Topological Classification of Symmetric Quantum Walks

Discrete Symmetry Types and Chiral Symmetric Protocols

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Abstract

In this thesis, we study the topological classification of symmetric quantum walks. These describe the discrete time evolution of single quantum particles on the lattice with additional locally acting symmetries. The thesis consists of three parts:

In the first part, we discuss discrete symmetry types for self-adjoint and unitary operators from an abstract point of view, i.e. without assuming an underlying physical model. We reduce any abstract finite group of involutive symmetries and their projective representations to a smaller set of symmetry types, eliminating elements that are redundant for topological classifications. This reduction process leads to the well-known tenfold way for self-adjoint operators, and for unitary operators, we identify 38 non-redundant symmetry types. For these, we define a symmetry index, which labels equivalence classes of finite-dimensional representations up to trivial direct summands. We show that these equivalence classes naturally carry a group structure and finish the discussion by explicitly computing the corresponding index groups for all non-trivial symmetry types.

Second, we develop a topological classification for symmetric quantum walks based on the symmetry index derived in the first part. We begin without a locality condition on the unitary time evolution operator but only assume an underlying discrete spatial structure. Unlike continuous-time systems, quantum walks exhibit non-gentle perturbations, i.e. local or compact perturbations that cannot be undone continuously. Using the symmetry index, we provide a complete topological classification of such perturbations of unitary operators on any lattice or graph. We add a locality condition on the one-dimensional lattice and detail the implications of such assumption on the classification. The spatial structure of the one-dimensional lattice allows us to define the left- and right symmetry index, which characterise a walks topological properties on the two half-chains. The sum of these two indices equals the overall symmetry index, which provides a lower bound on the number of symmetry protected eigenstates of the walk. For the symmetry types of the tenfold way, a subset of three different symmetry indices is complete with respect to norm-continuous deformations and compact perturbations.

In the third part, we consider quantum walk protocols instead of single time-step unitaries. We show that any unitary operator with finite jump length on a one-dimensional lattice can be factorised into a sequence of shift and coin operations. We then provide a complete topological classification of such protocols under the influence of chiral symmetry. The classification is in terms of the half-step operator, i.e. the time evolution operator at half of the driving period, which is singled out by the chiral symmetry. We also show that a half-step operator can be constructed for every chiral symmetric single time-step unitary without a pre-defined underlying protocol. This renders the classification via the half-step operator valid for periodically driven continuous-time (Floquet systems), discretely driven protocols, and single time-step quantum walks.

Keywords: Quantum walks, topological classification, discrete symmetry types

Zusammenfassung

In dieser Arbeit untersuchen wir die topologische Klassifikation symmetrischer Quantenwalks. Diese beschreiben die diskrete Zeitentwicklung einzelner Quantenteilchen auf dem Gitter mit zusätzlichen lokal wirkenden Symmetrien. Die Arbeit besteht aus drei Teilen:

Im ersten Teil diskutieren wir diskrete Symmetrietypen für selbstadjungierte und unitäre Operatoren von einem abstrakten Standpunkt aus, ohne ein zugrundeliegendes physikalisches Modell anzunehmen. Wir reduzieren eine abstrakte endliche Gruppe involutiver Symmetrien und deren projektive Darstellungen auf eine kleinere Menge von Symmetrietypen, wobei Elemente, die für topologische Klassifikationen redundant sind, eliminiert werden. Für selbstadjungierte Operatoren führt dieser Reduktionsprozess zum wohlbekannten "tenfold way", und für unitäre Operatoren identifizieren wir 38 nicht-redundante Symmetrietypen. Für diese definieren wir einen Symmetrie-Index, welcher Äquivalenzklassen endlichdimensionaler Darstellungen bis auf triviale direkte Summanden kennzeichnet. Wir zeigen, dass diese Äquivalenzklassen auf natürliche Weise mit einer Gruppenstruktur versehen sind und schließen die Diskussion mit der expliziten Berechnung dieser Indexgruppen für alle nichttrivialen Symmetrietypen.

Basierend auf dem im ersten Teil hergeleiteten Symmetrie-Index entwickeln wir im zweiten Teil eine topologische Klassifikation für symmetrische Quantenwalks. Dabei beginnen wir ohne eine Lokalitätsbedingung für den unitären Zeitentwicklungsoperator, sondern lediglich eine zugrundeliegende diskrete räumliche Struktur anzunehmen. Anders als zeitkontinuierliche Systeme, weisen Quantenwalks unsanfte Störungen auf, d.h. lokale oder kompakte Störungen, die nicht auf stetige Weise eliminiert werden können. Mithilfe des Symmetrie-Index gelingt uns die vollständige topologische Klassifikation solcher Störungen unitärer Operatoren auf beliebigen Gittern oder Graphen. Anschließend fügen wir eine Lokalitätsbedingung auf dem eindimensionalen Gitter hinzu und untersuchen den Einfluss einer solchen Annahme auf die topologische Klassifikation. Die räumliche Struktur des eindimensionalen Gitters erlaubt uns die Definition eines links- und rechtsseitigen Symmetrie-Index, welche die topologischen Eigenschaften des Walks auf den jeweiligen Halbachsen charakterisieren. Die Summe dieser beiden Indizes ist gleich dem Symmetrie-Index des gesamten Walks, welcher eine untere Schranke für die Anzahl der durch die Symmetrien geschützten Eigenzustände liefert. Zudem liefert eine Teilmenge von drei dieser Symmetrie-Indizes einen vollständigen Satz von Invarianten für die Klassifikation bis auf normstetige Deformationen und kompakte Störungen.

Im dritten Teil widmen wir uns Quantenwalk-Protokollen anstelle von Unitären, welche einen einzelnen diskreten Zeitschritt beschreiben. Wir zeigen zunächst, dass jeder unitäre Operator mit endlicher Sprungweite auf dem eindimensionalen Gitter in eine Sequenz von "shift"- und "coin"-Operatoren faktorisiert werden kann. Anschließend liefern wir eine vollständige topologische Klassifikation solcher Protokolle mit chiraler Symmetrie. Diese Klassifikation findet anhand des durch die chirale Symmetrie ausgezeichneten Halbschritt-Operators, d.h. des Zeitentwicklungsoperators nach einer halben Periode statt. Wir zeigen, dass auch für unitäre Operatoren ohne zugrundeliegendes Protokoll immer ein Halbschritt-Operator konstruiert werden kann, wodurch sich die Klassifikation über den Halbschritt-Operator sowohl auf periodisch getriebene Systeme in kontinuierlicher Zeit (Floquet-Systeme), diskrete Protokolle, als auch einen einzelnen Zeitschritt beschreibende Quantenwalks anwenden lässt.

Schlagworte: Quantenwalks, topologische Klassifikation, diskrete Symmetrietypen

Contents

Introduction

Motivation

It is the matter of physics to systematically describe the behaviour of nature, i.e. to translate observed phenomena into the language of mathematics. Only when we are equipped with a mathematical model that explains observed phenomena and predicts new ones, we claim to understand a physical process. However, sometimes it is the model itself, which sparks further research interest without being bound to observations in the lab. Studying the details of a model may be driven more by mathematical interest than by physical motivation, but only when we understand a model in all its details, can we pin down its predictive power and, even more importantly, its limitations. Hence, the study of models in their own right belongs to physics in the same way as the pure descriptions of phenomena do. The combination and, in particular, the interplay between these two disciplines enables us to claim to understand the processes in nature.

The model systems we study in this thesis are called quantum walks. These describe the dynamics of single particles on discrete spatial structures such as lattices or graphs in discrete time. Another way of seeing quantum walks is as the quantum mechanical counterparts of classical random walks. These two pictures correspond to two different lines of research in the quantum walk community. On the one hand, seen as quantum mechanical generalisations to random walks, quantum walks have many algorithmic applications. After being introduced by Aharonov et al. in 1993 [ADZ93], quantum walks became famous with the well known Grover search algorithm [Gro96] in 1996. Since then, quantum walk based algorithms have appeared in various topics, like cryptography [VRM$^+$15], pseudo-random number generation [SC19], graph classification [CMC20], neural networks [DMKP$^+$19], and have been shown to provide a universal platform for quantum computation [LCE$^+$10]. On the other hand, interpreted as the dynamics of single particles [Mey96], quantum walks exhibit a variety of physical phenomena, such as dynamical localisation [ASW11], mimicking the dynamics under the Dirac equation [BB94], Bloch-oscillations [RBH$^+$11], molecular binding [AAM$^+$12], and the coupling of a quantum mechanical particle to electromagnetic fields [CRW$^+$13, CGWW19].

We here approach quantum walks from the perspective of a topological classification with symmetries. This is motivated by topological phases of matter in solid-state physics. Sparked by the observation of the well-known integer quantum Hall effect [KDP80], the search for topological phases of matter as well as their rigorous classification became a highly active area of research [SRFL08, SRFL09, RSFL10,

HK10, QZ11]. Quantum walks were found to serve as a well-suited model system for this topic, providing examples for all non-trivial topological phases in the so-called tenfold way [KRBD10]. Since then, many quantum walk models and examples with non-trivial topological properties have been studied [Kit12, Asb12, AO13, ATD14, OANK15, CMM$^+$16, CGS$^+$16] and were also experimentally realised on various platforms [KBF$^+$12, GBA$^+$16, RFR$^+$17, BNE$^+$17, NGS$^+$19]. However, a profound topological classification beyond specific models with a satisfying level of rigour was missing when we first approached the topic. This motivated us to fill this gap and provide a topological classification of symmetric quantum walks from a mathematical point of view [CGG$^+$18, CGS$^+$18, CGWW21].

Generally speaking, the ingredients for such a topological classification are (1.) a set of systems, (2.) a set of assumptions, respectively restrictions, and (3.) a set of transformation rules. The task is to precisely label the connected components of the systems under the set of transformations that obey the assumptions and restrictions. In a sense, a topological classification is motivated by trying to pin down the most fundamental structure of a model at hand without letting unnecessary details stand in the way. In our case, the systems will be (1.) quantum walks on the one-dimensional lattice, obeying (2.) a locality condition, certain symmetries and a gap condition. In particular, we do not assume translation invariance or a restricted type of disorder in an otherwise translation-invariant system. The classification is then up to (3.) norm-continuous deformations and compact perturbations.

We focus on two aspects: First, we generalise the ten discrete symmetry types typically considered in the literature. The tenfold way provides an exhaustive set of non-trivial symmetry types for self-adjoint operators, i.e. the generators of the time evolution in continuous time. Quantum walks do not necessarily stem from such continuous-time evolution. Hence, considering only these ten types is not necessarily exhaustive in our setting. To pin this down, we study the possible projective representations for finite groups of involutive symmetries, i.e. symmetry types, from an abstract point of view, which leads to 38 non-trivial different symmetry types for unitary operators. Building on this, we provide a complete classification of compact perturbations for unitaries that fulfil the respective symmetry condition for all these 38 types. Taking a locality condition with respect to a one-dimensional lattice into account, we apply the classification to quantum walks. For these, we define spatial symmetry indices, the left and right symmetry index. These can be computed arbitrarily far to the left and right, respectively, and therefore only depend on the half infinite bulks to the left and the right. Moreover, they add up to the overall symmetry index and therefore predict whether a system consisting of two joined half-systems in possibly different topological classes hosts symmetry-protected edge states at the boundary. This equality of the sum of two bulk indices on the one hand, and an invariant that characterises the symmetry protected eigenstates of the system without being bound to the underlying spatial structure, can be interpreted as a version of the well-known bulk-boundary correspondence for one-dimensional symmetric quantum walks. Moreover, we provide a complete topological classification of one-dimensional quantum walks subject to the symmetry types of the tenfold way. While we could not fully generalise these far-reaching results to all symmetry types, we provide a partial classification and discuss the problems one encounters

beyond the tenfold way.

The fundamental question that will accompany us along the way is: What exactly is meant by a "quantum walk"? A discrete-time system that evolves by recurring application of the same unitary operator can be thought of in different ways. An idea that comes to mind is periodically driven, i.e. Floquet systems. When observed only stroboscopically at integer multiples of the period, such systems provide the so-called Floquet operator as the recurring unitary time evolution operator. Another ansatz is to axiomatically assume the time evolution as a recurring application of a unitary operator with a locality condition, that is, without any underlying driving process whatsoever. The standard concept for quantum walks in the literature lies somewhat in between these two points of view. Quantum walks are usually defined as a sequence of shift and coin operations, i.e. in terms of two fundamental building blocks.

We discuss the differences between the three points of view throughout this thesis and elaborate on their consequence on the topological classification. While not every abstractly defined discrete-time quantum walk can be realised as the Floquet operator of a periodically driven system, the two remaining definitions coincide. We show that every unitary with finite jump-length on the one-dimensional lattice can be factorised into a sequence of shift and coin operations, proving two of the three settings outlined above equivalent. With this, we affirmatively answer a long-standing question, the answer to which was previously known only in the translation invariant case [Vog09], where the walks can be factorised in momentum space using techniques from the theory of filter banks.

We proceed by studying the influence of chiral symmetry on a driving process. There is a mismatch between our complete topological classification of single time-step quantum walks [CGG$^+$18] and other results from the literature [Asb12, AO13]. We resolve this mismatch by showing how it originates in different underlying definitions of a quantum walk. Insisting on a protocol structure in the presence of chiral symmetry introduces a second timeframe, i.e. an equally valid second quantum walk that does not necessarily share the same topological invariants. This enlarges the set of describing indices, which must be equal for homotopies to exist between two protocols. We provide a complete classification of chiral symmetric protocols, which also applies to continuously driven systems, by focussing on the half-step operator, i.e. the time evolution operator after half of the driving period. This half-step operator is singled out by the chiral symmetry, which always contains a time-reversing action. In a periodically driven process, this time reversing action causes the unitary at the full driving period T to be of the form $U(T) = \gamma U(T/2)^* \gamma^* U(T/2)$, where γ denotes the chiral symmetry operator. Hence, the half-step operator already contains all information needed for the classification. We show that the norm-continuously connected components of half-step operators are labelled by five integer-valued indices, in contrast to only three for quantum walk operators. For axiomatically defined quantum walks without an underlying driving process but chiral symmetry, we show that a half-step operator also always exists, such that the classification in terms of those captures both pictures simultaneously.

We end the last chapter by studying the aforementioned compact perturbations for chiral symmetric protocols and chiral symmetric protocols in finite systems. We find that a non-gentle compact perturbation of a chiral symmetric quantum walk, i.e.

a perturbation that cannot be reached via a continuous path, always stems from a bulk-boundary scenario of half-step operators. That is, a half-step operator, which is a crossover between two topologically distinct halves of the system. Moreover, differently from spatially infinite systems, single non-gentle perturbations prevent the existence of an underlying protocol in finite systems. However, we find that locally non-gentle perturbations can occur in pairs that "annihilate" each other globally.

Outline

In Chapter 1 we introduce the basic theory and mathematical facts needed in the following chapters. We start with the essentials of quantum theory, that is, Hilbert spaces, states, measurements, and time evolution in Section 1.1, followed by a selection of mathematical concepts and tools in Section 1.2. We continue with a closer look at the time evolution in quantum mechanics and introduce periodically driven systems, so-called Floquet systems, in Section 1.3. Having set the stage, we introduce the main topic for this theses, i.e. quantum walks, in Section 1.4. We end the chapter with an introduction to the projective representations of symmetries in quantum mechanics.

In Chapter 2 we classify the equivalence classes of projective representations of groups of involutive symmetries. We begin with the general definition of these symmetry types in Section 2.1 and discuss their possible action on operators in Section 2.2, where we derive the reduction to the 38 non-trivial classes. We finish the chapter with the definition and computation of the symmetry index for finite-dimensional representations in Section 2.3.

In Chapter 3 we provide a topological classification of essentially gapped unitaries and quantum walks, which are subject to one of the symmetry conditions of the 38-fold way. First, in Section 3.1, we apply the symmetry index to essentially gapped unitary operators on infinite-dimensional systems and prove its homotopy invariance. We use this invariant for a complete classification of compact perturbations of symmetric unitary operators on the lattice in Section 3.2. In Section 3.3 we add a locality condition to the picture and discuss its implications on the topological classification. An essential tool for the proof of the main theorem in Section 3.3 is the decoupling construction, which allows splitting an essentially local unitary into two independent half-space systems. In Section 3.4 we discuss this construction in the presence of symmetries and identify necessary and sufficient conditions for the existence of such decoupling for all 38 symmetry types. We define the left and right symmetry index and formulate the bulk-boundary correspondence for one-dimensional quantum walks in Section 3.5. In Section 3.6 we end the chapter with a sketch of the proof for the completeness of the symmetry indices for the symmetry types of the tenfold way.

In Chapter 4 we prove that every strictly local quantum walk on the one-dimensional lattice can be factorised into a finite sequence of shift and coin operations.

Finally, in Chapter 5 we provide a complete classification of chiral symmetric protocols instead of single time step unitaries. We start by precisely defining the setting and discussing the questions we are going to address in Section 5.1. In Section 5.2 we introduce the half-step operator and discuss the conditions for such an operator and, therefore, an underlying protocol to exist for an arbitrary chiral symmetric quantum

walk. In Section 5.3 we identify a set of five independent indices for the half-step operator and prove their completeness. We apply the theory to a well-known example system with an inherent protocol structure, the so-called split-step quantum walk in Section 5.4, and discuss the connection of the set of five indices for the half-step operator to the symmetry indices of the underlying quantum walks in Section 5.5. In Section 5.6, we discuss compact perturbations of chiral symmetric protocols, as well as protocols on finite systems.

1 Preliminaries

Before we delve into the topic and tackle the tasks and questions outlined above, let us introduce some of the concepts and techniques that we need. This chapter is dedicated to laying a minimal foundation for the upcoming journey. We start with the basic concepts of **quantum theory**, followed by a section dedicated to purely mathematical concepts, which we need later. This includes C^***-algebras**, **compact operators**, **Fredholm operators**, the **Fredholm index** and the **essential spectrum** of an operator. Of course, a preliminary section like this cannot contain a full course on the needed mathematical concepts, but instead, one has to choose a starting point, assuming knowledge of the needed basics. We here only present a small selection of mathematical objects and some of their properties, thereby keeping this section very short and referring the interested reader to the literature. We continue with a discussion on **time evolution** in **driven systems** and in particular, **Floquet drivings**. Building on this, we introduce the main concept for this thesis: **Quantum walks**, also discussing one of the standard examples in the literature, the **split-step walk**, which we will meet more than once during this thesis. We end this preliminary chapter with a closer look at the representation of **symmetries in quantum mechanics**, via **unitary or antiunitary operators**. The last section also transitions to the following chapter on discrete symmetry types for unitary operators.

1.1 Essentials of quantum theory

We only give a rough overview of the basics of quantum mechanics in order to set the stage for the considerations to follow. For this, we chose an axiomatic point of view, following [Wer16]. Since this thesis is not on the foundations of quantum theory, we will not detail the numerous implications of the axioms and, in particular, do not touch their possible interpretations. For a detailed study of quantum theory and its mathematical framework, we recommend the textbooks [Kra83, Per02, Tes09, Bal14].

The underlying philosophy for the postulates in [Wer16] is a purely statistical interpretation of quantum theory, together with the ansatz of keeping the theory's postulates as general (and therefore arguably also as simple) as possible. A statistical physical theory rests on the following fundamental building blocks: **Preparation** and **measurement**. In a physical experiment, the system is first prepared in a reproducible and well controllable state. Secondly, a measurement of any kind is performed on the system, producing some outcomes. The outcomes are stored, analysed, and the process is re-

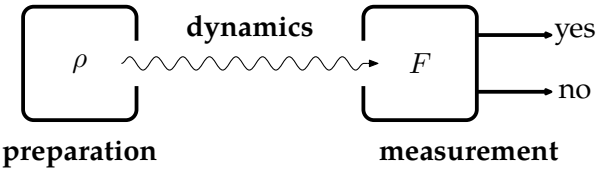


Figure 1.1: Schematic of a statistical experiment with outcomes "yes" and "no" (compare [Wer16, Abb. 1.5]).

peated to build up evidence for the findings to truly originate in an underlying physical phenomenon and not some random fluctuation of the lab environment. The last step is crucial and gives rise to the statistical nature of the interpretation: We do not demand our theory to give specific absolute values on a process, but rather expectation values, i.e. the likeliness of a specific outcome to occur. A crucial point omitted in the rough description above is the **dynamics** of the system. No measurement is instantaneous, and there is always some timespan between the preparation and the measurement, i.e. the system undergoes some dynamics in the meantime. In addition, it is usually the dynamic properties that unveil the physical concepts in a system process. Thereby it is crucial that the time intervals between the two steps are equal in each repetition of the experiment. Figure 1.1 shows a schematic of a statistical experiment outlined above.

According to the description above, there are three fundamental concepts a theory needs to postulate: **states**, **detectors** and the **dynamics** of the system. We here present the five postulates from [Wer16]. The first one sets the mathematical framework, the second defines the states and preparation step of a system, whereas the third and fourth ones are concerned with the measurement process. Finally, the last one defines the dynamics of the theory.

Postulate 1. *Each quantum mechanical system gets assigned a Hilbert space $\mathcal{H}$.*

The Hilbert space might be finite-dimensional, e.g. for a spin $1/2$ particle without further degrees of freedom we have $\mathcal{H} = \mathbb{C}^2$ with the two states "spin up"$\equiv (1, 0)$ and "spin down"$\equiv (0, 1)$. Typically the Hilbert space is infinite-dimensional and might even be non-separable. However, throughout this thesis, we assume all Hilbert spaces to be separable, i.e. to exhibit a countable orthonormal basis. The set of bounded operators on a Hilbert space $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$.

Postulate 2. *The preparation of a quantum mechanical state corresponds to a density operator $\rho \in \mathcal{B}(\mathcal{H})$, with $\rho > 0$ and $\operatorname{tr} \rho = 1$. For pure states, ρ is a one-dimensional projection $|\psi\rangle\langle\psi|$, defined by a normalized vector $\psi \in \mathcal{H}$.*

The pure states on $\mathcal{H}$ are in one-to one correspondence with the rays in a Hilbert space, i.e. the set of orthonormal vectors up to multiplication with a phase. Moreover, the state space for any Hilbert space is a convex set with the pure states as the extremal points. In particular, we can write any state ρ as a convex combination of pure states, i.e.

$$\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|, \quad \text{with} \quad \lambda_i \geq 0 \quad \text{and} \quad \sum_i \lambda_i = 1. \tag{1.1}$$

Postulate 3. *A detector with the possible outcomes "yes" and "no" (also called effect [Kra83]) corresponds to an operator* $0 \leq F \leq \mathbb{1}$.

The detector alone says relatively little without a way of retrieving outcomes from a prepared state ρ, which is provided by the fourth postulate.

Postulate 4. *The detection probability for a detector* F *and a prepared state* ρ *is given by* $\mathrm{tr}(\rho F)$. *For pure states, this can be written as* $\langle \psi, F\psi \rangle$.

Restricting the measurement framework to the outcomes "yes" and "no" seems a little oversimplified at first sight. Of course, a generic physical measurement can have more complex outcome-sets than just these two possibilities, but we can always trace back any measurement outcome-set to simple yes/no-questions: Let X be the set of possible outcomes for a physical measurement (e.g. the set of possible positions of a pointer on some scale). For each measurable subset $S \subset X$, we can ask whether the measurement outcome $x \in X$ lies in S or not. Hence, by Postulate 3, there exists an operator F_S for this yes/no question. For disjoint sets $S \subset X$ and $T \subset X$ it is then reasonable to demand $F_{S \cup T} = F_S + F_T$, and we set $F_X = \mathbb{1}$. This turns $S \mapsto F_S$ into a positive operator-valued measure (POVM), which is called an **observable**. The outcome statistics of a POVM for a state ρ is then completely determined by Postulate 4.

In many standard textbooks, measurements are postulated as projection valued measures, and observables are identified with self-adjoint operators. It is often argued that the reason for these assumptions is that physical measurements always yield real-valued outcomes. However, it has been shown that there exist measurements, e.g. arrival-time measurements, which cannot be realised by projection valued measures [Wer87]. Let us, nevertheless, briefly comment on how this special case emerges from a POVM. Let all Fs of an observable be projections, i.e. $F = F^* = F^2$. If, additionally, $X \subset \mathbb{R}$, i.e. all measurement outcomes are real, we can define the self-adjoint operator $A = \int_X x dF$, from which we get the distribution of expectation values via $\mathrm{tr}(\rho A)$. This means that the projection valued measure F is the spectral measure of the operator A.

Finally, the dynamics of a quantum mechanical system is provided via the fifth and last postulate:

Postulate 5. *Each system is characterized by a self-adjoint Hamiltonian* $H \in \mathcal{B}(\mathcal{H})$ *(i.e.* $H^* = H$*) that determines the time evolution operator* $U_t = \exp(-iHt)$[1]. *Applying a measurement* F *on a system that is initially prepared in the state* ρ *after a time* t, *the expectation value is given by*

$$\mathrm{tr}(U_t \rho U_t^* F) = \mathrm{tr}(\rho U_t^* F U_t). \tag{1.2}$$

The two sides of the equation in the postulate above are equivalent due to the invariance of the trace under swaps of the argument, i.e. $\mathrm{tr}(AB) = \mathrm{tr}(BA)$. We portrayed both, in order to emphasise two different views onto the time evolution in quantum mechanics. According to Postulate 4, the left hand side can be interpreted as the expectation value $\mathrm{tr}(\rho_t F)$ for the detector F in the time evolved state

$$\rho_t = U_t \rho U_t^*. \tag{1.3}$$

[1] Where we set $\hbar = 1$ by an appropriate choice of units.

This point of view of evolving the state without changing the detector is known as the **Schrödinger picture**. In contrast to that, we can interpret the right-hand side as the expectation value $\mathrm{tr}(\rho F_t)$ of the initially prepared state ρ with the (backwards) time evolved detector

$$F_t = U_t^* F U_t, \tag{1.4}$$

which is known as the **Heisenberg picture**. Of course, the two points of view are equivalent and is a matter of taste which to use.

The physical ingredient to the theory is the assignment of the correct Hamiltonian to a system. One way of doing this is to quantise a classical Hamilton function, which is often a highly non-unique process. We omit the details of this discussion here and think of the Hamiltonian as part of the definition of a quantum mechanical system from the outset. Note that in general the generator of a quantum mechanical time evolution might well be unbounded, but for the purpose of this thesis it suffices to only consider bounded operators.

The last postulate implicitly includes the well-known Schrödinger equation.

Corollary 1.1.1 (Schrödinger equation)**.** *The time evolution operator U_t from Postulate 5 fulfils the **Schrödinger equation***

$$\partial_t U = -iHU_t. \tag{1.5}$$

We will discuss the solution of this equation in detail for time-dependent and periodically driven systems $H(t)$ in Section 1.3.

Of course, the five postulates presented above only provide a rough framework on which one builds to describe actual physical systems. Nevertheless, we close our discussion on the general framework of quantum theory and move on to some needed mathematical concepts.

1.2 Mathematical concepts: C^*-algebras, compact operators and Fredholm index

Let us introduce some of the mathematical concepts we need throughout this thesis.The following list of definitions and results is by no means intended to serve as a basis for studying the contained concepts but should only serve as a collection of facts for later reference. We follow [Con07] and [Dix77].

Let us start with the definition of a **C^*-algebra** and the functional calculus on such.

Definition 1.2.1. (C^**-algebra*) *A C^*-**algebra** $\mathcal{A}$ is an associative algebra over $\mathbb{C}$ with a norm $\|\cdot\|$ and a map $A \mapsto A^*$, $A \in \mathcal{A}$, such that*

i) *$\mathcal{A}$ is norm-closed with respect to $\|\cdot\|$.*

ii) *For all $A, B \in \mathcal{A}$:*

$$\|AB\| \leq \|A\|\|B\|. \tag{1.6}$$

iii) *For all $A, B \in \mathcal{A}$, $\lambda \in \mathbb{C}$):*

$$\begin{aligned} (A^*)^* &= A & (A+B)^* &= A^* + B^* \\ (AB)^* &= B^* A^* & (\lambda A)^* &= \overline{\lambda} A^*. \end{aligned} \tag{1.7}$$

iv) *For all* $A \in \mathcal{A}$*:*

$$\|A^*A\| = \|A^*\|\|A\| = \|A\|^2. \tag{1.8}$$

If $\mathcal{A}$ *has an identity, it is called unital.*

If only *i*) and *ii*) are embraced, $\mathcal{A}$ is called a Banach algebra, which, including *iii*) becomes a $*$-algebra and a C^*-algebra with *iv*). The most prominent example of a C^*-algebra is the set of bounded operators $\mathcal{B}(\mathcal{H})$ on a Hilbert space $\mathcal{H}$. In fact, any C^*-algebra is isomorphic to a subalgebra of $\mathcal{B}(\mathcal{H})$ on some Hilbert space $\mathcal{H}$, which is known as the Gelfand-Naimark theorem [GN43].

