiral block form* via chiral reduction. After that, we will analyse statements of completeness for the different symmetry types where this theorem holds.

Chiral reduction

For the rest of this chapter, ρ represents any of the symmetry types AIII, BDI and CII with $\gamma^2 = \mathbb{1}$. This allows to use P_+, the projection onto the $+1$-eigenspace of $\gamma = 2P_+ - \mathbb{1}$, to bring every admissible ELEU U to block matrix form w.r.t. P_+ and $P_- = \mathbb{1} - P_+$ and the respective subspaces $\mathcal{H}_\pm = P_\pm \mathcal{H}$. Thus for the moment, we return to the general setting that does not demand translation invariance.

Definition 7.4 (Chiral block form)
Let ρ be a representation for AIII, BDI *or* CII *with $\gamma = P_+ - P_-$ on $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, s.t. $\dim(\mathcal{H}_+) = \dim(\mathcal{H}_-)$. Furthermore, let U be an ELEU on $\mathcal{H}$. With respect to P_+ and P_-, we can write U in* **chiral block form**, *s.t.*

$$U = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \text{and} \quad \gamma = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}. \tag{7.22}$$

Since ρ-admissibility in these cases reduces to $\gamma U = U^* \gamma$ (besides the essential gap condition), the additional conditions for U can easily be deduced.

Lemma 7.5 (Chiral block form: ELEU)
Let U be an ELEU in chiral block form that fulfils the commutation relation with γ. Then, $A = A^*$, $D = D^*$ and $C = -B^*$. Furthermore, U is essentially gapped iff B is Fredholm.

That is, the lemma collects the algebraic properties of a ρ-admissible ELEU U. Let us continue with the case that U is exactly unitary, not merely *essentially* unitary, before proving both lemmas together.

Lemma 7.6 (Chiral block form: unitary)
Let U be an essentially local unitary operator in chiral block form that fulfils the commutation relation with γ. Then,

(0) $BB^* + A^2 = \mathbb{1}, \qquad B^*B + D^2 = \mathbb{1}, \qquad AB = BD$

(1) *U is gapped at $+1$ and -1 iff B has a bounded inverse.*

(2) *U is in* flat-band form *iff B is unitary and $A = D = 0$.*

Proof. The algebraic relations for the ELEU follow directly from the definition of the *chiral block form* and the admissibility relation. (0) are precisely the unitarity conditions for U in chiral block form. Note that for U merely essentially unitary, (0) holds after projecting into the Calkin algebra, hence holds *essentially*.

To prove (1) (⇒), let U be properly gapped at ±1. Then, the imaginary part of U

$$\operatorname{Im} U = \frac{1}{2i}(U - U^*) = \begin{pmatrix} 0 & -iB \\ iB^* & 0 \end{pmatrix} \tag{7.23}$$

has a proper gap at 0, and is hence invertible. This is exactly the case if B has a bounded inverse. For the converse (⇐), let B be invertible. Then, $\operatorname{Im} U$ is invertible and therefore properly gapped at 0, implying a properly gapped U at ±1, proving (1).

This already proves Lemma 7.5 through demanding (1) to hold only for $\pi(U)$ instead of U. That is, for the image of U in the Calkin algebra, the gap becomes an essential gap and the invertibility of B becomes *invertibility up to a compact operator*, which is the definition of a Fredholm operator.

In order to prove (2), recall that a flat-band unitary U fulfils $U^2 = -\mathbb{1}$ as in Lemma 7.1. Then, (⇒) follows by using the unitarity of U to write $U = -U^*$ and reading off the relations. (⇐) follows directly from the unitarity of B and the computation of U^2. □

In the translation invariant case, we know from Lemma 7.1 that the topological classification of U is the same as the classification of $U_\flat$, since they are homotopic even within the set of bulks. This result will be crucial in discussing the completeness of our classification of bulks, e.g. in Proposition 7.10 for AIII. These two lemmas have thus shown, that the *chiral block form* of U effectively reduces the classification of admissible unitary operators U to the classification of unitary operators B. More precisely, since the flat-band condition guarantees a proper gap for U, there is no (essential) gap condition for B, and the admissibility for γ is covered completely. That is, in the case of AIII, there are no other symmetries and hence no further restrictions for B. In the cases BDI and CII, there are additional constraints stemming from the admissibility for η. Then, the admissibility for τ follows from our choice that all the represented symmetries commute with each other.

Let us now check which conditions are imposed on B stemming from a flat-band $U_\flat$ due to the presence of η. Since the construction around (2.30) shows that η takes block diagonal form with identical blocks (after choosing a suitable basis in the second block), we can write

$$\eta = \begin{pmatrix} \eta_b & 0 \\ 0 & \eta_b \end{pmatrix}, \qquad \begin{aligned} \text{BDI}: \ \eta_b^2 &= +\mathbb{1} \\ \text{CII}: \ \eta_b^2 &= -\mathbb{1}. \end{aligned} \tag{7.24}$$

η-admissibility of U then demands $\eta_b B = B\eta_b$. The question at hand is now: Did the chiral block form reveal that BDI and CII can after all be reduced to D and C, respectively, contradicting completeness of the index and our index construction in general?

Luckily this is not the case. The substantial condition we overlooked is the *essential gap*: classifying B with corresponding symmetry rela-

tions for η is *not* the same as classifying *admissible* essentially unitary operators B of symmetry type D or C, since *admissibility* demands an essential gap. Hence without this condition, more paths are allowed which connect different subsets, rendering their index identical[5].

Index formulas

In the following, we investigate how the *chiral block form* simplifies the computation of $\mathrm{si}(U)$ (and hence $\vec{\mathrm{si}}(U)$ etc.).

Lemma 7.7 (Chiral block form: si)
Let ρ represent AIII, BDI *or* CII, *and let U be a ρ-admissible essentially local unitary operator in chiral block form. Then, the symmetry index can be expressed as a Fredholm index*

$$\mathrm{si}(U) = -\operatorname{ind}_{\mathrm{F}}(B). \tag{7.25}$$

It is interesting to note that for chiral symmetries squaring to $+\mathbb{1}$, this expression reduces si to a Fredholm index of the matrix block B, which represents that part of γ, which maps positive to negative chirality. This resembles the definition of ind, which uses a block from the block-decomposition with respect to a projection onto the half-line of positive positions.

Proof. As was shown in (7.5) and (7.23), the imaginary part of U is

$$\operatorname{Im} U = \begin{pmatrix} 0 & -iB \\ iB^* & 0 \end{pmatrix}. \tag{7.26}$$

Using Definition 5.7 and Proposition 5.3, we know that B is Fredholm and $\mathrm{si}(U) = \operatorname{tr}_{\mathcal{N}} \gamma$, where $\mathcal{N} = \ker(\operatorname{Im} U) = \ker(U - U^*)$. The simple form of $\operatorname{Im} U$ allows to read off the kernel as

$$\mathcal{N} = \left\{ \phi_1 \oplus \phi_2 \,\middle|\, B^*\phi_1 = 0 \wedge B\phi_2 = 0 \right\} = \ker(B^*) \oplus \ker(B). \tag{7.27}$$

But since this decomposition is in the same basis as the chiral block form, we know that γ acts like σ_3 on $\phi_1 \oplus \phi_2$ and hence

$$\mathrm{si}(U) = \operatorname{tr}_{\mathcal{N}} \gamma = \dim\ker(B^*) - \dim\ker(B) = -\operatorname{ind}_{\mathrm{F}}(B). \tag{7.28}$$

□

We know from Table 1 and Section 4.4 that in the case of CII, $\mathrm{si}(U)$ must be an even integer. This is now easily confirmed, since the restricted η_b-symmetry for B with $\eta_b^2 = -\mathbb{1}$ forces $\ker(B)$ and $\ker(B^*)$ to be of even dimension, respectively. To see this, let ϕ lie in the kernel of B. Then, the admissibility implies

$$\eta_b B\phi = B(\eta_b \phi) = 0. \tag{7.29}$$

5 This is very similar to the forget homomorphisms from Section 4.4. There, not knowing about a symmetry (or *forgetting* about its existence) allows for transformations that connect formerly different classes, thus reducing the number of equivalence classes.

But since $\eta_b^2 = -\mathbb{1}$, we have

$$\langle \phi, \eta_b \phi \rangle = \overline{\langle \eta_b \phi, \eta_b^2 \phi \rangle} = -\langle \phi, \eta_b \phi \rangle = 0. \tag{7.30}$$

Thus, $\eta_b \phi$ is an independent eigenvector and the kernel is even dimensional. The argument for $\ker(B^*)$ is completely analogous.

We have already commented on the similarity between the definition of the index $\mathrm{ind}(U)$ and the value of $\mathrm{si}(U)$ if U is in chiral block form. In the following, we will return to the translation invariant case and extend this similarity to deduce a representation of $\mathrm{si}(U)$ as a *winding number* in much the same way as $\mathrm{ind}(U)$ can be written as a winding of the eigenvalues $\omega_\alpha(k)$ as remarked after (3.48).

In the very beginning, we assumed that every symmetry considered is compatible with the cell structure, i.e. they act on translation invariant operators through the one-cell symmetries as described in (7.3). Moreover, we can use the chiral block form of Definition 7.4 to split the d-dimensional coin-space further into two subspaces of dimension $d' = {}^{d}/_{2}$, such that after Fourier transform, $\widehat{U}(k)$ is in *chiral block form*:

$$\widehat{U}(k) = \begin{pmatrix} \widehat{A}(k) & \widehat{B}(k) \\ -\widehat{B}^*(k) & \widehat{D}(k) \end{pmatrix}. \tag{7.31}$$

The admissibility of a translation invariant U demands a gap at ± 1, s.t. by Lemma 7.6, B is invertible, and hence $\widehat{B}(k)$ is invertible for all k as well. Moreover, the essential locality of U is equivalent to continuity of $\widehat{U}(k)$ for all $k \in \mathbb{T}$ (with periodic boundary conditions) by Theorem 6.1, which makes $\widehat{B}(k)$ depend continuously on k as well. This is exactly the minimal condition one needs for a winding number to make sense. Let $f : [-\pi, \pi] \to \mathbb{C}$ be a continuous function that never vanishes. Then, $\mathrm{wind}(f)$ denotes the *winding number* of f around the origin. The following result from [AS01, Thm. 7] connects the Fredholm index to a winding number:

Theorem 7.8 ($\mathrm{ind}_{\mathrm{F}}$ as winding)
Let T_f be a continuously differentiable Toeplitz operator. Then, T_f is Fredholm iff its symbol f is non-zero on the whole unit circle. In that case, the Fredholm index is minus the winding number of f around the origin, namely

$$\mathrm{ind}_{\mathrm{F}}(T_f) = -\mathrm{wind}(f) = \frac{-1}{2\pi i} \int_{\mathbb{T}} \frac{\mathrm{d}f}{f}. \tag{7.32}$$

In order to proof our statement in full generality, we need a more general form of this statement. A version of the theorem for matrix-valued f' is e.g. provided by [Pel03, Thm. 4.8], which amounts to replacing f in the above theorem with f', and with $\det(f')$ in the denominator of the integrand. The full form is found in [GGK90, XXXII.5: Thm. 5.1], where the assumption of continuous differentiability is weakened to demand mere continuity, and which treats matrices as well.

This allows us to prove Theorem 7.3 and hence finally express $\vec{\mathrm{si}}$ as a winding number.

Proof of Theorem 7.3. By Definition 5.8, we know that $\vec{\mathrm{si}}(U) = \mathrm{si}(PUP)$. Since U is a bulk in chiral block form, we can apply Lemma 7.7 to PUP, which is an ELEU on the half-space $P\mathcal{H}$, and get

$$\vec{\mathrm{si}}(U) = -\operatorname{ind}_{\mathrm{F}}(PBP). \tag{7.33}$$

By Definition 6.4, the half-space compression of a translation invariant operator yields a Toeplitz operator with *symbol* $\widehat{B}(k)$. Since U is gapped, B is invertible due to Lemma 7.6. Therefore, $\widehat{B}(k)$ never vanishes and we can apply Theorem 7.8 to get

$$\vec{\mathrm{si}}(U) = \operatorname{wind}(k \mapsto \det \widehat{B}(k)), \tag{7.34}$$

finishing the first part of the proof.

In order to prove the additional formula, let $\widehat{U}(k)$ be continuously differentiable. Then, $f(k) = \det \widehat{B}(k)$ is continuously differentiable as well and we can write the winding as in (7.32):

$$\begin{aligned} 2\pi i \operatorname{wind}(f) &= \int_{-\pi}^{\pi} \mathrm{d}k \, \frac{f'(k)}{f(k)} = \int_{-\pi}^{\pi} \mathrm{d}k \, \frac{\mathrm{d}}{\mathrm{d}k} \log \det \widehat{B}(k) \\ &= \int_{-\pi}^{\pi} \mathrm{d}k \, \operatorname{tr}\left(\widehat{B}^{-1}(k) \frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k} \right), \end{aligned} \tag{7.35}$$

where in the last step we used the derivative of the determinant from Lemma 3.7. Using the unitarity of $\widehat{B}(k)$ then leads to the final result

$$\vec{\mathrm{si}}(U) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \, \operatorname{tr}\left(\widehat{B}^{*}(k) \frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k} \right). \tag{7.36}$$

□

It was mentioned in the introduction, that e.g. in the quantum hall effect, the classifying topological invariant can be expressed as the total Chern number of the quasi-energy bands, computed e.g. via an integral over the quasi-momentum space.

Since we are rooted in one spatial dimension, the best candidate for a geometrical expression of our symmetry index is the Berry phase (or first Chern number), introduced in [Ber84] (for a more recent review, see [XCN10]). There, Berry shows that a continuous transformation of the Hamiltonian can lead to an eigenstate acquiring a phase-difference. If the transforming path is a loop, this phase-difference β_α is shown to be a homotopy-invariant that takes values in the integers (up to 2π), that can be expressed as an integral over the Berry connection

$$\beta_\alpha = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \, \left\langle \phi_\alpha(k), \frac{\mathrm{d}}{\mathrm{d}k} \phi_\alpha(k) \right\rangle, \tag{7.37}$$

where $\phi_\alpha(k)$ represents the eigenstate which changes differentiably while the time evolution changes continuously from $k = -\pi$ to π, which is a loop in the Brillouin zone.

Applied to our situation, this leads to the following definition of the total Berry phase β, acquired by summing over all eigenfunctions of a d-dimensional matrix-valued function:

$$\beta = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \sum_{\alpha=1}^{d} \left\langle \phi_\alpha(k), \frac{\mathrm{d}}{\mathrm{d}k} \phi_\alpha(k) \right\rangle . \tag{7.38}$$

Returning to our symmetry index, we show that $\vec{\mathrm{si}}(U)$ can be expressed as twice the Berry phase of the upper band, if $\widehat{U}(k)$ is continuously differentiable and *flat-band*:

Corollary 7.9 ($\vec{\mathrm{si}}$ as Berry phase)
Let $U = U_\flat$ be a flat-band bulk for symmetry type AIII, BDI *or* CII. *Then, for all $\alpha = 1, \ldots, d'$, there is a continuously differentiable eigenfunction of U to the eigenvalue i, denoted by $\phi_\alpha(k)$, that spans the projection $Q_\alpha(k)$ s.t. together, they sum up to the upper band projection $Q(k)$ as defined in Lemma 7.1.*
In this case, $\vec{\mathrm{si}}(U)$ is twice the Berry phase for the upper band, i.e.

$$\vec{\mathrm{si}}(U) = \frac{2}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \sum_{\alpha=1}^{d'} \left\langle \phi_\alpha(k), \frac{\mathrm{d}}{\mathrm{d}k} \phi_\alpha(k) \right\rangle . \tag{7.39}$$

Proof. From Lemma 7.6 we know, that a flat-band bulk $\widehat{U}(k)$ in chiral block form has vanishing diagonal blocks $\widehat{A}$ and $\widehat{D}$, and unitary antidiagonal blocks s.t.

$$\widehat{U}(k) = \begin{pmatrix} 0 & \widehat{B}(k) \\ -\widehat{B}(k)^* & 0 \end{pmatrix} . \tag{7.40}$$

Let $\{\chi_\alpha\}_{\alpha=1}^{d'}$ denote a (fixed, k-independent) basis of $\mathcal{H}_-$, the -1-eigenspace of γ on $\mathcal{H}$ from Definition 7.4 (after Fourier transform). Then, for all $\alpha = 1, \ldots, d'$,

$$\phi_\alpha(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} i\widehat{B}(k)\chi_\alpha \\ -\chi_\alpha \end{pmatrix} \tag{7.41}$$

is a suitable eigenfunction as described in the Corollary. It inherits continuous differentiability (respecting the boundary conditions) directly from $\widehat{B}(k)$. Furthermore, due to the unitarity of $\widehat{B}(k)$,

$$\begin{aligned} \widehat{U}(k)\phi_\alpha(k) &= \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & \widehat{B}(k) \\ -\widehat{B}(k)^* & 0 \end{pmatrix} \begin{pmatrix} \widehat{B}(k)\chi_\alpha \\ i\chi_\alpha \end{pmatrix} \\ &= \frac{i}{\sqrt{2}} \begin{pmatrix} i\widehat{B}(k)\chi_\alpha \\ -\chi_\alpha \end{pmatrix} = i\phi_\alpha(k). \end{aligned} \tag{7.42}$$

Moreover, unitarity of $\widehat{B}(k)$ guarantees that the $\phi_\alpha(k)$ are an orthonormal basis with cardinality d'. That is, they span the $+i$-eigenspace

of $\widehat{U}$, and therefore their corresponding projections sum up to $Q(k)$. Anticipating the Berry formula, we note

$$\frac{\mathrm{d}}{\mathrm{d}k}\phi_\alpha(k) = \frac{i}{\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}k}\widehat{B}(k)\begin{pmatrix}\chi_\alpha\\ 0\end{pmatrix}. \tag{7.43}$$

Now, the trace in (7.36) evaluates to

$$\begin{aligned}
&\operatorname{tr}\left(\widehat{B}^*(k)\frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k}\right)\\
=&\sum_{\alpha=1}^{d'}\left\langle \widehat{B}(k)\chi_\alpha,\ \frac{\mathrm{d}}{\mathrm{d}k}\widehat{B}(k)\chi_\alpha\right\rangle\\
=&2\sum_{\alpha=1}^{d'}\left\langle \frac{1}{\sqrt{2}}\begin{pmatrix}i\widehat{B}(k)\chi_\alpha\\ -\chi_\alpha\end{pmatrix},\ \frac{i}{\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}k}\widehat{B}(k)\begin{pmatrix}\chi_\alpha\\ 0\end{pmatrix}\right\rangle\\
=&2\sum_{\alpha=1}^{d'}\left\langle \phi_\alpha(k),\ \frac{\mathrm{d}}{\mathrm{d}k}\phi_\alpha(k)\right\rangle,
\end{aligned} \tag{7.44}$$

finishing the proof. □

At this point, it makes sense to look back and relate the result to the *bulk-boundary-correspondence* from Section 5.3. Recall that in Definition 5.10, we defined a *bulk* as a translation invariant ρ-admissible ELEU. But since every bulk defined this way is already *unitary* (not merely *essentially unitary*), the winding formula just obtained allows to quickly determine $\vec{\mathrm{si}}(U)$ for every bulk given.

As explained in the introduction, the first approaches regarding bulk-boundary correspondence in quantum walks was more of an exploring kind [Kit+10; Asb12], where effective Hamiltonians of specific examples were analysed with corresponding specific formulas to compute *relative* phases between two systems. Then, a *crossover* between two systems is implemented on a small finite lattice, and an initial state on the boundary is driven by the crossover-walk, which indicates topological protection if some probability remains around the origin after a small number of time steps. Hence the often assumed bulk-boundary correspondence was verified by identifying a lower bound on the probability in a small area at the edge of two systems, which is stable for a few time steps. Later, a winding number like the one stated in Theorem 7.3 was stated (see e.g. [AO13]) as a candidate for a *bulk-invariant*, i.e. a number denoting an *absolute* topological phase, which was *assumed* to be robust w.r.t. some class of admissible perturbations.

Our result is hence not the discovery of the winding formula, but on one hand, the statement that this winding number matches a precisely defined symmetry index $\vec{\mathrm{si}}$, which was shown to be robust under a sharply defined, broad class of perturbations. On the other hand, it confirms the common interpretation of the bulk-boundary-correspondence in the following sense: Topological invariants are *bulk-*

invariants, in the sense that their values can be computed from the bulk alone. On joining two bulks, these values predict the occurrence of *edge states* at the interface if they differ.

Clearly, this is not new to us, since our result in Theorem 5.12 was stated within a setting that contained all these systems, and thoroughly *proven*, not merely conjectured or verified along a few examples. Furthermore, we know, that the homotopy invariance and stability w.r.t. perturbations of our symmetry indices simply carry over to the more restricted subset of bulks. But the converse, i.e. the question of completeness within the setting of bulks in chiral block form, is not answered yet and has to be analysed:

We know from Theorem 5.9 that $\mathrm{si}(U) = 0$ for translation invariant U. Since $\mathrm{si}(U) = \vec{\mathrm{si}}(U) + \overleftarrow{\mathrm{si}}(U) = 0$, we have found all classifying topological invariants from our general, non translation invariant theory, since translation invariance of the bulks ensures that $\mathrm{si}_{\pm}(U) = 0$ because of the gap condition. But as already mentioned in the introduction of Section 7.1, restricting our setting by demanding translation invariance for all objects under considerations does not change the classification provided by Chapter 5. That is, the assigned symmetry indices in the restricted setting are invariant w.r.t. every perturbation described, since the translation invariant objects were already included in the setting. But the completeness result might not be as simply transferred to the translation invariant settings, since adding additional constraints might disconnect formerly connected subsets, since *bridges* between them might require the breaking of translation invariance, or at least the breaking of translation invariance w.r.t. to the rigid cell structure (that is, allow for *regrouping*). Hence, in the following subsection, we analyse whether for every U_1, U_2 that share the same value of $\vec{\mathrm{si}}$, we can find gentle perturbations within the set of bulks on a rigid cell structure that connect them. In cases where this is impossible, we introduce the additional invariant necessary, and show that allowing to regroup adjacent cells once does restore completeness in this more *flexible* setting.

7.3 COMPLETENESS

The extensive simplifications that the chiral block form, as well as the flattening construction provide can now be used to answer the questions about completeness directly. Let us begin with AIII, where there is only one symmetry, i.e. γ with $\gamma^2 = \mathbb{1}$.

Proposition 7.10 (Completeness: TI, AIII)
Let ρ be a representation of AIII *and let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ be a rigid cell structure.*
Then, the classification of bulks on $\mathcal{H}$ through $\vec{\mathrm{si}}$ is complete.
That is, any two bulks U, U' such that $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$ are gentle perturbations

of each other that keep translation invariance w.r.t. the cell structure along the way.

Proof. The Fourier transform maps U to $\widehat{U}(k)$, which is a continuous periodic function on $\mathbb{T}$ due to the essential locality of U and Theorem 6.1. Following Lemma 7.1, for every $\widehat{U}(k)$, there is a gentle perturbation that keeps translation invariance w.r.t. the cell structure, which brings $\widehat{U}(k)$ to $\widehat{U}_\flat(k)$, its unique *flat-band form*. Now we can transform $\widehat{U}(k)$ into chiral block form, which by Lemma 7.6 is block-antidiagonal with a unitary $\widehat{B}(k)$ that hence completely determines $\widehat{U}_\flat(k)$. The γ-admissibility (including the gap condition due to its flat-band form) is fulfilled automatically due to the chiral block form for any $\widehat{V}_\flat(k)$ that stems from a continuous unitary loop $\widehat{B}_V(k)$.

Since the determinant of a loop in the unitary group $\mathcal{U}(d')$ induces a loop from the unit circle to the unit circle, it has a winding number. We need the following well-known properties about $\mathcal{U}(d')$, that can e.g. be found in [Nak03, (4.56)]: The unitary group is path-connected, but not simply connected, since the fundamental group is $\pi_1\big(\mathcal{U}(d')\big) \cong \mathbb{Z}$. By definition, the fundamental group is formed by the homotopy classes of loops and hence two loops in $\mathcal{U}(d')$ are homotopic iff the windings of their determinants coincide.

Summing up, if we are given two bulks U, U' such that $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$, we bring them into flat-band and chiral block form, s.t. $\widehat{B}(k)$ and $\widehat{B}'(k)$ are two arbitrary unitary loops in $\mathcal{U}(d')$ that share the same winding number due to Theorem 7.3 and $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$. Therefore they are homotopic. Moreover, the continuity of the loop guarantees continuity of the flattened path along the way. Therefore, essential locality is again implied by Theorem 6.1, finishing the proof. □

Note that the result can be stated within the stricter class of quantum walks as well. The only adjustment needed is that for strict locality, one needs to ensure the uniformly bounded jump length *along the way*, which can be done exactly as in the proof of (3.13), found in [Gro+12, Prop. 6].

In the other cases, namely BDI and CII, there is an η-symmetry present, which translates to an η_b-symmetry for B in chiral block form as explained in (7.24). This then implies that $\widehat{B}(k)$ fulfils the same symmetry relations with η_b as explained in (7.3), that is

$$\widehat{B}(k) = \eta_b^* \widehat{B}(-k) \eta_b. \tag{7.45}$$

The effect of this additional symmetry on $\det \widehat{B}(k)$ is shown by a simple computation:

$$\det \widehat{B}(k) = \det\left(\eta_b^* \widehat{B}(-k) \eta_b\right) = \overline{\det \widehat{B}(-k)}. \tag{7.46}$$

In the last step, we used that the effect of conjugation with an antiunitary operator is complex conjugation of the eigenvalues and rotation of the eigenvectors with a unitary operator, due to (2.12). The determi-

nant is invariant under unitary conjugations, hence what remains is the complex conjugation of the eigenvalues and hence of their product, the determinant.

To clarify the notation, let us introduce c to denote the curve that leads to $\vec{\mathrm{si}}$, that is

$$c : [-\pi, \pi] \to \mathbb{C}, \quad c(k) = \det \widehat{B}(k), \quad c(k) = \overline{c(-k)}. \tag{7.47}$$

Here, the last relation follows from (7.46).

As we will show, this constraint prevents the completeness of $\vec{\mathrm{si}}$ in the case of BDI. In the simplest case of $d = 2$, we have one dimensional chiral "blocks". Let $\widehat{B}(k) = +1$ and $\widehat{B}'(k) = -1$ be two of these blocks. Since they are constant in k, their winding numbers vanish, respectively. If completeness of $\vec{\mathrm{si}}$ held, we would be able to connect them within the set of bulks.

The additional symmetry constraint from (7.46) forces $c(0)$ and $c(\pi)$ to be real. To satisfy the gap condition *along the way*, $\widehat{B}_t$ has to keep a bounded inverse by Lemma 7.6, which forbids a path between $\widehat{B}$ and $\widehat{B}'$ that crosses the origin, that is $\widehat{B}_t(k) \neq 0$ for all t and k. But this is impossible, since at the same time, $\widehat{B}_t$ has to fulfil the reality condition at $k_0 \in \{0, \pm\pi\}$, that is $c_t(k_0)$ has to continuously connect $+1$ and -1 along the real line without crossing 0. Therefore, there is no admissible path within this set, and $\vec{\mathrm{si}}$ is not complete for BDI.

The lack of completeness hints at an additional invariant, which stems from the tighter constraint to fix a cell structure. As we will show shortly, by allowing to *regroup* the system as described in Definition 7.2, this additional invariant trivializes.

Definition 7.11 (Regrouping sign)
Let U be a bulk for BDI *with corresponding curve c as above. Then, the* **regrouping sign** *of U is defined as*

$$\mathrm{rs}(U) = \mathrm{sign}(c(0)). \tag{7.48}$$

As was already explained in the completeness-contradicting example above, the reality condition from (7.46) shows, that no gentle perturbation $c_t(0)$ can change the value of $\mathrm{rs}(U_t)$, since the determinant cannot change its sign without crossing 0 while satisfying the reality condition.

The following proposition now fixes the completeness of bulks on a rigid cell structure in the case of BDI:

Proposition 7.12 (Completeness: TI, BDI)
Let ρ be a representation of BDI *and let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ be a rigid cell structure. Then, the classification of bulks on $\mathcal{H}$ through $\vec{\mathrm{si}}$ and* rs *is* complete. *That is, any two bulks U, U' such that $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$ and $\mathrm{rs}(U) = \mathrm{rs}(U')$ are gentle perturbations of each other that keep translation invariance w.r.t. the cell structure along the way.*

Proof. The general outline of the proof matches the proof of Proposition 7.10 for AIII, but the presence of η and rs complicate the pathfinding, as will be seen shortly.

Analogously to Proposition 7.10, Lemma 7.1 guarantees that there is a gentle perturbation within the set of translation invariant bulks on a rigid cell structure, that transports $\widehat{U}(k)$ to $\widehat{U}_\flat(k)$, its *flat-band form*. In chiral block form, this yields a unitary $\widehat{B}(k)$ that completely determines $\widehat{U}_\flat(k)$. Furthermore, γ-admissibility and the gap condition are satisfied in chiral block form for any $\widehat{U}_t(k)$ that stems from a continuous unitary loop $\widehat{B}_t(k)$. The consequence is that a curve c as defined in (7.47) is restricted to the unit circle, and we can identify the phase function $\varphi(k) \in \mathbb{R}$ via

$$c(k) = e^{2\pi i\varphi(k)}, \qquad \varphi(\pi) = \varphi(-\pi) + \mathrm{wind}(c). \tag{7.49}$$

Now, adding the η_b-admissibility from (7.24) to the picture restricts the allowed loops $\widehat{B}_t(k)$ even further:

The particle-hole symmetry η_b is an antiunitary operator with $\eta_b^2 = \mathbb{1}$, hence by (2.12), there is an η_b-real basis where η_b acts as complex conjugation. As was already used in the example above, (7.46) shows that $c(k_0) = \pm 1$ for $k_0 \in \{0, \pm\pi\}$. Furthermore, defining $\widehat{B}_t(k)$ on $[0, \pi]$ fixes $\widehat{B}_t(k)$ on the whole interval $[-\pi, \pi]$ by (7.45). Hence, it suffices to determine $\widehat{B}_t(k)$ at the interval $[0, \pi]$.

With these preliminary considerations at hand, let us show that $\widehat{U}_\flat$ and $\widehat{U}'_\flat$ are homotopic within the set of admissible translation invariant essentially local unitary operators with rigid cell structure. Since $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$, their winding numbers coincide as well, and we have

$$e^{2\pi i\varphi(k)} = c(k) = \overline{c(-k)} = e^{-2\pi i\varphi(-k)}. \tag{7.50}$$

This implies that

$$2\varphi(0) = \varphi(k) + \varphi(-k) = \varphi(\pi) + \varphi(-\pi) \in \mathbb{Z}, \tag{7.51}$$

and we get with $k = \pi$ and (7.49)

$$2\varphi(\pi) = 2\varphi(0) + \mathrm{wind}(c), \tag{7.52}$$

finally leading to

$$c(\pi) = c(0)e^{\pi i\cdot \mathrm{wind}(c)} = c(0)\cdot(-1)^{\mathrm{wind}(c)} = \mathrm{rs}(U)\cdot(-1)^{\vec{\mathrm{si}}(U)}. \tag{7.53}$$

Hence $c(\pi)$ is completely determined by $c(0)$ and $\mathrm{wind}(c)$, or $\mathrm{rs}(U)$ and $\vec{\mathrm{si}}(U)$, respectively. Since both invariants are assumed to coincide for U and U', we have deduced that in this case, $c(\pi)$ and $c'(\pi)$ match as well.

What is left now is to connect $\widehat{B}(k)$ and $\widehat{B}'(k)$ with a suitable $\widehat{B}_t(k)$ on the interval $[0, \pi]$. Since we already know, that the matching of $\vec{\mathrm{si}}$ and rs implies that $c(0) = c'(0)$ and $c(\pi) = c'(\pi)$, the endpoints of c_t are fixed by these values.

The orthogonal group has two connected components [Nak03, 4.7]. These are distinguished by the determinant, which takes values on the

intersection of the real axis with the unit circle, that is ± 1. Since rs is given by the sign of $c(0)$, and $\mathrm{rs}(U)$=$\mathrm{rs}(U')$, we know that the endpoints both have the same determinant and hence the corresponding $\widehat{B}(0)$ and $\widehat{B}'(0)$ lie in the same connected component of $O(d')$. But admissibility precisely allows for paths $\widehat{B}_t(0)$, that lie in the orthogonal group, thus we can interpolate between $\widehat{B}(0)$ and $\widehat{B}'(0)$ in $O(d')$. $\widehat{B}(\pi)$ and $\widehat{B}'(\pi)$ follow completely analogously.

What remains is to show the existence of the homotopy $\widehat{B}_t(k)$ that interpolates between $\widehat{B}(k)$ and $\widehat{B}'(k)$ for $k \in (0, \pi)$. Given $k_0 \in \{0, \pi\}$, we know that the endpoints $\widehat{B}(k_0)$ and $\widehat{B}'(k_0)$ lie in the same connected component of the orthogonal group $O(d')$, since their determinants, given by $c(k_0)$ and $c'(k_0)$ coincide. Hence there is a path within this connected component that connects $\widehat{B}(k_0)$ and $\widehat{B}'(k_0)$. The additional constraint of η_b-admissibility is exhausted by restricting to half the Brillouin zone, hence the path $\widehat{B}_t(k)$ for $k \in (0, \pi)$ simply lies in the unitary group $\mathcal{U}(d')$, without additional constraints. That is, similar to the case AIII, since the winding numbers of $\widehat{B}(k)$ and $\widehat{B}'(k)$ coincide, they can be contracted one onto the other within the unitary group and the result follows. □

For symmetry type BDI, in the translation invariant case with rigid cell structure, we have thus shown, that $\vec{\mathrm{si}}$ is not complete by itself, but that we need to introduce the $\mathbb{Z}_2$-valued invariant rs. However, as the following Lemma shows, if we loosen the rigid cells constraint by allowing to regroup at least once, rs trivializes to depend only on the winding of $c(k)$, s.t. $\vec{\mathrm{si}}$ becomes a complete invariant in this more *flexible* setting.

Lemma 7.13 (Regrouping for BDI)
Let U be a bulk for BDI *and let U_r be its regrouped pendant as in Definition 7.2. Then,* $\mathrm{rs}(U_r)$ *depends only on* $\vec{\mathrm{si}}(U)$.

Proof. From Definition 7.2, we know that

$$\widehat{U}_r(k) = H(k/2) \begin{pmatrix} \widehat{U}(k/2) & 0 \\ 0 & \widehat{U}(k/2 + \pi) \end{pmatrix} H(k/2)^*. \tag{7.54}$$

In each of these regrouping-blocks, we can find a basis s.t. $\widehat{U}$ is in *chiral block form*. This change of basis does not change H, since it acts like the identity on the regrouping-blocks. Hence writing $\widehat{U}_r$ in regrouping blocks with chiral sub blocks yields

$$\widehat{U}_r(k) = H(k/2) \begin{pmatrix} A & B & 0 & 0 \\ C & D & 0 & 0 \\ 0 & 0 & A_\pi & B_\pi \\ 0 & 0 & C_\pi & D_\pi \end{pmatrix} H(k/2)^*, \tag{7.55}$$

where we shortened notation such that e.g. A denotes $\widehat{A}(k/2)$ and e.g. B_π denotes $\widehat{B}(k/2 + \pi)$.

Since γ_r on a new cell is just the direct sum of $\gamma = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ on the old cells, we transition to the chiral block form for the regrouped setting by conjugation with the unitary V, that is

$$\gamma_r = V \begin{pmatrix} \gamma & 0 \\ 0 & \gamma \end{pmatrix} V^* = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \qquad V = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{7.56}$$

The second factor on the right hand side of (7.55) is then transformed to

$$V \begin{pmatrix} A & B & 0 & 0 \\ C & D & 0 & 0 \\ 0 & 0 & A_\pi & B_\pi \\ 0 & 0 & C_\pi & D_\pi \end{pmatrix} V^* = \begin{pmatrix} A & 0 & B & 0 \\ 0 & A_\pi & 0 & B_\pi \\ C & 0 & D & 0 \\ 0 & C_\pi & 0 & D_\pi \end{pmatrix} \tag{7.57}$$

Hence, the relevant chiral block up to the action of H is

$$\widehat{B}_H(k) = \begin{pmatrix} \widehat{B}(k) & 0 \\ 0 & \widehat{B}(k+\pi) \end{pmatrix}. \tag{7.58}$$

In the case of H, conjugation with V leads to

$$\begin{aligned} \sqrt{2}\, V\, H(k) V^* &= V \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ e^{-ik}\mathbb{1} & -e^{-ik}\mathbb{1} \end{pmatrix} V^* \\ &= \begin{pmatrix} 1 & 1 & 0 & 0 \\ e^{-ik} & -e^{-ik} & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & e^{-ik} & -e^{-ik} \end{pmatrix}. \end{aligned} \tag{7.59}$$

In a slight abuse of notation, this allows us to write

$$V H(k) V^* = \begin{pmatrix} H(k) & 0 \\ 0 & H(k) \end{pmatrix}, \tag{7.60}$$

where on the right hand side, $\mathbb{1}$ in $H(k)$ has to be replaced by 1. But in this basis, H is block-diagonal and acts on each block identically. That is, the conjugation with $H(k/2)$ to get $\widehat{U}_r$ translates to a conjugation with $H(k/2)$ on each block separately. We get

$$\widehat{B}_r(k) = H(k/2)\widehat{B}_H(k/2)H^*(k/2). \tag{7.61}$$

H is unitary and the determinant is a homomorphism w.r.t. multiplication, therefore we have

$$\det\left(\widehat{B}_H(k)\right) = \det\left(\widehat{B}(k)\right) \cdot \det\left(\widehat{B}(k+\pi)\right), \tag{7.62}$$

and thus for c_r

$$c_r(k) = c(k/2) \cdot c(k/2 + \pi). \tag{7.63}$$

Using the result from (7.53) allows us to write

$$c_r(0) = c(0) \cdot c(\pi) = c(0)^2 \cdot (-1)^{\mathrm{wind}(c)} = (-1)^{\mathrm{wind}(c)} \tag{7.64}$$

and finally compute $\mathrm{rs}(U_r)$

$$\mathrm{rs}(U_r) = \mathrm{sign}\big(c_r(0)\big) = \begin{cases} 1 & \mathrm{wind}(c) \text{ even}, \\ -1 & \mathrm{wind}(c) \text{ odd}. \end{cases} \tag{7.65}$$

Hence we have thus shown, that regrouping makes $\mathrm{rs}(U_r)$ a function of $\mathrm{wind}(c)$, i.e. a dependent invariant which is completely covered by $\vec{\mathrm{si}}(U)$, finishing the proof. □

Therefore we now proved that the *regrouping sign* is needed for a complete classification of BDI-admissible bulks U, if we fix the cell structure and do not allow regrouping. If we *do* allow regrouping, we can regroup U and U' after flattening, making rs useless, since it depends only on $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$ respectively, and thus is the same for U_r and U'_r. That is, in the setting of *flexible* cell structures, $\vec{\mathrm{si}}$ is a complete homotopy invariant for BDI.