Arguably the most important property of a C^*-algebras is that there exists a **functional calculus for C^*-algebras** (see, e.g. [Dix77, Theorem 1.5.1]):

Theorem 1.2.2 (Functional calculus for C^*-algebras)**.** *Let* $\mathcal{A}$ *be a* C^**-algebra with identity* 1 *and* $A \in \mathcal{A}$ *a normal element* (*i.e.* $A^*A = AA^*$) *with spectrum* $\sigma(A)$*. Moreover, denote by* $C(\sigma(A))$ *the the* C^**-algebra of continuous complex-valued functions on* $\sigma(A)$*, and by* $C^*(A, 1) \subset \mathcal{A}$ *the sub* C^**-algebra generated by* A *and* 1 (*containing only normal elements*)*. Then there exists a unique isometric isomorphism* $\varphi\colon C(\sigma(A)) \to C^*(A, 1) \subset \mathcal{A}$*, such that* $\varphi(1) = 1$ *and* $\varphi(\mathrm{id}) = A$*, where* id *denotes the identity map on* $\sigma(A)$*. Moreover, for any complex valued function* $f \in C(\sigma(A))$ *on* $\sigma(A)$*, the element* $\varphi(f)$ *is denoted by* $f(A)$ *and we have*

$$\sigma\left(f(A)\right) = f\left(\sigma(A)\right). \tag{1.9}$$

The functional calculus for C^* algebras provides a way to "apply" continuous functions on elements $A \in \mathcal{A}$. Specific C^*-algebras other than $\mathcal{B}(\mathcal{H})$ will be the band dominated and essentially local operators on a Hilbert space with a one-dimensional local structure (see Section 3.3). Identifying these sets as C^*-sub-algebras of $\mathcal{B}(\mathcal{H})$ and using the functional calculus, we are guaranteed that applying continuous functions on band dominated or essentially local operators, we always stay in the set we started with. We will use the functional calculus for many arguments of this type throughout this thesis.

We now come to two particular classes of operators that will be important later on, namely **compact operators** and **Fredholm operators**. On a Hilbert space, the former can be thought of as the closure of finite rank operators, that is, matrices. The latter generalises the concept of invertible operators to those invertible up to a compact perturbation. We first give the respective definition and then collect some properties for later use for both classes of operators.

Definition 1.2.3 (Compact operator)**.** *An operator* $K \in \mathcal{B}(\mathcal{H})$ *is called* ***compact****, if for any bounded subset* $\mathcal{M} \subset \mathcal{H}$*,* $\overline{K(\mathcal{M})}$ *is a compact subset of* $\mathcal{H}$*.*

The following Lemma collects some well-known properties of compact operators:

Lemma 1.2.4 (Properties of compact operators)**.** *Denote by* $\mathcal{B}(\mathcal{H})_{\mathcal{K}}$ *the set of compact operators and let* $K \in \mathcal{B}(\mathcal{H})_{\mathcal{K}}$*. Then*

i) *An operator* $K \in \mathcal{B}(\mathcal{H})_{\mathcal{K}}$ *is compact if the image of the unit ball in* $\mathcal{H}$ *under* K *is precompact.*

ii) *There is a norm convergent sequence of finite rank operators $A_n \in \mathcal{B}(\mathcal{H})$, such that $\lim A_n = K$. Conversely, any norm limit of finite rank operators is compact.*

iii) *$\mathcal{B}(\mathcal{H})_\mathcal{K}$ is a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. In particular, $\mathcal{B}(\mathcal{H})_\mathcal{K}$ is a closed two-sided ideal in $\mathcal{B}(\mathcal{H})$.*

iv) *$\sigma(K) \setminus \{0\}$ consists of eigenvalues with finite multiplicity and for $\dim \mathcal{H} = \infty$ we have $0 \in \sigma_e(K)$*[2]*.*

Compact operators will play an important role later, when we discuss the different notions of possible perturbations of a symmetric unitary on a one-dimensional lattice. Thereby, "compact perturbations" are the natural generalisation of strictly local perturbations, which only act on a finite number of finite-dimensional subspaces of the whole lattice, and are therefore of finite rank (see Section 3.2). Moreover, compact operators are critically involved in our standing assumption for locality of an operator on the one-dimensional lattice, namely "essential locality" (see Section 3.3).

An important structure arising from the observations above is the so-called Calkin algebra.

Definition 1.2.5 (Calkin algebra)**.** *The factor C^* algebra $\mathcal{B}(\mathcal{H})/\mathcal{B}(\mathcal{H})_\mathcal{K}$ is called the **Calkin algebra**. We denote by $\pi\colon \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})_\mathcal{K}$ the natural map from $\mathcal{B}(\mathcal{H})$ into the Calkin algebra.*

Establishing the Calkin algebra as an object on its own simplifies some of the proofs later on. Many statements formulated for operators "up to compact perturbations" can be transferred to the Calkin algebra. If e.g. an operator is gapped up to some finite-dimensional eigenspaces inside the gap, it suffices to show that the corresponding image of the operator in the Calkin algebra is properly gapped (see, e.g. the proof of Lemma 5.2.1).

The second set of operators we introduce is the set of Fredholm operators. These are invertible up to compact operators, i.e. are given by the operators with an invertible image in the Calkin algebra. However, we do not use this as the defining property. Instead, we introduce Fredholm operators in a way that immediately leads to the definition of the so-called **Fredholm index**, which will be of great importance in various situations throughout the thesis.

Definition 1.2.6 (Fredholm operator and Fredholm index)**.** *An operator $F \in \mathcal{B}(\mathcal{H})$ is called **Fredholm** if its range is closed and $\ker F$, as well as $\ker A^*$ are finite-dimensional. The **Fredholm index** of F is defined as*

$$\operatorname{ind}(F) = \dim\ker F - \dim\ker F^*. \tag{1.10}$$

The following lemma collects some well known facts about Fredholm operators and the Fredholm index

Lemma 1.2.7 (Properties of Fredholm operators)**.** *Let A and B be Fredholm operators. Then*

i) *AB is Fredholm and*

$$\operatorname{ind}(AB) = \operatorname{ind}(A) + \operatorname{ind}(B). \tag{1.11}$$

[2]The essential spectrum is defined in Definition 1.2.8.

ii) $\mathrm{ind}\,(\cdot)$ *is norm-continuous on the set of Fredholm operators.*

iii) $\mathrm{ind}\,(A+K) = \mathrm{ind}\,(A)$ *for* K *compact.*

iv) A *is Fredholm if and only if its image* $\pi(A)$ *in the Calkin algebra is invertible.*

v) A *is Fredholm if and only if there exists a bounded operator* B*, such that* $AB = \mathbb{1} + K$ *and* $BA = \mathbb{1} + K'$*, with compact operators* K, K'*. That is,* A *is left and right invertible up to compact operators.*

In the sense of *v*) and *iv*) of Lemma 1.2.7, Fredholmness generalizes the concept of invertibility of an operator on a Hilbert space, which also leads to the following concept: The essential spectrum of an operator.

Definition 1.2.8 (Essential spectrum)**.** *Let* $A \in \mathcal{B}(\mathcal{H})$*. The essential spectrum* $\sigma_e(A) \subset \sigma(A)$ *is defined as*

$$\sigma_e(A) = \{\lambda \in \mathbb{C} \mid (A - \lambda\mathbb{1}) \text{ is not Fredholm}\} \tag{1.12}$$

This formulation for the definition of the essential spectrum is motivated by [Con07, Chap. XI, Prop. 4.3]. Usually, the essential spectrum is defined via the first item in the following Lemma, which collects some properties of the essential spectrum.

Lemma 1.2.9. *Let* $A \in \mathcal{B}(\mathcal{H})$ *and* $K \in \mathcal{B}(\mathcal{H})_{\mathcal{K}}$*. Then*

i) $\sigma_e(A+K) = \sigma_e(A)$*, or, equivalently* $\sigma_e(A) = \sigma(\pi(A))$*.*

ii) $\sigma_e(A \oplus B) = \sigma_e(A) \cup \sigma_e(B)$*.*

iii) *Let* A *be normal, then* $\sigma(A) \setminus \sigma_e(A)$ *is the set of isolated eigenvalues of finite multiplicity. Hence,* $\sigma_e(A)$ *is the set of limit points in* $\sigma(A)$*.*

Let us give an example for the concepts above, introducing the unilateral shift operator on $\ell^2(\mathbb{N}_0)$, which will also be important later on.

Example 1.2.10 (The shift operator)**.** *Let* $\mathcal{H} = \ell^2(\mathbb{N}_0)$*, i.e. the space of square summable sequences* $\phi\colon \mathcal{N}_0 \to \mathbb{C}$ *with inner product* $\langle\varphi,\psi\rangle = \sum_x \overline{\varphi_x}\psi_x$*. The unilateral shift* S *is defined via its action on elements* $\varphi \equiv (\varphi_0, \varphi_1, \varphi_2, \ldots) \in \mathcal{H}$ *via*

$$S\varphi = (0, \varphi_0, \varphi_1, \varphi_2, \ldots) \quad \textit{and} \quad S^*\varphi = (\varphi_1, \varphi_2, \varphi_3, \ldots). \tag{1.13}$$

S *is a Fredholm operator with* $S^*S = \mathbb{1}$ *and* $SS^* = \mathbb{1} - P_{\ker S^*} = \mathbb{1} - P_0$*, where* P_0 *is the rank one projection onto* $(1,0,0,\ldots) \in \mathcal{H}$*. The Fredholm index is therefore given by*

$$\mathrm{ind}\,(S) = -1. \tag{1.14}$$

Moreover, its spectrum $\sigma(S) = \{\lambda \in \mathbb{C} \mid |\lambda| \leq 1\} = \overline{\mathbb{D}}$ *is the full closed unit disk (thereby, for* $|\lambda| < 1$*,* $S - \lambda\mathbb{1}$ *is Fredholm, with index* -1 *[Con07, Sect. VII, Prop. 6.5]). But since its image in the Calkin algebra* $\pi(S)$ *is unitary, we get* $\sigma_e(S) \subset \{\lambda \in \mathbb{C} \mid |\lambda| = 1\}$*, i.e. its essential spectrum is the full unit circle [Con07, Sect. XI, Ex. 4.10].*

1.3 Time evolution

As discussed above, the time evolution in quantum mechanics is modelled by the Schrödinger equation $\partial_t U(t) = -iHU(t)$, where $U(t) \in \mathcal{B}(\mathcal{H})$ is unitary and H is self-adjoint. In many applications, e.g. a fine-tuned experimental setup, one has control over the driving process, i.e. the Hamiltonian H, and wants to investigate the generated time evolution. The setting we are aiming for are periodically driven systems, i.e. a driving process via a time-dependent Hamiltonian $H(t)$ with $H(t+T) = H(t)$ for some period T. In order to take a closer look at such a driving procedure, we revert the axiomatic point of view and start with the Schrödinger equation on $U(t)$

$$\partial_t U(t) = -iH(t)U(t), \quad \text{with} \quad U(0) = \mathbb{1}, \tag{1.15}$$

where $t \mapsto H(t) \in \mathcal{B}(\mathcal{H})$ is a measurable function into the self-adjoint bounded operators on $\mathcal{H}$. We assumed $H(t)$ to be bounded, which is indeed a major simplification. However, having in mind a well-controlled experimental environment, where the $H(t)$ only refers to a well separated, possibly even finite-dimensional subsystem, this assumption becomes feasible at least effectively. For details on more general scenarios we refer the reader to [Kre72, Kat53, Fri64, Tan60]

It is easy to see that the solution of (1.15) has to be unitary (assuming its existence for a moment). Indeed, $U(t)^*U(t)$ does not change in time, which can be seen by evaluating

$$\partial_t \big(U(t)^*U(t)\big) = iU(t)^*\big(H(t) - H(t)\big)U(t) = 0. \tag{1.16}$$

Hence, by the initial condition $U(0) = \mathbb{1}$, we get $U(t)^*U(t) = \mathbb{1}$ (and the same for $U(t)U(t)^*$) for all t.

The existence of a unique solution for $t \in [a,b] \subset \mathbb{R}$ is guaranteed by the well known Picard-Lindelöf theorem, also known as Chauchy-Lipschitz theorem (see, e.g. [Bre10, Theorem 7.3] or [Tol, Section 2]), given that $\|H(t)\|$ is bounded for all $t \in [a,b]$.

Theorem 1.3.1 (Picard-Lindelöf)**.** *Let $\mathcal{B}$ be a Banach space, $I = [a,b] \subset \mathbb{R}$ a closed interval and $F\colon I \times \mathcal{B} \to \mathcal{B}$ a map, such that*

i) $t \mapsto F(t, y(t))$ is measurable[3], and for all arbitrary but fixed $y \in C(I, \mathcal{B})$ there exists a $C = C(y) > 0$, such that $\|F(t, y(t))\| \leq C$ for $t \in I$.

ii) F fulfils a global Lipschitz condition in the second argument.

Then, for each $y_0 \in \mathcal{B}$ there exists a unique continuous solution $y\colon I \to \mathcal{B}$ to the initial value problem

$$\partial_t y(t) = F(t, y(t)), \qquad y(a) = y_0. \tag{1.17}$$

Proof. Let λ be the Lipschitz constant for F. Equipping the set of continuous functions $C(I, \mathcal{B})$ with the norm $\|y(t)\|_{C(I,\mathcal{B})} := \sup_t e^{-2\lambda t} \|y(t)\|_{\mathcal{B}}$ (which is equivalent to the

[3] We here omit the details concerning the measurability and integratability of Banach space valued functions. Details can be found in [Coh13].

usual supremum norm $\sup_t \|y(t)\|_{\mathcal{B}}$), $C(I,\mathcal{B})$ becomes a Banach space. Consider the operator $T\colon C(I,\mathcal{B}) \to C(I,\mathcal{B})$, defined via

$$\big(T(y)\big)(t) = y_0 + \int_a^t F(s,y(s))ds. \tag{1.18}$$

Thereby, $i)$ guarantees that T is well defined: For all t $\int_a^t F(s,y(s))ds$ exists and we have

$$\big\|\big(T(y)\big)(t_1) - \big(T(y)\big)(t_2)\big\|_{\mathcal{B}} = \left\|\int_{t_1}^{t_2} F(s,y(s))ds\right\|_{\mathcal{B}} \leq C|t_2 - t_1|, \tag{1.19}$$

wherefore $T(y) \in C(I,\mathcal{B})$ is indeed continuous.

Using the Lipschitz condition for F, we can now show, that T is a contraction with respect to $\|\cdot\|_{C(I,\mathcal{B})}$: For all t we have

$$\begin{aligned}\big\|\big(T(x)\big)(t) - \big(T(y)\big)(t)\big\|_{\mathcal{B}} &= \left\|\int_a^t F(s,x(s)) - F(s,y(s))ds\right\|_{\mathcal{B}} \\ &\leq \lambda \int_a^t \|x(s) - y(s)\|_{\mathcal{B}}\, ds \\ &\leq \lambda \int_a^t e^{2\lambda s}\, \|x-y\|_{C(I,\mathcal{B})}\, ds = \frac{e^{2\lambda t} - e^{2\lambda a}}{2}\, \|x-y\|_{C(I,\mathcal{B})} \\ &\leq \frac{e^{2\lambda t}}{2}\, \|x-y\|_{C(I,\mathcal{B})}\,,\end{aligned} \tag{1.20}$$

which gives

$$\|T(x) - T(y)\|_{C(I,\mathcal{B})} \leq \frac{1}{2}\|x-y\|_{C(I,\mathcal{B})}. \tag{1.21}$$

Now, since T is a contraction, by the Banach fixed point theorem, there exists a unique fixed point $y \in C(I,\mathcal{B})$ with $T(y) = y$. By construction $y(t)$ solves (1.17). □

In order to apply this to (1.15), we set $\mathcal{B} = \mathcal{B}(\mathcal{H})$, and define F via $(t, U(t)) \mapsto -iH(t)U(t)$. Thereby, $\|H(t)\| < \infty$ ensures $ii)$:

$$\|F(t,U(t)) - F(t,V(t))\| \leq \|H(t)\|\|U(t) - V(t)\|, \tag{1.22}$$

and, together with the measurability of $t \mapsto H(t)$ also $i)$, with $C = \sup_t \|H(t)U(t)\|$. The solution is then often referred to as the time ordered exponential

$$\begin{aligned}U(t) &= \mathcal{T}\exp\left(-i\int_0^t H(s)ds\right) \\ &= \mathbb{1} + \frac{1}{i}\int_0^t H(s)ds + \frac{1}{i^2}\int_0^t\int_0^s H(s)H(s')ds'ds + \dots.\end{aligned} \tag{1.23}$$

In particular, any C^*-algebra is a Banach space. Hence, whenever (1.15) is formulated in a C^*-subalgebra $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ of the bounded operators on $\mathcal{H}$, i.e. $H(t) \in \mathcal{A}$, $\forall t \in I$, the solution $U(t)$ is also contained in $\mathcal{A}$. This fact will turn out useful later, when we discuss the different locality conditions for operators on the one-dimensional lattice. In particular the set of **essentially local** operators (see Section 3.3) forms a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. Hence, any driving by an essentially local operator results in an essentially local time evolution.

1.3.1 Periodic driving: Floquet time evolution

The time evolution operator has a special property if the driving is periodic in time, i.e. if

$$H(t+T) = H(t), \quad \forall t, \tag{1.24}$$

for some period T. In this setting one speaks of Floquet time evolution [Flo83]. In general, $U(t)$ does not necessarily turn out to be periodic in time (i.e. $U(t+T) \neq U(t)$, $\forall t$), instead we get:

Lemma 1.3.2. *Let $U(t)$ be the time evolution operator for a periodically driven system, i.e. driven by $H(t)$ with (1.24). Then, for all t, $U(t)$ fulfils*

$$U(t+T) = U(t)U(T). \tag{1.25}$$

In particular, we have

$$U(nT) = U(T)^n, \quad n \in \mathbb{N}_0. \tag{1.26}$$

Proof. (1.25) follows from evaluating the right and side of (1.23), using an appropriate change of variables after splitting the integrals into the intervals $[0, t+T] = [0, T] \cup [T, t+T]$ (see, e.g. [Sal74]). (1.26) is a direct consequence of (1.25) and follows by iteratively replacing $U(nT) = U(nT-T)U(T)$. □

If we now consider the time evolution only stroboscopically at each whole period $t = nT$, we get the discrete time evolution operators via iterative multiplication with the so-called **Floquet operator** $U(T)$. Such a stroboscopic view onto a periodic driving process defines a **quantum walk** in the sense we discuss below[4]. Later we will see that the opposite is not true in general, i.e. not every discrete-time quantum walk can be realised as the Floquet operator of a periodic driving process (see Section 3.3.2, and Theorem 3.3.19 in particular).

1.4 Quantum walks

In this section, we introduce the central concept for this thesis: **quantum walks**. We begin with some remarks on the historical developments and some general properties before we particularise the notion of a quantum walk in one dimension and discuss two different ansatzes for their definition. We end the section with an example, the so-called split-step walk, which we will meet again in Chapter 5. The overview will, however, only be a brief one and we refer the interested reader to the review articles [Kem03] and [VA12]. We will also include time-continuous processes into the considerations later, but here focus on discrete-time quantum walks. Generally speaking, for our purpose, a quantum walk is the unitary time evolution operator for a discrete-time evolution on a discrete spatial structure such as the one-dimensional lattice. However, let us begin with the historical development:

[4] and further in Section 3.3, where the necessary generalisation to broader notions of locality are discussed

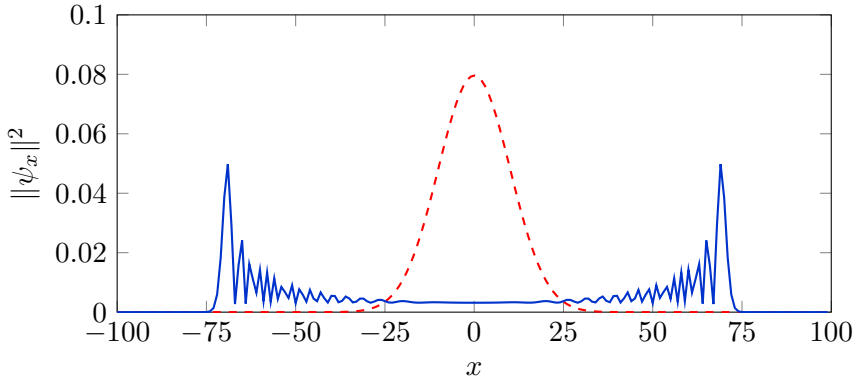


Figure 1.2: Position distribution for the split-step quantum walk (see Example 1.4.6) with $\theta_1 = \theta_2 = \pi/4$ and initial state $\psi_0 = 1/\sqrt{2}(1, i)$ (blue), and the probability distribution for a classical random walk with fair coin starting at $x = 0$ (red, dashed) after 100 time steps.

The concept of a quantum random walk was first introduced by Aharonov et al. in 1987 as a quantum mechanical version of a classical random walk [ADZ93]. Let us briefly describe the standard example of a classical random walk, i.e. a particle on the one-dimensional lattice, represented by $\mathbb{Z}$. The only degree of freedom for the particle is the position, and it evolves discretely in time according to the following rule. In each time step, a fair coin is tossed, and the particle moves one step to the left or one step to the right, depending on the coin toss outcome. After $t \in \mathbb{N}$ time steps, starting at $x_0 = 0$, the particle is at position $x_t = 2k - t$ for some $k = 0, \dots, t$. The probability of finding the particle at x_t is $P(x_t = 2k - t) = t!/(k!(t-k)!2^t)$, i.e. a binomial distribution with expectation value 0 and variance t. The expected travel distance of the particle is therefore given by $\sqrt{t}$, wherefore one speaks of **diffusive spreading**. Of course, this concept easily generalizes to higher-dimensional lattices or general graphs. Random walks have numerous applications, including stochastic algorithms [MR95, Sch99], biology and genetics [Ber84, LS91, vdEST92], neuroscience [TYZ+09], computer vision [WGW+19], and many more [XLN+20] (see also references therein).

In [ADZ93] a spin 1/2-particle is used instead of a classical one. The coin toss is then replaced by a measurement on the spin state, which determines the direction of movement. Measuring the S_z-eigenbasis and assigning the step to the left/right to the respective spin up/down outcomes, the protocol described in [ADZ93] reproduces the classical random walk. If the measurement basis is chosen differently, without changing the left/right assignments, a faster spreading of the position distribution t steps is observed due to interference effects.

Later, the measurement and preparation step was removed, and the classical coin toss dependent steps were replaced by state-dependent shift operations and local unitaries acting in each cell [Mey96, ABNW01]. This way, the dynamics are coherent, and it was soon observed that this model allows for ballistic instead of diffusive spreading (see Figure 1.2). In a seemingly different approach, formerly known as **unitary cellular automaton** or **quantum cellular automaton**, quantum walks were introduced more

axiomatically as unitary time evolution operators on a lattice with finite jump length [BB94, Mey96]. In modern terms, **quantum cellular automata** denote the many-particle generalization of quantum walks [SW04, GNVW12], i.e. automorphisms of the quasi-local algebra associated to some lattice structure, with a locality condition. The quantum cellular automata in [BB94, Mey96] would be called quantum walks today. Generally speaking, a **quantum walk** describes the discrete-time evolution of a single quantum particle on some lattice or other discrete structure like a graph. As such, quantum walks are similar to Floquet systems. Indeed, given a periodically driven system, the stroboscopic view onto the time evolution, i.e. the repeated application of the Floquet operator, is a quantum walk. However, not every discrete-time quantum walk can be realized via a periodically driven system in continuous time. We discuss the connections and differences between the two pictures in Section 3.3, Chapter 4, and particularly in Chapter 5.

Driven by the various applications of classical random walks and the observed spreading speed up in the quantum mechanical counterparts, quantum walks sparked interest as possible models for quantum algorithms. This was initiated by the famous quantum walk based search algorithm by Grover [Gro96] and is still an active area of research [SKW03, AKR05, Amb07, San08, MNRS11, Por16, KH18, BLP21]. Besides the application for search algorithms, also other properties of classical random walks, such as recurrence [ŠJK08, ŠKJ08, BGVW14, GVWW13] and mixing times [MPAD08, Kar10, MPA10, CLR20] have been investigated for quantum walks. Meanwhile, quantum walk based algorithms are found in a variety of different applications, including cryptography [VRM$^+$15, VKM$^+$18, SC20, AAEAAI20], pseudo-random number generation [SC19, AAEAAI20, BK21], graph classification [CMC20, DMKP$^+$19] and neural networks [DMKP$^+$19]. Quantum walks have even been shown to be universal for quantum computation [LCE$^+$10].

Besides the focus on algorithmic applications, quantum walks were also investigated from a more physical point of view. On the one hand, the ballistic spreading of quantum walks was formulated in terms of weak convergence of the random variable corresponding to the time evolved position operator X_t/t, scaled by t in contrast to $\sqrt{t}$ in case of the classical counterparts [GJS04, Kon05, WKKK08, AVWW11]. It was shown that in the translation invariant case, it is possible to define a group velocity operator that translates the properties of the dispersion relation of the walk into the spreading behaviour [AVWW11, Ahl13] (see also below). On the other hand, quantum walks are also of interest as simple and well controllable model systems for various physical phenomena, such as dynamical localisation [JM10, Joy12, ASW11, Wer13, CW21], Bloch oscillations [RBH$^+$11, APP20], Landau-Zener tunneling [RBH$^+$11], molecular binding [AAM$^+$12], Klein Paradox [Kur08] and the effects of coupling of a one-dimensional quantum walk to an electro magnetic field [CRW$^+$13, Arn17, SAM$^+$19, CGWW19, CW21, PFM20, CFGW20]. Moreover, specific quantum walk models have been shown to mimic relativistic particles in the continuum limit [BB94, DP14, ANF14, APAF19].

The growing interest in quantum walks soon lead to the first experimental implementations. Meanwhile, quantum walks have been realised or proposed on a variety of different platforms, building on different physical concepts. These include optical waveguide arrays [PLM$^+$10, SSV$^+$12, KBF$^+$12], superconducting qubits [RFR$^+$17, FRHG$^+$17, BCS18], single photons in free space [BFL$^+$10], trapped ions in phase space

[SMS+09, ZKG+10], wave packages in optical fibre loops [SCP+10, SGR+12, CDQ+18, NGS+19], and neutral atoms in optical lattices [KFC+09, AAM+12, GAS+13].

Of course, an experimental realization of a theoretical model comes with physical imperfections, and therefore the question arose how disorder, spatial and temporal fluctuations, or decoherence affect the predicted spreading behaviour of quantum walks. These questions were addressed in [RSA+05, Ken07, Joy11, AVWW11, KKNJ12, ACM+12, Ahl13, Wer13].

A recent development in the quantum walk community is the study of topological phases of matter from the perspective of quantum walks and their topological classification under the influence of discrete symmetries. This is the main topic of this thesis, and therefore we devote it its own introduction and literature overview in the introduction to Chapter 3, leaving it here with a mere mention.

Quantum walks describe the dynamics of single-particle systems. Hence, the obvious question about possible generalizations of the concepts to many-particle dynamics arises. There have been different approaches to many-particle quantum walks [EB05, VAB09, AAM+12, Toi20]. As already mentioned above, the general models for coherent discrete-time many-particle lattice systems with finite interaction length are known as **quantum cellular automata** and were first axiomatically described in [SW04]. In [Vog09] it has been shown that for any translation-invariant quantum walk, there exists a quantum cellular automaton, which exhibits the dynamics of the quantum walk as its single-particle sector. This ansatz has been further developed in [Ahl13], which provides a general construction for quantum cellular automata from interacting quantum walks. Quantum cellular automata have also been proven equivalent to time evolution via matrix product unitary operators [CPGSV17]. For an overview about quantum cellular automata, we recommend the two reviews [Arr19, Far20].

We end our short overview here and proceed with an introduction to the technical basics for quantum walks on the one-dimensional lattice.

1.4.1 Quantum walks: The technical basics

We informally introduced quantum walks as discrete-time evolution operators for single-particle dynamics on the lattice. This rather vague description leaves room for different definitions. Quantum walks can either be defined axiomatically, i.e. as a unitary operator equipped with a locality assumption or constructively, i.e. via a sequence of fundamental building blocks: Shift and coin operations. Let us formalise these two concepts, beginning with the axiomatic ansatz. In the first part of this thesis, we discuss results that hold without any locality condition. In the remainder (from Section 3.3 onwards), the focus lies on quantum walks on the one-dimensional lattice. We, therefore, restrict our considerations to one spatial dimension also in this preliminary section.