Let us now analyse completeness for CII. We know from (7.45) that $\eta_b \widehat{B}(k) = \widehat{B}(-k)\eta_b$, which is the same as for BDI. The difference is now that (7.24) implies $\eta_b^2 = -\mathbb{1}$ for symmetry type CII, which means that the chiral blocks are of even dimension. This restriction to even dimensions obviates the introduction of an additional invariant, as Proposition 7.14 shows. Before we state the proposition, let us explain why the *regrouping sign* is trivial in the case of CII:

The admissibility condition for $\widehat{B}(k)$ implies that for $k_0 \in \{0, \pm\pi\}$, $\widehat{B}(k_0)$ commutes with η_b. Furthermore, from (4.3) we learn, that for any ϕ s.t. $\widehat{B}(k_0)\phi = e^{i\omega}\phi$, there is $\eta_b\phi$ s.t.

$$\widehat{B}(k_0)(\eta_b\phi) = e^{-i\omega}(\eta_b\phi). \tag{7.66}$$

But since $\eta_b^2 = -\mathbb{1}$, ϕ and $\eta_b\phi$ are orthogonal and hence independent eigenvectors. This implies that the dimension d' is even and we can write it as $d' = 2d''$. Reordering the eigenvalues s.t. $\omega_{2j-1} = -\omega_{2j}$ for all $j = 1, \ldots, d''$, implies that

$$\det \widehat{B}(k_0) = \prod_{j=1}^{2d''} e^{i\omega_j} = \prod_{j=1}^{d''} e^{i\omega_{2j-1}} e^{-i\omega_{2j-1}} = 1. \tag{7.67}$$

Thus we showed, that the sign of $c(k_0)$ is an invariant for all bulks of CII, but with the same trivial value. Therefore, it does not contribute to a classification. The following proposition shows that $\vec{\mathrm{si}}$ suffices as the index for a complete classification:

Proposition 7.14 (Completeness: TI, CII)
Let ρ be a representation of CII *and let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ be a rigid cell structure. Then, the classification of bulks on $\mathcal{H}$ through $\vec{\mathrm{si}}$ is complete.*
That is, any two bulks U, U' such that $\vec{\mathrm{si}}(U) = \vec{\mathrm{si}}(U')$ are gentle perturbations

of each other that keep translation invariance w.r.t. the cell structure along the way.

Proof. Most of the proof is completely analogous to the proof of Proposition 7.10 for AIII. That is, we transition from U and U' to the *flat-band form* in *chiral block form*. These are each determined completely by unitary loops $\widehat{B}(k)$ and $\widehat{B}'(k)$, which are admissible for η_b in the sense of (7.45). Similarly to the BDI-case, admissibility reduces the analysis to $[0, \pi]$, since $[-\pi, 0]$ follows by symmetry. Hence for the endpoints $\widehat{B}(k_0)$ and $\widehat{B}'(k_0)$ for $k_0 \in \{0, \pm\pi\}$, we are left with paths in the orthogonal group of finite dimension d', denoted $O(d')$. But the discussion before this proposition showed, as opposed to BDI, that for CII, $c(k_0) = 1$. Hence the endpoints lie in the same connected component, namely the connected component of the identity in $O(d')$ denoted by $O^+(d')$, and can thus be connected.

The windings of $\widehat{B}(k)$ and $\widehat{B}'(k)$ coincide due to their matching $\vec{\text{si}}$, and therefore we are left with two paths within the unitary group $\mathcal{U}(d')$ which have the same winding number. In order to connect these two, we use that the set of η_b-commuting unitaries is connected to the identity in the case of CII. This is due to $\eta_b^2 = -\mathbb{1}$ which by (7.66) forces the eigenvalues to come in pairs, allowing to continuously move the spectrum to $+1$ without changing the eigenvectors, keeping the symmetry. This makes the case CII differ from BDI, where $\eta_b^2 = +\mathbb{1}$.

Returning to the overall path, since $O^+(d')$ is contained in $\mathcal{U}(d')$, there is a contraction $\widehat{B}_t(k)$ between $\widehat{B}(k)$ and $\widehat{B}'(k)$ for all $k \in [-\pi, \pi]$ which is periodic at the boundaries and fulfils all the required constraints, finishing the proof. □

We have thus seen that the chiral block form provides a significant simplification in proving completeness for symmetry types with a chiral symmetry γ present that squares to $\mathbb{1}$. In the cases AIII and CII, $\vec{\text{si}}$ provides a complete classification within the set of bulks, even if restricted to rigid cell structure. For BDI, if we allow flexible cell structures (or at least allow regrouping once), $\vec{\text{si}}$ provides a complete classification as well. Restricted to rigid cell structures, we had to introduce the regrouping sign rs. Together with $\vec{\text{si}}$, it provided a complete classification in the rigid setting for BDI.

In the following chapter, we will proceed to the examples and visualize the results of this thesis.

8 EXAMPLES

In this chapter, we provide multiple examples, applications and visualizations of the theory that was derived in this thesis.

In Section 8.1, we provide a translation invariant example that generates all values of the symmetry index. This shows that in every setting that was described, the sets that are labelled by symmetry indices are non-empty. After that, we consider the *Split-Step-Walk* in Section 8.2, which serves as the iconic example to show the splitting and joining of bulks (Section 5.5), the bulk-boundary correspondence (Section 5.3), forgetting about symmetries (Table 2), the index as a winding number (or bulk-invariant, Section 7.2) and the exponential decay at the boundary (Section 6.2). In Section 8.3, we introduce a browser-application called the *Split-Step-Explorer*, which we developed to visualize many of the aforementioned features of the *Split-Step-Walk*, together with a brief explanation on the corresponding web page [Sta15a]. The Four-Step-Example we introduce in Section 8.4 shows how the simple Split-Step-Walk can be generalized to a slightly more complicated example, that is still easily classified by our general theory. We modify the example to explicitly break two out of three symmetries, which leaves a larger, but also coarser class of less symmetry, that corresponds to forgetting about these two symmetries. Finally, in Section 8.5 we provide a non-translation invariant Split-Step-Walk that is described by our general theory and still permits precise statements about the symmetry indices, as long as the spatial position does not vary too wildly.

8.1 TRANSLATION-INVARIANT GENERATOR

The previous chapters provide a list of different (symmetry-) indices with corresponding results stating on the one hand the invariance of the indices w.r.t. perturbations that still follow certain constraints, on the other the completeness of these indices. Searching for the *best*[1] setting for every theorem, it was often necessary to adjust the assumptions for a given chapter. Throughout this thesis we learned, that quantum walks, which satisfy discrete symmetries of the tenfold-way, are not necessary the best object to look at for each part of the classification. Therefore, the assumptions of the setting regarding the basic objects ranged from essentially local essentially unitary operators (ELEU) to translation invariant strictly local unitary operators, i.e. translation invariant *quantum walks*. The allowed homotopies respectively ranged

1 Usually, *best* means *most general*. But if there are multiple parameters to tweak, it is often hard to find the right compromise between generality and applicability.

from gentle perturbations that are translation invariant w.r.t. a rigid cell structure along the way, to merely compact admissible perturbations that are essentially local.

Therefore, it is even more remarkable, that there is an example, that is compatible with all the different settings, the so called *translation-invariant generator* W_g. With slight adjustments, it serves as a generator for the index groups $\mathbf{I}(\mathsf{S})$ that correspond to the different (non-trivial) symmetry types of the tenfold way (see Table 1).

In order to write down the generating example, let $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ be the Hilbert space of a typical Qubit on the 1D-lattice. Then, for a suitable basis $|x, s\rangle$ with $x \in \mathbb{Z}$ and $s = \pm 1$, we define W_g as

$$W_g|x,+\rangle = i\,|x-1,-\rangle \qquad\qquad W_g|x,-\rangle = i\,|x+1,+\rangle. \tag{8.1}$$

As can be seen in Figure 8, W_g simply swaps basis elements of opposite spin in neighbouring cells and multiplies with i. The multiplication with i ensures that $W_g^2 = -\mathbb{1}$, and hence the whole spectrum of W_g lies at $\pm i$. Furthermore, W_g commutes with the simple translations

$$T|x,s\rangle = |x+1,s\rangle, \tag{8.2}$$

and is thus translation invariant w.r.t. the rigid cell structure.

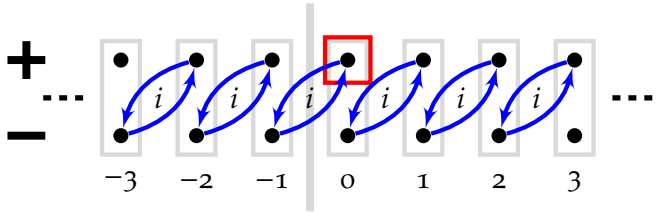


Figure 8: Schematic picture of the action of W_g on the basis elements $|x, s\rangle$, denoted by a black dot. The walk multiplies the coefficient with i and swaps the basis elements as indicated by the arrows. In this form, by following the arrows, one can clearly identify the red box as the kernel of PW_gP, where P denotes the projection onto the non-negative half-chain as indicated by the grey separation line.

This lucid choice of the basis has a disadvantage, namely that we cannot stick to our usual convention to pick an η-real basis. Let us look at how the complex conjugation[2] K commutes with W_g:

$$KW_g|x,s\rangle = K\,i|x+s,-s\rangle = -i|x+s,-s\rangle = W_g^*K|x,s\rangle, \tag{8.3}$$

where in the last step we used $W_g = -W_g^*$ due to $W_g^2 = -\mathbb{1}$. This shows, that in this choice of basis, K represents a time reversal symmetry τ, which squares to $+\mathbb{1}$. Furthermore,

$$\gamma\,|x,s\rangle = s\,|x,s\rangle \tag{8.4}$$

is an obvious choice for a chiral symmetry γ, since

$$W_g\gamma\,|x,s\rangle = s\cdot i\,|x+s,-s\rangle = -sW_g\,|x,s\rangle = \gamma W_g^*\,|x,s\rangle. \tag{8.5}$$

2 Note that we choose K s.t. the basis $|x, s\rangle$ is real w.r.t. K, i.e. $K|x, s\rangle = |x, s\rangle$.

Thus, γ squares to $+\mathbb{1}$ as well, and with $\eta = \tau\gamma$, we see that in this form, W_g is a translation invariant quantum walk of symmetry type BDI. Performing the Fourier transform w.r.t. T, we can read off

$$\widehat{W}_g(k) = \begin{pmatrix} 0 & ie^{ik} \\ ie^{-ik} & 0 \end{pmatrix}. \tag{8.6}$$

This allows us to easily determine the symmetry index $\vec{\mathrm{si}}(W)$ by using Theorem 7.3. Since γ is already diagonal in this basis, $\widehat{W}_g(k)$ is already in *chiral block form* and

$$\widehat{B}(k) = ie^{ik} \tag{8.7}$$

denotes the upper right block. Since it is a 1×1-matrix, its determinant and trace are trivial, and we get[3]

$$\vec{\mathrm{si}}(W_g) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} \mathrm{d}k \ \mathrm{tr}\left(\widehat{B}^*(k) \frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k}\right) = 1. \tag{8.8}$$

If W_g were not translation-invariant, we would have to determine $\vec{\mathrm{si}}(W_g)$ via Definition 5.8 and Definition 5.7 as

$$\vec{\mathrm{si}}(W_g) = \mathrm{si}\big(P \operatorname{Im} W_g P\big). \tag{8.9}$$

That is, we have to compute the trace of γ on the kernel of $P \operatorname{Im} W_g P$, as follows from the derivation of the symmetry index for BDI in Section 4.4. The definition of the imaginary part yields

$$\operatorname{Im} W_g = \frac{1}{2i}\big(W_g - W_g^*\big) = -iW_g, \tag{8.10}$$

which tells us that it acts only on its direct neighbours. Moreover, $\operatorname{Im} W_g$ simply swaps $|x, +\rangle$ and $|x-1, -\rangle$ with each other, while P acts like the identity on $|x, s\rangle$ for all $x \geq 0$. That leaves only one candidate for the kernel of $P \operatorname{Im} W_g P$ w.r.t. the Hilbert space $P\mathcal{H}$. That is $|0, +\rangle$, since it gets mapped by $\operatorname{Im} W_g P$ to $|-1, -\rangle$, which is projected away by P. This could similarly be deduced from Figure 8. Hence we identified the null space of $P \operatorname{Im} W_g P$ as the span of $|0, +\rangle$, and we can determine $\vec{\mathrm{si}}(W_g)$ as the trace of γ on this space by reading off the eigenvalue of γ for the eigenvector $|0, +\rangle$, that is

$$\vec{\mathrm{si}}(W_g) = 1. \tag{8.11}$$

If we choose ρ' as the inverse representation in the sense of Proposition 4.8, that is, we define

$$\gamma' = -\gamma \qquad \tau' = -\tau \qquad \eta' = \eta, \tag{8.12}$$

the whole argument runs as before with the only difference being that γ has flipped the eigenspaces, implying a sign flip in $\vec{\mathrm{si}}'(W_g)$. That is,

3 Clearly, one could have just as easily read off the winding of this trivial curve, leading to the same result.

with ρ and ρ', we can create a representation $\rho_0 = \rho \oplus \rho'$ such that for $W_g \oplus W_g$, we have

$$\vec{\mathrm{si}}(W_g \oplus W_g) = \vec{\mathrm{si}}(W_g) + \vec{\mathrm{si}}\,'(W_g) = 0. \tag{8.13}$$

Here, we choose the new basis in $\mathcal{H} \oplus \mathcal{H}$ such that we double the dimension of the coin space. That is,

$$(|x\rangle \otimes \phi) \oplus (|x'\rangle \otimes \psi) \mapsto |x\rangle \otimes (\phi \oplus 0) + |x'\rangle \otimes (0 \oplus \psi). \tag{8.14}$$

In Figure 8 this corresponds to combining both half-chains one below the other.

Similarly, we can combine an arbitrary number of ρ and ρ' to create a new representation ρ'' and a suitable direct sum of multiple W_g to create every value $\vec{\mathrm{si}}$ in $\mathbf{I}(\mathsf{BDI}) = \mathbb{Z}$. Hence we have fully generated the index group for BDI.

How can we use this example for other non-trivial symmetry types? As Table 2 shows, forgetting about the existence of τ (and hence η as well), leaves us with symmetry type AIII. In this case, the symmetry index is determined exactly as before, thus this case is already treated completely.

Forgetting about γ and τ, hence leaving only η leaves us with symmetry type D. This case is not covered by the winding formula, since it is not (recognized as being) chiral symmetric. But the general way works as before, and we determine the index as described for D in Section 4.4. That is, $\vec{\mathrm{si}}(W_g)$ is again determined via the null space of $P \operatorname{Im} W_g P$, which is the span of $|0, +\rangle$. On this space, ρ is one-dimensional and with $\mathrm{si}(\rho) = d \bmod 2$, we have $\vec{\mathrm{si}}(W_g) = 1$. Here, 1 denotes the generator for $\mathbf{I}(\mathsf{D}) = \mathbb{Z}_2$. In this case, doubling W_g as for BDI, we find $\vec{\mathrm{si}}(W_g \oplus W_g) = 0$. Hence we generated all values of the index group $\mathbf{I}(\mathsf{D}) = \mathbb{Z}_2$.

The remaining two non-trivial symmetry types are CII and DIII, which both possess an antiunitarily represented symmetry with square $-\mathbb{1}$. This causes the values of the symmetry indices to double, since the eigenvectors spanning the null spaces always occur in pairs. Therefore, it is plausible to look for examples that are direct sums of W_g (and W_g^*), similar to the way we generated the different values of $\mathbf{I}(\mathsf{S})$.

For symmetry type CII, we choose the new generator as

$$W_c = W_g \oplus W_g. \tag{8.15}$$

It is admissible for $\gamma_c = \gamma \oplus \gamma$, where γ (and likewise τ and η) denote the symmetries from the non-doubled example of W_g in (8.4). With $\eta = \gamma\tau$, we define

$$\eta_c = \begin{pmatrix} 0 & -\eta \\ \eta & 0 \end{pmatrix}, \quad \text{s.t.} \quad \eta_c^2 = \begin{pmatrix} -\eta^2 & 0 \\ 0 & -\eta^2 \end{pmatrix} = -\mathbb{1}, \tag{8.16}$$

and admissibility of W_c for η_c follows directly from admissibility of W_g for η, i.e. $W_g\eta = \eta W_g$, s.t.

$$\eta_c W_c = \begin{pmatrix} 0 & -\eta W_g \\ \eta W_g & 0 \end{pmatrix} = \begin{pmatrix} 0 & -W_g\eta \\ W_g\eta & 0 \end{pmatrix} = W_c\eta_c. \tag{8.17}$$

As always, τ_c is determined via (2.27) and we have

$$\gamma_c = \eta_c\tau_c \quad \Leftrightarrow \quad \eta_c\gamma_c = -\tau_c \quad \Rightarrow \quad \tau_c = \begin{pmatrix} 0 & \tau \\ -\tau & 0 \end{pmatrix}. \tag{8.18}$$

That is, admissibility for τ_c follows directly from admissibility[4] for τ, and we can conjugate with V from (7.56) to bring W_c into *chiral block form*. Completely analogous to Lemma 7.13, we can read off the relevant chiral block $\widehat{B}_c(k)$ from (8.6) and get

$$\widehat{B}_c(k) = \begin{pmatrix} \widehat{B}(k) & 0 \\ 0 & \widehat{B}(k) \end{pmatrix}. \tag{8.19}$$

Using Theorem 7.3 as in (8.8), we get

$$\vec{\mathrm{si}}(W_c) = \frac{1}{2\pi i}\int_{-\pi}^{\pi} \mathrm{d}k\ \mathrm{tr}\begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} = 2. \tag{8.20}$$

Comparing with the result from the general theory is even easier, as we quickly check. We have to determine the null space $\mathcal{N}$ in the doubled case, where

$$\mathrm{Im}\, W_c = \frac{1}{2i}\left(W_c - W_c^*\right) = -iW_c. \tag{8.21}$$

Hence the kernel is similarly spanned by $|0\rangle \otimes \left(|+\rangle \oplus 0\right)$ and $|0\rangle \otimes \left(0 \oplus |+\rangle\right)$. There, γ_c acts as γ on each eigenvector individually, and we have

$$\vec{\mathrm{si}}(W_c) = \mathrm{tr}_{\mathcal{N}}\,\gamma = 2 \tag{8.22}$$

as before. The algorithm to generate the whole index group that was used after (8.11) for BDI is now similarly applicable to CII, and yields $\mathbf{I}(\mathrm{CII}) = 2\mathbb{Z}$ as expected.

Finally, let us introduce a generator W_d for DIII,

$$W_d = W_g \oplus W_g^*. \tag{8.23}$$

To compare the action of W_d and W_c, see Figure 9. Similar to CII, we introduce doubled symmetries, but switch the roles of η and γ s.t. $\eta_d^2 = \mathbb{1}$ and $\gamma_d^2 = -\mathbb{1}$. That is, we choose[5]

$$\eta_d = \begin{pmatrix} \eta & 0 \\ 0 & \eta \end{pmatrix} \qquad \gamma_d = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \qquad \tau_d = \begin{pmatrix} 0 & -\eta \\ \eta & 0 \end{pmatrix}. \tag{8.24}$$

4 This is only shown directly to provide self-consistency. Admissibility for τ_c has to follow directly from admissibility of γ_c and η_c by construction.

5 In this case taking the squares into account, we have $\tau_d = \eta_d\gamma_d$.

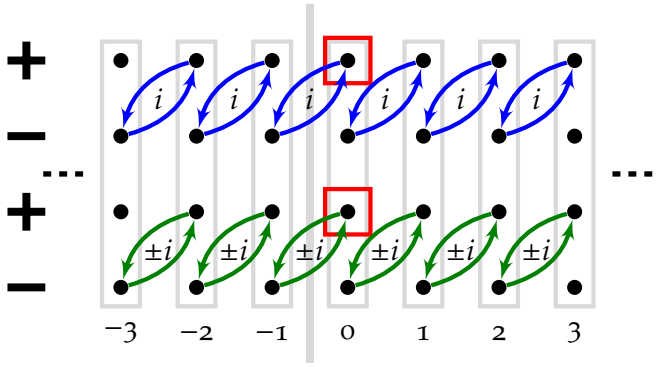


Figure 9: Schematic picture of the action of $W_c = W_g \oplus W_g$ for CII and $W_d = W_g \oplus W_g^*$ for BDI on the new basis elements that stem from the direct sum of two $|x, s\rangle$, denoted by a black dot. The blue arrow denotes the action of W_g, that is multiplication with i and swapping basis elements as indicated. The green arrow denotes the action of W_g or $W_g^* = -W_g$, depending on the sign of $\pm i$. Similar to Figure 8, one identifies the red boxes as the vectors that span $\ker\left(PW_cP\right) = \ker\left(PW_dP\right)$.

Note that this choice does not need a chiral or time-reversal symmetry of W_g, only η from symmetry type D is required. Since for DIII, we have not proven a translation-invariant formula, we have to use the general approach in this case as well. Thus, we compute the null space of $P \operatorname{Im} W_d P$ as before. Since $W_g^* = -W_g$,

$$\operatorname{Im} W_d = \frac{1}{2i}\left(W_d - W_d^*\right) = -iW_d, \tag{8.25}$$

and the kernel of W_d is computed using

$$\ker\left(W_g^*\right) = \ker\left(-W_g\right) = \ker\left(W_g\right). \tag{8.26}$$

We see that the vectors $|o\rangle \otimes \left(|+\rangle \oplus o\right)$ and $|o\rangle \otimes \left(o \oplus |+\rangle\right)$ span the null space as in the case of CII before. Using the index formula $\mathrm{si}(\rho) = d \bmod 4$ for DIII, we find that $\vec{\mathrm{si}}(W_d) = 2$, which serves as the generator of the group $2\mathbb{Z}_2$ as described in Section 4.4.

The simplicity of W_g should allow to generate similar examples for more intricate representations ρ. One would hope to be able to show that for every (non-translation invariant?) ρ, there is an element W_g that generates the full group $\mathbf{I}(\mathsf{S})$. But it is not clear whether such a general statement is even possible. Certainly, it is beyond the scope of this section.

8.2 THE SPLIT-STEP-WALK

The iconic example found throughout most of the literature regarding topology in quantum walks was (to our knowledge) introduced in [Kit+10], and treated in [Kit12; Asb12; AO13; TAD14]. It is called the Split-Step-Walk. For many authors, it served as a testing environ-

ment for topological phenomena like symmetry indices for translation invariant systems, or signatures of eigenstates localized at a boundary. In its typical form, it is a quantum walk which is admissible for symmetry representations of BDI, and by forgetting about symmetries, can serve as an example for D and AIII as well. Using the doubling procedures introduced in the previous section, it could even serve as an example for all symmetry types of the tenfold way.

As was already mentioned in the introduction, after defining the Split-Step-Walk, we will apply many techniques that were derived earlier in this thesis to join different bulks, verify the bulk-boundary correspondence, forget about symmetries, compute the symmetry index in multiple ways and finally determine the exponentially decaying eigenfunctions at the boundary, if present.

The Split-Step-Walk W is an alternating product of shifts and two-dimensional coin operations, i.e. a *coined quantum walk* as defined in Definition 3.3. More precisely, W is a translation invariant quantum walk on the line with two-dimensional coin space, that is a strictly local unitary operator on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ defined as

$$W = BS_{\downarrow}AS_{\uparrow}B. \tag{8.27}$$

On the canonical cell structure, the shift operations $S_{\downarrow}$, $S_{\uparrow}$ are minimal shifts in the sense of Definition 3.2. Thus, we fix a basis w.r.t. these shifts which we call *spin up* and *spin down* and denote with $+$ and $-$ respectively. We introduce the two shift operations

$$\begin{aligned} S_{\uparrow}|x,+\rangle &= |x+1,+\rangle & S_{\downarrow}|x,+\rangle &= |x,+\rangle \\ S_{\uparrow}|x,-\rangle &= |x,-\rangle & S_{\downarrow}|x,-\rangle &= |x-1,-\rangle, \end{aligned} \tag{8.28}$$

where $S_{\uparrow}$ shifts spin up vectors to the right while leaving spin down vectors untouched, and $S_{\downarrow}$ shifts spin down vectors to the left while leaving spin up vectors untouched. Note that the product $S_{\uparrow}S_{\downarrow}$ is the *standard shift* S in the quantum walk literature that was e.g. introduced in Section 3.1. The *coins* A and B are unitary operators that are block diagonal with respect to the spatial structure, i.e.

$$A = \bigoplus_{x\in\mathbb{Z}} A_x \qquad\qquad B = \bigoplus_{x\in\mathbb{Z}} B_x. \tag{8.29}$$

Thus in the general case, the coins can be chosen non-translation invariant, as we need later on the one hand for splitting and joining, on the other when transitioning to Section 8.5. Additionally, we assume that A and B themselves are admissible for the symmetries that will be introduced shortly. Since coins and symmetries are assumed to be block-diagonal, this admissibility constraint reduces to admissibility of A_x and B_x w.r.t. the on-cell symmetries.

The representation ρ on $\mathcal{H}$ for symmetry type BDI will now consist of

$$\eta = K \qquad \gamma = \bigoplus_{x\in\mathbb{Z}} \sigma_1 \qquad \tau = \eta\gamma = \bigoplus_{x\in\mathbb{Z}} \sigma_1 K \tag{8.30}$$

where K denotes complex conjugation which is real w.r.t. the basis chosen by the shifts, and σ_1 denotes the first Pauli-matrix $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ which flips the spin.

Since $\eta|x,s\rangle = |x,s\rangle$, η commutes with $S_\uparrow$ and $S_\downarrow$. The assumed admissibility of A and B for η then implies that A_x and B_x have real matrix elements w.r.t. the basis chosen. Therefore, the η-admissibility of each factor of W implies that W is admissible for η.

The chiral symmetry γ simply flips the spin, and we have

$$\begin{aligned} \gamma S_\uparrow|x,+\rangle &= |x+1,-\rangle = S_\downarrow^*\gamma|x,+\rangle \\ \gamma S_\uparrow|x,-\rangle &= |x,+\rangle = S_\downarrow^*\gamma|x,-\rangle. \end{aligned} \tag{8.31}$$

Exchanging $S_\uparrow$ and $S_\downarrow$ leads to a similar expression, and we get

$$\gamma S_\downarrow = S_\uparrow^*\gamma \qquad \gamma S_\uparrow = S_\downarrow^*\gamma. \tag{8.32}$$

The coin operations A and B are admissible for γ, if

$$A_x\sigma_1 = \sigma_1 A_x^* \qquad \text{and} \qquad B_x\sigma_1 = \sigma_1 B_x^*, \tag{8.33}$$

which from now on, we assume to hold. Then, we can simply see that W is admissible for γ, since

$$\gamma W = \gamma B S_\downarrow A S_\uparrow B = B^* S_\uparrow^* A^* S_\downarrow^* B^* = W^*\gamma. \tag{8.34}$$

This special alternating form, which is a concatenation of coins and shifts that is *symmetrical up to flips of the shifts* w.r.t. the central coin A, reminds of a *palindrome*. Thus, we refer to this form as ***γ-palindromic***.

Since η and γ square to $+\mathbb{1}$, and hence $\tau = \eta\gamma$ as well, we confirm that W is of symmetry type BDI, if η and γ are both part of ρ (and are thus not forgotten).

In the following, we choose different rules for A_x and B_x to allow different settings. Firstly, we choose the setting of *bulks*, which means that translation invariance fixes the coins for all x. Using the standard rotation matrix $R(\theta)$, i.e.

$$R(\theta) = e^{i\sigma_y\theta} = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}, \tag{8.35}$$

where σ_2 denotes the second Pauli-Matrix $\sigma_2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$, a BDI-admissible choice for the coins is

$$A_x = R(\theta_2) \qquad B_x = R(\theta_1/2). \tag{8.36}$$

This is easily checked: η-admissibility follows, since $R(\theta)$ has real entries. For γ, we see that

$$\sigma_x R(\theta) = \begin{pmatrix} -\sin(\theta) & \cos(\theta) \\ \cos(\theta) & \sin(\theta) \end{pmatrix} = R^*(\theta)\sigma_x, \tag{8.37}$$

implying admissibility of A and B for γ.

The translation invariance allows us to transition to momentum space by applying the Fourier transform as in Section 3.3. Since $R(\theta)$ is block diagonal in position space and independent of x, it is left unchanged by Fourier transform, and we have

$$\widehat{W}(k) = R(\theta_1/2)\begin{pmatrix} 1 & 0 \\ 0 & e^{-ik} \end{pmatrix} R(\theta_2)\begin{pmatrix} e^{ik} & 0 \\ 0 & 1 \end{pmatrix} R(\theta_1/2). \tag{8.38}$$

This can be decomposed into the right-moving, left-moving and still-standing parts, which correspond to the three non-vanishing coefficients in the Fourier expansion of $\widehat{W}(k)$. We get:

$$\begin{aligned} W_1 &= \frac{1}{2}\begin{pmatrix} (1+\cos\theta_1)\cos\theta_2 & \sin\theta_1\cos\theta_2 \\ -\sin\theta_1\cos\theta_2 & (1-\cos\theta_1)\cos\theta_2 \end{pmatrix} \\ W_{-1} &= \frac{1}{2}\begin{pmatrix} -(1-\cos\theta_1)\cos\theta_2 & \sin\theta_1\cos\theta_2 \\ -\sin\theta_1\cos\theta_2 & (1+\cos\theta_1)\cos\theta_2 \end{pmatrix} \\ W_0 &= \begin{pmatrix} -\sin\theta_1\sin\theta_2 & \cos\theta_1\sin\theta_2 \\ -\cos\theta_1\sin\theta_2 & -\sin\theta_1\sin\theta_2 \end{pmatrix}. \end{aligned} \tag{8.39}$$

To determine the spectrum of $\widehat{W}(k)$, we use the fact that in the non-trivial cases, there will always be γ or η (or both), even after forgetting symmetries. But (4.3) shows, that the spectrum is symmetrical w.r.t. the real axis, and hence (using (3.32)) we can diagonalize $\widehat{W}(k)$

$$\widehat{W}(k) = V^*(k)\begin{pmatrix} e^{i\omega(k)} & 0 \\ 0 & e^{-i\omega(k)} \end{pmatrix} V(k), \tag{8.40}$$

where $V(k)$ is the unitary matrix that diagonalizes $\widehat{W}(k)$. Using that the trace is invariant under cyclic permutations of factors, we have

$$\operatorname{tr}\widehat{W}(k) = \operatorname{tr}\left\{ V^*(k)\begin{pmatrix} e^{i\omega(k)} & 0 \\ 0 & e^{-i\omega(k)} \end{pmatrix} V(k) \right\} = 2\cos\omega(k). \tag{8.41}$$

The left hand side of this equation is easily computed from (8.38), leading to

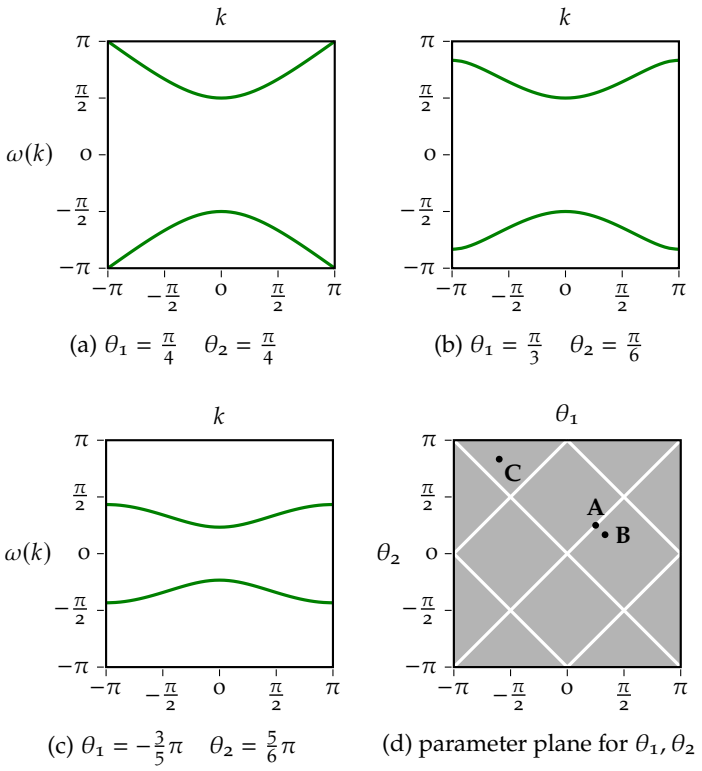
$$\cos\omega(k) = \cos k\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2. \tag{8.42}$$

For different values of θ_1, θ_2, we can analyse the dispersion relation. In order to satisfy the gap condition for W, there must not be any essential spectrum of W at ± 1. Since translation invariant operators have only essential spectrum, we need a proper gap at ± 1, or equivalently, $\omega(k)$ has to have a gap at 0 and $\pm\pi$. Values for θ_1 and θ_2 where this is not

the case do not create admissible walks and are hence excluded from our theory. Solving (8.42) for these values leads to

$$W_{\theta_1,\theta_2} \text{ admissible} \quad \Leftrightarrow \quad \nexists n \in \mathbb{Z} : \quad \theta_1 \pm \theta_2 = n \cdot \pi. \tag{8.43}$$

Figure 10 shows different dispersion relations for different values of θ_1 and θ_2, as well as the parameter plane with the excluded values.



(a) $\theta_1 = \frac{\pi}{4}$ $\theta_2 = \frac{\pi}{4}$ (b) $\theta_1 = \frac{\pi}{3}$ $\theta_2 = \frac{\pi}{6}$

(c) $\theta_1 = -\frac{3}{5}\pi$ $\theta_2 = \frac{5}{6}\pi$ (d) parameter plane for θ_1, θ_2

Figure 10: Dispersion relations for the Split-Step-Walk with different values of the angles θ_1 and θ_2 that fix the translation invariant walk. The walk in (a) is clearly not admissible, since it violates the gap condition at $\omega(k) = \pi \equiv -\pi$. The parameters for (b) are very close to (a) and we see that the gap just opened. (c) provides another walk which lies close to the gap at 0 but is still admissible. (d) shows the parameters of the different walks from (a)-(c). The white lines denote gap closures of the dispersion relation. Thus, the gap condition there is violated and walks from these parameters are excluded from our theory.

In the next step, we want to determine the symmetry index $\vec{\text{si}}(W)$ for the different values of θ_1 and θ_2, where the resulting W is admissible. Since W is a translation invariant quantum walk of symmetry type BDI, we have a chiral symmetry γ that squares to $+\mathbb{1}$ such that we can use the winding formula from Theorem 7.3 to determine $\vec{\text{si}}$.

We need to find the chiral block form for $\widehat{W}(k)$. γ acts like σ_1 on momentum space operators. σ_1 is then diagonalized by V:

$$\sigma_1 = V^* \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} V \qquad V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \tag{8.44}$$

Therefore, the chiral block form is given by

$$V\widehat{W}(k)V^* = \begin{pmatrix} \widehat{A}(k) & \widehat{B}(k) \\ -\widehat{B}^*(k) & \widehat{D}(k) \end{pmatrix}, \tag{8.45}$$

and we get

$$\widehat{B}(k) = \cos\theta_1 \sin\theta_2 + \cos\theta_2 \big(\sin\theta_1 \cos k + i \sin k \big) \tag{8.46}$$

with derivative

$$\frac{\mathrm{d}\widehat{B}(k)}{\mathrm{d}k} = -\cos\theta_2 \big(\sin\theta_1 \sin k + i \cos k \big). \tag{8.47}$$

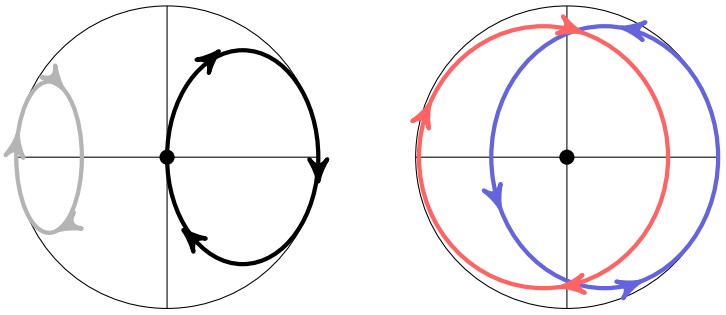
Even if $\widehat{B}(k)$ is continuously differentiable, it is easier to determine the value of $\vec{\mathrm{si}}(W)$ without using the integral formula. This is due to $\det \widehat{B}(k) = \widehat{B}(k)$, allowing us to read-off the winding number of this element easily, since it is an ellipse in the complex plane. It can be constructed from the unit circle by scaling it with $\cos\theta_2$, then scaling the real part by $\sin\theta_1$, and finally shift by $\cos\theta_1 \sin\theta_2$ along the real line, see (8.46). Figure 11 provides a visualization of the winding of the element, as well as the coloured parameter plane indicating $\vec{\mathrm{si}}(W)$ for each pair of θ_1 and θ_2. Now that we know the symmetry indices of W, considered as a translation invariant quantum walk of symmetry type BDI, we can deduce $\vec{\mathrm{si}}$ for the settings AIII and D. Since AIII is chiral symmetric with $\gamma^2 = \mathbb{1}$, the index formula for $\vec{\mathrm{si}}$ leads to the same result and we can refer to the parameter plane in Figure 11. Again, we can use the index formula

$$\vec{\mathrm{si}}(W) = \mathrm{si}\big(P \operatorname{Im} WP\big) \tag{8.48}$$

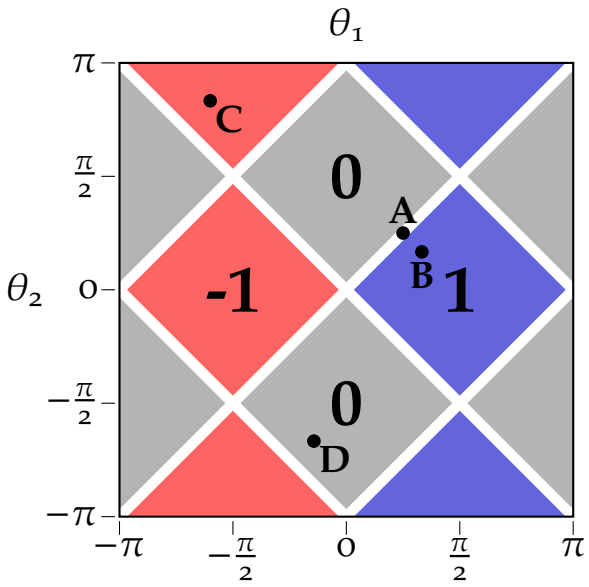
and deduce $\vec{\mathrm{si}}(W)$ for symmetry type D. That is, after determining $\ker P \operatorname{Im} WP$, we have to apply the index formula for symmetry type D from Section 4.4 to determine $\vec{\mathrm{si}}$ for D. In the case of BDI, we have $\mathrm{si}(\rho) = \operatorname{tr}\gamma$, and in the case of D it is $\mathrm{si}(\rho) = d \bmod 2$. This suffices to deduce $\vec{\mathrm{si}}$ for D from BDI, since

$$d \bmod 2 = (d_+ + d_-) \bmod 2 = (d_+ - d_-) \bmod 2 = \operatorname{tr}\gamma \bmod 2. \tag{8.49}$$

Hence $\vec{\mathrm{si}}$ for D follows from applying mod 2 to $\vec{\mathrm{si}}$ for BDI. Clearly, what we have done is, we verified the forget homomorphism from BDI to D from Table 2 by hand. The resulting parameter plane is shown in Figure 12. In the next step, we want to drop translation invariance and verify the *gentle decoupling theorem* from Theorem 5.20. More precisely, we find admissible unitary decouplings V s.t. $W' = VW$ differs from



(a) trivial / undefined winding (b) non-trivial winding of $\det \widehat{B}(k)$



(c) parameter plane for W

Figure 11: Winding of $\det \widehat{B}(k)$ for the translation invariant Split-Step Walk. The black winding in (a) stems from point A in the parameter plane of (c). It lies on a white line and is hence not covered by our setting. The winding number is undefined since it crosses the origin. The grey path for D does not wind around the origin and hence corresponds to $\vec{\mathrm{si}}(W) = 0$. The blue winding in (b) corresponds to B and $\vec{\mathrm{si}}(W) = 1$, while the red winding corresponds to C and $\vec{\mathrm{si}}(W) = -1$. We added colours in (c) to indicate the value of $\vec{\mathrm{si}}(W)$ matching the colour of the windings from (a) and (b). That is, red denotes -1, blue denotes 1 and grey denotes 0. The coordinates of A, B, C match with those in Figure 10, while D has $\theta_1 = -\frac{\pi}{7}$ and $\theta_2 = -\frac{2\pi}{3}$.