The underlying Hilbert space for a one-dimensional quantum walk consists of finite-dimensional local **cells** $\mathcal{H}_x$, labelled by $x \in \mathbb{Z}$. Axiomatically, a quantum walk is defined as a unitary with an upper bound on the jump length between the individual cells:

Definition 1.4.1 (Quantum walk (strictly local))**.** *Let $\mathcal{H}$ be a separable Hilbert space with a*

one-dimensional lattice structure and finitely many local degrees of freedom, i.e.

$$\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x \tag{1.27}$$

is the direct sum of finite-dimensional Hilbert spaces $\mathcal{H}_x$, where the cell dimensions $d_x = \dim \mathcal{H}_x$ are uniformly bounded, i.e. there exists a $d \in \mathbb{N}$, such that $d_x \leq d$ for all $x \in \mathbb{Z}$. If the local cells are pairwise isomorphic, e.g. for translation invariant systems, we can also write

$$\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d \quad \textit{for} \quad \mathcal{H}_x = \mathcal{H}_0 = \mathbb{C}^d, \ \forall x. \tag{1.28}$$

*On $\mathcal{H}$ a (strictly local) **quantum walk** is defined as a discrete time evolution operator U with finite interaction length L. More precisely, U is a unitary operator, such that there exists an $L \in \mathbb{N}$ with*

$$\langle \psi_y, U\psi_x \rangle = 0 \quad \textit{for all} \quad \psi_x \in \mathcal{H}_x \, \psi_y \in \mathcal{H}_y, \quad \textit{with} \quad |x-y| > L. \tag{1.29}$$

A single time step for a vector $\psi(t) \in \mathcal{H}$, $t \in \mathbb{Z}$ is implemented via

$$\psi(t+1) = U\psi_t. \tag{1.30}$$

The action of a quantum walk on a vector $\psi \in \mathcal{H}$ can be expressed locally via

$$(U\psi)_x = \sum_y U_{xy}\psi_y, \tag{1.31}$$

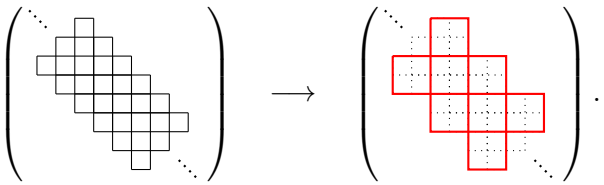
where U_{xy} is the part of U that maps from $\mathcal{H}_y$ to $\mathcal{H}_x$. With this in mind, and organising the basis accordingly, we can think of a walk as a doubly infinite matrix with non-zero entries around the main diagonal. With $L = 1$ for x around zero we get

$$U \equiv \begin{pmatrix} \ddots & U_{\text{-}2,\text{-}1} & & & \\ U_{\text{-}1,\text{-}2} & U_{\text{-}1,\text{-}1} & U_{\text{-}1,0} & & \\ & U_{0,\text{-}1} & U_{0,0} & U_{0,1} & \\ & & U_{1,0} & U_{1,1} & U_{1,2} \\ & & & U_{2,1} & \ddots \end{pmatrix} \tag{1.32}$$

Remark 1.4.2. *Any strictly local quantum walk can be thought of as a next-neighbour walk with $L = 1$ by regrouping the cell structure. Indeed, let U be a quantum walk on $\mathcal{H}$ with some local structure according to* (1.27)*. Reconsidering sets of $2L$ consecutive cells into one new cell along the whole lattice yields a new cell structure*

$$\mathcal{H} = \bigoplus_{y\in\mathbb{Z}} \widetilde{\mathcal{H}}_y \qquad \textit{with} \qquad \widetilde{\mathcal{H}}_y = \mathcal{H}_{2Ly} \oplus \mathcal{H}_{2Ly+1} \oplus \ldots \oplus \mathcal{H}_{2Ly+2L-1}. \tag{1.33}$$

With respect to the regrouped cells the walk has the new interaction length $\widetilde{L} = 1$. This can be depicted as



The local Hilbert spaces or cells are often called coin-space, which leads us to the constructive definition of quantum walks. For this, let us introduce two archetypical examples of quantum walks in the sense above, which serve as the fundamental building blocks for the constructive definition.

Definition 1.4.3 (Coin operations)**.** *A **coin operation** is a quantum walk with interaction length $L = 0$. That is, a direct sum of finite-dimensional unitary operators C_x:*

$$C = \bigoplus_{x\in\mathbb{Z}} C_x \equiv \begin{pmatrix} \ddots & & & \\ & C_{-1} & & \\ & & C_0 & \\ & & & C_1 \\ & & & & \ddots \end{pmatrix}, \qquad C_x \in \mathcal{U}(\mathcal{H}_x). \tag{1.34}$$

Coins are trivial in the sense that they do not contain any dynamics between the different cells. We can identify a coin operation with just a base-choice locally in each cell.

Definition 1.4.4 (Shifts)**.** *The prototype examples of quantum walks with interaction length $L > 0$ are shift operations. We begin with the simplest case: a Hilbert space with only one-dimensional cells $\mathcal{H}_x = \mathbb{C}$. In this case, $\mathcal{H}$ naturally equals $\ell^2(\mathbb{Z})$. On $\ell^2(\mathbb{Z})$, the **bilateral shift** S is defined as*

$$Se_x = e_{x+1}, \tag{1.35}$$

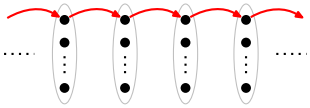
where $\{e_x\}_{x\in\mathbb{Z}}$ denotes the standard positional basis for $\ell^2(\mathbb{Z})$. S is clearly strictly local, with interaction length $L = 1$.

*The concept of S can easily be transferred to larger cell structures with more than one local degree of freedom, i.e. with $d_x > 1$: We choose a vector $\phi_x \in \mathcal{H}_x$ in each cell and embed the shift above into the subspace spanned by the collection $\{\phi_x\}_{x\in\mathbb{Z}}$ of these vectors. This defines a **partial shift** with*

$$S_\phi\phi_x = \phi_{x+1} \qquad \text{and} \qquad S_\phi\psi = \psi, \quad \text{for all} \quad \psi \perp \phi_x. \tag{1.36}$$

In the translation invariant case, choosing a basis for $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$, such that $\phi_x = (1, 0, \ldots, 0)$ is the first basis vector in each cell, we write

$$S_\phi = \begin{pmatrix} S & \\ & \mathbb{1}_{d-1} \end{pmatrix} \equiv \tag{1.37}$$



and similarly for other choices of ϕ_x, with the bilateral shift S from above.

Using the two examples above, discrete-time quantum walks are often defined constructively as finite sequences of these two basic operations:

Definition 1.4.5 (Coined quantum walk)**.** *On $\mathcal{H}$ from Definition 1.4.1 a **coined quantum walk** is define by a finite sequence of shifts S_i and coin operations C_i from Definition 1.4.3 and Definition 1.4.4:*

$$U = C_{n+1} S_{\phi_n} C_n \dots S_{\phi_1} C_1. \tag{1.38}$$

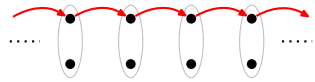
Clearly, any coined quantum walk is a quantum walk in the sense of Definition 1.4.1, with $L \leq n$. In Chapter 4 we prove that also the opposite is true, that is, any quantum walk in the sense of Definition 1.4.1 can be decomposed into a sequence of shifts and coins with respect to the given cell structure.

Example 1.4.6 (Split-step walk)**.** *The split-step walk is defined on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ via*

$$U_{ss} = S_{\downarrow} C_2 S_{\uparrow} C_1, \tag{1.39}$$

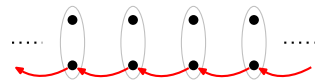
where $S_{\uparrow}$ ($S_{\downarrow}$) denotes the partial shift S_ϕ with $\phi_x = (1, 0)$ (resp. S_ϕ^* with $\phi_x = (0, 1)$), i.e.

$$S_{\uparrow} = \begin{pmatrix} S & 0 \\ 0 & 1 \end{pmatrix} \equiv \tag{1.40}$$



and

$$S_{\downarrow} = \begin{pmatrix} 1 & 0 \\ 0 & S^* \end{pmatrix} \equiv \tag{1.41}$$



similar to (1.37)*.*

Typically the local coins are chosen as real rotations $C_{i,x} = R(\theta_{i,x})$, with $R(\theta) = \exp(i\theta\sigma_y)$. Figure 1.2 shows the position distribution $\|\psi_x\|^2$ after 100 time-steps, for the coin-angles $\theta_{1,x} = \theta_{2,x} = \pi/4$, $\forall x$ and the the initial state $\psi_0 = (1, i)/\sqrt{2}$ at $x = 0$.

The split-step walk was first introduced in [KRBD10] and is one of the standard examples in the literature on topological phases in one-dimensional quantum walks [Kit12, Asb12, AO13, ATD14, TAD14, KBF+12, CGS+16, Sta15, CGG+18, CGS+18, CGG+21, CGWW21]. We discuss the topological classification of the split-step walk model in Chapter 5.

1.4.2 Translation invariant quantum walks

Above, we already broached translation invariance in the example of the partial shift. Let us give a brief overview about translation-invariant quantum walks in general. Translation invariant operators act especially simple in momentum space, that is, after Fourier transformation with respect to the one-dimensional lattice[5]. This opens various techniques to analyse quantum walks, e.g. their propagation behaviour or homotopy invariants.

In the translation invariant case, all cells $\mathcal{H}_x$ are isomorphic and we can write $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathcal{H}_0 = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$. Hence, we can consider any vector $\psi \in \mathcal{H}$ as a $\mathbb{C}^d$ valued

[5]Most results presented below are valid in any lattice dimension, but since we are concerned with on-dimensional systems in this thesis, we restrict our consideration to those systems also for this summary.

function $\psi\colon \mathbb{Z} \to \mathbb{C}$, with values $\psi(x) = \psi_x$. For such functions we can define the discrete Fourier transformation $\mathcal{F}\colon \ell^2(\mathbb{Z}) \to \mathcal{L}^2(\mathbb{T})$ on the first tensor factor, i.e.

$$(\mathcal{F}\psi)(k) = \widehat{\psi}(k) = \sum_x e^{ikx}\psi_x \qquad \text{and} \qquad \left(\mathcal{F}^*\widehat{\psi}\right)_x = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikx}\widehat{\psi}(k). \tag{1.42}$$

An operator A on $\mathcal{H}$ is called translation invariant if it commutes with the global lattice translation $T = S \otimes \mathbb{1}_d$, i.e. if $AT = TA$. This implies $A_{xy} = A_{x-y,0}$ for all $x, y \in \mathbb{Z}$ for the block-matrix elements in the decomposition according to (1.31). Moreover, any translation invariant bounded operator A becomes a d-dimensional k-dependent multiplication operator in momentum space [Ahl13, Lemma 3.2.2 and 3.2.3]. In particular, for a quantum walk, i.e. a unitary operator with only finitely many non-zero $U_{x,0}$ we get

$$\widehat{(U\psi)}(k) = \widehat{U}(k)\widehat{\psi}(k), \qquad \text{with} \qquad \widehat{U}(k) = \sum_x e^{ikx}U_{x,0}. \tag{1.43}$$

Example 1.4.7 (Shifts in momentum space)**.** *The bilateral shift S on $\ell^2(\mathbb{Z})$ from Definition 1.4.4 is obviously translation invariant. We get $S_{x,0} = \delta_{x1}$ and therefore*

$$\widehat{S}(k) = e^{ik}. \tag{1.44}$$

Consequently, the partial shift in (1.37) *takes the form*

$$\widehat{S}_\phi = \begin{pmatrix} e^{ik} & \\ & \mathbb{1}_{d-1} \end{pmatrix}. \tag{1.45}$$

Considering a translation invariant walk in momentum space via Fourier transformation opens the possibility for various techniques. In particular, it enables us to assign a band structure to the walk. Indeed, the Fourier transformed quantum walk $\widehat{U}(k)$ is a k-dependent finite-dimensional unitary matrix, which can be diagonalised, i.e.

$$\widehat{U}(k) = \sum_{\alpha=1}^{d} e^{i\omega_\alpha(k)}Q_\alpha(k), \tag{1.46}$$

where $\omega_\alpha(k)$ are the quasi-energies and $Q(k)$ the corresponding band-projections.

Winding numbers

For translation-invariant walks, many of the topological invariants can be expressed in terms of winding numbers over the Brillouin-zone [GNVW12, KRBD10, CGS$^+$18]. For some symmetry types, the right symmetry index (see Section 3.5) may be expressed via the Berry phase of the eigen-bundles $Q_\alpha(k)$ [CGS$^+$18]. Another index quantity, which we will discuss in great detail in Section 3.3, is the information flow index [Kit06, GNVW12]. It measures the net shift content of a one-dimensional quantum walk and is an integer-valued homotopy invariant. For translation-invariant walks, it can be obtained in a straightforward way, wherefore we already introduce it here in that case, in anticipation of the discussion in Section 3.3: By definition, any strictly local translation

invariant quantum walk U becomes a matrix-valued Laurent polynomial $\widehat{U}(k)$ in e^{ik}. Hence, its determinant $\det(\widehat{U}(k))$ is a scalar valued Laurent polynomial in e^{ik}. Moreover, by unitary of $\widehat{U}(k)$, $\det(\widehat{U}(k)^*) = 1/\det(\widehat{U}(k))$ is also a polynomial, and therefore $\det(\widehat{U}(k))$ has to be a monomial in e^{ik}:

$$\det(\widehat{U}(k)) = \lambda e^{ikn}, \quad \lambda \in \mathbb{T},\, n \in \mathbb{Z}. \tag{1.47}$$

A norm-continuous, translation invariance preserving deformation of the whole walk U always induces a norm-continuous deformation of the finite-dimensional matrices $\widehat{U}(k)$ and therefore also of $\det(\widehat{U}(k))$. At each point of the deformation, the determinant must be a monomial in e^{ik}, wherefore its power has to stay constant. Hence, n is homotopy invariant and can be identified with the information flow index [GNVW12]. This way, the index can be expressed as the total winding of the quasi-energy spectrum around the Brillouin zone

Definition 1.4.8. *Let U be a translation invariant quantum walk with continuously differentiable[6] Fourier transform $\widehat{U}(k)$. Then its index may be defined as*

$$\mathrm{ind}\,(\widehat{U}) = \frac{1}{2\pi i}\int_{-\pi}^{\pi} dk \left(\frac{\partial}{\partial k}\log\det(\widehat{U}(k))\right). \tag{1.48}$$

1.5 Symmetries in quantum mechanics

In this section, we introduce the basics for symmetries in quantum mechanics, and in particular, the concept of representations of symmetry groups via unitary and antiunitary operators. For the general concept of symmetry, we follow [Lan17, Chapter 5]. For a general introduction to the theory of group representations, we refer the reader to [BR86].

Symmetries play an essential role in most physical theories. Generally speaking, a symmetry is an invertible map that leaves the relevant physical model or mathematical structure invariant. Studying the action of such an operation in detail often enables one to reveal structures of the underlying theory or objects that remained hidden otherwise. One of the most prominent examples of this is the spin of a quantum mechanical particle, which emerges from the theory of projective representations of symmetries. Quantum mechanics comes with various concepts for symmetry, distinguished by the different structures that are left invariant. If the whole underlying Hilbert space $\mathcal{H}$ is under consideration, a symmetry is just a unitary operator, i.e. a base-choice. However, the relevant symmetries involve further mathematical structures on $\mathcal{H}$, carrying the physical information of the underlying system. Considering different physical structures results in different concepts of symmetries. These include ([Lan17]):

- The normal pure state space on $\mathcal{H}$, i.e. $\{p \in \mathcal{B}(\mathcal{H}) | p = p^* = p^2, \mathrm{rank}\,(p) = 1\}$ (Wigner symmetry)

[6]The Fourier transformation $\widehat{U}(k)$ of any stritcly local quantum walk is a Laurent poylonial in e^{ik} and therefore always continuously differentiable in k. We include this asusmption in anticipation of the weaker locality assumptions we introduce in Section 3.3.

- The normal state space on $\mathcal{H}$, i.e. $\{\rho \in \mathcal{B}(\mathcal{H}) | \rho \geq 0,\, \mathrm{tr}(\rho) = 1\}$ (Kadison symmetry)
- The self-adjoint operators on $\mathcal{H}$, i.e. $\{H \in \mathcal{B}(\mathcal{H}) | H = H^*\}$ (Jordan symmetry)
- The effects/detectors on $\mathcal{H}$, i.e. $\{e \in \mathcal{B}(\mathcal{H}) | 0 \leq e \leq \mathbb{1}\}$ (Ludwig symmetry)
- The projections on $\mathcal{H}$, i.e. $\{P \in \mathcal{B}(\mathcal{H}) | P^2 = P^* = P\}$ (von Neumann symmetry)
- The unital commutative C^*-subalgebras of $\mathcal{B}(\mathcal{H})$ (Bohr symmetry)

Each of these sets is equipped with an additional structure that defines what it means for a symmetry to leave the set invariant. However, by a remarkable result, which is shown in [Lan17, Chapter 5], these different notions are equivalent, and each symmetry acts in a specific way via unitary or antiunitary operators. Hence, we will only spell out the precise definition in case of a Kadison symmetry and move on to the theory of symmetry representations afterwards.

Definition 1.5.1 (Kadison symmetry)**.** *Let $\mathcal{D}(\mathcal{H}) = \{\rho \in \mathcal{B}(\mathcal{H}) | \rho \geq 0,\, \mathrm{tr}(\rho) = 1\}$ be the set of density operators on a Hilbert space $\mathcal{H}$. A **Kadison symmetry** is a bijection $S \colon \mathcal{D}(\mathcal{H}) \to \mathcal{D}(\mathcal{H})$ that preserves the convex structure of $\mathcal{D}(\mathcal{H})$, i.e. for $\lambda \in [0,1]$ and $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ it fulfils*

$$S\left(\lambda\rho + (1-\lambda)\sigma\right) = \lambda S(\rho) + (1-\lambda)S(\sigma). \tag{1.49}$$

Note that the set pure states for a Wigner symmetry is the boundary of the set of density operators for a Kadison symmetry. By the above definition, this boundary is preserved by a symmetry, wherefore we can treat both cases simultaneously. An important result for symmetries in quantum mechanics is **Wigner's theorem**, which, in adapted formulation, holds for every concept of symmetry above.

Theorem 1.5.2 (Wigner/Kadison)**.** *Every Kadison symmetry S of $\mathcal{D}(\mathcal{H})$ is of the form*

$$S(\rho) = u\rho u^*, \quad \forall \rho \in \mathcal{D}(\mathcal{H}), \tag{1.50}$$

where u is either a unitary or an antiunitary operator on $\mathcal{H}$ that is uniquely determined by the symmetry S up to a phase.

For a proof see, e.g. [Wig59, BR86, Lan17]. By Wigner's theorem and the equivalence of the different concepts for symmetry [Lan17, Chapter 5], the action of a symmetry can always be described via conjugation with a unitary or an antiunitary operator on $\mathcal{H}$, no matter which notion of symmetry is considered.

Before we turn to the representation of groups via unitary and antiunitary operators, let us introduce the concept of an **antiunitary operator**. First recall, what defines a unitary operator. Above we characterized unitary operators as the symmetries of the underlying Hilbert $\mathcal{H}$ space itself, i.e. an operator U on $\mathcal{H}$ is unitary if it leaves the scalar product on $\mathcal{H}$ invariant $\langle U\varphi, U\psi\rangle = \langle \varphi, \psi\rangle$, $\forall \varphi, \psi \in \mathcal{H}$. The relevant physical consequence of this property is that it leaves the transition probabilities between vectors in $\mathcal{H}$ invariant, i.e.

$$|\langle U\varphi, U\psi\rangle|^2 = |\langle \varphi, \psi\rangle|^2, \quad \forall \varphi, \psi \in \mathcal{H}. \tag{1.51}$$

This qualifies unitary operators as representatives for Wigner symmetries. However, invariance of the scalar product is not the only operation that does not change $|\langle\varphi,\psi\rangle|^2$. The second option $\langle\varphi,\psi\rangle \mapsto \overline{\langle\varphi,\psi\rangle}$ leads to the defining property of antiunitary operators.

Definition 1.5.3. (*Antiunitary operator*) *Let $\mathcal{H}$ be a Hilbert space. An operator A is called antiunitary if*

$$\langle A\varphi, A\psi\rangle = \overline{\langle\varphi,\psi\rangle} = \langle\psi,\varphi\rangle. \tag{1.52}$$

Equivalently, an antiunitary operator is an antilinear operator A, i.e. $A(\lambda\psi) = \overline{\lambda}A\psi$, such that $A^*A = AA^* = \mathbb{1}$, where the action of the conjugate operator A^* follows from (1.52) *via*

$$\langle\varphi, A^*\psi\rangle = \overline{\langle A\varphi, AA^*\psi\rangle} = \langle\psi, A\varphi\rangle. \tag{1.53}$$

Including antiunitary operators in Wigner's theorem, motivated by the property above, might seem like being overly mathematically meticulous in the context of physical symmetries. However, Wigner showed that one of the fundamental physical symmetries in quantum mechanics, namely **time reversal** can only be represented antiunitarily [Wig59].

The properties of antiunitary operators are summarised in two works by Wigner [Wig60a, Wig60b]. Let A an antiunitary operator on $\mathcal{H}$. Fixing a basis $\{\varphi_i\}$ for $\mathcal{H}$ allows us to write A in an especially simple form. Denote by K the complex conjugation of coefficients with respect to the basis $\{\varphi_i\}$, i.e.

$$K\psi = K\sum_i \lambda_i\varphi_i = \sum_i \overline{\lambda}\varphi_i \equiv \overline{\psi}. \tag{1.54}$$

Since K is obviously antilinear and fulfils $K^2 = K^*K = \mathbb{1}$, it is an antiunitary operator. It is easy to verify that the product of two antiunitary operators and therefore also $U_A := AK$ is unitary. Hence, writing $A = AK^2 = U_AK$ we can express A as the product of the unitary operator U_A and the complex conjugation K with respect to the chosen basis:

$$A\psi = (AK)\sum_i \overline{\lambda}_i\varphi_i = U_A\overline{\psi}. \tag{1.55}$$

This way, if we meet the convention of always writing the complex conjugation to the right, the unitary parts of two antiunitary operators A and A' multiply as

$$U_{AA'} \equiv AA' = U_AKU_{A'}K = U_A\overline{U_{A'}}. \tag{1.56}$$

Writing antiunitary operators like this is helpful when dealing with actual realisations on a Hilbert space. However, for the structure theory, we will usually work with antiunitary operators without splitting them into a unitary and a standard antiunitary part.

1.5.1 (Projective) Representation of groups via unitary and antiunitary operators

If more than one symmetry is present in a system, they naturally carry the structure of a group. Wigner's theorem lifts the abstract concepts of symmetries as invertible maps

on certain sets with some invariance condition to the level of representations via unitary and antiunitary operators. These operators are only fixed up to a phase, which defines a projective representation of the abstract symmetry group:

Definition 1.5.4 (Symmetry representation)**.** *Let G be a symmetry group and $\mathcal{H}$ a Hilbert space. A **projective symmetry representation** ρ of G on $\mathcal{H}$ is determined by a map $\rho\colon g \mapsto \rho_g$ from G to the set of unitary and antiunitary operators on $\mathcal{H}$ and a function $m\colon G \times G \to \mathbb{T}$, such that*

$$\rho_g \rho_h = m(g,h)\rho_{gh}, \quad \forall g,h \in G. \tag{1.57}$$

The function m accounts for the freedom of choosing a phase for a symmetry in Wigner's theorem. We will often drop the term "projective" and just call the above concept a **representation** or a representation that is **fixed up to phases**. In the next section, we will study the freedom of choosing phases for the operators of a representation and the multiplication function and, in particular, its interplay with the presence of antiunitary operators in great detail for groups of involutive symmetries. This will lead to one of the main concepts in this thesis: **symmetry types** for groups of involutive symmetries.

Leaving the discussion about the phase choices and the multiplication function for the next chapter, we close this preliminary section with the study of "ordinary representations" with unitary and antiunitary operators, that is, with trivial multiplication function m. In particular, following [Wig59] and Dimmock [Dim63], we characterise the possible irreducible representations in this setting.

Remark 1.5.5. *Note that in slight difference to the setting we present here, Wigner and Dimmock consider so-called **corepresentations**, in which antiunitary operators are represented by linear matrices with adapted multiplication rules (see* (1.56)*). The two seemingly different concepts become equivalent via* (1.55) *with the convention that we always write the complex conjugation with respect to the chosen basis to the right. With that in mind, we will stick to representations including antiunitary elements for the sake of coherence.*

Let G be a finite group of symmetries, which contains both unitary u_i and antiunitary elements a_j[7]. The product of two antiunitary and the product of two unitary operators is unitary, whereas the product of an antiunitary and a unitary operator is again antiunitary. Consequently, the unitaries form a proper subgroup $H \subset G$. Moreover, G contains an equal number of unitary and antiunitary elements. Indeed, let $\{a_0, a_1, \ldots, a_n\} \subset G$ be the set of antiunitary operators, $\{u_0, u_1, \ldots, u_m\} \subset G$ the set of unitaries and $n-1$, respectively $m-1$ be their cardinalities. Then $\{a_0^2, a_0a_1, \ldots, a_0a_n\}$ is a set of $n-1$ different unitaries, wherefore $n \leq m$. On the other hand $\{a_0u_0, a_0u_1, \ldots, a_0u_m\}$ is a set of $m-1$ different antiunitary operators, implying $m \leq n$. Hence, H has index two in G, i.e. $|G:H| = 2$.

By the argument above, any antiunitary operator can be written as $a_i = a_0u_i$, with $u_0 = id$, by singling out one antiunitary element a_0. Hence, the group is of the form

$$G = H \cup a_0H, \tag{1.58}$$

[7]We here call the abstract group elements unitary or antiunitary, referring to the property of being represented by such an operator in a representation. In the next chapter, we formalise this distinction on the abstract group level via a unitarity character (see Section 2.1).

i.e. a single antiunitary element is sufficient to infer the group from its unitary subgroup H.

Let ρ be a representation for G. Similar to the linear case, a representation including antiunitary operators is called **irreducible** if there is no basis, such that ρ_u and ρ_a admit a block diagonal decomposition

$$\rho_u = \begin{pmatrix} \rho'_u & 0 \\ 0 & \rho''_u \end{pmatrix} \qquad \rho_a = \begin{pmatrix} \rho'_a & 0 \\ 0 & \rho''_a \end{pmatrix},$$

for all $u, a \in G$. For usual linear representations of groups, the question whether a representation is irreducible is settled by Schur's Lemma [BR86, Ch. 5, Sec. 3, Prop. 4]:

Theorem 1.5.6 (Schur's Lemma)**.** *A unitary representation ρ of G on $\mathcal{H}$ is **irreducible** if and only if the only operators commuting with all the ρ_g, $g \in G$ are scalar multiples of the identity:*

$$\{A \in \mathcal{B}(\mathcal{H}) \mid A\rho_g = \rho_g A, \forall g \in G\} = \{\lambda \mathbb{1} \mid \lambda \in \mathbb{C}\}. \tag{1.59}$$

Another formulation of the result above is that the only non-trivial ρ_G-invariant subspaces of $\mathcal{B}(\mathcal{H})$ is $\mathcal{B}(\mathcal{H})$ itself.

Dimmock proves a similar result for finite-dimensional representations involving antiunitary operators [Dim63, Thm. II]:

Theorem 1.5.7. *Let ρ be a finite-dimensional representation of a finite group G via unitary and antiunitary operators. Then ρ is **irreducible** if and only if every self-adjoint matrix M with*

$$M\rho_g = \rho_g M \tag{1.60}$$

is constant, i.e. $M = \mu\mathbb{1}$, $\mu \in \mathbb{R}$.

Note that differently from the usual complex linear case, the matrices M are restricted to be self-adjoint. In the complex linear case, it is already sufficient to prove the general statement for self-adjoint operators, since every operator is of the form $M = H_1 + iH_2$, for self-adjoint H_i. Hence, if it holds for the self-adjoint operators $H_1 = (M + M^*)/2$ and $H_2 = -i(M - M^*)/2$, it also holds for an arbitrary M. However, in the presence of antiunitary operators, we cannot deduce the statement for arbitrary operators from self-adjoint ones since we would get an additional minus sign for the commutation relation of the anti-self-adjoint part of an arbitrary M with ρ_a.