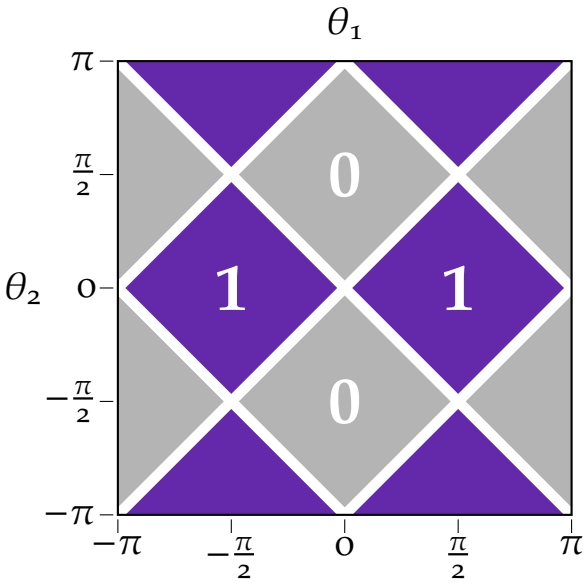


Figure 12: Parameter plane of the Split-Step-Walk for symmetry type D. The white lines denote non-admissible walks, while grey indicates $\vec{\mathrm{si}}(W) = 0$ and blue indicates $\vec{\mathrm{si}}(W) = 1$.

W only at a neighbourhood around the decoupling site $x = 0$. By definition, a decoupled operator W' is then given as

$$W' = W_L \oplus W_R, \tag{8.50}$$

where each half-space-walk acts only on $(\mathbb{1} - P)\mathcal{H}$ and $P\mathcal{H}$ respectively. The criterion for a decoupling is thus commutativity with P. Clearly, W and W' are compact admissible perturbations of each other. Hence the relative index of W' and W from Section 5.4 tells us, whether these perturbations are gentle or not. If $\mathrm{si}(W' : W) \neq 0$, we know that the absolute indices $\mathrm{si}_\pm$ of W and W' differ, rendering the perturbation non-gentle.

Let us now proceed to find minimal decouplings for W at $x = 0$. These are decouplings, where W is modified only on those $|x, s\rangle$, that are reached after applying W once to any vector localized at $x = 0$. For this argument, we return to the general setting of admissible W, which are not necessarily translation invariant, but where A and B are direct sums of potentially varying A_x and B_x. Since we only need commutativity with P, and B already commutes with P, because it is block-diagonal w.r.t. position, the decoupling at $x = 0$ is only decided by $S_\downarrow A S_\uparrow$. Due to the unitarity of W and V, we only need to check that $S_\downarrow A S_\uparrow$ leaves $P\mathcal{H}$ invariant, because the invariance of $(\mathbb{1} - P)\mathcal{H}$ then follows by unitarity.

W is a nearest neighbour quantum walk, and therefore we only have to look at the action of W on $|0, \pm\rangle$, because no element of $P\mathcal{H}$ that is orthogonal on $|0, \pm\rangle$ can be mapped to $(\mathbb{1} - P)\mathcal{H}$ due to the maximal

jump length of 1. Furthermore, we can rule out every contribution from $|0,+\rangle$, due to

$$S_\downarrow A S_\uparrow |0,+\rangle = S_\downarrow A |1,+\rangle \in P\mathcal{H}, \tag{8.51}$$

and the fact, that $S_\downarrow$ shifts at most by one step. Let A_0 denote the modified coin of the decoupled operator, s.t.

$$A_0 = \begin{pmatrix} a_{++} & a_{+-} \\ a_{-+} & a_{--} \end{pmatrix}. \tag{8.52}$$

Then, η-admissibility demands that the matrix elements are *real*, while γ-admissibility for A demands that

$$\sigma_1 A_0 = A_0^* \sigma_1 \qquad \Rightarrow \qquad a_{++} = a_{--}. \tag{8.53}$$

The action of $S_\downarrow A S_\uparrow$ on $|0,-\rangle$ can now easily be determined

$$S_\downarrow A S_\uparrow |0,-\rangle = S_\downarrow A |0,-\rangle = \big(a_{+-}|0,+\rangle + a_{--}|-1,-\rangle\big). \tag{8.54}$$

This lies in $P\mathcal{H}$ if and only if $a_{--} = 0$. Together with (8.53), this implies that A_0 has to be purely off-diagonal if W is supposed to be decoupled. Furthermore, unitarity of A demands that a_{+-} and a_{-+} lie on the unit circle, which leaves only four cases due to η-admissibility:

$$\begin{aligned} &\text{Case 1}: && A_0 = \begin{pmatrix} 0 & \pm 1 \\ \pm 1 & 0 \end{pmatrix} = \pm\sigma_1 \\ &\text{Case 2}: && A_0 = \begin{pmatrix} 0 & \pm 1 \\ \mp 1 & 0 \end{pmatrix} = \pm i\sigma_2 = \pm R(\pi/2). \end{aligned} \tag{8.55}$$

Figure 13 provides an explicit example of the matrix elements belonging to a Split-Step-Walk that was decoupled by $A_0 = -\sigma_1$, that is a non-gentle decoupling corresponding to case 1. Having found all minimal decouplings for the Split-Step-Walk even in the non-translation invariant case, let us now return to the translation invariant Split-Step-Walk, where $A_x = R(\theta_2)$ and $B_x = R(\theta_1/2)$ for all $x \in \mathbb{Z}$. In case 2, since the rotations $R(\theta)$ are all connected, admissible and continuous in θ, we can find a path

$$W_t := R\big(\theta_1/2\big) S_\downarrow R\big(\theta(t)\big) S_\uparrow R\big(\theta_1/2\big), \tag{8.56}$$

with $\theta(t) := (1-t)\theta_2 \pm t \cdot \pi/2$ such that the decoupled $W' = W_1$ is a gentle perturbation of $W = W_0$.

In the first case, note that the spectrum of $R(\theta_2)$ (that is, A_0 before the perturbation) consists of $e^{\pm i\theta_2}$. On the one hand, since $R(\theta_2)$ is admissible for η, an admissible and norm-continuous (i.e. gentle) perturbation can only move these eigenvalues symmetrically[6]. On the other hand, we see that A_0 has eigenvalues -1 and 1, with non-degenerate eigenvectors. Since BDI-admissibility fixes these eigenvalues, there is no way to move them without dropping either unitarity or admissibil-

6 This is the same argument as in the introduction to Section 4.3.

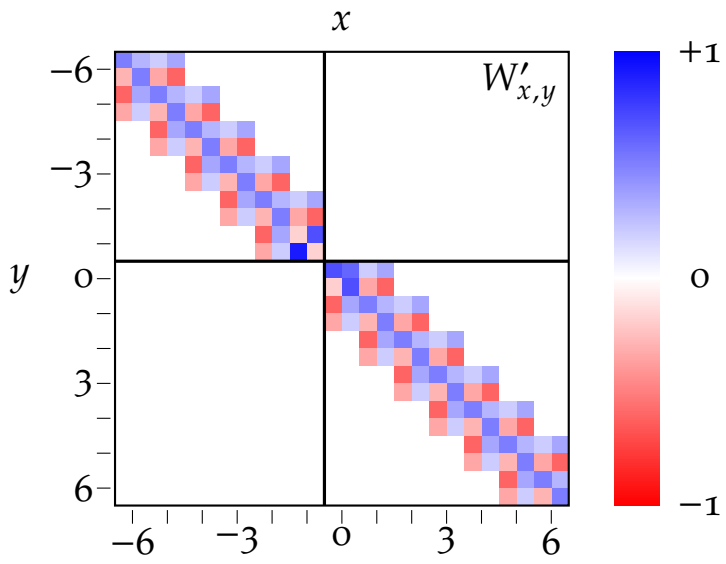


Figure 13: Matrix elements $W'_{x,y}$ of a decoupled Split-Step-Walk where $\theta_1 = \pi/3$ and $\theta_2 = \pi/4$. Each 2×2-block $W'_{x,y}$ represents the four spin-combinations in the coin space as in (8.52). η-symmetry forces each of them to be real. The black lines mark the block decomposition w.r.t. the projection P onto all cells $\mathcal{H}_x$ with $x \geq 0$ and its complement $\mathbb{1} - P$. The translation invariant walk W is modified only at $x = 0$ by setting $A_0 = -\sigma_1$. Due to the shifts $S_\uparrow$ and $S_\downarrow$, this changes only the matrix elements in a direct neighbourhood of $x = 0$. Since A_0 is a decoupling coin for the projection P, the off-diagonal blocks are empty. That is, no state localized in $P\mathcal{H}$ can be mapped to $(\mathbb{1} - P)\mathcal{H}$ and vice versa.

ity. Therefore, the compact (and local) admissible unitarity-preserving perturbation by $A_0 = \pm\sigma_1$ cannot be gentle.

In addition, we know that restricted to the ± 1-eigenspaces, γ and W commute, and we can choose the eigenvectors of W to be of definite chirality, that is they are eigenvectors of γ to eigenvalues $+1$ or -1. Let W denote the walk before the perturbation, and W' the walk after perturbing with A_0 from (8.55). Furthermore, denote by $\mathcal{N}_\pm$ and $\mathcal{N}'_\pm$ the ± 1-eigenspaces of W and W' respectively. Then,

$$\mathrm{si}_\pm(W) = \mathrm{tr}_{\mathcal{N}_\pm} \gamma \tag{8.57}$$

and W' analogously. For an admissible compact perturbation that is not necessarily gentle, the $\mathrm{si}_\pm$ themselves can change. But Theorem 5.9 guarantees that

$$\mathrm{si}_+(W) + \mathrm{si}_-(W) = \mathrm{si}(W) = \mathrm{si}(W') = \mathrm{si}_+(W') + \mathrm{si}_-(W'), \tag{8.58}$$

hence the overall change of the index has to vanish. Since W is a translation invariant operator, the overall symmetry index $\mathrm{si}(W)$ vanishes (see Theorem 5.9), and hence $\mathrm{si}(W')$ vanishes as well. In other words, whenever a perturbation creates (or removes) a W'-eigenvector at $\lambda \in \{\pm 1\}$ with chirality s, admissibility enforces that a second eigen-

vector emerges, which has opposing chirality $-s$, such that their contribution to $\mathrm{tr}_{\mathcal{N}'}\,\gamma$ vanishes. For a compact, non-gentle perturbation, the second eigenvector may emerge at $+1$ or -1, independent of λ.

But if the perturbation is *gentle*, we know from Theorem 5.5 that si_+ and si_- are each for themselves invariant. The consequence is, that for a gentle perturbation, the eigenvalues at λ must come (or go) in chirally opposite pairs.

Thus we have just created four different decouplings for W, two gentle and two non-gentle ones. Each of them modifies W only in three neighbouring single cells, arbitrarily chosen to be centred at $x = 0$. In addition, we know from Theorem 5.9 that $\overrightarrow{\mathrm{si}}(W) = \overrightarrow{\mathrm{si}}(W')$ and $\overleftarrow{\mathrm{si}}(W) = \overleftarrow{\mathrm{si}}(W')$, since both are invariant under arbitrary (admissible) compact perturbations. Therefore, the parameter planes for W denoting $\overrightarrow{\mathrm{si}}$ (and hence $-\overleftarrow{\mathrm{si}}$) from Figure 11 (and in the case of D from Figure 12) are both valid for W' as well.

We have now reached the point where we can finally analyse composed systems, that is join two different bulk systems and verify the *bulk-boundary-correspondence* from Theorem 5.12. But before we use the decoupling construction, let W_L and W_R be two translation-invariant ρ-admissible quantum walks. Furthermore, let W_c be a *crossover* (see Definition 5.11) between W_L and W_R. That is W_c agrees with W_L far to the left, and with W_R far to the right. Then, $\overleftarrow{\mathrm{si}}(W_c)$ coincides with $\overleftarrow{\mathrm{si}}(W_L)$, and $\overrightarrow{\mathrm{si}}(W_c)$ with $\overrightarrow{\mathrm{si}}(W_R)$. The bulk-boundary-correspondence now predicts

$$\mathrm{si}(W_c) = -\overrightarrow{\mathrm{si}}(W_L) + \overrightarrow{\mathrm{si}}(W_R). \tag{8.59}$$

Thus, if W_L and W_R are in different topological phases, i.e. $\overrightarrow{\mathrm{si}}(W_L) \neq \overrightarrow{\mathrm{si}}(W_R)$ and we have

$$\mathrm{si}(W_c) = \mathrm{si}(\mathrm{Im}\, W_c) \neq 0. \tag{8.60}$$

But a non-vanishing $\mathrm{si}(\mathrm{Im}\, W_c)$ demands that W_c has at least one eigenvector corresponding to eigenvalue $+1$ or -1, hence an eigenvalue in the gap. Since $\overrightarrow{\mathrm{si}}$ (and hence $\overrightarrow{\mathrm{si}}(W_R) - \overrightarrow{\mathrm{si}}(W_L)$) is invariant w.r.t. compact admissible perturbations, we can neither locally nor compactly perturb the walk s.t. this *topologically protected eigenvector* vanishes; at least not without breaking the symmetries. Moreover, Theorem 6.9 guarantees that these eigenvectors are localized at the boundary, and decay exponentially in the bulk. This is where a decoupling proves its strength: exponentially decaying eigenvectors of a decoupled walk are localized on one side of the cut, hence are supported only in one of the two bulks that were joined.

The gentle decoupling theorem allows us to decouple any admissible quantum walk W without changing its indices. That is, the resulting W' has the following form

$$W' = W_L \oplus W_R \qquad W_L = (\mathbb{1} - P)W'(\mathbb{1} - P) \qquad W_R = PW'P, \tag{8.61}$$

and the indices $\mathrm{si}_\pm$ and $\vec{\mathrm{si}}, \overleftarrow{\mathrm{si}}$ both coincide for W and W'. More precisely, we know from Definition 5.8 and Theorem 5.9 that

$$\begin{aligned}\overleftarrow{\mathrm{si}}(W) &= \mathrm{si}\big((\mathbb{1}-P)W(\mathbb{1}-P)\big) = \mathrm{si}(W_L) = \overleftarrow{\mathrm{si}}(W'),\\ \vec{\mathrm{si}}(W) &= \mathrm{si}\big(PWP\big) = \mathrm{si}(W_R) = \vec{\mathrm{si}}(W').\end{aligned} \tag{8.62}$$

Now, this allows for the simplest kind of composition. That is, we can create arbitrary pairs of W_L and W_R stemming from different quantum walks that are admissible for the same symmetry representation. The resulting *crossovers* W_c then represent any desired combination of $\vec{\mathrm{si}}(W_c)$ and $\overleftarrow{\mathrm{si}}(W_c)$. Furthermore, the decoupling simplifies searching for eigenfunctions considerably. That is, eigenvectors can always be chosen to be localized only on the left or right side of the cut, which makes the boundary conditions especially simple.

Returning to our example, we know that gentle and non-gentle decouplings for the translation invariant Split-Step-Walk are given by (8.56). Let W_L and W_R be left and right half-space quantum walks that stem from two different translation invariant Split-Step-Walks $\widehat{W}_L(k)$ and $\widehat{W}_R(k)$, which were decoupled by potentially different methods (e.g. by those derived before). Since these decoupled walks cannot be translation invariant any more, the restriction to essential spectrum alone is lifted and thus additional eigenvectors might have emerged in the process. But in general, one can simply construct a different perturbation and make these additional eigenvectors vanish or correspond to different eigenvalues. What we are interested in are eigenvectors that are *topologically protected*, that is, eigenvectors that cannot be removed by engineering the crossover between the two joined walks differently.

Their crossover $W_c = W_L \oplus W_R$ is then still a decoupled quantum walk, and hence eigenvectors of W_L and W_R become eigenvectors of W_c, corresponding to the same eigenvalue as before. With the help of Theorem 6.9, let us now explicitly determine the topologically protected eigenvectors of the translation invariant Split-Step-Walks that are decoupled by (8.55). By the above reasoning, if we then create crossovers W_c, we know that the topologically protected eigenvectors of the corresponding side of the cut simply carry over to the respective W_c.

In this approach we solve the eigenvalue equations for a translation invariant Split-Step-Walk W as a recursion relation in the bulk

$$W\phi = s\phi \qquad\qquad \gamma\phi = \chi\phi, \tag{8.63}$$

where $s = \pm 1$ and $\chi = \pm 1$. This yields exponential solutions, and selecting those solutions satisfying the boundary conditions imposed by the method of decoupling leaves us with the valid topologically protected eigenstates.

Let $\widetilde{W}(\lambda)$ be defined as in (6.48), that is

$$\widetilde{W}(\lambda) = \sum_{z\in\mathcal{N}} W_z \lambda^{-z}, \tag{8.64}$$

where W_z are the Fourier-coefficients of W that where computed in (8.39). The decay coefficients λ are then the solutions to

$$\det\left(\widetilde{W}(\lambda) - s\mathbb{1}\right) = 0, \tag{8.65}$$

as described in Theorem 6.9. In that section, no additional assumptions on admissibility were to be satisfied. But in this case, the fixed chirality χ from $\gamma\phi = \chi\phi$ simplifies the equations, since any solution ϕ has to satisfy

$$\phi(x) = c(x)\phi_0, \tag{8.66}$$

where ϕ_0 is an eigenvector of the action of γ on the single cells, that is σ_1, and $c(x)$ is a suitable complex coefficient that normalizes ϕ. The eigenvectors of σ_1 can be chosen as

$$\phi_0 = \left(|+\rangle + \chi|-\rangle\right) = \begin{pmatrix} 1 \\ \chi \end{pmatrix}, \tag{8.67}$$

such that $c(x)$ are real coefficients by the choice of η as complex conjugation, which leaves the basis elements $|x, s\rangle$ invariant. Thus, taking chirality into account, (8.65) is replaced by

$$\widetilde{W}(\lambda)\begin{pmatrix} 1 \\ \chi \end{pmatrix} = s\begin{pmatrix} 1 \\ \chi \end{pmatrix}. \tag{8.68}$$

The solutions to this equation are the decay coefficients $\lambda_{s\chi}$,

$$\begin{aligned} \lambda_{+\chi} &= \frac{\cos\theta_- - \chi\sin\theta_+}{\cos\theta_- + \chi\sin\theta_+} \\ \lambda_{-\chi} &= \frac{\sin\theta_- - \chi\cos\theta_+}{\sin\theta_- + \chi\cos\theta_+} \end{aligned} \tag{8.69}$$

where $\theta_\pm = \frac{1}{2}(\theta_1 \pm \theta_2)$. Since $\lambda_{s+} \cdot \lambda_{s-} = 1$, there is always[7] exactly one solution that provides exponential decay to the right $|\lambda| < 1$, and exactly one solution that provides exponential decay to the left $|\lambda| > 1$. Hence in our case we have only one decay coefficient λ for every candidate ϕ, and the ansatz from Theorem 6.9 yields up to normalization

$$\phi_R(x) = \left(\lambda_{s\chi}\right)^x \begin{pmatrix} 1 \\ \chi \end{pmatrix} \quad \forall x > 0, \tag{8.70}$$

if $|\lambda| < 1$, and $\phi_R(x) = 0$ for all $x < 0$. The ansatz for eigenvectors localized on the left-hand side is then

$$\phi_L(x) = \left(\lambda_{s\chi}\right)^{-x} \begin{pmatrix} 1 \\ \chi \end{pmatrix} \quad \forall x < 0, \tag{8.71}$$

if $|\lambda| > 1$, and $\phi_L(x) = 0$ for all $x > 0$.

7 The case $\lambda_{s+} = 1 = \lambda_{s-}$ is excluded since these values of θ_1 and θ_2 correspond to non-admissible walks, indicated by the white lines in Figure 10.

The fact that the walk is a nearest neighbour walk could make it necessary to determine the value of $\phi(0)$ differently, such that it satisfies the boundary condition imposed by the specific crossover. Theorem 6.9 and ρ-admissibility provided necessary conditions for the eigenvectors that correspond to eigenvalues in the gap, but if these vectors do not satisfy the constraints imposed by the decoupled walk at the boundary $x = 0$, they are no eigenvectors for W at all. As was already suggested in (8.58), the different choices of A_0 that determine how the decoupling is made now impose different boundary conditions for ϕ_L and ϕ_R.

Checking the eigenvalue-equation for every combination of s and χ for both ϕ_R and ϕ_L and all four different decouplings lead to an intricate case distinction that can be followed in all detail in the Mathematica™ file [Sta15b] which was published as supplementary material along [Ced+15]. The combinations of χ and s for the different choices of A_0 that satisfy the boundary condition are also represented shortly. Note that in this example, allowing for an arbitrary $\phi(0)$ never made ϕ satisfy a boundary condition it did not satisfy already by extending the definition of (8.70) to $\phi_R(0)$, or setting $\phi_L(0) = 0$. That is, the simplest choice for $\phi(0)$ always sufficed. This allows us to determine the normalization constant, which by the geometric series and $\|\phi_0\| = \sqrt{2}$ leads to

$$\begin{aligned} \phi_R(x) &= \sqrt{\frac{1-|\lambda_{s\chi}|^2}{2}}\,(\lambda_{s\chi})^x \begin{pmatrix} 1 \\ \chi \end{pmatrix} && \forall x \geq 0, \\ \phi_L(x) &= \sqrt{\frac{1-|\lambda_{s\chi}|^{-2}}{2}}\,(\lambda_{s\chi})^{-x} \begin{pmatrix} 1 \\ \chi \end{pmatrix} && \forall x < 0. \end{aligned} \tag{8.72}$$

The candidates for eigenfunctions on the respective side of the cut are represented in Table 3. We see that there are at most two topologically

ϕ_L	$\chi = 1$	$\chi = -1$
$s = 1$	$(1+, 2+)$	$(1-, 2-)$
$s = -1$	$(1-, 2-)$	$(1+, 2+)$
ϕ_R	$\chi = 1$	$\chi = -1$
$s = 1$	$(1+, 2-)$	$(1-, 2+)$
$s = -1$	$(1-, 2+)$	$(1+, 2-)$

Table 3: The different combinations of s and χ that are compatible with the boundary conditions imposed by the different A_0. Here, the digits with the sign denote the case from (8.55), with the corresponding sign for the Pauli matrix, e.g. the cell $(1-, 2+)$ denotes that decoupling with $-\sigma_1$ or with $+i\sigma_2$ yields an eigenfunction ϕ_R on the right hand side with eigenvalue $s = 1$ and chirality $\chi = 1$. Note that satisfying the boundary condition does not yet imply that the eigenvector exists for every θ_1 and θ_2.

protected eigenvectors at each side of the cut for each decoupling. But

for e.g. ϕ_R to exist, it has to be paired with $|\lambda_{s\chi}| < 1$, which strongly depends on θ_1 and θ_2. Hence only all constraints together decide about whether we have zero, one or two topologically protected eigenstates on each side of the cut. The areas where $|\lambda_{s\chi}| < 1$ are shaded in Figure 14.

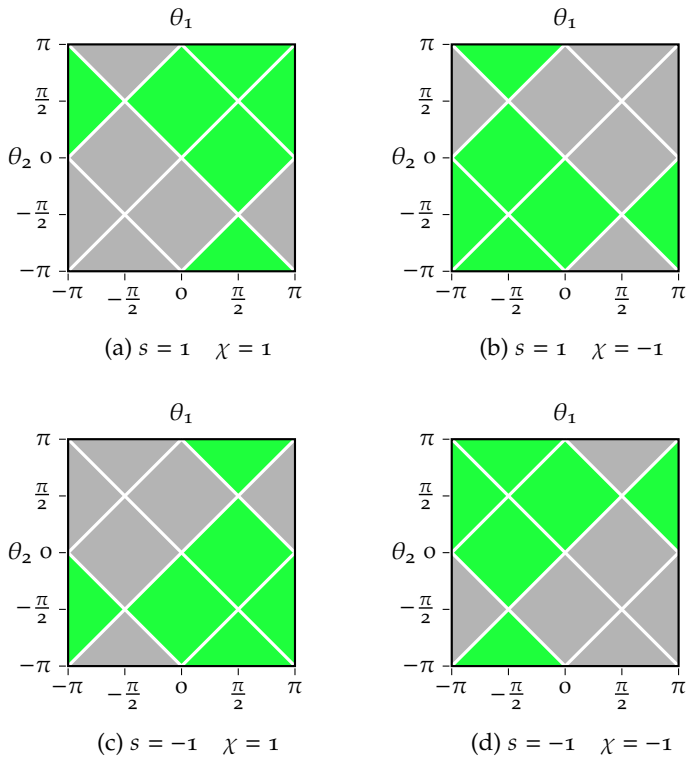
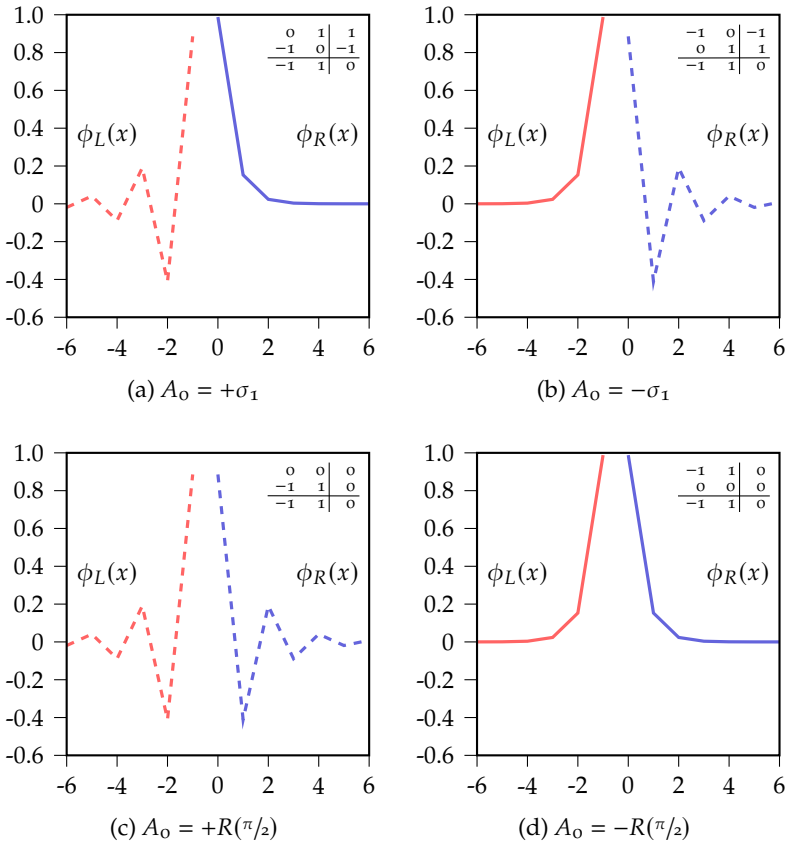


Figure 14: Parameter plane of the Split-Step-Walk. The green areas represent $|\lambda_{s\chi}| < 1$, while grey areas represent $|\lambda_{s\chi}| > 1$. Hence, if a Split-Step-Walk has a candidate for an eigenvector that is compatible with the boundary conditions of the decoupling as shown in Table 3, the corresponding parameter plane in this figure indicates whether the decay coefficient $\lambda_{s\chi}$ corresponds to a right eigenvector ($|\lambda_{s\chi}| < 1$) or a left eigenvector ($|\lambda_{s\chi}| > 1$).

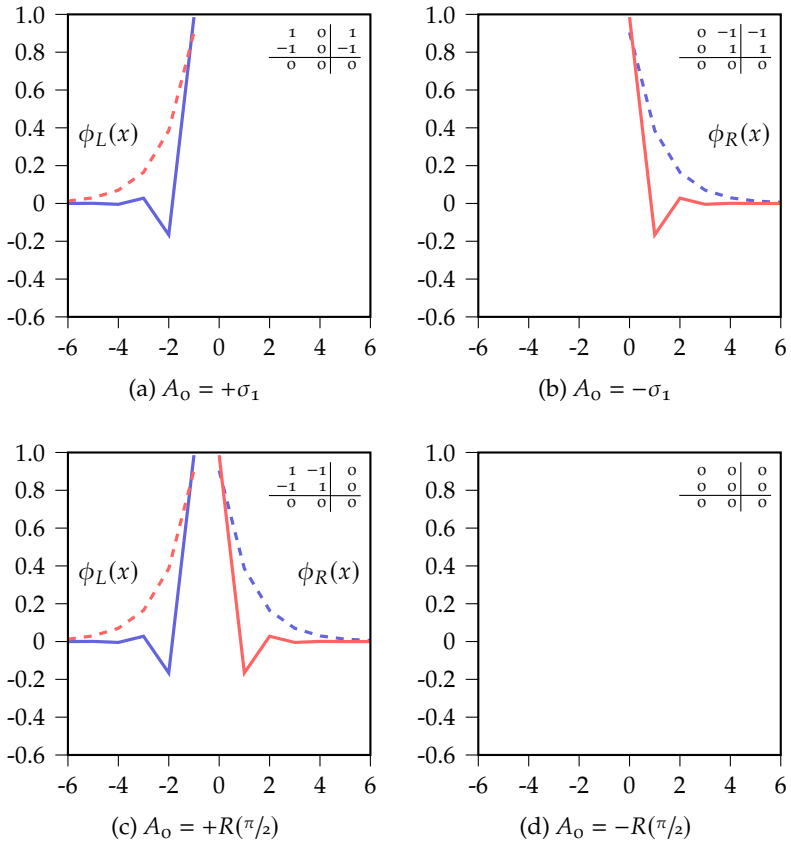
Finally, this allows us to plot the eigenfunctions for two examples of θ_1 and θ_2 for all four decouplings, see Figure 15 and Figure 16. More precisely, the plots show the real valued-coefficients $\phi_L(x)$, $\phi_R(x)$ up to the factor ϕ_0. This allows to distinguish whether the phase jumps from site to site indicating whether $\lambda_{s\chi}$ is negative or positive, as opposed to traditional plots that show only the probability $p(x) = \|\phi(x)\|^2$. The inset used in the figure gives a quick overview about the different symmetry indices as introduced in (5.57). Note that the overall symmetry index $\mathrm{si}(W)$ is always 0, which can be seen as follows: W is a compact perturbation of a *translation invariant* Split-Step-Walk, which has vanishing si by Theorem 5.9. But compact perturbations leave $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ invariant, and therefore their sum si as well. The marginal column sums lead to $\overleftarrow{\mathrm{si}}(W)$ and $\overrightarrow{\mathrm{si}}(W)$, whose value is also indicated



(a) $A_0 = +\sigma_1$ (b) $A_0 = -\sigma_1$

(c) $A_0 = +R(\pi/2)$ (d) $A_0 = -R(\pi/2)$

Figure 15: Exponentially decaying eigenfunctions at the cut point $x = 0$ for B from Figure 10. The exact values of $\phi_L(x)$ and $\phi_R(x)$ can be found in (8.72). The four different decoupling-coins A_0 generate different eigenfunctions at the respective sides as predicted. For each eigenfunction, a solid line denotes that the respective eigenvalue is $s = +1$, while a dashed line indicates $s = -1$. Furthermore, a blue colour refers to positive chirality $\chi = +1$, while a red colour indicates $\chi = -1$. Thus, the emergence of an eigenfunction has direct consequences for all relevant symmetry indices in the inset table. Due to the invariance of $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ w.r.t. compact admissible perturbations, all four decouplings leave $\overleftarrow{\mathrm{si}}(W) = -1$ and $\overrightarrow{\mathrm{si}}(W) = +1$ invariant, which is still the same value that the translation invariant walk had before decoupling. On the one hand, for non-gentle decouplings $A_0 = \pm\sigma_1$, the row-sums in the inset table show that si_+ and si_- can change, as opposed to $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$. On the other, gentle decouplings $A_0 = \pm R(\pi/2)$ change neither $\overleftarrow{\mathrm{si}}$, $\overrightarrow{\mathrm{si}}$, nor $\mathrm{si}_\pm$. The exponential decay, as well as the site-wise sign flip in the case of $-1 < \lambda < 0$ are readily seen in the graphs.



(a) $A_0 = +\sigma_1$ (b) $A_0 = -\sigma_1$

(c) $A_0 = +R(\pi/2)$ (d) $A_0 = -R(\pi/2)$

Figure 16: Exponentially decaying eigenfunctions at the cut point $x = 0$ for D from Figure 11. The same analysis as in Figure 15 applies for this example as well. Note that the Split-Step-Walk at these values of θ_1 and θ_2 is in an area of $\overrightarrow{\mathrm{si}}(W) = 0 = \overleftarrow{\mathrm{si}}(W)$, and thus the column sums of the 2×2-inset both have to vanish. That is, on each side of the cut the eigenfunctions have to occur in chirally opposite pairs, which is readily indicated by the differing colour on each side. While the gentle decouplings $A_0 = \pm R(\pi/2)$ may not change the row sums $\mathrm{si}_\pm(W)$ on the right, the non-gentle decouplings $A_0 = \pm\sigma_1$ again can. Nevertheless, all decouplings leave the overall sum of the indices, $\mathrm{si}(W)$, invariant.

by the colouring of the parameter plane. As explained in (8.58), since case 2 denotes a gentle perturbation, it does not change the marginal row sums $\mathrm{si}_\pm(W)$. But $\pm\sigma_1$ in case 1 is a non-gentle perturbation, and therefore $\mathrm{si}_\pm(W)$ can change. $\mathrm{si}_\pm(W_L)$ and $\mathrm{si}_\pm(W_R)$ reflect whether an eigenvector emerged at the left or the right side, whether it emerged at $s = +1$ or $s = -1$, and whether it had chirality $\chi = +1$ or $\chi = -1$, as denoted by the inset, known from (5.57):

$$\begin{array}{cc|c} \mathrm{si}_+(W_L) & \mathrm{si}_+(W_R) & \mathrm{si}_+(W) \\ \mathrm{si}_-(W_L) & \mathrm{si}_-(W_R) & \mathrm{si}_-(W) \\ \hline \overleftarrow{\mathrm{si}}(W) & \overrightarrow{\mathrm{si}}(W) & \mathrm{si}(W) \end{array} \tag{8.73}$$

In conclusion, we have thoroughly analysed the translation invariant Split-Step-Walk and applied many results from the translation invariant, as well as general theory of the thesis to great effect.

The following section will briefly describe how these results were visualized first in an interactive Mathematica-notebook, and then in an interactive web-application that accompanied papers and posters of this research.

8.3 SPLIT-STEP-EXPLORER

This interlude explains the motivation behind- and creation of the *Split-Step-Explorer*, that was repeatedly mentioned throughout this thesis. It is an important tool we used to properly understand, visualize and communicate many results and applications of our classification of quantum walks with discrete symmetries of the tenfold-way.

The everyday usage of Mathematica™ [Wol17] in our research motivated us to create a toolbox to test our predictions and conjectures against the well-known examples. That is, we implemented the basic building blocks that span the class of coined quantum walks, namely arbitrary spin-dependent shifts and position-dependent coins. Then, we implemented the algebraic relations to look at time evolutions of arbitrary initial states by any coined quantum walk. Using Mathematicas acceptably efficient implementation of sparse- and dense-array-algebra[8], we could perform a few thousand time steps on a typical lattice of a few thousand cells e.g. for a Split-Step-Walk, Four-Step-Walk or a similar Few-Step-Walk with arbitrarily position dependent coins in double precision within seconds on an average laptop. Due to the simplicity to switch to arbitrary precision, we could distinguish rare numerical artefacts from actual effects. As an example, 5000 decimal digits precision on a lattice with 2000 sites and a Split-Step-Walk performing 1000 time steps on an initially localized vector takes about one minute on a laptop.

8 In the Wolfram Language, arrays are called PackedArrays for some reason, while Arrays usually denote Lists of arbitrarily mixed objects or types.