According to Wigner [Wig59, Dim63] we can now deduce the irreducible representations of the whole group G from those of its unitary subgroup H. Let $\{\phi^i_\alpha\}$ be an orthonormal basis of the i'th irreducible representation σ^i of H, i.e.

$$\rho_u \phi^i_\alpha = \sum_\beta (\sigma^i_u)_{\alpha\beta} \phi^i_\beta, \quad u \in H \subset G,$$

and K the complex conjugation with respect to this basis. Moreover, let a_0 be a fixed antiunitary element of G, and consider G as $G = H \cup a_0 H$. The irreducible representations of G are then determined by the action of a_0 on the basis $\{\phi^i_\alpha\}$ for σ^i. Let $\psi^i_\alpha = \rho_{a_0}\phi^i_\alpha$. There are three cases to distinguish:

1. $\{\psi^i_\alpha\}$ reproduces the basis $\{\phi^i_\alpha\}$, i.e. $\langle\psi^i_\alpha, \phi^i_\beta\rangle$ are the elements of a unitary matrix. In this case the representation σ^i already defines an irreducible representation $\hat{\rho}$ of the whole group:

$$\hat{\rho}_u = \sigma^i_u \qquad \hat{\rho}_{a_0} = \sum_{\alpha\beta} |\psi^i_\alpha\rangle\langle\phi^i_\beta| K. \tag{1.61}$$

2. $\{\psi^i_\alpha\}$ is an independent set of vectors, which is the basis for an irreducible representation of H that is equivalent to σ^i. In this case the dimension is doubled and an irreducible representation $\hat{\rho}$ of G contains two copies of the same irreducible representation of H:

$$\hat{\rho}_u = \begin{pmatrix} \sigma^i_u & 0 \\ 0 & \sigma^i_u \end{pmatrix} \qquad \hat{\rho}_{a_0} = \sum_{\alpha\beta} \begin{pmatrix} 0 & |\phi^i_\alpha\rangle\langle\psi^i_\beta| \\ |\psi^i_\alpha\rangle\langle\phi^i_\beta| & 0 \end{pmatrix} K. \tag{1.62}$$

3. $\{\psi^i_\alpha\}$ is an independent set of vectors, which is the basis for an inequivalent irreducible representation σ^j of H. Similar to case 2, the dimension is doubled and an irreducible representation $\hat{\rho}$ of G contains two inequivalent irreducible representations of H:

$$\hat{\rho}_u = \begin{pmatrix} \sigma^i_u & 0 \\ 0 & \sigma^j_u \end{pmatrix} \qquad \hat{\rho}_{a_0} = \sum_{\alpha\beta} \begin{pmatrix} 0 & |\phi^i_\alpha\rangle\langle\psi^j_\beta| \\ |\psi^j_\alpha\rangle\langle\phi^i_\beta| & 0 \end{pmatrix} K. \tag{1.63}$$

Dimmock also describes a method to determine the case from the irreducible representations of the unitary subgroup [Dim63]:

Lemma 1.5.8. *Let σ be an irreducible representation of the unitary subgroup $H \subset G$ of a finite group G. Then*

$$\sum_k \mathrm{tr}\left(\sigma_{a_k^2}\right) = \begin{cases} |H| & \textit{in case } \mathbf{1} \\ -|H| & \textit{in case } \mathbf{2} \\ 0 & \textit{in case } \mathbf{3}. \end{cases} \tag{1.64}$$

This distinction criterion will be helpful later in Section 2.3, where the we compute the irreducible representations of various symmetry groups in order to use them as building blocks for the so-called index group. With this we close the preliminary section and turn our attention to the concept of symmetry type for groups of involutive symmetries.

2 Discrete symmetry types for unitary operators: The 38-fold way

The concept of symmetry types for topological insulators and superconductors originates in the study of symmetries for random matrix ensembles. It dates back to Wigner and Dyson [Wig55, Wig57, Wig59, Dys62a, Dys62b], who distinguish three fundamental symmetry classes. These are called **unitary**, **orthogonal** and **symplectic**, and correspond to the presence or absence of time-reversal symmetry. In case of its presence time-reversal symmetry is represented by an antiunitary operator, which either squares to the identity (orthogonal) or minus the identity (symplectic). These three classes are known as **Dysons threefold way**, and are the fundamental concept behind further studies.

Altland and Zirnbauer extended the work by Dyson and Wigner. With the motivation of systematically classifying novel and exotic phases of matter, they found ten different symmetry types in their work on mesoscopic normal-superconducting hybrid systems [AZ97, Zir15]. Their classification became known as **the tenfold way**. Thereby, they unveiled a one-to-one correspondence between these ten types and the ten families of symmetric spaces, classified by Cartan [Car26, Zir96].

Further work finally led to these ten symmetry types becoming the standard framework for topological insulators and superconductors, or, more generally speaking, lattice systems [HHZ05, SRFL08, SRFL09], leading to the so-called **periodic table of topological insulators and superconductors** [SRFL08, Kit09, SRFL09, RSFL10, KZ15]. This table lists the index groups for the topological invariants of said systems for all ten symmetry types and all lattice dimensions. The periodic structure for different dimensions is due to the correspondence between the symmetry types in a given dimension d and certain Clifford algebras [Kit09], which exhibit Bott-periodicity[1]. Thereby, the periodic table for $0 \leq d \leq 7$ already contains all information.

The considerations for the tenfold way started example-driven and where based on specific models. However, the ten types can be understood on a fairly basic group theoretic level, as the different possibilities of representing one or all of the time reversal symmetry, the particle hole symmetry, and their product: the chiral symmetry, each acting on some Hamiltonian. Let $H \in \mathcal{B}(\mathcal{H})$ be a symmetric self-adjoint operator on a Hilbert space $\mathcal{H}$. The three mentioned symmetries are then represented as unitary or

[1] With period 2 for the complex classes A and AIII and period 8 for the remaining classes involving antiunitary symmetries.

antiunitary operators and the symmetry conditions on H are characterized as follows:

$$\begin{aligned} \textbf{Time reversal:} \quad & \tau H \tau^* = H, && \tau \text{ antiunitary} \\ \textbf{Particle hole:} \quad & \eta H \eta^* = -H, && \eta \text{ antiunitary} \\ \textbf{Chiral:} \quad & \gamma H \gamma^* = -H, && \gamma \text{ unitary} \end{aligned} \tag{2.1}$$

Thereby, each symmetry is involutive, i.e. applying it twice leaves invariant the operator under consideration. This leaves an arbitrary phase $\gamma^2 = \lambda \mathbb{1}$ for the chiral symmetry and the two distinct possibilities $\tau^2 = \pm\mathbb{1}$ and $\eta^2 = \pm\mathbb{1}$ for the time-reversal and particle-hole symmetry, respectively (see Section 1.5). Hence, counting the different possibilities of representing the full group generated by these three symmetries and its subgroups amounts to ten different symmetry types.

We chose this abstracted ansatz for the tenfold way for our topological classification of quantum walks [CGG$^+$18, CGS$^+$18, CGG$^+$21, CGWW21]. On the one hand, it allowed us to keep computations and proofs on a level, which can be grasped with basic knowledge about the theory of groups and their representations. On the other, it leaves enough room for profound statements, like completeness results for the topological invariants we define on the fundament paved by the basic group-theoretic considerations.

While the ansatz via representations of involutive symmetries is not example- or model-driven, it still contains an unsatisfactory arbitrariness in the ad hoc choice of the three symmetries under consideration. Moreover, it relies on the action on Hamiltonians, i.e. self-adjoint operators and is therefore not built for discrete-time quantum walks, i.e. unitary operators, without a necessary connection to a Hamiltonian in the first place. Bernard and LeClair found that waiving hermiticity leads to 38 instead of ten types [BL02], however, introducing an additional generator in a rather ad hoc way. We here approach the situation "from the outside": Instead of adding more generators to the picture and arguing that these are exhaustive afterwards, we start with an arbitrary group of involutive symmetries and show that each emerging type can be reduced to one of a specific finite list, namely the tenfold way for Hamiltonians and the 38-fold way for unitaries. In doing so, we provide a systematic picture and avoid the ad hoc choice of certain generators.

The antiunitarity of certain representatives enters already on the level of the abstract group G via a **unitarity character** $u\colon G \to \pm 1$, which decides whether a group element is represented unitarily or antiunitarily. This technique is similar to the approach by Freed and Moore [FM13], who also start with a group G of involutions, equipped with a unitarity character. Freed and Moore then proceed with a K-theoretic discussion, leading to twisted K-theory. However, K-theoretic tools require a high level of abstraction, wherefore a classification of walks via such tools might not be appreciated by a great audience among the quantum walk community[2]. Therefore, we here choose to follow the basic group-theoretic ansatz as long as possible to make our theory more applicable to the quantum walks community.

We begin by re-deriving the tenfold way from a minimal set of assumptions. We present a reduction procedure for any arbitrary group of involutions G consisting of

[2]There are further arguments, which led us to not use a K-theoretic ansatz for our classification, which we discuss in the introduction of Chapter 3.

symmetries equipped with a unitarity character. We first define what we mean by a symmetry type for those groups, namely the different equivalence classes of projective representations. For the symmetry representations ρ, we then assume a quite general action on Hamiltonians, namely

$$\rho_g H \rho_g^* = f_g(H), \tag{2.2}$$

for a group of continuous involutions $f_g \colon \mathbb{R} \to \mathbb{R}$, acting on H via the spectral calculus. Based on this, we discuss a systematic reduction procedure, which reduces every representation type of a group of involutive symmetries with these actions to a type of the tenfold way by eliminating redundancies in the symmetry conditions step by step.

Aiming for quantum walks, we then apply the tenfold way approved reduction procedure to unitary operators. For this, we adjust the action to

$$\rho_g U \rho_g^* = f_g(U), \tag{2.3}$$

such that the f_g are continuous involutions on the unit circle $\mathbb{T}$ instead of $\mathbb{R}$. Similar to Bernard LeClair [BL02] we find 38 symmetry types[3]. However, since we started with an arbitrary group of involutions, with arbitrary involutive action on the unitary operators under consideration, we can conclude that the 38 types for unitary operators are indeed exhaustive.

We close this chapter by defining the fundamental index map for our topological classification of quantum walks: The symmetry index assigns an element of an abelian index group to any finite-dimensional representation of one of the symmetry types. Thereby, the index group depends on the type and labels the equivalence classes of specific representations. This generalizes our construction in [CGS$^+$16, CGG$^+$18] from the tenfold way to all 38 symmetry types for unitary operators.

2.1 Projective representations and symmetry types

Our starting point for this section is an abstract group of involutions, without considering its action on states or operators on a Hilbert space, nor its possible representations on the latter. On this level, the structure is pretty simple and can be inferred from basic group theory:

Lemma 2.1.1. *Let G be a finite group of involutions, i.e. $g^2 = e$ for all $g \in G$, where $e \in G$ denotes the neutral element. Then G is abelian and $|G| = 2^n$, where n is the minimal number of elements $g_1, \dots, g_n \in G$ generating G. Moreover, for a fixed choice of generators $\{g_i\}$, every element $g \in G$ can be labelled by a subset $\Lambda \subset \{1, \dots, n\}$, such that $g = g_\Lambda = \prod_{i \in \Lambda} g_i$.*

Proof. Since any element of G fulfils $g^2 = e$, the following shows that G is abelian:

$$gh = h^2 ghg^2 = h(hg)^2 g = hg.$$

Choosing a minimal generating set $\{g_i\}$ of n generators, every group element can be written as a product of these n generators. Because G is abelian and we have $g^2 = e$

[3]The details of the connection between their an our ansatz will be discussed below (see Interlude on page 56)

for all $g \in G$, each $g \in G$ can be labelled by a subset $\Lambda \subset \{1, \dots, n\}$ of the $\{g_i\}_{i=1}^n$ without repeating elements. For each subset, each g_i is either present or not, wherefore $|G| = 2^n$. □

In order to speak of some group G as the symmetry group of a physical system, we have to specify a set and an action leaving this set invariant. This might for example be the set of pure states, i.e. $\{e \in \mathcal{B}(\mathcal{H}) | e = e^* = e^2, \operatorname{rank}(e) = 1\}$, in which case on speaks of Wigner symmetries (see Section 1.5), or the set of density operators, i.e. $\{\rho \in \mathcal{B}(\mathcal{H}) | \rho \geq 0, \operatorname{tr}(\rho) = 1\}$ (Kadison symmetries). However, by Wigner's theorem and the observation that the different notions of symmetries are equivalent [Lan17, Chapter 5], the structures we really need to investigate, are projective representations of G via unitary or antiunitary operators,, i.e. representation that are fixed up to phases (see Section 1.5.1):

$$\rho \colon g \mapsto \rho_g \quad \text{with} \quad \rho_g \rho_h = m(g,h)\rho_{gh}, \tag{2.4}$$

where the multiplication phases are encoded into a function $m \colon G \times G \to \mathbb{T}$. The choice of unitarity vs. antiunitarity of the representing operators can be expressed via equipping the abstract group with a unitarity character (see also [FM13])

$$u \colon G \to \pm 1, \quad u(g) = \begin{cases} +1 & \rho_g \text{ is unitary} \\ -1 & \rho_g \text{ is antiunitary.} \end{cases} \tag{2.5}$$

Since the product of two unitary or antiunitary operators is antiunitary if and only if one of them is antiunitary, (2.5) indeed defines a homomorphism. The unitarity character influences the multiplication phases m: When we evaluate the associativity of the product $\rho_g \rho_h \rho_k$, we get

$$m(g,h)m(gh,k) = m(h,k)^{u(g)} m(g,hk), \tag{2.6}$$

which is called the cocycle equation. For the concept of a **symmetry type**, we are not interested in the specifics of the possible representations but merely equivalence classes with respect to the choices for m and u. Hence, given a unitarity character u, the possible symmetry types for G are given by the solutions to the cocycle equation (2.6). Not all such solutions are fundamentally different: There are equivalence classes, which correspond to choosing phases for the representing operators. The multiplication function m always refers to such a choice of representatives for the projective representation of G. Indeed, choosing other phases, i.e. switching to $\widetilde{\rho}_g = \phi_g \rho_g$ results in the multiplication phases

$$\widetilde{m}(g,h) = \frac{\phi_g \phi_h^{u(g)}}{\phi_{gh}} m(g,h). \tag{2.7}$$

Note that $\widetilde{m}$ fulfils the cocycle condition (2.6) if and only if m does. This defines an equivalence relation, the equivalence classes of which become the possible symmetry types for a given pair (G, u)

Definition 2.1.2 (Symmetry type)**.** *Two multiplication functions m and $\widetilde{m}$ are equivalent if they are related as in* (2.7)*. The equivalence classes of solutions to* (2.6) *with respect to* (2.7) *are called the **symmetry types** of the underlying group G equipped with u. We denote a symmetry type by $\mathsf{S} \equiv (G, u, m)$, or, on the level of the representation, by $[\rho]$.*

Before we continue, let us take a short detour and investigate the general structure lying behind the concept of a symmetry type, namely the **second cohomology group** $H^2_u(G, \mathbb{T})$, associated with the possible extensions of a group G by $\mathbb{T}$.

Interlude: Group extensions and the second cohomology group The properties of projective representations of a group G can be understood on an abstract level via the group extensions of G by $\mathbb{T}$, which respects the action of the antiunitary character. For this interlude, we will loosely follow [BR86, Chapter 21, C], but adapt the general formulation there to our needs. The unitarity character u induces an action $\alpha\colon G \to \mathrm{Aut}(\mathbb{T})$ of G on $\mathbb{T}$ via

$$\alpha_g(\phi) = \phi^{u(g)}.$$

The corresponding group extensions of G by $\mathbb{T}$ is defined via the split exact sequence

$$0 \to \mathbb{T} \xrightarrow{\iota} \widehat{G} \underset{\nu}{\overset{\pi}{\rightleftarrows}} G \to 0, \tag{2.8}$$

where $\widehat{G}$ is a group and ι, π and ν are homomorphisms with $\mathrm{im}(\iota) = \ker(\pi)$ and $\pi \circ \nu = \mathrm{id}_G$, such that the inner automorphisms of $\widehat{G}$, restricted to $\mathbb{T}$ coincide with $\alpha \circ \pi$. Note that zeros on the left and right boundary of an exact sequence guarantee that ι is injective and π is surjective. Thus, $\widehat{G}$ is of the form $\widehat{G} = \{(g, \varphi) | g \in G, \varphi \in \mathbb{T}\}$, with the group multiplication

$$(g, \varphi)(h, \psi) = (gh, \varphi\alpha_g(\psi)m(g, h)) = (gh, \varphi\psi^{u(g)}m(g, h))$$

encoded into the multiplication function $m\colon G \times G \to \mathbb{T}$. In [FM13], $\widehat{G}$ is called the twisted central extension of G by $\mathbb{T}$, where "twisted" refers to the altered (no longer central) group multiplication induced by the action of the unitarity character.

For a trivial multiplication function, i.e. $m \equiv 1$, $\widehat{G}$ simply is the semidirect product $G \rtimes_\alpha \mathbb{T}$. The associativity in $\widehat{G}$ translates into the cocycle condition (2.6) on m and the inverse on $\widehat{G}$ is given by

$$(g, \varphi)^{-1} = \left(g^{-1}, \alpha_{g^{-1}}\left(m(g, g^{-1})^*\varphi^*\right)\right).$$

It is straightforward to check that this is a right inverse for (g, φ). To see that it is also a left inverse, one has to use $\alpha_{g^{-1}}\left(m(g, g^{-1})\right) = m(g^{-1}, g)$, which follows from applying the cocycle condition (2.6) to $g^{-1}gg^{-1}$ using $m(g, e) = m(e, g) = 1$, $\forall g \in G$.

By construction, the automorphisms α_g on $\mathbb{T}$ become inner on $\widehat{G}$ restricted to $\iota(\mathbb{T})$:

$$(g, 1)(e, \varphi)(g, 1)^{-1} = (e, \alpha_g(\varphi)).$$

We want to determine the different ways of realizing the action α induced by u of G on $\mathbb{T}$ via an inner automorphism in an extension $\widehat{G}$. This task is answered by the following proposition [BR86, Chapter 21 §4.C, Proposition 1]

Proposition 2.1.3. *The second cohomology group $H^2_u(G, \mathbb{T})$ is exactly the group of all (equivalence classes of) those extensions $\widehat{G}$ of G by $\mathbb{T}$ which realize the group action α induced by u of G on $\mathbb{T}$.*

The set of multiplication functions $M := \{m_\mu \colon G \times G \to \mathbb{T}\}$ can be equipped with a multiplication via the pointwise multiplication:

$$m_{\mu\nu}(g,h) := (m_\mu \circ m_\nu)(g,h) = m_\mu(g,h) m_\nu(g,h). \tag{2.9}$$

It is easy to check, that $m_{\mu\nu}$ fulfils the cocycle condition (2.6) if m_μ and m_ν do. With this, M becomes an abelian group. We identify the subgroup $N := \{n \colon G \times G \to \mathbb{T}\} \subset M$ of multiplication functions which are obtained from "just choosing phases" or, more precisely, choosing different representatives $\widehat{g}, \widehat{h} \in \widehat{G}$ with $\pi(\widehat{g}) = g$ and $\pi(\widehat{h}) = h$, i.e.

$$n(g,h) = \frac{\phi_g \phi_h^{u(g)}}{\phi_{gh}}.$$

This identifies the second cohomology group as the factor group

$$H^2_u(G, \mathbb{T}) = M/N, \tag{2.10}$$

and it becomes clear why it labels the different symmetry types for a given group G equipped with a unitarity character u as in Definition 2.1.2.

2.1.1 Labelling the symmetry types

Having defined the concept of a symmetry type raises the task of characterizing them for a given group of involutions. In order to tackle this task, we need to find data, which is independent of specific phase choices for the group elements. We address this in the remainder of this section. Thereby we introduce two different phase convention with their own advantages and caveats, respectively. One turns out to be convenient to work with in specific realizations and the other is better suited for a structural analysis of the different symmetry types.

To find data, which is independent under phase modification of a group of operators, commutation phases $c(g,h),\ g,h \in G$ are typically good candidates. These are defined as follows

$$c \colon G \times G \to \mathbb{T}, \qquad c(g,h) = \frac{m(g,h)}{m(h,g)}, \tag{2.11}$$

i.e. in a representation we have $\rho_g \rho_h = c(g,h)\rho_h \rho_g$. Indeed, c is invariant if $u \equiv 1$, i.e. if there are no antiunitary elements in a representation. When a non-trivial unitarity character is involved, c transforms as follows under phase choices $\rho_g \mapsto \phi_g \rho_g$:

$$\widetilde{c}(g,h) = \phi_g^{1-u(h)} \phi_h^{u(g)-1} c(g,h). \tag{2.12}$$

This seems to render the commutation phases $c(g,h)$ inappropriate as data fixing a type. However, note that in (2.12) $1-u(h)$ as well as $1-u(g)$ are both even for all values of u. This means, c stays invariant if we manage to reduce the phases ϕ_g to signs, which will be done in the following proposition. Other, more robust quantities are the

squares of the antiunitary operators. Being involutive, each element of ρ_G squares to a multiple of the identity. Evaluating $(\rho_a\rho_a)\rho_a = \rho_a(\rho_a\rho_a)$ for $u(a) = -1$, one finds that $\rho_a^2 = \pm\mathbb{1}$. Moreover, this sign cannot be changed by choosing different phases: $\phi_a\rho_a\phi_a\rho_a = \phi_a\phi_a^*\rho_a^2 = \rho_a^2$.

Proposition 2.1.4. *Let G be a finite group of involutions and ρ be a projective representation with unitarity character u and the multiplication function m. Then there is a choice of phases $\{\phi_g\}$ for ρ_g, $g \in G$, such that $\rho_g^2 = \pm\mathbb{1}$, $m(g,h) = \pm 1$, and $c(g,h) = \pm 1$ for all $g, h \in G$.*

Proof. The first step is to fix a set of generators for the group. Let H be the subgroup of unitarily represented elements, i.e. the kernel of u. We choose generators for H and label them via $g_1, \dots g_{n-1}$. If $H \neq G$, pick one element $a \in G$ with $u(a) = -1$. Then G is generated by $g_1, \dots g_{n-1}, a$ and we set $a = g_n$. To reduce notation, we write ρ_j instead of ρ_{g_j}, when referring to the representing operators for the generators.

Next, we adjust the phases for the unitary generators $\rho_1, \dots \rho_{n-1}$, such that every ρ_i squares to the identity. This can be achieved by choosing $\phi_i = m(g_i, g_i)^{-1/2}$, such that $(\phi_i\rho_i)^2 = m(g_i,g_i)\phi_i^2\mathbb{1} = \mathbb{1}$. Note that, as discussed above, the square $\rho_a^2 = \pm\mathbb{1}$ cannot be changed for the antiunitary operators. Having fixed the squares to $\pm\mathbb{1}$, the commutation phases $c(g_i, g_j) = c_{ij}$ for the generators must be real as well. Indeed, assuming ρ_i to be unitary we get

$$\rho_i^2\rho_j = c_{ij}\rho_i\rho_j\rho_i = c_{ij}^2\rho_j\rho_i^2,$$

where we used the unitarity of ρ_i for $\rho_i c_{ij} = c_{ij}\rho_i$. Since $\rho_i^2 = \pm\mathbb{1}$, we conclude that $c_{ij}^2 = 1$ and hence $c_{ij} = \pm 1$. A similar computation gives the same result, when ρ_j is assumed to be unitary. Since we chose at most one antiunitary generator, the case of two antiunitary operators does not occur.

We proceed by fixing a standard representation for every $g \in G$: according to Lemma 2.1.1 we write $\rho_g = \prod_{j\in\Lambda}^{\rightarrow}\rho_j$, where the arrow indicates that the generators are multiplied from left to right with increasing indices. We can bring any product of generators, into normal form by successively commuting generators and replacing squares ρ_j^2 by $\pm\mathbb{1}$. Since both operations only add factors ± 1, they do not change the commutation relation of the product with the antiunitary generator. Therefore we get $\rho_g\rho_h = \pm\rho_{gh}$ and $\rho_g^2 = \pm 1$ for all $g, h \in G$.

□

Choosing phases according to Proposition 2.1.4 turns $c\colon G \times G \to \{\pm 1\}$ into a **symmetric bicharacter** on G, i.e. $c(\cdot, g) = c(g, \cdot)$ are homomorphisms $G \to \{\pm 1\}$. However, it does not fix the actual values for $c(g,h)$ for arbitrary g, h. Indeed, we can change these values quite liberally without harming the arguments in the proof. Whereas the squares of the antiunitary elements cannot be changed by choosing different phases, we can still modify the signs of the unitary squares: Let ρ_g be unitary and consider $\rho_g \mapsto i\rho_g$ instead. This does not alter the arguments in Proposition 2.1.4 but changes the square $\rho_g^2 \mapsto -\rho_g^2$ and the values of the commutation character $c(g,\cdot)$. For unitarily represented h, $c(g,h)$ stays the same, but for ρ_h antiunitary we get $c(g,h) \mapsto -c(g,h)$. Hence, we can exchange the signs of the squares of the unitary elements for their commutation signs with the antiunitary generator. Fixing this freedom with a phase convention can be achieved in different ways.

Phase conventions:

The first phase convention we introduce involves relatively little further modifications. It is motivated by the attempt to make the representation of a symmetry type as commutative as possible:

Lemma 2.1.5 (**Phase convention I**). *In the setting of Proposition 2.1.4, pick $a \in G$ with $u(a) = -1$ as the antiunitary generator. Then we can adjust phases, such that for all g with $u(g) = 1$ we get $\rho_{ga} = \rho_g\rho_a = \rho_a\rho_g$, i.e. $c(g, a) = 1$. Moreover, this implies that the squares for the unitary elements are fixed by data which is independent of phase choices, since, for every g we can write $\rho_g^2 = \rho_{ga}^2\rho_a^2$.*
This fixes all phases up to arbitrary signs for each unitary element ρ_g and an arbitrary phase for the antiunitary generator ρ_a.

Proof. In the setting of Proposition 2.1.4, $c\colon G \times G \to \pm 1$ is already a real symmetric bicharacter. We further adjust the phase for every unitary element ρ_g with $c(g, a) = -1$ via $\rho_g \mapsto i\rho_g$, which yields $c(g, a) = 1$ for all unitarily implemented g. This implies

$$\rho_{ga}^2\rho_a^2 = (m(g, a)\rho_g\rho_a)^2 \rho_a^2 = m(g, a)^2\rho_g^2\rho_a^4 = \rho_g^2,$$

where we used $m(\cdot, \cdot) = \pm 1$ and $c(g, a) = 1$. □

This convention is the plausible choice for dealing with explicit representations in a given setting, since it makes the representations as commutative as possible. For this reason, it was our convention of choice in [CGG$^+$18], where at most one unitary and one antiunitary generator are considered. For such small groups representations in phase convention I are always abelian.

However, phase convention I is not helpful for the structure theory, because it does not incorporate the commutation character as a structural element. Instead of focussing on commutativity, our second phase convention is centred around the commutation character, and turns out to be the better choice for labelling the symmetry types for an arbitrary pair (G, u). Let us first investigate what structure the existence of a given symmetric bicharacter $c\colon G \times G \to \{\pm 1\}$ imposes on a finite group of involutions:

Lemma 2.1.6. *Let G be a finite group of involutions with a symmetric bicharacter $c : G \times G \to \{\pm 1\}$, such that $c(g, g) = 1$ for all $g \in G$. Then there is a set of generators $g_1, h_1, \ldots, g_n, h_n$, $r_1, \ldots, r_m \in G$, such that $c(g_j, h_k) = 1 - 2\delta_{jk}$, and $c(\cdot, \cdot) = 1$ on all other combinations of generators.*

Proof. We start by identifying the generators $r_1, \ldots, r_m$. Consider the set $G_c = \{g \in G | c(g, h) = 1\, \forall h \in G\}$. Since G_c is the intersection of kernels of the homomorphisms $c(\cdot, h)$, it is a subgroup of G. Hence, we can pick generators for G_c, providing us the wanted $r_1, \ldots, r_m$. Denoting by G_1 the group generated by a remaining set of generators, which, together with $r_1, \ldots, r_m$ generates G, we get $G \cong G_c \times G_1$. Now, by construction, we find for every element $g \in G_1$ an element $h \in G_1$ with $c(g, h) = -1$. Note that by $c(g, g) = 1$, h is different from g. Pick any such pair g_1, h_1, add it to the list of the m central generators, and consider the subgroup $G_2 \cong \{k \in G_1 |\, c(g_1, k) = c(h_1, k) = 1\}$. We get $G \cong G_c \times \langle g_1, h_1\rangle \times G_2$. In G_2 we repeat the last step, picking generators g_2, h_2,

with $c(g_2, h_2) = -1$, which cannot be in the subgroup generated by g_1, h_1 by definition of G_2. We proceed like this, until $G_n = \{e\}$, providing us with the desired list of generators $g_1, h_1, \dots g_n, h_n, r_1, \dots, r_m$ for G. □

Hence, a symmetric bicharacter with a trivial diagonal allows for a choice of generators, which is split into two classes: On the one hand, a set of anti-commuting pairs (g_i, h_i), which commute with all remaining generators, respectively; and on the other, a remaining set of central generators r_k. We can now use this structure and incorporate it into a phase convention, while additionally trying to makes as many unitary elements square to $+1$ as possible. Note that we cannot, in general, avoid $\rho_g^2 = -\mathbb{1}$ for all unitary elements since the relation

$$\rho_{gh}^2 = c(g, h)\rho_g^2\rho_h^2 \tag{2.13}$$

cannot be changed by phase factors if both elements are unitary. However, it is possible to achieve ρ_g^2 for all unitary generators:

Lemma 2.1.7 (**Phase convention II**). *In the setting of Proposition 2.1.4, there is a set of generators according to Lemma 2.1.6 and a further adjustment of phases, resulting in at most one generator being antiunitary, and $\rho_g^2 = +\mathbb{1}$ for all unitary generators g.*
This fixes the phases of all generators up to arbitrary signs for each unitary generator ρ_g and an arbitrary phase for the antiunitary generator ρ_a. Fixing a standard presentation $\rho_g = \prod_{j\in\Lambda}^{\rightarrow} \rho_j$ for each group element[4] then also fixes the phases for all remaining group elements. In particular, this uniquely determines the values of the multiplication function m in terms of the commutation character c.

Proof. In the setting of Proposition 2.1.4 we first pick generators ρ_{g_i}, ρ_{h_i} and ρ_{r_k} according to Lemma 2.1.6 for the unitary subgroup H. We then further adjust the phases, such that all these generators square to $+\mathbb{1}$, by multiplying with i if necessary. If there are no antiunitary generators, there is nothing left to do.

Otherwise, we can always pick an antiunitary generator, which commutes with all the generator pairs ρ_{g_i}, ρ_{h_i} with $c(g_i, h_i) = -1$. Indeed, pick any antiunitary element ρ_a and consider the first of these pairs g, h. Then $\rho_g^2 = \rho_h^2 = (i\rho_{gh})^2 = \mathbb{1}$ by (2.13) and the phase adjustments described above. Now, since c is a bicharacter, $c(\cdot, a)$ is a homomorphism on G. Hence we have $c(g, a)c(h, a)c(gh, a) = 1$, which implies that the product of the commutation phases of ρ_a with ρ_g, ρ_h and $(i\rho_{gh})$ is equal to -1. But this is only possible if either one or all three commutation phases are equal to -1. In the first case we pick the two unitaries which commute with ρ_a, replacing the pair ρ_g, ρ_h, without harming the commutation relations with the remaining generators of the unitary subgroup. In the second case, we replace a by ga, which changes two of the three commutation phases and leaves us with the first case: $c(g, ga) = c(g, a), c(h, ga) = -c(h, a)$ and $c(gh, ga) = -c(gh, a)$. Proceeding in this way, we fix the commutation phases between all pairs (ρ_{g_i}, ρ_{h_i}) and ρ_a. In the central unitary subgroup H_c, generated by $r_1, \dots, r_m$, every element ρ_r squares to $+\mathbb{1}$ by (2.13) and the fact, that we set this for the generators. Moreover, this does not change, no matter which elements we choose as the generators r_k. There are now two cases to distinguish: the character $r \mapsto c(r, a) \in \{\pm 1\}$ on the

[4]The generators may for example be ordered as $g_1 < h_1 \dots < g_n < h_n < r_1 \dots < r_m < a$.

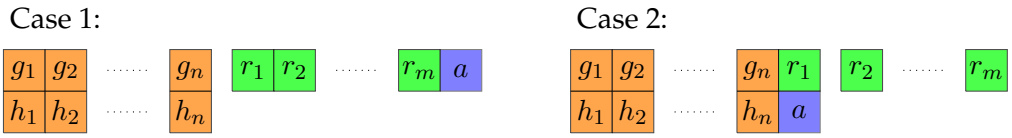


Figure 2.1: Adding the antiunitary generator in the setting of Lemma 2.1.6.

center is either trivial or takes the value -1 on exactly $|H_c|/2 = 2^{m-1}$ elements. In the first case a becomes an additional central generator $r_{m+1} = a$. In the second, pick any element r with $c(r, a) = -1$ (w.l.o.g. $r = r_1$), which together with a forms an additional pair of anti-commuting generators $g_{n+1} = r_1, h_{n+1} = a$ for the whole group.

The last statement of the lemma follows by similar arguments as in the proof of Proposition 2.1.4. □

Phase convention II will be our standard convention from now on. In particular, we use it in Table 2.1, which tabulates all symmetry types without redundant symmetries (see Section 2.2.2). However, sometimes phase convention I from Lemma 2.1.5 simplifies computations, wherefore we will switch the convention occasionally.

Having sufficiently fixed the phases, following the structure given by Lemma 2.1.6, we can now tackle the question of how to label the equivalence classes of representations for a pair (G, u). Since the multiplication function is uniquely determined by the commutation character and the square of the antiunitary generator, this data singles out a unique representative for each symmetry type and therefore labels the equivalence classes. Organizing the generators and their phases according to phase convention II makes it especially easy to count the number of symmetry types for a group G equipped with a unitarity character u:

Corollary 2.1.8. *In phase convention II from Lemma 2.1.7, the equivalence classes of representations are labelled by the values of the commutator bicharacter c on the generators and the square of the antiunitary generator a. Hence, if G is generated by n elements, the number of equivalence classes N is given by*

$$N = \begin{cases} 2^{\binom{n}{2}} & \text{if } u(g) = 1 \,\forall g \in G \\ 2^{\binom{n}{2}+1} & \text{if } \exists\, a \in G \text{ with } u(a) = -1 \end{cases} \tag{2.14}$$

Proof. There are $\binom{n}{2}$ sign-choices for the values of c on the n generators and one additional sign-choice for the square of the antiunitary generator, if present. □

Later, we will only consider symmetry groups with at most two unitary generators. For those, the different symmetry types coincide with the different possible combinations of squares for antiunitary elements (if present). This can be seen in Table 2.1, where for each group, each combination of antiunitary squares occurs. In general, however, multiplying by a factor of two for each antiunitary element would exceed the number of symmetry types many times over. Indeed, for $n > 3$ we get $2^{2^{n-1}} > 2^{\binom{n}{2}+1}$, which are equal for $n \leq 3$.

2.1.2 Realizations on a Hilbert space

It remains to verify that all the possibilities in Lemma 2.1.6 and Lemma 2.1.7 are realizable on a Hilbert space $\mathcal{H}$, i.e. that each symmetry type admits a projective representation, which realizes a representative of the equivalence class of $m(\cdot,\cdot)$. We answer this question in the affirmative by explicitly writing down finite-dimensional representations in the structure of Lemma 2.1.6 and Lemma 2.1.7. We will also connect the resulting possibilities to the theory given by Wigner, and Dimmock [Wig59, Dim63] (see also Section 1.5.1). Similar to Wigner, and in line with the proof of Lemma 2.1.7, we will first write down representations for the unitary subgroup and add an antiunitary element afterwards. There are three cases to distinguish, which are equivalent to the three cases in Section 1.5.1: The antiunitary generator is either of type h_i in Lemma 2.1.6, i.e. it forms an anti-commuting pair with one of the central generators of the unitary subgroup, or it is of type r_i, in which case the square of ρ_a distinguishes two different scenarios.

Let H be the unitary subgroup of a group of involutions G, with n anti-commuting pairs of generators (g_i, h_i) and m_H central generators r_k according to Lemma 2.1.6. We start with the anti-commuting pairs of generators (g, h). Each such pair singles out a tensor factor $\mathbb{C}^2$ of the underlying Hilbert $\mathcal{H}$ space. On this tensor factor g, h and gh are represented via a copy of the Pauli matrices σ_i. Indeed, let ψ be an eigenvector of ρ_g corresponding to the eigenvalue $+1$ (recall $\rho_g^2 = \mathbb{1}$). Since g and h anti-commute, $\rho_h\psi$ must be an eigenvector of ρ_g corresponding to the eigenvalue -1, and vice versa. Since all other generators commute with g, h and gh, they must be realized in a different tensor factor. This implies $\mathcal{H} = \mathbb{C}^2 \otimes \mathcal{H}'$ and without loss of generality we set $\rho_g = \sigma_z \otimes \mathbb{1}'$, $\rho_h = \sigma_x \otimes \mathbb{1}'$ and $\rho_{gh} = i\sigma_y \otimes \mathbb{1}'$.

The central generators, on the other hand, all commute with each other. Hence, the Hilbert space decomposes into a direct sum of joint eigenspaces $\mathcal{H}_{\mathbf{r}}$, indexed by the m_H-tuples $\mathbf{r} = (r_1, \ldots, r_{m_H}) \in \{\pm 1\}^{m_H}$, labelling the eigenvalues of the central unitary generators. Note that not every possible combination $(\pm 1, \ldots, \pm 1)$ has to be part of a specific representation, the most trivial example being $\{\mathbf{r}\} = \{(1, 1, \ldots, 1)\}$, where every central generator is represented trivially. The direct sum of these common eigenspaces $\mathcal{H}_{\mathbf{r}}$ is thus another tensor factor of the underlying Hilbert space.

Combining those arguments, we get

$$\mathcal{H} = \left(\bigotimes_{j=1}^{n} \left(\mathbb{C}^2\right)\right) \otimes \left(\bigoplus_{\mathbf{r}} \mathcal{H}_{\mathbf{r}}\right), \tag{2.15}$$

on which the generators of the unitary subgroup H are represented as

$$\rho_{g_j} = \sigma_3^{(j)} \otimes \mathbb{1}, \qquad \rho_{h_j} = \sigma_1^{(j)} \otimes \mathbb{1}, \qquad \text{and} \qquad \rho_{r_k} = \mathbb{1} \otimes \bigoplus_{\mathbf{r}} r_k \mathbb{1}_{\mathbf{r}}, \tag{2.16}$$

where $j = 1, \ldots, n$, $k = 1 \ldots, m_H$ and $A^{(j)}$ denotes an operator, acting as A on the j'th tensor factor and as $\mathbb{1}$ on the others, i.e. $A^{(j)} = \ldots \otimes \mathbb{1} \otimes A \otimes \mathbb{1} \otimes \ldots$.

Let us now add an antiunitary generator a. It follows from the proof of Lemma 2.1.7 that a can be chosen to act "trivially" on the first tensor factor in (2.15). However, since the tensor product between linear and anti-linear operators is ill-defined, we cannot just

take the ansatz $\mathbb{1} \otimes X$. Instead, we have to define what "trivial" in this sense means. Fortunately, there is only one antiunitary operator on $\mathbb{C}^2$, which commutes with σ_z, σ_x and $i\sigma_y$: the complex conjugation K with respect to the chosen basis (w.l.o.g. the σ_3-eigenbasis). Hence, we set $K \otimes X$ instead of $\mathbb{1} \otimes X$ to realise an antiunitary operator acting on the second tensor factor into the whole space. a is now either of type r_k or becomes a part of a pair g_j, h_j.

Case 1, $\underline{a = r_m}$**:** In this case we get $m = m_H + 1$ central generators for he whole group and we set $\rho_{r_m} = \rho_a$. ρ_a leaves all eigenspaces of the ρ_{r_j} invariant and acts as K on the fist tensor factor in (2.15). Hence, we only need to choose an antiunitary operator $\rho_a(\mathbf{r})$ in each eigenspace and get

$$\rho_a = \rho_{r_m} = K^{\otimes n} \otimes \bigoplus_{\mathbf{r}} \rho_a(\mathbf{r}),$$

with $\mathbf{r} \in \{\pm 1\}^{m-1}$. Taking the square of this operator $\rho_a^2 = \mathbb{1} \otimes \bigoplus_{\mathbf{r}} \rho_a(\mathbf{r})^2$, we find, that all the antiunitary operators $\rho_a(\mathbf{r})$ have to have the same square as ρ_a^2. Moreover, since the eigenspaces are left invariant, the representation is either of type **1**, for $\rho_a^2 = \mathbb{1}$, or of type **2** for $\rho_a^2 = -\mathbb{1}$, in the sense of Dimmock (Section 1.5.1). In the latter case, each of the eigenspaces $\mathcal{H}_{\mathbf{r}}$ is even dimensional, in accordance with (1.62).

Case 2, $\underline{a = h_n}$**:** In this case, a forms an anti-commuting pair together with one of the central generators of the unitary subgroup, say with r_1. In order to achieve this in a representation, ρ_a has to swap $+1$ the -1 eigenspace of ρ_{r_1}. That is, $\mathcal{H}_{\mathbf{r}}$ with $\mathbf{r} = (1, r_2, \ldots, r_{m_H})$ is mapped to $\mathcal{H}_{\mathbf{r}'}$ with $\mathbf{r}' = (-1, r_2, \ldots, r_{m_H})$ and vice versa. We can then choose the basis in $\mathcal{H}_{\mathbf{r}'}$, such that ρ_a effectively acts as the complex conjugation in this mapping, and only get an additional minus sign when mapping back, depending on the square of ρ_a^2. Without r_1, we are left with $m = m_H - 1$ central generators, which we relabel according to $j \mapsto j - 1 \in \{1, \ldots, m\}$. ρ_a is then of the form

$$\rho_a = K^{\otimes n} \otimes \begin{pmatrix} 0 & \pm K \\ K & 0 \end{pmatrix} \otimes \bigoplus_{\mathbf{r}} K, \tag{2.17}$$

with $\mathbf{r} \in \{\pm 1\}^m$. For both signs $\rho_a = \pm\mathbb{1}$, this situation corresponds to type **3** in the sense of Dimmock (Section 1.5.1).

The considerations above allow us to determine all irreducible representations of the symmetry types, depending on the generators involved:

Corollary 2.1.9. *In each of the cases above, the irreducible representations of a symmetry type are characterized by the fact, that only one of the $\mathcal{H}_{\mathbf{r}}$ is non-zero and one-dimensional (or two-dimensional for $\rho_a^2 = -\mathbb{1}$ in case 1). I.e. for a given symmetry type, there is exactly one irreducible representation for each possible sign combination $\mathbf{r} \in \{\pm 1\}^m$, resp. $\mathbf{r}\{\pm 1\}^{m-1}$. The dimensions of the irreducible representations are determined by the number of anti-commuting pairs and in case 1 the square of the antiunitary generator. Each anti-commuting pair contributes a factor of two and so does the antiunitary generator if it is central and squares to $-\mathbb{1}$. This leads*

to the following three possibilities:

	#irreps	$\dim \mathcal{H}$
only unitaries or $a = h_n$	2^m	2^n
$a = r_m$, $\rho_a^2 = \mathbb{1}$	2^{m-1}	2^n
$a = r_m$, $\rho_a^2 = -\mathbb{1}$	2^{m-1}	2^{n+1}

(2.18)

2.2 Action on operators

We now come to the action of the symmetry representations on the operators describing the dynamics, i.e., the properties, which justify naming the group elements **symmetries**. We first concentrate on their action on Hermitian operators, i.e. Hamiltonians. For these, we will derive the tenfold way as the set of "interesting" symmetry types, after eliminating redundant symmetries. After that, we come to the action on the type of operators, which are more prominent throughout this thesis: quantum walks or, for this purpose, just unitary operators. We will apply the techniques developed for the hermitian case and find a set of 38 different symmetry types. In both cases, we derive our techniques from minimal principles, and we deduce the sets of non-trivial symmetry types from an arbitrary symmetry group of involutions, using a minimal set of assumptions. This ansatz is different from the techniques we found in the literature, where usually a more ad hoc way is chosen. Typically specific models are under consideration, or the set of symmetries is fixed from the outset [AZ97, BL02, RSFL10, KRBD10].

2.2.1 Action on Hamiltonians

The symmetries act on operators under consideration via conjugation with the representing operator ρ_g (see Section 1.5). Speaking of a symmetry of a system, the action on a Hamiltonian is typically assumed as $g(H) = \rho_g H \rho_g^* = H$, that is, the symmetry operation leaves the Hamiltonian invariant. This, however, does not include well known physical symmetries, e.g. particle-hole symmetry η, represented by an antiunitary operator ρ_η with $\eta(H) = \rho_\eta H \rho_\eta^* = -H$. Such symmetry action emerges from the standard assumption above, e.g. via second quantization of the underlying system [Zir15]. However, we here want to include the possibility of such symmetry from the outset without referring to its possible physical origin. In the end, it turns out that this additional sign is all we need to add to the considerations, but we aim to deduce this from as few assumptions as feasible. Given a symmetry group G, for every g we therefore choose the ansatz

$$g(H) := \rho_g H \rho_g^* = f_g(H),$$

with a continuous function $f_g \colon \mathbb{R} \to \mathbb{R}$, evaluated on H in the spectral calculus. For a single H, it would be sufficient to specify f_g only on the spectrum of H. However, since we aim for a homotopy classification of families of symmetric operators, we need to allow for deformations of Hamiltonians H, and therefore the symmetry-action formulated independently of H.

Since the symmetries are assumed to be part of a group of involutions G, the set of functions $f_G = \{f_g | g \in G\}$ also carries a group structure, and in particular, f_g has to be

involutive for all $g \in G$. I.e. f_G is a group of involutive homeomorphisms on the real line. The following proposition characterizes such groups.

Proposition 2.2.1. *Let G be a finite group of involutions, and $g \mapsto f_g$ a homomorphism into the group of homeomorphisms on $\mathbb{R}$. Then there is a homeomorphism h and a character $r : G \to \{\pm 1\}$ such that*

$$h \circ f_g \circ h^{-1}(x) = r(g)\, x \tag{2.19}$$

for all g.

This reduces a group of involutive homeomorphisms to a single character $r(g)$ on G by classifying the conjugacy classes of these groups. Note that conjugating the action of a symmetry with an invertible continuous function h does not change the task of classifying the symmetric hermitian operators with respect to homotopy. The key observation is that the conjugating homeomorphism h is independent of g. We can therefore classify the symmetric Hamiltonians H, by studying instead $H' = h(H)$, which satisfies a much simpler symmetry condition, namely $(g(H))' = \pm H'$. A particular case of this are affine functions $f_g(x) = ax + b$, where $a = \pm 1$ by the involution property, and it suffices to adjust the origin of the energy axis by $H' = H - b/2\mathbb{1}$.

Proof. Let $f\colon \mathbb{R} \to \mathbb{R}$ be a continuous involution. Then f is invertible and, in particular, bijective. Hence, f is either strictly monotonically increasing or strictly monotonically decreasing. Since, conjugation $h \circ f_g \circ h^{-1}$ in (2.19) does not change the direction of monotonicity, we can define a character $r\colon G \to \pm 1$, which takes the value $+1$, if f_g increasing and -1 if f_g is decreasing.

The only increasing function on $\mathbb{R}$, which is also an involution, is the identity. To see this, consider the graph of f. The involutive property translates into the symmetry of the graph of f, namely invariance under reflection at the main diagonal. Let $(x, f(x)) \in \mathbb{R} \times \mathbb{R}$ be a point in the graph of f, which is not on the main diagonal. Without loss of generality, assume $f(x) > x$. i.e. the point lies above the main diagonal. Then its mirror image under the reflection symmetry is below the diagonal, and therefore f has to be decreasing between these two points to connect them.

Moreover, suppose that the group f_G contains two decreasing elements. Then their product is increasing, hence the identity. Since f_G is a group of involutions, the two decreasing functions are the same. It follows that f_G contains at most one decreasing element.

Since the identity is invariant under conjugation, we only have to find a homeomorphism h that satisfies (2.19) for this one decreasing element. Note that f has a unique fixed point x_0, because its graph has to intersect the main diagonal precisely once. In a first step we shift this point to $x_0 = 0$ by a conjugation with $h_1(x) = x - x_0$. For $\widetilde{f} = h_1 \circ f \circ h_1^{-1}$ we then have $\widetilde{f}(0) = 0$. The appropriate conjugating homeomorphism h_2, which further simplifies the action of $\widetilde{f}$ is then found in [O'F04]:

$$h_2(x) = \begin{cases} x & x \leq 0 \\ -\widetilde{f}(x) & x > 0, \end{cases} \tag{2.20}$$

which is increasing. It is easy to check that

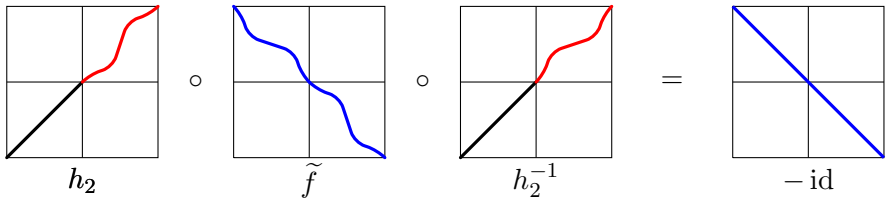


Figure 2.2: Schematic flattening of a decreasing involution via $h_2 \circ \widetilde{f} \circ h_2^{-1} = -\mathrm{id}$.

$$h_2 \circ \widetilde{f}(x) = \begin{cases} \widetilde{f}(x) & \widetilde{f}(x) \leq 0 \\ -x & \widetilde{f}(x) > 0 \end{cases} = \begin{cases} \widetilde{f}(x) & x \geq 0 \\ -x & x < 0 \end{cases} = -h_2(x), \tag{2.21}$$

where we used that $\widetilde{f}(x) < 0 \Leftrightarrow x > 0$. This last condition is due to the fact that $\widetilde{f}$ is a strictly monotonically decreasing function with $\widetilde{f}(0) = 0$.

Finally, (2.21) is equivalent to (2.19) with $h = h_2 \circ h_1$ and $r(g) = -1$, which proves the Lemma. □

We can hence describe the action of the symmetries on a Hamiltonian by a function $r\colon G \to \{\pm 1\}$. By definition the function r is a character on G, similar to the unitarity character u. We call it the **reversing character** and accordingly a symmetry with $r(g) = -1$ reversing. The two possibilities $g(H) = \pm H$ are the standard assumptions that lead to the tenfold way from a group theoretical point of view (see, e.g. [FM13]). On the other hand, in the tenfold way, every combination of the character pair $(u(g), r(g))$ occurs. Vice versa, as we will show below, any symmetry of the tenfold way is uniquely characterized by u and r. Adding r to our setting of a symmetry type, we can now define what it means for a Hamiltonian to be **admissible** for a symmetry type:

Definition 2.2.2. *Let ρ be a representation of a symmetry type and $r\colon G \to \{\pm 1\}$ a reversing character. A Hamiltonian, which satisfies*

$$g(H) = \rho_g H \rho_g^* = r(g) H, \tag{2.22}$$

*is called **admissible** for the ρ with respect to r.*

2.2.2 Redundant symmetries

So far, we considered arbitrarily large symmetry groups of involutions, and hence, a symmetry group might contain multiple symmetries with the same character combination (u, r). However, classification problems do not necessarily become more interesting with larger symmetry groups. Consider for example two anti-commuting unitary symmetries g, h with $r(g) = r(h) = 1$. Then the Hilbert space can always be written as the tensor product $\mathcal{H} = \mathbb{C}^2 \otimes \mathcal{H}'$, on which ρ_g and ρ_h act as Pauli operators in the first tensor factor and as the identity in the second (see the discussion on realisations on a Hilbert space in Section 2.1.2). Any admissible Hamiltonian on this Hilbert space, by $r(g) = r(h) = 1$, commutes with these symmetries and hence is of the form $H = \mathbb{1} \otimes H'$. This reduces the problem of classifying H to classifying H', and since admissibility for g and h is taken care of by this decomposition, H' only needs to be admissible for a

smaller symmetry group. Our goal for this section is to formalise this notion of redundancy and to establish a reduction procedure, which reduces any symmetry type $[\rho]$ to a type with less symmetries and without such redundancy. For Hamiltonians this leads to the well known tenfold way of symmetries, as the set of symmetry types for involutive symmetry groups that do not contain any redundant symmetries. Applying the reduction procedure, as well as further phase choices, to unitary operators in the next section leads to 38 symmetry types without redundancies.

To this end, let us first investigate the influence of any unitary symmetry on the structure of the whole group:

Lemma 2.2.3. *Let G be a group of involutions and $g \in G$, with $u(g) = 1$. Then in every representation ρ of a fixed type $[\rho]$, ρ_g imposes a direct sum decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ of the underlying Hilbert space into its eigenspaces, for which the following holds*

- *Whether the representatives of the other group elements ρ_h leave these eigenspaces invariant is independent of the representation ρ.*
- *The elements ρ_h with the property above form a subgroup $G' \subseteq G$, which inherits representations $\rho'_\pm$ from ρ on $\mathcal{H}_\pm$, respectively.*
- *This induces a symmetry type $[\rho'] = [\rho'_+] = [\rho'_-]$, which is uniquely specified by $[\rho]$ and g.*

*We call $[\rho']$ the **restriction of** $[\rho]$ **induced by** g.*

Proof. First, note that the above statements are independent of the phase convention we choose. Indeed, the eigenspaces of an operator and the condition of leaving a certain space invariant do not change when that operator is multiplied by any phase. Hence, we are free to choose any phase convention for the representation ρ of the symmetry type $[\rho]$. For convenience, we choose phase convention II (see Lemma 2.1.7).

Since $\rho_g^2 = \pm\mathbb{1}$, the Hilbert space decomposes into $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, where $\mathcal{H}_\pm$ denote the ± 1, respectively the $\pm i$ eigenspaces of ρ_g. In phase convention II it is then easy to see, that there are only two possibilities for the remaining symmetry operators: they either leave these eigenspaces invariant or they swap them. For a unitary symmetry ρ_h this is decided by the commutation character: for $c(g,h) = +1$ the eigenspaces are invariant and for $c(g,h) = -1$ they are swapped. In case of an antiunitary symmetry ρ_a, also the square of ρ_g has to be taken into account. Let $\rho_g^2 = -\mathbb{1}$ and $\psi \in \mathcal{H}_+$. Then

$$\rho_g \rho_a \psi = c(g,a)\rho_a(i\psi) = -ic(g,a)\rho_a\psi,$$

i.e. $\rho_a\psi \in \mathcal{H}_\pm$ for $c(g,a) = \mp 1$. In general, we get the following condition for ρ_h:

$$\rho_h \mathcal{H}_+ = \mathcal{H}_\pm \quad \Leftrightarrow \quad c(g,h)\rho_g^{1-u(h)} = \pm\mathbb{1}, \tag{2.23}$$

and the analogous statement for $\rho_h\mathcal{H}_-$.

Using $1 - ab \equiv 2 - a - b \bmod 4$ for $a, b \in \{\pm 1\}$ we see, that (2.23) actually defines another character $\varphi^g \colon G \to \{\pm 1\}$: For for $g, h, k \in G$ we get

$$\begin{aligned} c(g,hk)\rho_g^{1-u(hk)} &= c(g,h)c(g,k)\rho_g^{1-u(h)u(k)} \\ &= \left(c(g,h)\rho_g^{1-u(h)}\right)\left(c(g,k)\rho_g^{1-u(k)}\right), \end{aligned}$$

i.e.

$$\varphi^g(hk) = \varphi^g(h)\varphi^g(k). \tag{2.24}$$

This character is independent of the phase convention, after adjusting the phases according to Proposition 2.1.4: For $u(h) = 1$ only $\varphi^g(h) = c(g,h)$ remains, which cannot be changed by phase choices if both elements are represented unitarily. For $u(h) = -1$ a different choice of phases might change the square ρ_g^2 to $-\rho_g^2$ due to a factor of i. However, this changes $c(g,h)$ to $-c(g,h)$ at the same time, and hence, (2.23) is invariant.

The kernel of this character defines a subgroup G', which leaves the eigenspaces of ρ_g invariant, and all operators ρ_h with $h \in G'$ are block diagonal with respect to the direct sum decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, i.e. $\rho_h = \rho_{h+} \oplus \rho_{h-}$. Hence, in each block the commutation relations and squares of the operators have to be the same as for ρ, wherefore $\rho'_\pm$ are representatives of the same symmetry type $[\rho']$ for the group G'. In general, $\mathcal{H}_+$ and $\mathcal{H}_-$ do not have to be of the same dimension. However, if $\dim \mathcal{H}_+ \neq \dim \mathcal{H}_-$, we get $G' = G$ because Hilbert spaces of different dimension cannot be mapped to each other by a unitary (or antiunitary) operator.

Since, as we checked above, this reduction only depends on the symmetry type $[\rho]$, and not on the specific representation, the restriction $[\rho']$ is uniquely specified by $[\rho]$ and g. □

With this in mind, we can define a notion of redundancy, which will lead to the tenfold way for Hamiltonians, respectively the 38-fold way for unitary operators. Roughly speaking, a symmetry of a symmetry type $[\rho]$ is redundant, if the above procedure of inducing a smaller symmetry type $[\rho']$ is compatible with the operators, that are admissible for $[\rho]$. I.e. if no information concerning a classification task is lost due to reducing considerations to a smaller symmetry type. Note that g is still part of the reduced symmetry type since the swapping character φ^g is trivial on g. Since the restriction of ρ'_g to $\mathcal{H}_\pm$ is just a multiple of the identity, it has no non-trivial action on admissible operators. This suggests to further reduce the symmetry type by removing g from G'. However, since there is, in general, no unique way of removing an element of a group, we did not include this further reduction in the lemma above and instead included it in the following definition.

Definition 2.2.4. *Let G be a finite group of involutions, $g \in G$, with $u(g) = 1$ and $[\rho]$ a symmetry type of G. Denote by $[\rho']$ the restriction of $[\rho]$ induced by g, according to Lemma 2.2.3, with the corresponding subgroup $G' \subset G$. Moreover, let $\widetilde{G}' \subset G'$ be a maximal subgroup not containing g. We call g, as well as all other symmetries $h \in G \setminus \widetilde{G}'$ **redundant**, if, in any representation ρ, a Hamiltonian $H \in \mathcal{B}(\mathcal{H})$ is admissible for ρ if and only if the following conditions are met:*

i) $H = H_+ \oplus H_-$ is block diagonal with respect to the direct sum decomposition of $\mathcal{H}$.

ii) H_+ is admissible for the symmetry type $[\widetilde{\rho}']$, restricted to $\widetilde{G}'$.

iii) If there is a symmetry $h \in G \setminus G', h \neq g$, H_- is determined by H_+, via the action of h.