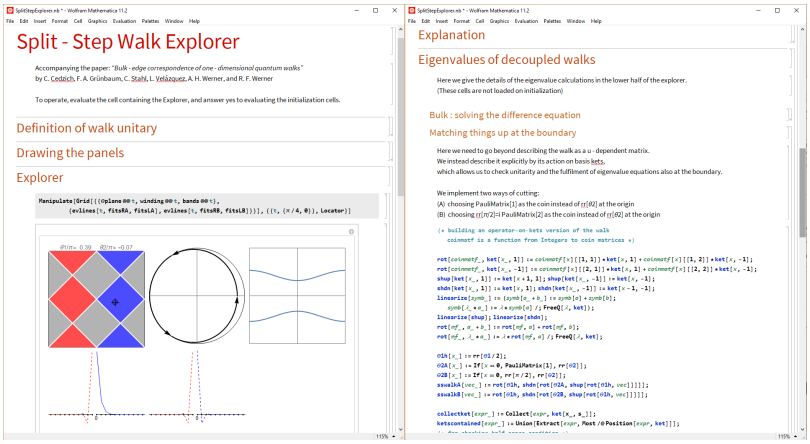


Figure 17: The first version of the Split-Step-Explorer, published [Sta15b] along the announcement of our classification [Ced+15]. It contains all intermediate steps and definitions of the deductions in Section 8.2. In addition, the interactive panel allows to choose a Split-Step-Walk via the parameter plane, and see the winding of $\det \widehat{B}(k)$, the quasi-energy-spectrum $\omega(k)$ and the topologically protected eigenvalues in the gap, depending on the decoupling chosen. Moreover, there is an implementation of the Split-Step-Walk that allows for arbitrary, non-translation invariant coins, and acts on general basis elements, or *kets*. Additionally, it serves to verify the boundary conditions for every decoupling imaginable.

To *exactly* verify a pen-and-paper calculation, we wrote a *symbolic* algebraic implementation *on kets*, e.g. to check boundary conditions or periodic effects stemming from coins with angles that are rational multiples[9] of π. This was done by defining a basic symbolic object called *ket*, on which operators are defined just as on paper. Time evolution with a quantum walk acting on these kets then leads to larger and larger sums of kets, leaving us with an intricately nested tree of objects. Such an approach is feasible for a few hundred time steps if one starts from a single (or a few) kets.

For translation invariant systems, we used the Fourier transform to translate the algebra of coined quantum walks into the algebra of matrix-valued Laurent polynomials in e^{ik}. This allowed us to determine spectrum and windings analytically, which is necessary e.g. if we want to distinguish *essential* and *discrete* spectrum.

Synthesizing all these approaches, we created the Split-Step-Explorer in Mathematica [Sta15b] (see Figure 17) to follow the examples in our (and others') papers. The openness and modularity of the notebook allows everyone to modify the tools and methods presented to his or her needs.

In talking with other groups and through discussions after talks and poster-sessions at conferences we learned, that providing a notebook

9 More precisely, a walk that is translation invariant w.r.t. a shift of q-cells, if q denotes the denominator of the angle of the coin in multiples of π.

for Mathematica is not yet accessible enough for many researchers, since most universities do not provide licenses for the researchers, or that any other similarly powerful tool like MATLAB [Mat17] or SciPy [JOP+01] is used for their research, such that installing and starting Mathematica was too much of an effort. Thus in the 21th century, it turned out to be appropriate to create a web-application [Sta15a] that is supported by any sufficiently modern web-browser, which we hence did. Figure 18 shows a screenshot of the Split-Step-Explorer web-application. This was favoured over a separate application for Smartphones or Tablets, since a web-application was simply the most accessible solution, even if this meant to lower one's sights regarding the performance.

We decided to use Bootstrap [OT16] to provide good accessibility of the controls, a clean interface and make everyone feel right at home as if navigating any major website. Since our approach to topological phases did not need to perform large-scale time evolutions of walks, or diagonalization of large unitary matrices, we did not need to do any *heavy load* on the hosting backend, but could simply rely on the client browser to do necessary computations. D3.js [Bos16], the JavaScript library for producing dynamic, interactive data visualizations in websites provided the necessary framework to do beautiful plotting and allow to interact with mouse and touch. To parse LaTeX-based input, we used MathJax [Soc09], which made typesetting beautiful equations in web pages as easy as in a paper. The final Split-Step-Explorer [Sta15a] shows most of the results from Section 8.2, as is seen in Figure 18.

While preparing a poster for an annual Quantum Walk conference in Prague [Sta+16], we decided to make the poster interactive by mounting a Tablet-PC to the wall, right on the poster. This required a few adjustments to the Split-Step-Explorer web-application, since it should also function as a screensaver-like slideshow of our results. It turned out that this version serves equally well to visualize our results using a video projector in a presentation. A screenshot of the final version [Sta16] is found in Figure 19.

Note that the Split-Step-Walk W' in the explanation of the Split-Step-Explorer differs from the Split-Step-Walk W in Section 8.2 by conjugation with B. That is,

$$W' = B^* W B = S_\downarrow A S_\uparrow B^2. \tag{8.74}$$

The reason is, that this is the most commonly found form of the Split-Step-Walk, even if it has disadvantages (see the previous section for the details). This requires to modify the symmetry representation ρ by conjugation with B, making ρ site-dependent, and potentially parameter dependent, if B has any of these dependencies. η is not changed by conjugation with B, since we restricted ourselves to η-admissible coin matrices B, which means that B and η commute.

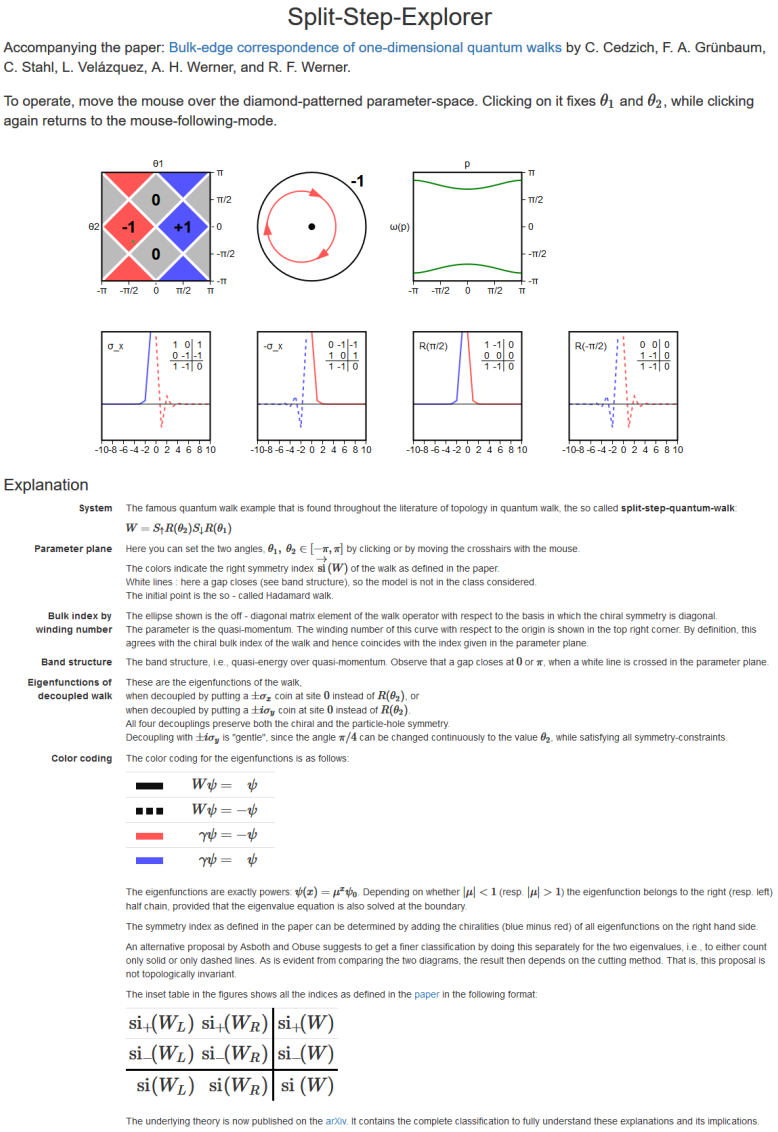


Figure 18: Screenshot of the Split-Step-Explorer as a web-application. By moving the mouse over (or touching / clicking) the parameter plane, one can modify the underlying, translation invariant Split-Step-Walk. The parameter plane is statically drawn from the known data, while the winding of the chiral block, the quasi-energy spectrum, as well as the topologically protected eigenstates in the four differently decoupled cases are generated on-the-fly in the browser, using the results from Section 8.2. It is found at [Sta15a].

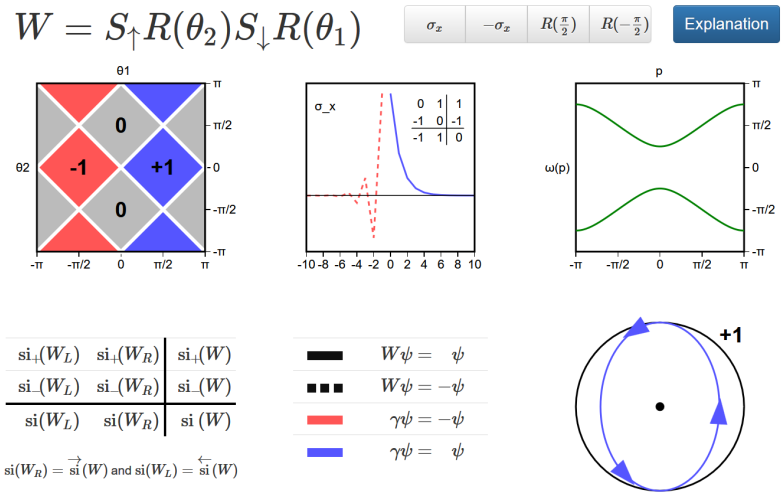


Figure 19: Screenshot of the *reduced* Split-Step-Explorer as a web-application that is optimized for presentation on a video projector or tablet. Usage is identical to the full-version from Figure 18, except that one has to choose the decoupling coin that is shown in the top panel. The explanation is displayed if one clicks on the corresponding blue button. Zooming in the browser leaves the panel untouched, while trying to optimize the space for the plots. This version of the Split-Step-Explorer is found at [Sta16].

But for γ (and hence τ), this is not the case. Thus, on the one hand, this modification makes the new chiral symmetry B-dependent. On the other, we know that conjugation with a unitary operator does not change the spectrum of any operator, but only changes the basis in which we build our quantum walks. Hence, after a relabelling of all states $\psi \in \mathcal{H}$ with $B^*\psi \in \mathcal{H}$, we are again describing the (almost) γ-palindromic Split-Step-Walk, since

$$\langle B^*\phi, S_\downarrow A S_\uparrow B^2 B^* \psi \rangle = \langle \phi, B S_\downarrow A S_\uparrow B \psi \rangle. \tag{8.75}$$

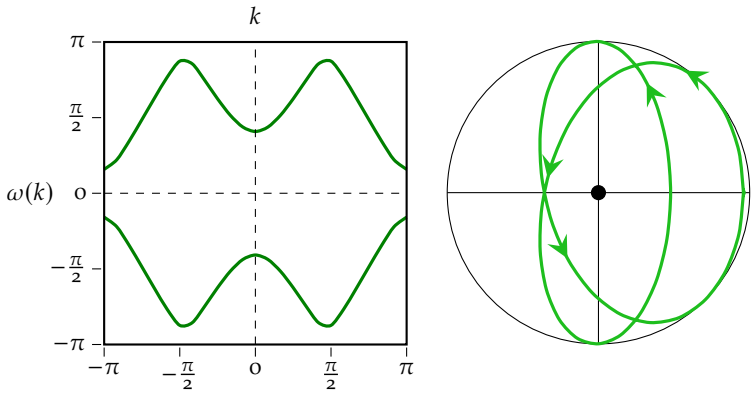
In the following section, we extend the Split-Step-Walk by adding another set of coins and shifts in the *Four-Step-Example*.

8.4 FOUR-STEP-EXAMPLE

Due to the modularity of the analysis of the Split-Step-Walk in Section 8.2, we can simply extend these results to similar examples containing more shifts and coins. In order to satisfy γ-symmetry stepwise, we have to keep the example γ-palindromic, which is satisfied by

$$W = C S_\downarrow B S_\downarrow A S_\uparrow B S_\uparrow C, \tag{8.76}$$

where A, B and C are coins, i.e. unitary operators that are block-diagonal w.r.t. position. ρ-admissibility follows exactly as before, and



(a) dispersion relation of $\widehat{W}(k)$ (b) winding of $\det \widehat{B}(k)$

Figure 20: A particular example of the Four-Step-Walk as defined in (8.76), with $\theta_0 = \pi/5$, $\theta_1 = \pi/16$ and $\theta_2 = \pi/12$. Similar to the Split-Step-Walk in Figure 10, the quasi-energy $\omega(k)$ in (a) indicates the admissibility of $\widehat{W}(k)$ since it leaves the gap at 0 and π open, and is symmetric w.r.t. the gap. (b) shows that $\det \widehat{B}(k)$ winds twice around the origin, which leads to $\vec{\mathrm{si}}(W) = +2$. Note that due to η-symmetry, the winding of $\det \widehat{B}(k)$ is symmetrical w.r.t. the real axis, as is shown in (7.46). Furthermore, the dispersion relation has all three symmetries from (7.5), that are axial symmetries w.r.t. the dashed lines (τ and γ), as well as their composition (η), which imposes point symmetry w.r.t. the origin.

the decoupling theory applies by choosing A_0 and B_0 both as the decoupling coin from (8.52).

As an example, let us first look at the translation invariant case where A, B and C are rotations as in Section 8.2:

$$A_x = R(\theta_2) \qquad B_x = R(\theta_1) \qquad C_x = R(\theta_0/2) \qquad \forall x \in \mathbb{Z}. \tag{8.77}$$

Similar to (8.42), we derive the dispersion relation via

$$\cos \omega(k) = \frac{1}{2} \operatorname{tr} \widehat{W}(k) = c_0 + c_1 \cos k + c_2 \cos 2k, \tag{8.78}$$

where

$$\begin{aligned} c_0 &= -\cos\theta_0 \sin^2\theta_1 \cos\theta_2 - \sin\theta_0 \cos(2\theta_1) \sin\theta_2 \\ c_1 &= -\sin(2\theta_1) \sin(\theta_0 + \theta_2) \\ c_2 &= \cos\theta_0 \cos^2(\theta_1) \cos\theta_2. \end{aligned} \tag{8.79}$$

An example of the dispersion relation and (following Theorem 7.3) the winding of $\det \widehat{B}(k)$ is shown in Figure 20. In principle, this allows us to analyse the gap closings and hence find the non-admissible angles for the Four-Step-Walk. But it turns out to be easier to use an equivalent criterion for this purpose, as described shortly. To apply it, we need the chiral block $\widehat{B}(k)$, which additionally serves to determine the symmetry index $\vec{\mathrm{si}}(W)$. It is computed exactly as in (8.46).

The symmetry index as a winding number can only change if the path $\widehat{B}(k)$ crosses the origin. But this case is excluded, not only because the winding number (and hence the index) is undefined in these cases, but also because $\widehat{B}(k_0) = 0$ implies that $\widehat{W}(k_0)$ violates the gap condition. This can easily be seen, since $\widehat{B}(k_0) = 0$ implies that $\widehat{W}(k_0)$ is block diagonal in γ-eigenbasis, hence commutes with γ. On the other hand, $\widehat{W}(k_0)$ is γ-admissible which implies that it is real. But if $\widehat{W}(k_0)$ is a real diagonal matrix, its eigenvalues are clearly real and unitary, hence ± 1 - violating the gap condition at k_0.

We find all k_0 s.t. $\widehat{B}(k_0) = 0$ in two steps. Firstly, we analyse the necessary condition of vanishing imaginary part $\operatorname{Im}\widehat{B}(k_0) = 0$. Then, we find the zeros to the remaining equation within the set of k_0 s.t. $\widehat{B}(k_0)$ is real. The solutions to

$$\operatorname{Im}\widehat{B}(k_0) = \frac{1}{2i}\left(\widehat{B}(k_0) - \widehat{B}^*(k_0)\right) = 0 \tag{8.80}$$

are $k = 0$, $k = \pi$ or

$$\cos k + i \sin k = \frac{\sin\theta_1 \cdot \sin\theta_2 \pm \sqrt{-\cos(2\theta_1) - \cos(2\theta_2)}}{\sqrt{2}\cos\theta_1 \cos\theta_2}. \tag{8.81}$$

Inserting them back into $\widehat{B}(k_0)$ leaves only two cases to distinguish:

$$\begin{aligned} &\widehat{B}(k_0) = 0 = \sin(\theta_0 \pm 2\theta_1 + \theta_2) \quad \text{or} \\ &\widehat{B}(k_0) = 0 = \sin(\theta_0 - \theta_2). \end{aligned} \tag{8.82}$$

That is, we have to exclude the following non-admissible values for the Four-Step-Walk

$$\exists n \in \mathbb{Z}: \quad \theta_0 \pm 2\theta_1 + \theta_2 = n\pi \quad \text{or} \quad \theta_0 - \theta_2 = n\pi. \tag{8.83}$$

Now that we have identified the phase boundaries at which the winding number of $\det\widehat{B}(k)$ can change, we determine $\vec{\mathrm{si}}(W)$ for all translation invariant admissible Four-Step-Walks by computing it for a representative on each octahedron or tetrahedron that the constraints from (8.83) form. This can either be done by inspecting the winding of $\widehat{B}(k)$, or by computing the winding number directly via the integral from Theorem 7.3. Figure 21 shows the non-admissible values for the Four-Step-Walk, as well as the (surface of) the three-dimensional parameter-cube with the symmetry index $\vec{\mathrm{si}}(W)$ indicated by the colour similar to the Split-Step-Walk in Figure 11. Note that the doubling of the shift operations now increases the range of the symmetry index to

$$\vec{\mathrm{si}}(W) \in \{-2, -1, 0, 1, 2\}. \tag{8.84}$$

In what follows, we want to modify the Four-Step-Walk from above such that it explicitly breaks η-symmetry, and hence yields an example of AIII.

Both the Split-Step-Walk and the Four-Step-Walk we considered were BDI-admissible, and therefore had an η-symmetry that squared to $+\mathbb{1}$. As was mentioned in Figure 20, the direct implications of the

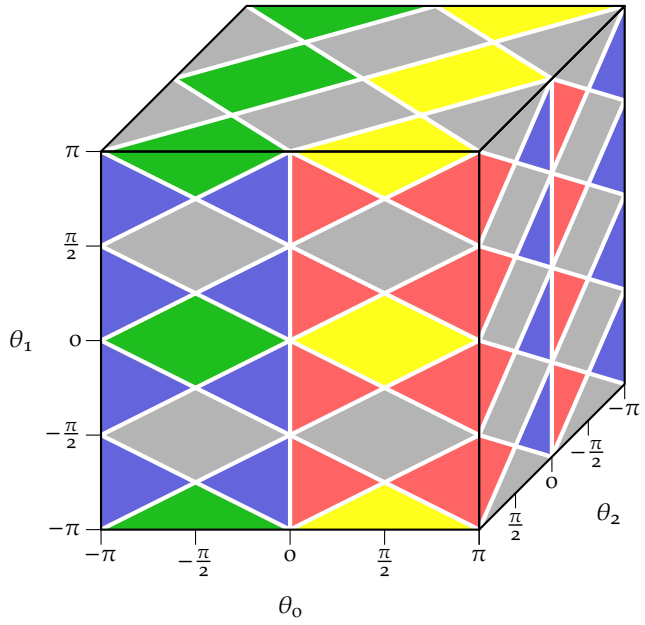


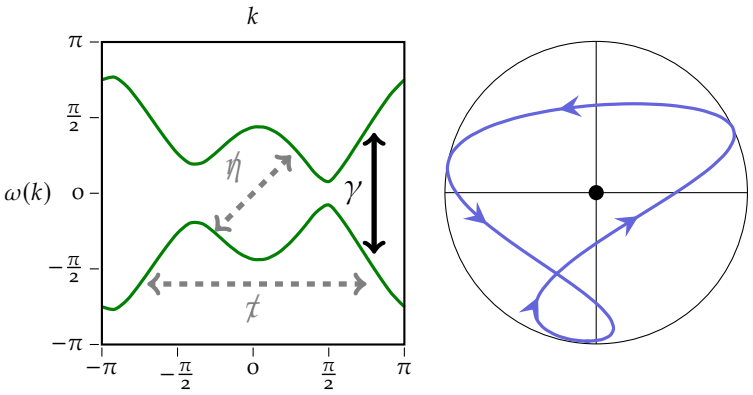
Figure 21: The three dimensional parameter cube for the Four-Step-Walk. White lines denote the parameters that lead to non-admissible Four-Step-Walks and are hence excluded. The colour coding corresponds to the one from the Split-Step-Walk, where grey denotes trivial index, while blue and red indicate $\vec{\text{si}}(W) = +1$ and $\vec{\text{si}}(W) = -1$ respectively. Due to the fact that the number of shifts is doubled compared to the Split-Step-Walk, the maximum (and minimum) value of $\vec{\text{si}}$ doubles as well. Hence we denote $\vec{\text{si}}(W) = +2$ in green and $\vec{\text{si}}(W) = -2$ in yellow.

presence of an η-symmetry are the point-symmetry of the dispersion relation w.r.t. the origin and the axial symmetry of the winding of the determinant of the chiral block $\widehat{B}(k)$ w.r.t. the real axis. Both properties were computed in (7.5) and visualized in Figure 7.