The purpose of this definition is to get rid of unnecessary symmetries in a classification task. If an operator H is admissible for a redundant symmetry in the above sense, a

topological classification reduces to the classification of H_+ and H_- separately. If there is a swapping symmetry $h \in G \setminus G'$ according to *iii*) above, it suffices to consider only one of the blocks, because they are images of each other under h. Note that by this definition the identity $e \in G$ is never redundant, since there is no subgroup $\widetilde{G}'$ not containing it. But, as already mentioned, $\widetilde{G}'$ is not uniquely defined, which the following example demonstrates:

Example 2.2.5. *Consider the Klein four group $G = \{e, g_1, g_2, g_3\}$, with $g_i^2 = e$ and $g_i g_j = g_k$ for $i \neq j \neq k$, from which we want to remove g_3. Then both, $\widetilde{G}_1 = \{e, g_1\}$ and $\widetilde{G}_2 = \{e, g_2\}$ are valid maximal subgroups.*

However, the goal is to remove all redundant symmetries in a symmetry type, i.e. to further reduce $[\widetilde{\rho}']$ until "there is no redundancy left". The following Proposition shows that the result of such complete reduction process is independent of the "intermediate" groups $\widetilde{G}'$.

The distinguished group elements, which we use to reduce the symmetry type step by step, are unitary symmetries that commute with the Hamiltonian. These symmetries are thus the non-trivial elements of the subgroup

$$G_{11} = \{g \in G | u(g) = r(g) = 1\}, \tag{2.25}$$

i.e. the common kernel of the unitarity character u and the reversing character r.

Theorem 2.2.6. *Let $[\rho]$ be a symmetry type of a symmetry group G without redundant symmetries. Then $G_{11} = e$, and every symmetry $g \in G$ is uniquely characterized by the pair $(u(g), r(g))$.*

Proof. Let $e \neq g \in G_{11}$. Then g is redundant in the sense of Definition 2.2.4: Since $u(g) = 1$, it induces a restriction according to Lemma 2.2.3 and by $r(g) = 1$, it commutes with any admissible Hamiltonian. Hence, condition *i*) in Definition 2.2.4 is met. Moreover, since for H_+, ρ'_g acts trivially, so is *ii*). By Lemma 2.2.3, item *iii*) is automatically fulfilled and the only thing we need to check is, that different symmetries $h, h' \in G \setminus G'$ produce the same H_-. Since their product must be part of G', this is guaranteed by the admissibility of H_+ for ρ'_+. This proves $G_{11} = e$ for a symmetry type which doesn't contain redundant symmetries.

In order to show the uniqueness statement, let $g, h \in G$, with $g \neq h$, $u(g) = u(h)$ and $r(g) = r(h)$. Then their product $k = gh$ would be a non-trivial element of G_{11}, since $u(gh) = u(g)u(h) = 1 = r(gh) = r(g)r(h)$. Hence every combination of (u, r) can only occur once. □

The remaining non-trivial symmetries after the reduction procedure described above can now precisely be identified with the symmetries from the tenfold way, which enables us to state the following corollary, highlighting the unique role of the tenfold way for the topological classification of quantum systems:

Corollary 2.2.7. *For Hamiltonians, the set of all symmetry types without redundant symmetries is the tenfold way.*

Proof. Every symmetry in a symmetry type is uniquely labelled by the pair (u, r), which are identified with the symmetries from the tenfold way according to (compare (2.1))

$$\begin{aligned} \textbf{Time reversal symmetry:} \quad & \tau \equiv (-1, +1) \\ \textbf{Chiral symmetry:} \quad & \gamma \equiv (+1, -1) \\ \textbf{Particle hole symmetry:} \quad & \eta \equiv (-1, -1) \end{aligned} \quad . \tag{2.26}$$

The symmetry group either consists of one non-trivial or all three symmetries, together with the identity. If τ or η are contained in the symmetry group, we have to distinguish the signs of their square. Since there is at most one unitary operator, i.e. γ, we can always choose it to be a generator. In that case, phase convention I in Lemma 2.1.5 is the convenient choice, because it renders the representation commutative, and the square of the unitary operator is determined by the product of the squares of the anti unitary ones. Counting the types according to (2.14) leads to one type for $\{\gamma, \mathrm{id}\}$ (AIII), two types for $\{\eta, \mathrm{id}\}$ (D, C) and $\{\tau, \mathrm{id}\}$ (AI, AII), respectively, and four types for $\{\gamma, \eta, \tau, \mathrm{id}\}$ (BDI, CI, CII, DIII). Adding the trivial group $\{\mathrm{id}\}$ (A) finally leads to ten different types without redundant symmetries for Hamiltonians. □

The symmetry types and their defining properties, as well as the corresponding symmetry groups (which will be defined later in Section 2.3) are listed in Table 2.1, where we subsumed them into the 38-fold way for unitary operators. The types are systematically numbered according to their defining properties (the commutation character $c(\cdot, \cdot)$ on the set of generators and, if present, the square of the antiunitary generator ρ_a^2). The symmetry types of the tenfold way are labelled by $1, 3, 4, 5, 8, 9, 20, 21, 22$ and 23. However, for easier identification the Cartan-labels for the corresponding symmetric spaces [Car26, Zir96] are also listed in the table (A, AIII, AI, AII, D, C, BDI, CII, CI and DIII, in the same order).

2.2.3 Action on unitary operators

The ansatz for unitary operators will be the same as for Hamiltonians. We assume the symmetries to act on a unitary operator via

$$g(U) = \rho_g U \rho_g^* = f_g(U), \tag{2.27}$$

where $f_g : \mathbb{T} \to \mathbb{T}$ is some family of continuous involutions on the unit circle, evaluated in the spectral calculus, which carries the group structure of G. In the Hamiltonian case, we reduced these actions to a single character $r(s)$ by conjugating with a fixed homeomorphism h (Proposition 2.2.1). A similar simplification is possible in the case of unitary operators, with two instead of one character:

Proposition 2.2.8. *Let G be a finite group of involutions, and $G \ni g \mapsto f_g$ a homomorphism into the group of homeomorphisms on the circle. Then there is a homeomorphism h and characters $s, ur : G \to \{\pm 1\}$ such that*

$$h \circ f_g \circ h^{-1}(z) = s(g)\, z^{ur(g)} \quad \textit{for all} \quad g \in G. \tag{2.28}$$

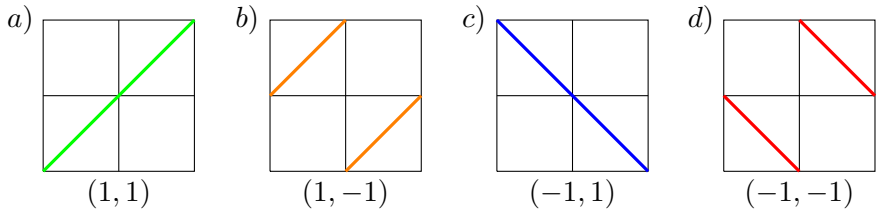


Figure 2.3: Graphs of representatives of the four classes of involutive homeomorphisms on the circle. By the involution property they are all mirror symmetric with respect to the main diagonal. The identity $a)$ has an infinite number of fixed points, the shift $b)$ has no fixed points and the two decreasing elements have exactly two fixed points ($(0,0)$ and (π,π) for $c)$ and $\pm(\pi/2,\pi/2)$ and for $d)$). The graphs are labelled by the character values (ur, s) of the corresponding involutions.

The distinguishing feature for continuous involutions on $\mathbb{R}$ was the monotonicity character r, which indicated whether a given involution is increasing or decreasing. A similar concept appears for involutions of the unit circle: the winding number, labelled by the character ur[5].

Proof. The concatenation of two functions on the unit circle induces the multiplication of their winding numbers. Hence, since f_g carry the group structure of a group of involutions, the only possible winding numbers for the f_g are ± 1. Moreover, conjugation with h does not change the winding number. We define the character $ur\colon g \mapsto \pm 1$, via to be the winding number of f_g. We can represent the graph of any function $f\colon \mathbb{T} \to \mathbb{T}$ on a square $(-\pi,\pi] \times (-\pi,\pi]$ with periodic boundary conditions, i.e. $-\pi \equiv \pi$. Then ur again distinguishes whether f_g is monotonically increasing or decreasing, of course, interpreted apart from jumps between the identified points $-\pi$ and π. We will keep this representation in mind and identify points on the circle by angles in $(-\pi,\pi]$. Accordingly, we call functions f_g with $ur(g) = \pm 1$ increasing or decreasing. In this picture the involution property of a function f is again equivalent to the graph of f being reflection symmetric with respect to the main diagonal, similar to the Hamiltonian case. Due to the periodic boundary conditions, however, there are now increasing involutions which are different from the identity (see, e.g. Figure 2.3 $b)$).

For the group $f_G = \{f_g | g \in G\}$ there are three cases to distinguish:

1. The trivial case $f_G = \{\mathrm{id}\}$.
2. f_G contains exactly one decreasing element.
3. f_G contains at least one increasing element distinct from the identity.

These capture all possibilities for f_G. Indeed, if f_G contains more than one decreasing element, the product of two of them is increasing, and we are in case 3. In the first case, there is nothing to do. Hence we start with the first non-trivial case.

Case 2:

[5]The choice of notation for the character ur is explained below the proof.

Let f be the decreasing involution. Then, apart from the identity, this must be the only element in f_G, since any non-trivial increasing involution would produce another decreasing one after concatenating it with f. An involution on the circle has either zero, two or infinitely many fixed points (see e.g. [Pfe74]). Hence, since f is decreasing, it has exactly two fixed points[6]. We start by moving one of these fixed points to $0 \in (-\pi, \pi]$ by conjugating with a shift h_1. Without loss of generality, we can assume the second fixed point x_0 to be greater than zero (otherwise move the second fixed point to zero in the first step). In a second step, we can now move x_0 to π, without changing $f(0) = 0$. This can be done by conjugating with

$$h_2(x) = \begin{cases} \frac{x_0}{\pi} x & -\pi \leq x < 0 \\ \frac{\pi}{x_0} x & 0 \leq x < x_0 \\ x - (\pi + x_0) & x_0 \leq x < \pi \end{cases} .$$

We are left with a decreasing involution $\widetilde{f} = h \circ f \circ h^{-1}$, $h = h_2 \circ h_1$, the graph of which connects the points $(-\pi, \pi)$ and $(\pi, -\pi)$, passing though $(0, 0)$. In a final step, we straighten this graph by conjugating with the homeomorphism

$$h_3(x) = \begin{cases} x & -\pi \leq x \leq 0 \\ -\widetilde{f}(x) & 0 < x \leq \pi, \end{cases} \tag{2.29}$$

as in the proof of Proposition 2.2.1.

We get $\widehat{f}(x) = h \circ f \circ h^{-1}(x) = -x$, with $h = h_3 \circ h_2 \circ h_1$, which gives $\widehat{f}(z) = z^{-1}$ on the circle in the complex plane. Hence, $\widehat{f} \in f_G$ is characterized by $ur(g) = -1$.

Case 3:

Let f be an increasing element in f_G different from the identity. Then, it cannot have any fixed points[7], and since the number of fixed points is constant under conjugation it can also not be transformed into the identity this way. However, it can be deformed to the π-shift via conjugation. For this, we first conjugate with a shift h_1, such that $(0, \pi) \equiv (0, -\pi)$ lies on the graph of $\widetilde{f} = h_1 \circ f \circ h_1^{-1}$. Note that this also fixes $(\pi, 0) \equiv (-\pi, 0)$, due to the mirror symmetry with respect to the main diagonal. Secondly, we straighten the connecting path between $(-\pi, 0)$ and $(0, \pi)$ in the graph of $\widetilde{f}$, as well as its mirror image, by conjugation with

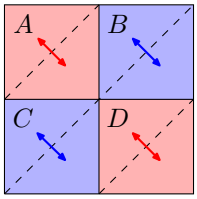
$$h_2(x) = \begin{cases} \widetilde{f}(x) - \pi & -\pi \leq x < 0 \\ x & 0 \leq x < \pi \end{cases} . \tag{2.30}$$

The resulting $s := h \circ f \circ h^{-1}$, $h = h_2 \circ h_1$ is the shift $x \mapsto x + \pi$ (see Figure 2.3 (b)) or, the rotation $z \mapsto e^{i\pi} z = -z$, when the circle is considered in the complex plane.

[6] A decreasing involutions f has at least one fixed point, because its graph intersects the main diagonal at least once, but cannot have infinitely many ones. Hence, the only possibility for a decreasing involution is to have two fixed points.

[7] The only increasing, continuous and mirror symmetric graph that intersects the main diagonal is the main diagonal itself.

Since f_G is abelian, any further element f_g has to commute with this shift. This π-shift invariance is equivalent to the equality of the graph of f_g in the off-diagonal tiles, as well as the diagonal tiles respectively in the square $[-\pi,\pi]\times[-\pi,\pi]$. I.e. equality of the graph in the tiles $A=[-\pi,0]\times[0,\pi]$ and $D=[0,\pi]\times[-\pi,0]$, and the same for B and C:



Combining this with the mirror symmetry with respect to the main diagonal, we also find that the graph is mirror-symmetric in each quadrant with respect to the reflection on the quadrants diagonal. This means that, by the same reasoning as in the proof of Proposition 2.2.1, there is no further increasing element in f_G, besides the identity and s. Moreover, this also restricts the possible number of decreasing elements in f_G because these would form a conjugacy class, which has to be of the same size as the increasing functions. Hence, there are either no or exactly two further elements in f_G, which are decreasing. However, it suffices to take only one of these into further consideration, since the second one is automatically taken care of by the group structure of f_G ($f_{g_2}=f_{g_1}\circ s$).

Let $d\in f_G$ be one of the decreasing elements. We will bring this into standard form, again by conjugating with suitable homeomorphisms h_i. In this case, however, we need to pay attention that each h_i is π-shift invariant, i.e. commutes with s. As a first step, we move one of the fixed points of d to $\pi/2$. This can be done by conjugating with an appropriate shift h_3. Both being shifts, s and h_3 certainly commute, and hence, we keep the π-shift invariance during this process. Moreover, this automatically moves the second fixed point to $-\pi/2$ due to the symmetry described above. We can now conjugate with a final homeomorphism h_4, which transforms the graph of $\widetilde{d}=h_4\circ d\circ h_4^{-1}$ to straight lines between $(0,\pi)$ and $(\pi,0)$, and $(-\pi,0)$ and $(0,-\pi)$ (see Figure 2.3 (d)). This can be archived via

$$h_4(x)=\begin{cases}\pi-\widetilde{d}(x) & -\pi\le x<-\pi/2\\ x & \pi/2\le x<0\\ \pi-\widetilde{d}(x) & 0\le x<\pi/2\\ x & \pi/2\le x<\pi\end{cases}, \tag{2.31}$$

which is invariant under shifts by π and hence, commutes with s. One checks by direct computation, that the result coincides with $x\mapsto\pi-x$ for $x>0$ and $x\mapsto-x-\pi$ for $x<0$, i.e. $\widetilde{d}(z)=-z^{-1}$ on the unit circle. The second decreasing involution is then given by $s\circ d(z)=z^{-1}$.

In summary, we constructed in each case a homeomorphism h, which transforms each element in f_G to one of the four standard involutions shown in Figure 2.3. Defining the character $s\colon G\to\{\pm1\}$ by

$$s(g)=(-1)^{f_g(0)/\pi},$$

which measures the "π-shift content" of f_g, allows us to label each of these possibilities by the character pair (ur, s), as in (2.28). □

The choice of notation for ur becomes clear by considering the time evolution operator $U_t = \exp(iHt)$ for an admissible Hamiltonian H. In this case, $ur(g) = u(g)r(g)$, where $r(g)$ is the reversing character for the Hamiltonian. We can use this relationship to define the reversing character for general unitaries without referring to the Hamiltonian case:

$$r(g) := u(g)ur(g).$$

In this sense, the new element in the unitary case is the sign $s(g)$. Similarly as before, we henceforth reduce our considerations to the actions induced by these three characters (u, r, s):

Definition 2.2.9. *Let ρ be a representation of a symmetry type, together with two characters $r, s\colon G \to \{\pm 1\}$. Then a unitary operators, which satisfies*

$$g(U) = \rho_g U \rho_g^* = s(g)\, U^{ur(g)}, \tag{2.32}$$

*with $ur = u \circ r$ is called **admissible** for ρ.*

The notion of redundancy of the Hamiltonian case directly transfers to unitary operators, and we will not state it again here. Similar to the above, the obvious candidate for a subgroup of redundant symmetries is

$$G_{111} = \{g \in G | u(g) = r(g) = s(g) = 1\},$$

i.e. the common kernel of the three characters in the unitary setting. Note that additionally taking the character s into account does not change the proof of Theorem 2.2.6. Hence:

Proposition 2.2.10. *Let $[\rho]$ be a symmetry type of a symmetry group G without redundant symmetries for unitary operators. Then $G_{111} = e$ and every symmetry $g \in G$ is uniquely characterized by the triple $(u(g), r(g), s(g))$.*

This leads to the following 8 possible symmetries:

g	(u,r,s)	g	(u,r,s)
e	(1, 1, 1)	τ	(-1, 1, 1)
σ	(1, 1, -1)	σ_τ	(-1, 1, -1)
γ	(1, -1, 1)	η	(-1, -1, 1)
σ_γ	(1, -1, -1)	σ_η	(-1, -1, -1)

, (2.33)

which allow for 16 possible symmetry groups: There are 7 groups with just one non-trivial element, 7 with three non-trivial elements, the full group and the trivial one. We can now count the number of possible symmetry types according to Corollary 2.1.8. The groups with one non-trivial element lead to one symmetry type if the element is unitary and two otherwise, whereas the group with three non-trivial elements lead to two symmetry types in the purely unitary case and four, if antiunitary elements are

n	$\varphi(n)$	group elements	# types
1		e	1
2		σ	1
3	13	γ	1
4		τ	2
5		σ_τ	2
6	14	η	2
7		$\sigma, \gamma, \sigma_\gamma$	2
8		$\sigma, \tau, \sigma_\tau$	4
9		$\sigma, \eta, \sigma_\eta$	4
10	15	γ, τ, η	4
11	16	$\gamma, \sigma_\tau, \sigma_\eta$	4
12		$\sigma, \gamma, \sigma_\gamma, \tau, \sigma_\tau, \eta, \sigma_\eta$	16
			$\Sigma : 43$
13	3	σ_γ	1
14	6	σ_η	2
15	10	$\sigma_\gamma, \tau, \sigma_\eta$	4
16	11	$\sigma_\gamma, \sigma_\tau, \eta$	4
			$\Sigma : 54$

Figure 2.4: List of different symmetry groups generated by the three character values (u, r, s) according to (2.33). The lower four groups are the images of four of the upper 12 groups under φ. A missing entry in the φ-column indicates $\varphi(G) = G$. The right column counts the number of different symmetry types for each group.

contained. Finally, for the whole group there are 16 different symmetry types. Together with the trivial group these add up to 54 different symmetry types (see Table 2.4).

However, not all of these 54 cases are fundamentally different when it comes to the task of topological classification of unitaries, since there is yet another phase freedom we can use to reduce the number of cases. Multiplying a family of unitary operators with a constant phase $\mathcal{U} \mapsto \lambda\mathcal{U}$ does not change its topological properties, i.e. we are free to choose this phase in a convenient way. The operation $\mathcal{U} \mapsto \lambda\mathcal{U}$ is reflected in the following action of the symmetries on $\widehat{U}$:

$$g(\widehat{U}) = \lambda^u g(U) = \lambda^{u(1-r)} s\widehat{U}^{ur} = \begin{cases} s\widehat{U}^{ur}, & r = 1 \\ \lambda^{2u} s\widehat{U}^{ur}, & r = -1. \end{cases} \tag{2.34}$$

We could now again apply Proposition 2.2.8 and investigate which possibilities emerge from this. However, we can equivalently only allow those λ, which keep the form of Proposition 2.2.8 ($g(\widehat{U}) = \pm\widehat{U}^{\pm 1}$) in the first place. It is easily verified that this is only the case for $\lambda = \pm 1$ and $\lambda = \pm i$. For $\lambda = \pm 1$ the symmetry conditions are unchanged, but for $\lambda = i$ (and equivalently also for $\lambda = -i$) we get a different action.

Lemma 2.2.11. *Let G be a symmetry group without redundant symmetries. Then the map*

$U \mapsto \widehat{U} = iU$ induces an isomorphism

$$\varphi\colon G \to G', \qquad (u, r, s) \mapsto (u, r, rs) \tag{2.35}$$

Proof. For $\lambda = i$ the u-dependence in (2.34) vanishes and we get $g(\widehat{U}) = rs\widehat{U}^{ur}$. Hence, g acts on $\widehat{U}$ with the character values (u, r, rs). Because G does not contain any redundant symmetries, i.e. every group element is uniquely labelled by the character triple (u, r, s) by Theorem 2.2.10, this induces a map $\varphi\colon (u, r, s) \mapsto (u, r, rs)$ from G to a possibly different group G'. Since u, r and s are characters with $r^2 = 1$, φ clearly is a homomorphism, which is one to one and onto due to $r^2 = 1$ and therefore $\varphi \circ \varphi = \mathrm{id}$. Hence G and G' are isomorphic. □

The possible group elements on which φ acts non-trivially are the pairs (γ, σ_γ) and (η, σ_η). These are mapped to each other respectively, i.e. $\varphi(\gamma) = \sigma_\gamma$, $\varphi(\eta) = \sigma_\eta$, with $\varphi \circ \varphi = \mathrm{id}$. Consequently, 11 of the groups we identified are affected by φ. If only one element of the pairs is part of a group, the whole group gets mapped to another one, which is the case for 8 groups, wherefore we can drop four of them (the lower part in Table 2.4), together with all their corresponding types. This leaves us with the 12 symmetry groups listed in the upper part of Table 2.4. Counting the possible symmetry types for these 12 groups according to Corollary 2.1.8 would lead to 43 types (see the last column in Table 2.4 for the number of types for each group).

Moreover, φ does not only affect the general group structure, it also induces a mapping on the level of symmetry types. Since G and G' are isomorphic, each representation $g \mapsto \rho_g$ of G defines a representation $g' \mapsto \rho_{\varphi^{-1}(g')}$ of G', with

$$\rho_g U \rho_g^* = s_g U^{ur_g} \qquad \Leftrightarrow \qquad \rho_{\varphi(g)}(iU)\rho_{\varphi(g)}^* = s_{\varphi(g)}(iU)^{ur_{\varphi(g)}}. \tag{2.36}$$

Therefore, each symmetry type $[\rho]$ of G gets assigned a unique symmetry type $[\rho \circ \varphi]$ of G' by φ, with $[\rho] \neq [\rho \circ \varphi]$ in general.

Three of the remaining 12 groups either contain one of the pairs (γ, σ_γ) and (η, σ_η) or both, i.e. the groups 7, 9 and 12 in Table 2.4. These are affected differently by φ:

- Group 7 is represented purely unitary, wherefore, according to Lemma 2.1.7, there are two types corresponding to the sign $c = \pm 1$ of the commutation character on the two generators. Usually we chose σ and γ as generators, but for the sake of the current discussion, choosing γ and σ_γ is more convenient. In this way it becomes clear that the two symmetry types of group 7 are invariant under the action of φ, because $c(\gamma, \sigma_\gamma) = c(\sigma_\gamma, \gamma) = c(\varphi(\gamma), \varphi(\sigma_\gamma))$. This argument also applies to group 12, which also contains γ and σ_γ.

- Group 9 and 12, on the other hand, contain the pair η and σ_η, for which the action of φ on the symmetry type becomes non-trivial. Since there is only one antiunitary generator, which we choose to be η here, the effect on the symmetry type is determined by the square of η alone. Hence, whenever $\eta^2 \neq \sigma_\eta^2$, we get $[\rho] \neq [\rho \circ \varphi]$, because the sign of the antiunitary generator changes under φ. This maps two of the types of group 9 and eight types of group 12 pairwise onto each other, respectively.

The relation between the types $[\rho]$ and $[\rho \circ \varphi]$ originates from a simple phase multiplication $U \mapsto iU$ of admissible unitaries. Therefore, a classification of the set of admissible unitaries has to be equivalent for both types: There exists an admissible unitary for $\rho' = \rho \circ \varphi$, if and only if there exists one for ρ. Moreover, the spectral orbits (which we introduce in the next section) and the corresponding gap conditions are similarly related via a rotation by $\pi/2$ in the complex plane, i.e. multiplication by i. In particular, the index groups (see Proposition 2.3.8) of the two types will be the same. Hence, we consider the symmetry types in the five pairs mentioned in the second bullet point above to be equivalent, respectively. Consequently, we drop one type of each pair from the list of distinct types in the following discussions, which further reduces the number of distinct types from 43 to 38.

Corollary 2.2.12 (38-fold way)**.** *The number of independent symmetry types induced by the characters u, r and s is 38.*

All groups and types, together with their spectral orbit, their defining properties, their images under φ as well as further quantities, which will be discussed in the following are listed in Table 2.1.

Connection to the Bernard LeClair symmetry classes [BL02]

Let us particularise the connection of the considerations here to the work by Bernard and LeClair [BL02], which we already mentioned in the introduction to the present chapter. The authors discuss symmetry classes for complex (non-hermitian) matrices M, obeying one or more of the following set of symmetries[8]:

$$\begin{aligned} &\text{C sym.}: \quad cMc^* = \epsilon_c \overline{M}, \quad c\bar{c} = \pm 1 \\ &\text{P sym.}: \quad pMp^* = -M, \quad p^2 = 1 \\ &\text{Q sym.}: \quad qMq^* = M^*, \quad q^2 = 1 \\ &\text{K sym.}: \quad kMk^* = M^T, \quad k\overline{k} = \pm 1, \end{aligned} \tag{2.37}$$

where c, p, q and k are unitary operators, implementing the symmetries. The symmetry transformations are assumed to commute, which, on the level of the unitary operators, implies

$$\begin{aligned} pc &= \pm c\bar{p}, \qquad pk = \pm k\bar{p}, \qquad qp = \pm pq, \\ qc &= \pm c\bar{q}, \qquad qk = \pm k\bar{q}, \qquad c\overline{k} = \pm k\bar{c}. \end{aligned} \tag{2.38}$$

Bernard and LeClair identify 38[9] different symmetry classes, based on the involved sign choices and equivalences they find. These classes correspond to the symmetry types we identified above.

In order to translate the conditions to our setting, we first have to get rid of the basis dependent operations $\overline{(\cdot)}$ and $(\cdot)^T$. This can be done by taking c and k to be antiunitary instead of unitary operators. We get

$$\begin{aligned} &\text{C sym.}: \quad cMc^* = \epsilon_c M, \quad c^2 = \pm 1 \\ &\text{K sym.}: \quad kMk^* = M^*, \quad k^2 = \pm 1 \end{aligned} \tag{2.39}$$

[8] Note that the notation is adjusted to the convention here.

[9] In the first version (2001) they identify 43 classes and corrected it to 38 in a second version (2020).

and all commutation relations also boil down to just the sign choices, representing the commutation character from our setting.

The symmetry transformations are then easily identified via the character values (u, r, s). For unitary M we get

$$\begin{aligned} C &\equiv (-1, 1, \epsilon_c), & P &\equiv (1, 1, -1), \\ Q &\equiv (1, -1, 1), & K &\equiv (-1, -1, 1). \end{aligned} \tag{2.40}$$

Comparing these with (2.33), we get $C \equiv \tau$ for $\epsilon_c = 1$, $C \equiv \sigma_\tau$ for $\epsilon_c = -1$, $P \equiv \sigma$, $Q \equiv \gamma$ and $K \equiv \eta$. Together with the trivial symmetry, these are six of our eight non-redundant symmetries. The missing ones ($\sigma_\gamma \equiv (1, -1, -1)$ and $\sigma_\eta \equiv (-1, -1, -1)$) could be included by introducing signs ϵ_q and ϵ_k. But, as Bernard an LeClair argue, this would not lead to fundamentally different symmetry transformations, since these can also be archived from the given ones by considering iM instead of M, which exactly matches the action of φ on γ and η in our approach (see e.g. Table 2.4).

To conclude this interlude, let us comment on the differences between the two approaches. While, in the end, considering an isomorphic set of symmetry transformations and counting the same number of different types emerging from these, Bernard and LeClairs ansatz lacks the generality our approach provides. We start with an arbitrary number of involutive symmetries, with an arbitrary continuous action on time evolution operators, discuss the possible different types of representations and reduce these to a minimal set of non-redundant types.

This way, we can be sure that the 38 symmetry types are indeed an exhaustive list of structurally different symmetry types for unitary operators. In [BL02] on the other hand, the authors define the symmetry transformations in a rather ad hoc way, without going into great detail about the origin of such assumptions. Moreover, in our approach, we chose to represent the symmetries by unitary and antiunitary operators, which, together with the different levels of generality our approach exhibits (group, symmetry type, representation), gives a clearer picture as opposed to the corepresentations with modified multiplications laws Bernard and LeClair use for their considerations. This is, however, more a matter of taste than an actual difference.

2.3 The symmetry index

Having identified the possible symmetry types for the specific settings (Hamiltonians, i.e. continuous-time systems and unitaries, i.e. discrete-time systems), we now proceed with the classification task by defining an index for finite-dimensional representations of any symmetry type. This will eventually lead to a classification of operators on separable Hilbert spaces by applying this index classification to the symmetry protected finite-dimensional eigenspaces. The key structure for this task is the so-called **symmetry index**, which labels the equivalence classes of finite-dimensional representations up to trivial direct summands for each symmetry type. These equivalence classes naturally form a group, which we call the index group, and the symmetry index assigns a unique element of this group to each finite-dimensional representation of a symmetry type. The formal definition of the symmetry index originated in [CGS$^+$16] and was further

developed and fully exploited for the symmetry types of the tenfold way in [CGG$^+$18]. Here, we extend this definition to all 38 distinct symmetry types and compute the corresponding symmetry groups.

In order to define the index group and the symmetry index, we need to investigate how the action of the symmetries influences the spectrum of the admissible operators under consideration. Although we are only dealing with finite-dimensional representations of the symmetry groups under considerations at the moment, we will, in foresight of the following classification tasks, formulate the following also for operators on an infinite-dimensional Hilbert space.

Lemma 2.3.1. *Let H and U be an admissible Hamiltonian, respectively unitary for a symmetry g with the character values (u, r) and (u, r, s), respectively. Then:*

- *When $z \in \sigma(H) \subset \mathbb{R}$, we also have $rz \in \sigma(H)$. I.e. symmetries with $r = -1$ impose a reflection symmetry on the spectrum with respect to the origin.*
- *When $\lambda \in \sigma(U) \subset \mathbb{C}$, we also have $s\lambda^r \in \sigma(U)$. I.e. symmetries with $r = -1$ impose a reflection symmetry with respect to the real line and symmetries with $s = -1$ impose a reflection symmetry with respect to the origin on the spectrum of U.*

Proof. **Hamiltonians H:** Let z be in the spectrum of H, i.e. $(H - z)$ is not invertible and let ρ_g be the representing operator for g. Then

$$\begin{aligned}(H - z)^{-1} \notin \mathcal{B}(\mathcal{H}) &\Leftrightarrow \left(\rho_g(H - z)\rho_g^*\right)^{-1} \notin \mathcal{B}(\mathcal{H}) \\ &\Leftrightarrow (rH - z)^{-1} \notin \mathcal{B}(\mathcal{H}) \\ &\Leftrightarrow (H - rz)^{-1} \notin \mathcal{B}(\mathcal{H}),\end{aligned}$$

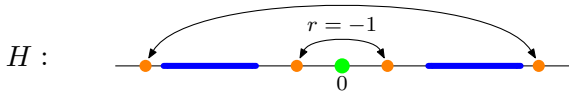
where we used $z \in \mathbb{R}$ in the second step.

Unitaries U: Let λ be in the spectrum of U. Then

$$\begin{aligned}(U - \lambda)^{-1} \notin \mathcal{B}(\mathcal{H}) &\Leftrightarrow \left(\rho_g(U - \lambda)\rho_g^*\right)^{-1} \notin \mathcal{B}(\mathcal{H}) \\ &\Leftrightarrow (sU^{ur} - \lambda^u)^{-1} \notin \mathcal{B}(\mathcal{H}) \\ &\Leftrightarrow (U - s\lambda^r)^{-1} \notin \mathcal{B}(\mathcal{H}),\end{aligned}$$

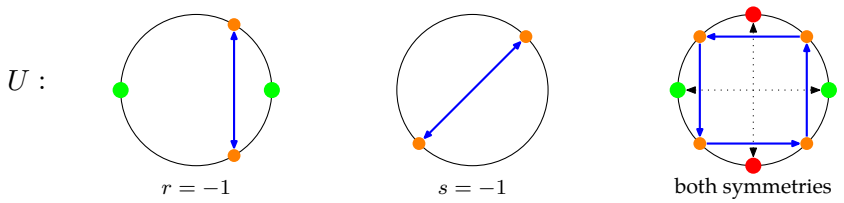
where, in the last step, we used $U^{-1} = U^*$ and $\lambda^{-1} = \overline{\lambda}$. □

For Hamiltonians the chiral symmetry (with $(u, r) = (1, -1)$) as well as the particle hole symmetry (with $(u, r) = (-1, -1)$) impose a reflection with respect to the origin.



This singles out the zero as the only invariant point in the spectrum of admissible operators. For unitaries, the actions on the spectrum are slightly more complex. Symmetries with $r = -1$ impose a reflection on the real line, whereas symmetries with $s = -1$ impose a reflection on the origin. For a symmetry group with more than one symmetry,

these relations impose certain orbits of eigenvalues of an admissible unitary under the action of the whole group. Given an eigenvalue $\lambda \neq \pm 1, \pm i$, each symmetry group imposes one of the following orbits: $\{\lambda\}$, $\{\lambda, \lambda^*\}$,$\{\lambda, -\lambda\}$ or $\{\lambda, \lambda^*, -\lambda, -\lambda^*\}$. Pictorially these orbits are represented by a point, a vertical line, a diagonal line passing through the origin or a rectangle.

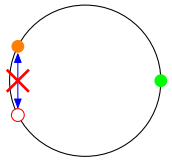


In principal, also the orbit $\{\lambda, -\lambda^*\}$ is possible, but all symmetry groups, with this orbit can be mapped to other ones via $U \mapsto iU$ (see the discussion before Corollary 2.2.12). However, note that as a limit case of a rectangle, the horizontal line with $\{\lambda\} = \{\pm 1\}$, as well as the vertical line $\{\pm i\}$ are still contained.

This singles out certain elements of the spectrum in two of the situations. For $r = -1$, the eigenspaces at ± 1 are invariant under the symmetry. For the rectangular orbits, we get two pairs of eigenspaces, each of which is invariant as a pair. On the one hand, the combined ± 1-eigenspaces $\mathcal{H}_{+1} \oplus \mathcal{H}_{-1}$ are invariant under the symmetry and on the other, so are $\mathcal{H}_{+i} \oplus \mathcal{H}_{-i}$, the eigenspaces corresponding to $\pm i$. One might now argue that this last property is also true for the reflection on the origin. However, the reflection symmetry has the same action on every other point and, therefore, does not single out specific eigenspaces. For the vertical reflection and the rectangular orbit, on the other hand, the described parts of the spectrum are special because the orbit is reduced on these points. Similar to Hamiltonians, our classification of admissible operators builds on these invariant eigenspaces. In contrast to self-adjoint operators, however, there are more than one of these invariant spaces, resulting in a richer classification.

In order to come up with the relevant equivalence relation between representations of an arbitrary but fixed symmetry type, we will start by delimiting the concept of a trivial representation with respect to the symmetry index we are aiming for. To motivate the following definition, let us consider two simple examples.

Example 2.3.2. *Let $\mathcal{H} = \mathbb{C}^2$ and consider a representation of the particle-hole symmetry $\eta \equiv (-1, -1, 1)$, which we assume to act as the complex conjugation with respect to the standard basis, i.e. $\eta = K$. Hence, by $\eta U \eta^* = U$, an admissible U must have real matrix elements. Moreover, by $r(\eta) = -1$, η imposes a vertical orbit on the eigenvalues of U (see Lemma 2.3.1). This means that all eigenvalues except those at ± 1 must appear in pairs $\{\lambda, \lambda^*\}$. Hence, for any continuous deformation of U in the set of admissible unitaries, the non-real eigenvalues are moved in pairs. Consequently, e.g. σ_z cannot be continuously connected with $\mathbb{1}$ without breaking the symmetry on the way, since the -1 eigenspace is one-dimensional and therefore pinned to the eigenvalues -1.*



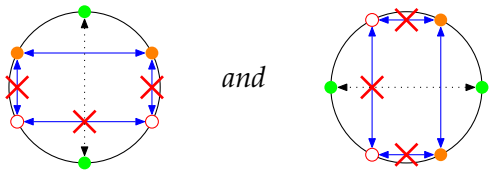
Therefore, the set of η-admissible unitaries is split into two connected components, distinguished by the -1 eigenspace dimension parity. This prototype of an invariant will later turn out to be the only necessity also in arbitrary dimensions.

Example 2.3.3. *We double the Hilbert space dimension, i.e. $\mathcal{H} = \mathbb{C}^4$, but keep $\eta = K$. Moreover, let us add another symmetry, namely $\sigma \equiv (1, 1, -1)$, represented by $\sigma = \sigma_z \otimes \mathbb{1}$. The resulting symmetry type imposes a rectangular orbit on the eigenvalues of an admissible U. Consider the following two examples:*

$$U_1 = \begin{pmatrix} 0 & R(\theta) \\ R(\theta) & 0 \end{pmatrix} \qquad \text{and} \qquad U_2 = \begin{pmatrix} 0 & \mathbb{1} \\ \sigma_z & 0 \end{pmatrix}, \tag{2.41}$$

where $R(\theta) = \exp(-ix\sigma_y)$ denotes the standard 2×2 real rotation matrix. Both unitaries have real matrix entries and are off-diagonal with respect to the σ-eigenbasis, and hence, admissible for the symmetry representation under consideration.

While the eigenvalues of U_1 ($\{\pm e^{\pm i\theta}\}$) can realize any rectangular orbit by varying θ, those of U_2 ($\{\pm 1, \pm i\}$) are pinned to the symmetry invariant points of the spectrum.



Again, there is more than one connected component of admissible unitaries: one without eigenvalues, pinned to the symmetry invariant points and possibly multiple ones with "symmetry protected" eigenspaces. Moreover, we again find, that while a reduced representation on one of the symmetry invariant eigenspaces might allow for admissible unitaries, it leaves no room for non-trivial homotopies.

In both examples above, we encountered unitaries, which did not allow for any continuous deformation without breaking the symmetry. In both cases, these unitaries hosted sub-representations on their symmetry protected eigenspaces, on which only special admissible unitaries exist (a one-dimensional one with $U = \pm 1$ in the first case and a two-dimensional one with $U \in \{\pm\sigma_z, \pm i\sigma_z\}$ in the second). These, in this sense, non-trivial representations are what we will base our classification on. To this end, let us specify what we mean by trivial in this context, or as we will call it **balanced**:

Definition 2.3.4 (Balanced)**.** *We call a representation of a symmetry type balanced if there exists an admissible unitary operator, which is gapped at the symmetry protected points of the spectrum.*

Whenever a sub-representation on one of the symmetry protected parts of the spectrum of an admissible operator is balanced, we can continuously deform these eigenspaces of the spectrum away from ± 1 and $\pm i$. Indeed, the existence of a gapped admissible unitary on these spaces leaves enough room for the deformations that where excluded in the examples above. In general, picking the eigenbasis of the gapped unitary inside the respective eigenspace, we can continuously connect the ± 1 or $\pm i$ eigenvalues

of the original operator with the eigenvalues of the gapped one, without changing the eigenvectors.

Note that in this definition, we only include the existence of admissible unitaries and do not address Hamiltonians. However, restricting ourselves to only unitaries is sufficient for the following considerations. Indeed, the tenfold way is contained in the 38 distinct symmetry types for unitary operators. Moreover, we have the following correspondence between Hamiltonians an unitaries for the symmetry types of the tenfold way.

Lemma 2.3.5. *Let ρ be a finite-dimensional representation of a symmetry type of the tenfold way, i.e. $s(g) = 1$ for all $g \in G$. Then there exists an admissible (and gapped) Hamiltonian if and only if there exists an admissible (and gapped) unitary.*

Proof. Let $g \in G$ with character values $u = \pm 1$, $r = \pm 1$ and $s = 1$, and U be an admissible unitary U. Then

$$H_U = i(U - U^*) \tag{2.42}$$

defines a Hamiltonian, which is admissible for g in the Hamiltonian sense:

$$g(H_U) = g(iU) - g(iU^*) = ui(U^{ur} - (U^*)^{ur}) = rH_U,$$

where we used $i^u = ui$ for $u = \pm 1$ in the second and $u^2 = 1$ as well as $(U - U^*)^r = r(U - U^*)$ for $r = \pm 1$ in the last step. On the other hand, given an admissible Hamiltonian H, denote by $P_\pm$ and P_0 the eigenprojections corresponding to positive/negative and zero eigenvalues of H, respectively. Then

$$U_H = i(P_+ - P_-) + P_0 \tag{2.43}$$

defines an admissible unitary:

$$g(U_H) = g(i(P_+ - P_-)) + g(P_0) = i^u(P_r - P_{-r}) + P_0 = urU = U^{ur},$$

where we used $g(P_\pm) = P_{\pm r}$, which follows from $g(H) = rH$.

Note that in particular, the symmetry protected eigenspaces of U and H result in the symmetry protected eigenspace of H_U and U_H, respectively. Therefore, H_U and U_H are gapped if and only if U and H are. □

Because of this observation, we restrict our considerations to unitary operators for the rest of the chapter, keeping in mind that we could equally well work with Hamiltonians in the tenfold way. Later, however, when we address physical systems in one dimension, i.e. quantum walks, considering unitaries instead of Hamiltonians makes a difference also in case of the tenfold way. On the one hand, having two symmetry protected eigenspaces instead of one introduces an additional invariant for unitary operators compared to the Hamiltonian setting. On the other, for symmetry types containing symmetries with $s = -1$, there is no such correspondence between unitaries and Hamiltonians. For this reason, many of the stability properties of the topological classification of operators, which are admissible for the tenfold way, do not transfer to the symmetry types of the 38-fold way (see, e.g. Section 3.2, in particular, Proposition 3.2.8 and also Section 3.5, in particular the subsections 3.4.3 and 3.5.1).

The definition of a balanced representation leaves room for both situations discussed earlier. On the one hand, the symmetry types, which leave invariant ± 1 respectively and on the other also the types, for which $\mathcal{H}_{+1} \oplus \mathcal{H}_{-1}$ and $\mathcal{H}_{+i} \oplus \mathcal{H}_{-i}$ are invariant. We will specify which of these situations is present when we compute the index groups for the different scenarios. As already stated, balanced representations take the role of the trivial class in our index classification and the index will, roughly speaking, measure how much a given finite-dimensional representation differs from a balanced one. The equivalence relation between two representations is defined as follows:

Definition 2.3.6 (Equivalence)**.** *Two finite-dimensional representations ρ and ρ' of the same symmetry type* S (*possibly with different dimensions*) *are called* ***equivalent****, if there are finite-dimensional balanced representations β and β' of the same symmetry type, such that $\rho \oplus \beta$ and $\rho' \oplus \beta'$ are unitarily equivalent, i.e. there is a unitary V, such that*

$$\rho \oplus \beta = V(\rho' \oplus \beta')V^*. \tag{2.44}$$

Note that this relation is obviously symmetric and reflexive and transitivity follows from the observation, that the direct sum of balanced representations is balanced.

Given a symmetry type, the set of equivalence classes of finite representations with respect to Definition 2.3.6, equipped with the direct sum of representatives as the operation naturally forms a commutative monoid. The neutral element is the equivalence class of balanced representations. A natural step in this situation would be to construct the Grothendieck group (see, e.g. [WO93, Appendix G]) from this monoid, which would then serves as the classifying structure for the given symmetry type. However, as we will show now, for every representation ρ, there exist another representation $\widetilde{\rho}$, such that $\rho \oplus \widetilde{\rho}$ is balanced. In other words: the set of equivalence classes already forms an abelian group with respect to the direct sum. This group will be called the **index group** of the symmetry type and is the crucial structure underlying our topological classification of quantum walks.

Lemma 2.3.7. *Let ρ be a representation of some symmetry type $[\rho]$. Then there is a representation $\widetilde{\rho}$ of the same type, such that $\rho \oplus \widetilde{\rho}$ is balanced.*

The Lemma holds for both possibilities for the definition of a balanced representation. On the one hand, for the case, where "balanced" refers to the existence of a unitary which is gapped at ± 1 and on the other for the definition of balanced, with respect to unitaries gapped at ± 1 and $\pm i$. Since it includes the first case, it suffices to prove the latter case.

Proof. First note that we have to at least quadruple the dimension of the system, since the representation we start with could be one-dimensional, and the smallest dimension allowing for an admissible unitary with gaps at all symmetry protected points $\{\pm 1, \pm i\}$ is four-dimensional (see e.g. Example 2.3.3). Given ρ, consider $\widetilde{\rho} = (ur \cdot \rho) \oplus (s \cdot ur \cdot \rho) \oplus (s \cdot \rho)$, where $ur \cdot \rho$ denotes the representation, where every ρ_g is replaced by $ur(g)\rho_g$. Every $\widetilde{\rho}_g$ is a direct sum of $\pm\rho_g$ with possibly different signs. Since multiplying with ± 1 does not change the commutation character, $\widetilde{\rho}$ is of the same type as ρ and we get

$\rho \oplus \widetilde{\rho} = \mathrm{diag}(\rho, ur \cdot \rho, s \cdot ur \cdot \rho, s \cdot \rho)$, which allows for the admissible unitary $U = \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right)$:

$$g(U) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} s \cdot ur & -s \\ s & s \cdot ur \end{pmatrix} = sU^{ur}$$

Note that in order to streamline the notation, we used just ur, s or 1 to denote the respective multiplication operators on the finite-dimensional Hilbert space ρ is defined on. The eigenvalues of U are $\pm e^{\pm i\pi/4}$, and hence, $\rho \oplus \widetilde{\rho}$ is balanced.

Note that if we are faced with a symmetry type with vertical eigenvalue orbit, i.e. one where balancedness refers to gaps only at ± 1, we can choose the simpler $\widetilde{\rho} = ur \cdot s \cdot \rho$. With this $U = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ turns out to be admissible for $\rho \oplus \widetilde{\rho}$ and gapped at ± 1. □

With this at hand, we are now able to formulate the main result of this section.

Proposition 2.3.8. *Let* S *be a symmetry type and* ρ *be a finite-dimensional representation of* S*. Then there exists an abelian group* $\mathbf{I}(\mathsf{S})$ *and a map* $\mathrm{si}\colon \rho \mapsto \mathrm{si}(\rho) \in \mathbf{I}(\mathsf{S})$*, such that*

i) si *is surjective.*

ii) $\mathrm{si}(\rho) = \mathrm{si}(\rho')$*, if* $\rho = U\rho'U^*$ *for a unitary operator* U*.*

iii) $\mathrm{si}(\rho \oplus \rho') = \mathrm{si}(\rho) + \mathrm{si}(\rho')$*.*

iv) $\mathrm{si}(\rho) = 0$ *if and only if* ρ *is balanced.*

We call $\mathbf{I}(\mathsf{S})$ *the index group of the symmetry type* S *and* $\mathrm{si}(\rho)$ *the symmetry index of the representation* ρ*.*

Note that we write the abelian group $\mathbf{I}(\mathsf{S})$ additively with neutral element 0.

Proof. Let $\mathbf{I}(\mathsf{S})$ be the set of equivalence classes of finite-dimensional representations with respect to the equivalence relation from Definition 2.3.6. Then si can be defined as the natural projection, mapping a finite-dimensional representation onto its equivalence class. This already guarantees *i*). *ii*) follows from the definition of the equivalence relation. The direct sum is an associative operation between finite-dimensional representation and since $\rho \oplus \rho'$ is unitarily equivalent to $\rho' \oplus \rho$, it establishes a commutative operation on $\mathbf{I}(\mathsf{S})$. Since we already established the existence of an inverse in Lemma 2.3.7, the only thing we need to check is, that *iii*) does not depend on the representatives ρ and ρ'. This also follows from Definition 2.3.6, since the equivalences $\rho_1 \sim \rho_2$ and $\rho_1' \sim \rho_2'$ imply the equivalence $\rho_1 \oplus \rho_1' \sim \rho_2 \oplus \rho_2'$. Hence, $\oplus$ is a well defined operation on the equivalence classes, which turns the set of those into an abelian group. *iii* and *iv*) are then a direct consequences of writing this abelian group additively with neutral element 0. □

2.3.1 Index groups

Before we use the symmetry index for the topological classification of symmetric essentially gapped unitaries, we compute the symmetry groups $\mathbf{I}(\mathsf{S})$ for all non-trivial symmetry types S. To this end, let us collect some useful facts and assumptions, which simplify these computations. In order to reduce notation, we denote the represented symmetries simply by the symbols for the abstract group elements, given in (2.33), e.g. σ instead of ρ_σ. It will be clear from the context, in which cases we consider the abstract group elements or the actual (anti-) unitary operators on the Hilbert space.

Since an index group is defined via equivalence classes of finite-dimensional representations with the group operation induced by the direct sum, the obvious strategy to compute the index groups is to determine their generators: the irreducible representations (**irreps**) of the symmetry types. However, there is a subtlety to take into account. In some cases, there exist representations, which do not allow for admissible unitaries at all. This happens for example for the irreducible representations of some groups containing $\sigma \equiv (1,1,-1)$ or $\tau \equiv (-1,1,1)$ with $\tau^2 = -\mathbb{1}$ (see Lemma 2.3.10 for the precise conditions). Since we aim for the classification of admissible unitary time evolution operators, such irreducible representations do not contribute any valuable structure. Therefore, we make the following assumption.

Assumption 2.3.9. *We only consider representations of symmetry types, for which admissible unitaries exist.*

Besides computing such minimal representations, we need to characterize the balanced representations for each type. On the one hand, the following lemma collects some necessary conditions to fulfil Assumption 2.3.9. On the other, it collects necessary conditions for balanced representations, which will be helpful for the actual computations later.

Lemma 2.3.10. *Let ρ be a representation of some symmetry type S, such that there exist admissible unitaries. Then:*

i) If $\sigma \equiv (1,1,-1)$ is part of S, we must have $\operatorname{tr}\sigma = 0$.

ii) If S imposes a rectangular eigenvalue-orbit on admissible unitaries, $\dim\rho = 0 \bmod 2$.

iii) If $\tau \equiv (-1,1,1)$ with $\tau^2 = -\mathbb{1}$ is part of S, we have

$$\dim\rho \equiv 0 \bmod \big(2\cdot|O_1(\mathsf{S})|\big), \tag{2.45}$$

where $|O_1(\mathsf{S})|$ denotes the number of elements in the eigenvalue-orbits of the eigenvalue 1 under the action of the whole symmetry type S.

Moreover, let ρ be balanced. Then:

a) If $\gamma \equiv (1,-1,1)$ is part of S, we have $\operatorname{tr}\gamma = 0$.

b) If $\sigma_\gamma \equiv (1,-1,-1)S$ is part of S, we have $\operatorname{tr}\sigma_\gamma = 0$.

c) If $\tau \equiv (-1,1,1)$ with $\tau^2 = -\mathbb{1}$ is part of S, we have

$$\dim \rho \equiv 0 \bmod \big(2 \cdot |O_\lambda(\mathsf{S})|\big), \tag{2.46}$$

where $|O_\lambda(\mathsf{S})|$ denotes the number of elements in the orbit of any eigenvalue $\lambda \notin \{\pm 1, \pm i\}$ of admissible unitaries under the action of the whole symmetry type S.

Proof. *i)*: Let U be admissible. Then, in the σ-eigenbasis we have

$$\sigma = \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & -\mathbb{1}_m \end{pmatrix} \qquad \text{and} \qquad U = \begin{pmatrix} 0 & U_{nm} \\ U_{mn} & 0 \end{pmatrix},$$

where U_{nm}, U_{mn} are $n \times m$, resp. $m \times n$ matrix blocks. By unitarity of U, each U_{kl} must be unitary, which is only possible for $n = m$. Hence, we get $\operatorname{tr} \sigma = n - m = 0$.

ii): The extremal cases of rectangular eigenvalue-orbits are those containing only ± 1 or $\pm i$. Both contain at least two elements, wherefore an admissible U needs an even number of eigenvalues.

a): Let $\operatorname{tr} \gamma \neq 0$, (w.l.o.g. $\operatorname{tr} \gamma > 0$) and U be admissible, then there exists a basis, such that

$$\gamma = \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & -\mathbb{1}_m \end{pmatrix} \qquad \text{and} \qquad U = \begin{pmatrix} U_n & U_{nm} \\ U_{mn} & U_m \end{pmatrix},$$

with $n > m$ and, the U_{kl} are $n \times m$, resp. $m \times n$ matrix blocks. Admissibility of U is now equivalent to $U_{nm} = -U_{mn}^*$, $U_n^* = U_n$ and $U_m^* = U_m$. Unitarity of U implies $U_n^* U_n + U_{mn}^* U_{mn} = \mathbb{1}_n$. Moreover, since $n > m$, U_{mn} has a non-trivial kernel $\mathcal{K} \subset \mathcal{H}_n$. From this it follows that restricted to $\mathcal{K}$, U_n is unitary and due to the chiral symmetry also self-adjoint. Therefore, U_n and consequently also U have an eigenvalue at $+1$ or -1. Hence, the representation cannot be balanced.

b): We can apply the same arguments as for γ, only with slight modifications: the admissibility conditions are now $U_{nm} = U_{mn}^*$, $U_n^* = -U_n$ and $U_m^* = -U_m$. With similar reasoning, this forces U to have an eigenvalue at $+i$ or $-i$, which is not balanced, since every type containing σ_γ imposes a rectangular orbit on unitaries and hence, balanced refers to an existing unitary with gaps at ± 1 and $\pm i$.

c) and iii): Let U be admissible and $U\psi = \lambda U$. Then by

$$U\tau\psi = \tau U^*\psi = \tau\lambda^*\psi = \lambda\tau\psi,$$

τ leaves the eigenspaces of U invariant. Hence, by $\tau^2 = -\mathbb{1}$, each of these eigenspaces has even degeneracy. For *iii)* note that the $\lambda = 1$ (or equivalently $\lambda = -1$ or $\lambda = \pm i$) orbit is minimal. □

Following Section 1.5.1 (in particular Lemma 1.5.8) and Section 2.1.2, we can now easily identify the irreps of the symmetry types. Since we have to deal with at most two unitary generators and one antiunitary one, there are, according to Corollary 2.1.9, either at most four irreps maximally of dimension 2, or at most two irreps of dimension four.

We will often determine index groups of the form $n\mathbb{Z}$ or $n\mathbb{Z}_2$, with $n \in \mathbb{N}$. Of course, these are isomorphic to $\mathbb{Z}$ and $\mathbb{Z}_2$, respectively, and we could equally well drop the factor n. However, n refers to the dimensions of the minimal possible representations and therefore carries an extra bit of information.

Index group computations:

This section contains the computation of the non-trivial index groups for all 38 distinct symmetry types. We collect the results in Table 2.1 on page 75.

Group 1 only contains the identity.

Group 2 is generated by $\sigma \equiv (1, 1, -1)$, which does not single out an invariant point in the spectrum. Hence, there exists no index group in the above sense.

Group 3 is generated by the chiral symmetry $\gamma \equiv (1, -1, 1)$. Since γ is unitary, there is only one symmetry type, with $\gamma^2 = \mathbb{1}$.

Type 3 (AIII), γ: There are two one-dimensional irreps $\rho_\pm$ for this type, which are defined by $\gamma = \pm 1$. By Lemma 2.3.10 $\operatorname{tr}\gamma = 0$ is a necessary condition for a representation to be balanced. Moreover, by Lemma 2.3.7, the two irreps are inverses of each other in $\mathbf{I}(\mathsf{S}_3)$. Indeed, $U = i\sigma_x$ is admissible for $\gamma = \sigma_z$ and gapped[10]. Hence, setting $\mathrm{si}(\rho_\pm) = \pm 1$, we get

$$\mathbf{I}(\mathsf{S}_3) = \mathbb{Z} \qquad \mathrm{si}(\rho) = \operatorname{tr}\gamma. \tag{2.47}$$

Groups 4 and 5: are generated by $\tau \equiv (-1, 1, 1)$ and $\sigma_\tau \equiv (-1, 1, -1)$, respectively, which do not single out an invariant point in the spectrum. Hence, there exists no index groups in the above sense. There are two types, corresponding to $\tau^2 = \pm\mathbb{1}$ and $\sigma_\tau^2 = \pm\mathbb{1}$, respectively.

Group 6: is generated by $\eta \equiv (-1, -1, 1)$, which imposes a vertical orbit on the spectrum of an admissible U. There are two types, corresponding to $\eta^2 = \pm\mathbb{1}$.

Type 8 (D), $\eta^2 = \mathbb{1}$: By $\eta^2 = \mathbb{1}$, there is always an invariant basis, with respect to which η acts as the complex conjugation. Hence, there is only one one-dimensional irrep with $\eta = K$. The only admissible unitaries are $U = \pm 1$, which are clearly not gapped. However, combining two copies of the irrep admits the admissible and gapped unitary $U = i\sigma_y$. Hence, the index group and symmetry index are given by

$$\mathbf{I}(\mathsf{S}_8) = \mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 2. \tag{2.48}$$

As already anticipated in Example 2.3.2.

[10] This is not the unitary suggested by Lemma 2.3.7 ($i\sigma_y$), but a unitarily equivalent one. We chose $i\sigma_x$ here because it enables us to directly reuse the present type later for some types of group 10 without changing the generators.