As a second example, we insert an additional coin $M = i(\sigma_2 + \sigma_3)/\sqrt{2}$ between C and $S_\downarrow$ (and $S_\uparrow$ respectively) to explicitly *break* η- (and hence τ-) symmetry, and not only *forget* about them. Thus, we are left with a chiral symmetry γ alone and get

$$W_M = CMS_\downarrow BS_\downarrow AS_\uparrow BS_\uparrow MC, \qquad M = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -1 & -i \end{pmatrix}. \tag{8.85}$$

We choose the coins A, B and C exactly as in the Four-Step-Walk which was BDI-admissible, see (8.77). Even if a complete analysis of this modified Four-Step-Walk is beyond the scope of this section, we can easily compute the properties by example. Figure 22 shows the dispersion relation and the winding of $\det \widehat{B}_M(k)$ for a set of parameters, where the breaking of η- and τ-symmetry is evident. This example proves that there is indeed *no* set of operators η or τthat made W_M an operator of symmetry type BDI for all parameters that lead to a gapped W_M. Furthermore, by counting the winding around the origin,



(a) dispersion relation of $\widehat{W}_M(k)$ (b) winding of $\det \widehat{B}_M(k)$

Figure 22: Dispersion relation and winding of $\det \widehat{B}_M(k)$ for W_M, the modified Four-Step-Walk which is of symmetry type AIII. Comparing the dispersion relation in (a) to Figure 7, one notes that η and τ are explicitly *broken*, not merely *forgotten*. This is confirmed by the winding in (b), which is not symmetric w.r.t. the horizontal axis. See Figure 20 for an opposing example where this symmetry is unbroken. The blue colour of the winding indicates that $\vec{\text{si}}(W_M) = +1$.

the symmetry index $\vec{\text{si}}$ in the example is determined as $+1$. In the next section, we leave the (mostly) translation invariant examples and analyse a Split-Step-Walk, where the angles θ_1 and θ_2 are allowed to depend on x.

8.5 NON-TRANSLATION INVARIANT SPLIT-STEP-WALK

In this section, we return to the Split-Step-Walk from (8.38)

$$\widehat{W}(k) = R(\theta_1/2)\begin{pmatrix} 1 & 0 \\ 0 & e^{-ik} \end{pmatrix} R(\theta_2) \begin{pmatrix} e^{ik} & 0 \\ 0 & 1 \end{pmatrix} R(\theta_1/2). \tag{8.86}$$

The difference is, that we do not only change the coin at $x = 0$ as in the *decoupling* case, but we allow θ_1 and θ_2 to vary. The area where for each x, θ_i is allowed to be chosen from, is a rectangle that lies in one of the tilted squares of constant $\vec{\text{si}}$ in the Harlequin-like pattern from Figure 11. If we chose a larger area, e.g. an area which contains parts of a *forbidden line* representing a gap closure, we could approach the line from both sides at different positions, producing arbitrarily many phase boundaries which closes the essential gap.

In contrast, staying within one square (and keeping a suitable distance to the forbidden lines as explained later) allows us to admissibly and continuously deform W into an appropriate W_0, with $W_0^2 = -\mathbb{1}$, whose index is readily computed and matches the index of W due to W_0 being a gentle perturbation of W.

Case	$\theta_1(x)$	$\theta_2(x)$
1	$\left[-\frac{\pi}{2}-\varepsilon_1, -\frac{\pi}{2}+\varepsilon_1\right]$	$[-\varepsilon_2, +\varepsilon_2]\cup[\pi-\varepsilon_2, \pi+\varepsilon_2]$
2	$\left[\frac{\pi}{2}-\varepsilon_1, \frac{\pi}{2}+\varepsilon_1\right]$	$[-\varepsilon_2, +\varepsilon_2]\cup[\pi-\varepsilon_2, \pi+\varepsilon_2]$
3	$[-\varepsilon_1, +\varepsilon_1]\cup[\pi-\varepsilon_1, \pi+\varepsilon_1]$	$\left[-\frac{\pi}{2}-\varepsilon_2, -\frac{\pi}{2}+\varepsilon_2\right]$
4	$[-\varepsilon_1, +\varepsilon_1]\cup[\pi-\varepsilon_1, \pi+\varepsilon_1]$	$\left[\frac{\pi}{2}-\varepsilon_2, \frac{\pi}{2}+\varepsilon_2\right]$

Table 4: The four different cases determining how the angles θ_1 and θ_2 are allowed to vary from cell to cell. The values ε_1 and ε_2 fulfil (8.87) to ensure that the intervals do not cross the forbidden lines, preserving the essential gap condition. Satisfying this constraint, case 1 and 4 are depicted in Figure 23, while case 2 and 3 can be inferred, noting that case 2 matches case 1 with θ_1 shifted by π, and case 3 matches case 4 with θ_2 shifted by π.

Thus, let us consider four different cases for W. That is for every $x \in \mathbb{Z}$, the angles for the coins $\theta_1(x)$ and $\theta_2(x)$ are allowed to take any value within the range shown in Table 4. Then, as long as the length and width of the rectangle $2\varepsilon_1$ and $2\varepsilon_2$ is subject to

$$\sin\frac{\varepsilon_1}{2} + \sin\frac{\varepsilon_2}{2} < \sqrt{2}, \tag{8.87}$$

we show that the corresponding walks W_j in case $j = 1, \ldots, 4$ are gapped and have BDI-index of the corresponding pair of squares these values are chosen from:

Case j	1	2	3	4
$\vec{\mathrm{si}}(W_j)$	-1	+1	0	0

(8.88)

The allowed regions for the different cases are marked in Figure 23. A crucial step in proving the statement is that in every tilted square that is enclosed by forbidden lines, there is a Split-Step-Walk W_0 that squares to $-\mathbb{1}$. This is easily seen if we look at what happens to W if we choose $\varepsilon_1 = \varepsilon_2 = 0$. Let us start with W_3 and W_4. Then, vanishing ε_2 leads to $R(\theta_2)$ being a decoupling coin as described in (8.55), case 2. Hence, we have a Split-Step-Walk that is decoupled in every cell, and acts like $W_0 = \pm i\sigma_y$, depending on whether we chose θ_1 as 0 or π. Clearly, for this W_0 we have $W_0^2 = -\mathbb{1}$.

In the case of W_1 and W_2, the argument is a bit trickier. Again, we encounter a decoupling coin, but this time, since the decoupling stems from the outer coin $R(\theta_1/2)$, it is *skew* w.r.t. the cell structure, similar to the generating example from Section 8.1, depicted in Figure 8. More precisely, choosing $\theta_2 = 0$ and θ_1 as in case 3 or 4 and $\varepsilon_1 = \varepsilon_2 = 0$, we have

$$W_0 = \begin{pmatrix} i\sin p & \mp\cos p \\ \pm\cos p & -i\sin p \end{pmatrix}. \tag{8.89}$$

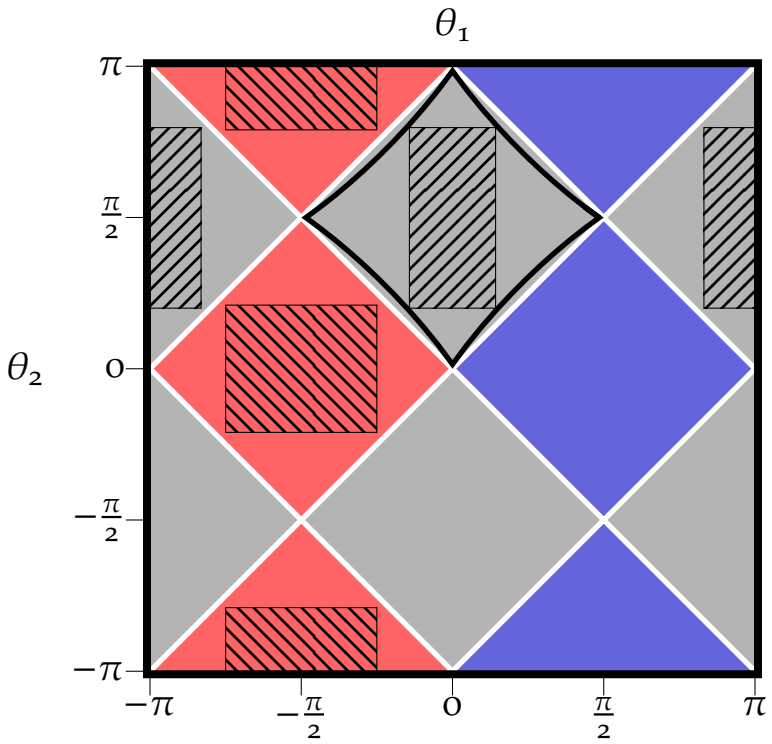


Figure 23: Parameter plane for the Split-Step-Walk as in Figure 11. The diagonally hatched rectangles denote case 1 from Table 4, where each coin is picked from walks with $\vec{\mathrm{si}}(W) = -1$. The anti-diagonally hatched rectangles denote case 4, which represents $\vec{\mathrm{si}}(W) = 0$. Note that case 2 and 3 follow by shifting θ_1 in case 1 and θ_2 in case 4 by π, and represent $\vec{\mathrm{si}}(W) = +1$ and $\vec{\mathrm{si}}(W) = 0$ respectively. Exemplary for one rectangle, the black line denotes the constraint from (8.87) on which the corners of the rectangle has to lie if we want to preserve the essential gap.

If we choose $\theta_2 = \pi$, the overall sign changes, i.e. $W_0 \mapsto -W_0$. Independent of these case distinctions, W_0 always fulfils $W_0^* = -W_0$ and hence $W_0^2 = -\mathbb{1}$.

What we have thus shown is that for every W_j and every $\theta_i(x)$, there is a Split-Step-Walk W_0 whose angles differ from those of W_j at most by ε_i for every x. Therefore, we have the estimate:

$$\begin{aligned}\|A - A_0\| &= \sup_{x\in\mathbb{Z}} \|R\big(\theta_2(x)\big) - R\big(\theta_{2,0}(x)\big)\| \\ &= \sup_{x\in\mathbb{Z}} \|R\big(\theta_2(x) - \theta_{2,0}(x)\big) - \mathbb{1}\| \\ &\leq \|R(\varepsilon_2) - \mathbb{1}\| = |e^{i\varepsilon_2} - 1| = 2\sin\frac{\varepsilon_2}{2}, \end{aligned} \tag{8.90}$$

since A and A_0 are block diagonal w.r.t. the cell structure, and multiplying with $R\big(-\theta_{2,0}(x)\big)$ as an element of the orthogonal group does not change the norm.

The estimate for $B^2 - B_0^2$ is identical if one again uses the group structure of the rotation matrices s.t. $R^2(\theta) = R(2\theta)$, and we get

$$\|B^2 - B_0^2\| \leq 2\sin\frac{\varepsilon_1}{2}. \tag{8.91}$$

Using both estimates, as well as the fact that W_j and W_0 are both Split-Step-Walks, we get from (8.86):

$$\begin{aligned}\|W - W_0\| &= \|S_\downarrow\| \cdot \|(A - A_0)S_\uparrow B^2 + A_0 S_\uparrow B^2 - A S_\uparrow B_0^2\| \\ &\leq \|(A - A_0)S_\uparrow B^2\| + \|S_\uparrow(B^2 - B_0^2)\| \\ &= \|A - A_0\| + \|B^2 - B_0^2\| \\ &\leq 2\sin\frac{\varepsilon_1}{2} + 2\sin\frac{\varepsilon_2}{2} < \sqrt{2}. \end{aligned} \tag{8.92}$$

We can use this estimate to show that in every case, $W = W_j$ is gapped at $+1$ (-1 follows analogously). Similar to the proof of the homotopy invariance of $\mathrm{si}_\pm$ in Theorem 5.5, the second resolvent identity from (5.11) is $R(\mathbb{1} - (W - W_0)R_0) = R_0$ and yields a geometric series for R, with $R = (\mathbb{1} - W)^{-1}$ and $R_0 = (\mathbb{1} - W_0)^{-1}$, if

$$\|(W - W_0)R_0\| < 1. \tag{8.93}$$

We know that W_0 has constant blocks w.r.t. two dimensional cells[10], and hence the norm of $\mathbb{1} - W_0$ coincides with the norm of the single blocks, leading to

$$\|R_0\| = |(1 \pm i)^{-1}| = \frac{1}{\sqrt{2}}. \tag{8.94}$$

Combining this with (8.92), we see that (8.93) is sharply satisfied, and we learn that R exists as a bounded operator whence $+1$ lies in the resolvent set of W. Furthermore, since the spectrum is closed, it cannot approach $+1$ arbitrarily, hence there has to be a finite distance between

10 In case 3 and 4, these cells coincide with the cells from the spatial structure, while in case 1 and 2, the cells are shifted by one basis-element, thus they are skew. But since the identity is diagonal in every basis, this does not make a difference.

$+1$ and the spectrum of W. The argument for -1 is completely analogous, and thus we know that W is a *gapped* admissible operator.

Now, by continuously contracting each θ_i to the respective $\theta_{i,\mathrm{o}}$, we create a homotopy between W_j and W_o. The estimate from above guarantees, that on the way to W_o, each intermediate walk is itself an admissible gapped Split-Step-Walk, fulfilling the same conditions as W_j and W_o. Hence, W_j is a gentle perturbation of W_o and we conclude, that $\vec{\mathrm{si}}(W_j) = \vec{\mathrm{si}}(W_\mathrm{o})$.

Then, we get $\vec{\mathrm{si}}(W_\mathrm{o})$ from Figure 11 for each case j:

Case j	1	2	3	4
$\vec{\mathrm{si}}(W_j)$	-1	+1	0	0

(8.95)

This finishes the example of a non-translation invariant Split-Step-Walk and the examples as a whole.

9

CONCLUSION AND OUTLOOK

In the beginning of this thesis, we were looking for a rigorous non-trivial theory that describes quantum walks that are admissible for the symmetries of the tenfold way. Striving for the most general setting, we identified the larger class of essentially local essentially gapped unitary operators as the right object of classification instead of merely looking at translation invariant gapped quantum walks.

Without further assumptions on these objects we found three symmetry indices whose values lie in the groups predicted by the Hamiltonian theory, depending on the symmetry type. We showed that there are non-gentle but compact perturbations that can be distinguished by one of our indices, which is a unique feature that distinguishes our theory from the Hamiltonian case. The other two indices are insensitive to compact perturbations and measure the asymptotic behaviour far to the left and far to the right, respectively. All three symmetry indices are proven to be stable under gentle perturbations and are hence homotopy invariants. Remarkably, these three homotopy invariants are a complete set of invariants in the sense that two classified objects are connected to each other within the classification if and only if their sets of invariants match. That is, there is no finer classification or additional hidden invariants, at least not based on these assumptions. This is the best result one could hope for in our attempt to connect quantum walks with the tenfold way and thus confirmed our choice of classifying objects and symmetry indices.

Restricting to translation invariant operators, we prove that demanding essential locality is equivalent to continuity in momentum space. This strengthens our choice even further, because continuity is exactly the necessary condition for winding numbers to make sense. Furthermore, we were able to express the symmetry index in three of the five non-trivial cases as a winding number of a determinant in momentum space after bringing them to a standard form. In two of these cases, we even succeeded in showing completeness of this symmetry index within the class of bulks with a fixed cell structure. In the third case, we proved that completeness in this setting only holds if we either add a parity-valued additional index or allow for a single pairwise regrouping of neighbouring cells along the paths.

Since we chose a sufficiently general setting, we were able to prove a precise statement of bulk-boundary correspondence. That is, we showed that joining two bulks in different phases leads to the emergence of exponentially decaying eigenfunctions in the gap. What distinguishes our result from earlier work is that the bulks to be joined as

well as the joined system together with its emerged eigenvalues in the gap are all described within a single theory.

The translation invariant generator was introduced as an example that generates all index groups, showing by example that all values predicted by our theory can be realized. Our exhaustive examples visualized many aspects of our classification, which is still enhanced by the accessible web-tool [Sta15a] we developed for demonstration purposes.

We conclude this thesis with a few suggestions of possible directions of future research:

- **Translation invariance:** In Chapter 7 we restricted ourselves to symmetry types where $\gamma^2 = +\mathbb{1}$. Meanwhile, most of the issues we had with the other cases are resolved and a publication of these results is in preparation [Ced+18a].

- **Additional symmetries:** In our attempt to find a suitable setting for a theory of topological phases in quantum walks, we used the tenfold way as an anchor which kept us in an area of comfort we know from the Hamiltonian case. Now that we finished our classification in these cases, a natural generalization we are working on [Ced+18b] is to go back to Section 2.3 and instead of restricting ourselves to the choices that lead to the tenfold way, to allow for the abstract group of n involutions $\{S_i\}_{i=1}^n$, and to exhaust the full range of phases $m_{ij} \in \mathbb{T}$ s.t. $V_i V_j = m_{ij} V_{ij}$. We expect that a proper identification of equivalent symmetries should on the one hand lead to the tenfold way in the purely Hamiltonian case, and on the other hand to a larger set of symmetry types in the unitary case, which clearly contains the tenfold way.

- **Higher dimensions:** Even if we considered it an advantage that our theory requires only elementary group theoretic methods, being able to apply K-theoretic methods to quantum walks could allow us to classify $d > 1$ as well. Using Bott periodicity, [Kit09] covers all dimensions in his periodic table, not only $d = 1$. A good starting point might be the work of Prodan and Schulz-Baldes [PSB16; SB16; SB15; GSB16] whose results also helped us to understand the translation invariant classification for DIII.

- **QCA:** Possibly the largest impact is expected from a theory that breaks the limits of quantum walks as a one-particle theory by extending to interacting systems. That is, we transition to quantum cellular automata (QCA) where *every* cell can host a particle s.t. the Hilbert space is a tensor product rather than a direct sum. The analogue of the index theory without symmetries from Section 3.4 has been successfully transferred to QCA [Gro+12] leading to a positive rational instead of an integer, so this might be worth an attempt.

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