Type 9 (C), $\eta^2 = -\mathbb{1}$**:** Again, there is only one irrep, which is two-dimensional due to $\eta^2 = -\mathbb{1}$. We can choose a basis in which $\eta = i\sigma_y K$. Again, $U = i\sigma_y$ is admissible and gapped. Hence, we conclude

$$\mathbf{I}(\mathsf{S}_9) = 0. \tag{2.49}$$

Group 7 is generated by the two unitary symmetries $\sigma \equiv (1, 1, -1)$ and $\gamma \equiv (1, -1, -1)$, which impose a rectangular orbit on eigenvalues of admissible unitary operators. There are two different types, corresponding to $c(\sigma, \gamma) = \pm 1$ (which we abbreviate by $c_{\sigma\gamma}$ and similarly for the other cases in the following). Depending on this sign, the representation is either abelian, i.e. the irreps are one-dimensional and given by $(\gamma, \sigma) = (\pm 1, \pm 1)$ or the irreps are given by a copy of the Pauli matrices.

Type 10, $c_{\sigma\gamma} = 1$**:** This is the abelian case, where the irreps are characterized by $(\sigma, \gamma) = (\pm 1, \pm 1)$. However, by Lemma 2.3.10, whenever $\operatorname{tr}\sigma \neq 0$, no admissible unitary exists at all. Let π_{ij}, $i, j = \pm$ be the direct sum of two irreps respectively, such that $\sigma = \sigma_z$ for all i, j and i and j denote the respective signs of γ. I.e. in π_{ij} we have $\sigma = \sigma_z$, $\gamma = \operatorname{diag}(i, j)$, and $\sigma_\gamma = \operatorname{diag}(i, -j)$:

ρ	π_{++}	π_{+-}	π_{-+}	π_{--}
γ	$\mathbb{1}$	σ_z	$-\sigma_z$	$-\mathbb{1}$
σ_γ	σ_z	$\mathbb{1}$	$-\mathbb{1}$	$-\sigma_z$

. (2.50)

One readily checks that for each π_{ij} there exists an admissible unitary. However, the representations can nevertheless not be balanced since they are two-dimensional, and we need at least dimension four for a unitary with four gaps to exist.

By Lemma 2.3.10 a necessary condition for an admissible U, which is gapped at ± 1 and $\pm i$ to exists is $\operatorname{tr}\gamma = \operatorname{tr}\sigma_\gamma = 0$. Furthermore, by going through the possible direct sums of building blocks π_{ij}, we verify that this condition is also sufficient. In the following table, the check marks denote that an admissible unitary with gaps at ± 1 and $\pm i$ exists, and the crosses mean that no admissible unitary is gapped:

$\oplus$	π_{++}	π_{+-}	π_{-+}	π_{--}
π_{++}	×	×	×	✓
π_{+-}	×	×	✓	×
π_{-+}	×	✓	×	×
π_{--}	✓	×	×	×

(2.51)

For $\pi_{++} \oplus \pi_{--}$ a possible unitary is given by $U = 1/\sqrt{2}(\mathbb{1} + i\sigma_y) \otimes \sigma_x$, and for $\pi_{+-} \oplus \pi_{-+}$ by $U = 1/\sqrt{2}(i\sigma_z \otimes \sigma_y + \sigma_x \otimes \sigma_x)$. The other two combinations with a check mark are obviously unitarily equivalent to these two cases.

Consequently, the symmetry group is given by

$$\mathbf{I}(\mathsf{S}_{10}) = 2\mathbb{Z} \times 2\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = (\operatorname{tr}\gamma, \operatorname{tr}\sigma_\gamma). \tag{2.52}$$

Type 11, $c_{\sigma\gamma} = -1$**:** There is only one irrep ρ, which is given by the Pauli matrices. Choose, e.g., $\sigma = \sigma_z$ and $\gamma = \sigma_x$. Being two-dimensional, ρ cannot be balanced, since a rectangular orbit without ± 1 and $\pm i$ needs at least four dimensions. But $U = 1/\sqrt{2}(\sigma_x \otimes \sigma_x + i\sigma_y \otimes \sigma_y)$ is admissible for $\rho \oplus \rho$ and gapped at ± 1 and $\pm i$. Hence, the index group is given by

$$\mathbf{I}(\mathsf{S}_{11}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = \dim \rho \bmod 4. \tag{2.53}$$

Group 8 is generated by $\sigma \equiv (1, 1, -1)$ and $\tau \equiv (-1, 1, 1)$. These symmetries do not single out invariant points in the spectrum, wherefore there are no index groups in the sense defined above for the four different symmetry types of this group.

Group 9 is generated by $\sigma \equiv (1, 1, -1)$ and $\eta \equiv (-1, -1, 1)$, which impose a rectangular orbit on the eigenvalues of admissible unitaries. Since there is only one unitary generator, the unitary subgroup is irreducibly represented by $\sigma = \pm 1$. There then are four types, corresponding to $c(\eta, \sigma) = \pm 1$ and $\eta^2 = \pm 1$.

Type 16, $(c_{\sigma\eta}, \eta^2) = (1, \mathbb{1})$**:** Symmetry type 16 is of type one in Lemma 1.5.8. Therefore, the irreps are one-dimensional and can be chosen as $\sigma = \pm 1$ and $\eta = K$, the complex conjugation with respect to the eigenbasis of σ. However, by Lemma 2.3.10, the irreps do not allow for admissible unitaries. There is only one minimal representation π, with $\sigma = \mathrm{diag}(1, -1)$ and $\eta = K$. Being two-dimensional π cannot be balanced, because of the rectangular orbit of admissible eigenvalues under the action of the whole group. $\pi \oplus \pi$ on the other hand is balanced, since $U = 1/\sqrt{2}\left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right) \otimes \sigma_y$ is admissible and gapped at ± 1 and $\pm i$. Consequently, the index group is isomorphic to $\mathbb{Z}_2$. In order to keep track of the fact, that a balanced representation has to be at least four-dimensional, we write it as

$$\mathbf{I}(\mathsf{S}_{16}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = \dim \rho \bmod 4. \tag{2.54}$$

Type 17, $(c_{\sigma\eta}, \eta^2) = (1, -\mathbb{1})$**:** Symmetry type 17 is of type two in Lemma 1.5.8. Hence, σ must be of the form $\sigma = \pm\mathbb{1}$ and, by $\eta^2 = -\mathbb{1}$, $\eta = i\sigma_y$. We denote these two irreps by $\rho_\pm$, where the sign distinguishes the sign of σ. By Lemma 2.3.10, none of the irreps allows for unitaries to exist. Again, the minimal possible representation is given by the direct sum of the two irreps $\pi = \rho_+ \oplus \rho_-$. But in this case π is already balanced, with the same unitary U as for type 16. Consequently:

$$\mathbf{I}(\mathsf{S}_{17}) = 0. \tag{2.55}$$

Type 18, $(c_{\sigma\eta}, \eta^2) = (-1, \mathbb{1})$**:** This type falls under case three in Lemma 1.5.8. Hence, there is only one irrep ρ, with $\sigma = \sigma_z$ and, by $\eta^2 = \mathbb{1}$, $\eta = \sigma_x K$. The irrep allows for admissible unitaries (i.e. $U = \sigma_x$), but since eigenvalue orbits are rectangular, it cannot

be balanced. $\rho \oplus \rho$ on the other hand is balanced, as considering $U = 1/\sqrt{2} \left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right) \otimes \sigma_x$ shows. Similar to type 16, the index group is given by

$$\mathbf{I}(\mathsf{S}_{18}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = \dim \rho \bmod 4. \tag{2.56}$$

Type 19, $(c_{\sigma\eta}, \eta^2) = (-1, -\mathbb{1})$**:** Type 19 is the image of type 18 under φ from Lemma 2.2.11. The gap property at ± 1 and $\pm i$ is invariant under multiplication by i, and therefore the index group is the same. Since the symmetry index is determined from the dimension of the representation, the formula is not affected by φ.

Group 10 is generated by $\gamma \equiv (1, -1, 1)$ and $\tau = (-1, 1, 1)$, which impose a vertical orbit on the eigenvalues of admissible unitaries. The unitary subgroup is represented by $\gamma = \pm 1$ (compare type 3) and there are four types, corresponding to the choices $c(\gamma, \tau) = \pm 1$ and $\tau^2 = \pm\mathbb{1}$.

Type 20 (BDI)**,** $(c_{\gamma\tau}, \tau^2) = (1, \mathbb{1})$**:** Type 20 is of case 1 in Lemma 1.5.8, wherefore its irreps $\rho_\pm$ are one-dimensional, with $\gamma = \pm 1$ and τ acting as the complex conjugation in each irrep. Hence, we can apply the same arguments as for type 3, which again gives

$$\mathbf{I}(\mathsf{S}_{20}) = \mathbb{Z}\,, \qquad \mathrm{si}(\rho) = \mathrm{tr}\,\gamma. \tag{2.57}$$

Type 21 (CII)**,** $(c_{\gamma\tau}, \tau^2) = (1, -\mathbb{1})$**:** For this type γ and τ still commute, but because of $\tau^2 = -\mathbb{1}$ the type falls under case two in Lemma 1.5.8. Therefore, we again get two irreps $\rho_\pm$, which are of dimension 2 and correspond to $\gamma = \pm\mathbb{1}$ with $\tau = i\sigma_y K$ in both cases. However, the arguments of type 3 are still valid and, since $U = i\sigma_x \otimes \mathbb{1}$ is gapped and admissible for $\rho_+ \oplus \rho_-$, $\mathrm{tr}\,\gamma = 0$ is again necessary and sufficient for a representation to be balanced. Hence:

$$\mathbf{I}(\mathsf{S}_{21}) = 2\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = \mathrm{tr}(\gamma). \tag{2.58}$$

Type 22 (CI)**,** $(c_{\gamma\tau}, \tau^2) = (-1, \mathbb{1})$**:** Because γ and τ anti-commute, this type is of case three in Lemma 1.5.8. Hence, there is only one irrep ρ, with $\gamma = \sigma_z$ and $\tau = \sigma_x K$. This is balanced, due to the existence of the gapped and admissible unitary $U = i\sigma_x$. Consequently:

$$\mathbf{I}(\mathsf{S}_{22}) = 0. \tag{2.59}$$

Type 23 (DIII)**,** $(c_{\gamma\tau}, \tau^2) = (-1, -\mathbb{1})$**:** This type is again of case three in Lemma 1.5.8, wherefore there is again only one irrep ρ, with $\gamma = \sigma_z$ and $\tau = i\sigma_y K$. The only admissible unitaries for ρ are $\pm\mathbb{1}$, which are clearly not gapped. Combining two copies of ρ on the other hand, admits the gapped unitary $U = i\sigma_y \otimes \sigma_x$, wherefore we get

$$\mathbf{I}(\mathsf{S}_{23}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 4. \tag{2.60}$$

Group 11 is generated by the two symmetries $\gamma \equiv (1,-1,1)$ and $\sigma_\tau \equiv (-1,1,-1)$, which impose a rectangular orbit on the eigenvalues of admissible unitaries. The symmetry types are distinguished by the two signs $c(\gamma,\sigma_\tau)=\pm 1$ and $\sigma_\tau^2=\pm\mathbb{1}$.

Type 24, $(c_{\gamma\sigma_\tau},\sigma_\tau^2)=(1,\mathbb{1})$**:** The irreps of the unitary subgroup are given by $\gamma=\pm 1$. Since symmetry type 24 is if type one in Lemma 1.5.8, the basis can be chosen such that $\sigma_\tau = K$ is the complex conjugation in each irrep. Because the spectrum of any admissible operator follows a rectangular orbit under the symmetries, no one-dimensional representation allows for any admissible unitary. The same holds for any odd dimension. Hence, similar as for type 10, we define the minimal representations π_{ij}, in which $\gamma=\left(\begin{smallmatrix} i & 0 \\ 0 & j\end{smallmatrix}\right)$ and $\sigma_\tau = K$. It is then straight forward to find admissible unitaries for each π_{ij}. However, being two-dimensional, none of these can be gapped at ± 1 and $\pm i$ simultaneously. The following table shows whether the pairwise direct sums of the π_{ij} are balanced or not.

$\oplus$	π_{++}	π_{+-}	π_{-+}	π_{--}
π_{++}	×	×	×	✓
π_{+-}	×	✓	✓	×
π_{-+}	×	✓	✓	×
π_{--}	✓	×	×	×

(2.61)

Note that since $\pi_{+-}\oplus(\pi_{+-}\oplus\pi_{-+}) \simeq \pi_{-+}\oplus(\pi_{+-}\oplus\pi_{+-})$ are unitarily equivalent, $\pi_{+-}\sim\pi_{-+}$ are equivalent modulo balanced representations. $\operatorname{tr}\gamma = 0$ is still necessary for a representation to be balanced, but because of the considerations above it is not sufficient. Instead, as the table shows, we also need the eigenspaces of γ to be even dimensional. Hence, mapping $\rho\mapsto(\operatorname{tr}\gamma, \dim\ker(\gamma-\mathbb{1}) \bmod 2) = (\operatorname{tr}\gamma, d_\gamma^+ \bmod 2)$ we get

$$\mathbf{I}(\mathsf{S}_{24}) = 2\mathbb{Z}\times\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = \big(\operatorname{tr}\gamma, d_\gamma^+ \bmod 2\big). \tag{2.62}$$

Type 25, $(c_{\gamma\sigma_\tau},\sigma_\tau^2)=(1,-\mathbb{1})$**:** Symmetry type 25 falls under case two in Lemma 1.5.8. Consequently the irreps $\rho_\pm$ are given by $\gamma=\pm\mathbb{1}$ and $\sigma_\tau = i\sigma_y K$. None of the irreps is balanced, due to Lemma 2.3.10. However, the direct sum $\rho=\rho_+\oplus\rho_-$ of the two different irreps admits the admissible unitary $U=1/\sqrt{2}\left(\begin{smallmatrix}\sigma_x & i\cdot\sigma_z \\ i\cdot\sigma_z & -\sigma_x\end{smallmatrix}\right)$, which is gapped at ± 1 and $\pm i$. This renders the index group to be isomorphic to $\mathbb{Z}$ and setting the index map to be $\operatorname{tr}\gamma$, we find

$$\mathbf{I}(\mathsf{S}_{25}) = 2\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = \operatorname{tr}\gamma. \tag{2.63}$$

Type 26, $(c_{\gamma\sigma_\tau},\sigma_\tau^2)=(-1,\mathbb{1})$**:** In symmetry type 26 the antiunitary generator σ_τ anti-commutes with the unitary one (γ). Therefore, it falls under case three in Lemma 1.5.8, leaving only one one irrep ρ, defined by $\gamma=\sigma_z$ and $\sigma_\tau=\sigma_x K$. Since ρ is two-dimensional, it cannot be balanced. However, the sum of two copies $\rho\oplus\rho$ is balanced, because it allows for the admissible unitary $U=1/\sqrt{2}\left(\begin{smallmatrix}0 & \sigma_x - i\cdot\mathbb{1} \\ i\cdot\mathbb{1}-\sigma_x & 0\end{smallmatrix}\right)$. Consequently, the index group is given by

$$\mathbf{I}(\mathsf{S}_{26}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 4. \tag{2.64}$$

Type 27, $(c_{\gamma\sigma_\tau}, \sigma_\tau^2) = (-1, -\mathbb{1})$**:** Type 27 is similar to type 26, with the difference, that the (single) irrep is defined by $\gamma = \sigma_z$ and $\sigma_\tau = i\cdot\sigma_y K$. Again, the sum of two irreps is balanced, which is shown by admissibility of $U = 1/\sqrt{2}\left(\begin{smallmatrix}\sigma_z & -i\cdot\sigma_x \\ -i\cdot\sigma_x & -\sigma_z\end{smallmatrix}\right)$. Therefore, we again get

$$\mathbf{I}(\mathsf{S}_{27}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 4. \tag{2.65}$$

Group 12 is generated by the three symmetries $\gamma \equiv (1, -1, 1)$, $\sigma \equiv (1, 1, -1)$ and $\tau \equiv (-1, 1, 1)$ and therefore contains all possible combinations of the character values (u, r, s), which impose a rectangular orbit on the eigenvalues of admissible unitaries. The symmetry types are distinguished by the four signs $c(\sigma, \gamma)$, $c(\sigma, \tau)$ $c(\gamma, \tau)$ and τ^2. The first eight types $(28 - 35)$ contain an abelian unitary subgroup. Therefore, we can start the considerations with one of the previous types and add σ or τ appropriately, by multiplying the dimension if needed. For the remaining types $(36 - 43)$ the unitary subgroup exhibits two anti-commuting generators, wherefore the unitary irreps are always given by a copy of the Pauli matrices. We choose this as $\sigma = \sigma_z$ and $\gamma = \sigma_x$. The representation ρ of the whole type is then always unique (up to equivalence) and can be obtained by adding τ appropriately, again by multiplying the dimension if necessary.

Type 28, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, 1, 1, \mathbb{1})$**:** Type 28 falls under case one in Lemma 1.5.8. Therefore, we can tread it exactly as type 10, with an additional antiunitary generator. It is the simplest to choose $\eta = \gamma\tau = K$ as the complex conjugation, which yields $\tau = \gamma\eta = \gamma K$. Since the gapped admissible unitaries we considered for type 10 are real, they remain admissible also in this case, wherefore we again get

$$\mathbf{I}(\mathsf{S}_{28}) = 2\mathbb{Z} \times 2\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = (\mathrm{tr}\,\gamma, \mathrm{tr}\,\sigma_\gamma). \tag{2.66}$$

Type 29, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, 1, 1, -\mathbb{1})$**:** This type is an example of case two in Lemma 1.5.8. We can again start with the considerations for type 10 and double the dimension for each representation in order to add τ. The specific realizations for σ and γ can be obtained from those for type 10 via $(\sigma, \gamma) \mapsto (\sigma \otimes \mathbb{1}_2, \gamma \otimes \mathbb{1}_2)$ and we set $\tau = (\gamma \otimes i\sigma_y)K$. We can then again use the same admissible gapped unitaries as before, to construct unitaries for this type via $U_i \mapsto U_i \otimes \mathbb{1}_2$. This gives

$$\mathbf{I}(\mathsf{S}_{29}) = 4\mathbb{Z} \times 4\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = (\mathrm{tr}\,\gamma, \mathrm{tr}\,\sigma_\gamma). \tag{2.67}$$

Type 30, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, 1, -1, \mathbb{1})$**:** Type 30 is similar to type 22 (CI), (with the unique irrep $\gamma = \sigma_z$ and $\tau = \sigma_x K$), with an additional generator σ. By $c_{\sigma\gamma} = c_{\sigma\tau} = 1$ this additional generator can only be represented by $\sigma = \pm\mathbb{1}$, resulting in two inequivalent irreps $\rho_\pm$. However, by Lemma 2.3.10, the minimal representation admitting admissible unitaries is $\rho = \rho_+ \oplus \rho_-$, with $\gamma = \mathbb{1} \otimes \sigma_z$, $\tau = (\mathbb{1} \otimes \sigma_x)K$ and $\sigma = \sigma_z \otimes \mathbb{1}$. For ρ we find the admissible gapped unitary $U = 1/\sqrt{2}\left(\sigma_x \otimes \left(\begin{smallmatrix}1 & -1 \\ 1 & 1\end{smallmatrix}\right)\right)$. Consequently, we get

$$\mathbf{I}(\mathsf{S}_{30}) = 0. \tag{2.68}$$

Type 31, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, 1, -1, -\mathbb{1})$**:** Type 31 contains type 23 (DIII), which has only one irrep with $\gamma = \sigma_z$ and $\tau = i\sigma_y K$. By $c_{\sigma\gamma} = c_{\sigma\tau} = 1$, we can simply add $\sigma = \pm\mathbb{1}$, resulting in two irreps $\rho_\pm$. However, by Lemma 2.3.10, these do not allow for any admissible unitaries, wherefore we get one minimal representation via $\rho = \rho_+ \oplus \rho_-$, with $\sigma = \sigma_z \otimes \mathbb{1}$, $\gamma = \mathbb{1} \otimes \sigma_z$ and $\tau = (\mathbb{1} \otimes i\sigma_y)K$. By Lemma 2.3.10, ρ is not balanced, since $2 \cdot |\mathcal{O}(S)| = 8$. For $\rho \oplus \rho$, on the other hand, we certainly find an admissible and gapped unitary. Indeed, note that $\rho_- = s \cdot \rho_+$ and $\sigma_x \rho_\pm \sigma_x = ur \cdot \rho_\pm$. Hence, $\rho \oplus \rho = \rho_+ \oplus \rho_- \oplus \rho_+ \oplus \rho_-$ is unitarily equivalent to $\rho_+ \oplus (ur \cdot \rho_+) \oplus (ur \cdot s \cdot \rho_+) \oplus (s \cdot \rho_+)$, which is balanced for any choice of ρ_+, by the arguments given in the proof of Lemma 2.3.7. We get

$$\mathbf{I}(\mathsf{S}_{31}) = 4\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 8. \tag{2.69}$$

Type 32, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, -1, 1, \mathbb{1})$**:** Starting with type 20 (BDI) (with the one-dimensional irreps $\gamma = \pm 1$, $\tau = K$) we need to add σ, such that $c_{\sigma\gamma} = -c_{\sigma\tau} = 1$. Since type 32 falls under case three in Lemma 1.5.8, we get the two irreps $\rho_\pm$ with $\sigma = \sigma_z$, $\gamma = \pm\mathbb{1}$ and $\tau = \sigma_x K$. By Lemma 2.3.10 these cannot be balanced ($\mathrm{tr}\,\gamma \neq 0$). Their sum $\rho = \rho_+ \oplus \rho_-$ on the other hand admits the gapped unitary $U = 1/\sqrt{2}\left(\begin{smallmatrix} 1 & i \\ i & 1 \end{smallmatrix}\right) \otimes \sigma_x$, which yields

$$\mathbf{I}(\mathsf{S}_{32}) = 2\mathbb{Z}\,, \qquad \mathrm{si}(\rho) = \mathrm{tr}\,\gamma. \tag{2.70}$$

Type 33, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, -1, 1, -\mathbb{1})$**:** For this type we will make use of two previous types. On the one hand, type 33 contains type 24 and on the other type 21 (CII). The latter has two inequivalent irreps given by $\gamma = \pm\mathbb{1}$ and $\tau = i\sigma_y K$. We need to add σ, such that $c_{\sigma\gamma} = -c_{\sigma\tau} = 1$. This can be done by choosing $\sigma = \sigma_z$ (or σ_x, which would result in a unitarily equivalent irrep), yielding the two irreps $\rho_\pm$. However, similar to case 24, these irreps do not allow for any admissible unitaries: Admissibility for σ and γ forces any admissible unitary to be of the form $U = \mu\sigma_x + \nu\sigma_y$, for appropriate $\mu, \nu \in \mathbb{R}$. But on such unitaries τ would impose the condition $U = -U$. From this we can also conclude that the same holds for any sum of an odd number of irreps. Indeed, this would imply a two-dimensional subspace, of the $\pm 1/\pm i$ eigenspaces of U, carrying an irrep and we get the same contradiction as above. Instead, similar to type 24, we define minimal representations π_{ij} via $\sigma = \mathbb{1} \otimes \sigma_z$, $\gamma = \left(\begin{smallmatrix} i & 0 \\ 0 & j \end{smallmatrix}\right) \otimes \mathbb{1}$ and $\tau = (\mathbb{1} \otimes i\sigma_y)K$, none of which can be balanced due to $\tau^2 = -\mathbb{1}$ and $2 \cdot |\mathcal{O}(S)| = 8$. In fact, the consideration from type 24 directly transfer to this case and we get the same combination table as before (see (2.61)), with the only difference, that the dimensions of the involved representations are doubled. Consequently, we get

$$\mathbf{I}(\mathsf{S}_{33}) = 4\mathbb{Z} \times 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = \left(\mathrm{tr}\,\gamma, d_\gamma^+ \bmod 4\right). \tag{2.71}$$

Types 34 and 35, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (1, -1, -1, \mathbb{1})$ **and** $(1, -1, -1, -\mathbb{1})$**:** Type 34 and 35 are the images of type 32 and 33 under φ from Lemma 2.2.11, respectively. Since the gap property at ± 1 and $\pm i$ is invariant under multiplication by i, the index groups are the same. In the formulas for the symmetry index γ has to be replaced by $\varphi(\gamma) = \sigma_\gamma$.

Type 36, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, 1, 1, \mathbb{1})$**:** Type 36 falls under case one in Lemma 1.5.8, wherefore τ can simply be added to the unitary irrep. We get ρ via $\sigma = \sigma_z$, $\gamma = \sigma_x$ and $\tau = K$. Being two-dimensional, ρ cannot be balanced, but for $\rho \oplus \rho$ we find the admissible gapped unitary $U = 1\sqrt{2}(\sigma_z \otimes \sigma_x + i\sigma_y \otimes \sigma_y)$. Hence, we get

$$\mathbf{I}(\mathsf{S}_{36}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 4. \tag{2.72}$$

Type 37, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, 1, 1, -\mathbb{1})$**:** Adding τ to the unitary subgroup, we find that type 37 is of case two in Lemma 1.5.8. Hence, we get one irrep ρ with $\sigma = \mathbb{1} \otimes \sigma_z$, $\gamma = \mathbb{1} \otimes \sigma_x$ and $\tau = i\sigma_y \otimes \mathbb{1}$. ρ is four-dimensional and by Lemma 2.3.10, it cannot be balanced ($2 \cdot |\mathcal{O}(S)| = 8$). For two copies $\rho \oplus \rho$, on the other hand, we find the unitary $U = 1/\sqrt{2}(\sigma_y \otimes \sigma_y \otimes \sigma_x + i \cdot \mathbb{1} \otimes \sigma_z \otimes \sigma_y)$, which is admissible and gapped. Consequently, we get

$$\mathbf{I}(\mathsf{S}_{37}) = 4\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 8. \tag{2.73}$$

Types 38 and 39, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, 1, -1, \mathbb{1})$ **and** $(-1, 1, -1, -\mathbb{1})$**:** Type 38 and 39 are the images of type 36 and 37 under φ from Lemma 2.2.11, respectively. The gap property at ± 1 and $\pm i$ is invariant under multiplication by i, and therefore index groups are the same. Since the symmetry indices are determined from the dimensions of the representation, the formulas are not affected by φ.

Type 40, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, -1, 1, \mathbb{1})$**:** Type 40 is of case one in Lemma 1.5.8, wherefore we can simply add $\tau = \sigma_x K$ to the irrep of the unitary subgroup without doubling the dimension. Being two-dimensional ρ is not balanced. $\rho \oplus \rho$, on the other hand, admits the gapped unitary $U = 1/\sqrt{2}(\sigma_x \otimes \sigma_x + i\sigma_z \otimes \sigma_y)$, which yields

$$\mathbf{I}(\mathsf{S}_{40}) = 2\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 4. \tag{2.74}$$

Type 41, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, -1, 1, -\mathbb{1})$**:** Type 41 is similar to type 37. Here, the irrep ρ can be chosen as $\sigma = \mathbb{1} \otimes \sigma_z$, $\gamma = \mathbb{1} \otimes \sigma_x$ and $\tau = (i\sigma_y \otimes \sigma_x)K$, and is again not balanced. For $\rho \oplus \rho$ we find the gapped unitary $U = 1/2\left[\left(\begin{smallmatrix} 1 & 1 \\ 1 & -1 \end{smallmatrix}\right) \otimes \mathbb{1} \otimes \sigma_x + \left(\begin{smallmatrix} -1 & 1 \\ 1 & 1 \end{smallmatrix}\right) \otimes \mathbb{1} \otimes \sigma_y\right]$ and we get

$$\mathbf{I}(\mathsf{S}_{41}) = 4\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 8. \tag{2.75}$$

Type 42, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, -1, -1, \mathbb{1})$**:** Type 42 is an example of case two in Lemma 1.5.8. Hence, the dimension doubles and we find an irrep by setting $\sigma = \mathbb{1} \otimes \sigma_z$, $\gamma = \mathbb{1} \otimes \sigma_x$ and $\tau = (\sigma_y \otimes \sigma_y)K$. Since $\tau^2 = \mathbb{1}$, τ does not enforce a dimensional restriction for the representation to be balanced. In fact, the irrep is already balanced, since there exists the admissible and gapped unitary $U = 1/\sqrt{2}\left(\begin{smallmatrix} i\sigma_y & \sigma_x \\ \sigma_x & -i\sigma_y \end{smallmatrix}\right)$. Consequently:

$$\mathbf{I}(\mathsf{S}_{42}) = 0. \tag{2.76}$$

Type 43, $(c_{\sigma\gamma}, c_{\sigma\tau}, c_{\gamma\tau}, \tau^2) = (-1, -1, -1, -\mathbb{1})$**:** This last type is an example of case one in Lemma 1.5.8. Hence, we can simply add τ to the irrep of the unitary subgroup without doubling the dimension. The irrep ρ is given by $\sigma = \sigma_z$, $\gamma = \sigma_x$ and $\tau = (i\sigma_y)K$. However, since $\tau^2 = -\mathbb{1}$ forces each eigenspace of admissible unitaries to be of even degeneracy and every unitary has to have at least two eigenspaces (± 1 or $\pm i$), there are no admissible unitaries for this irrep. Hence, the minimal representation is given by $\rho \oplus \rho$. Being four-dimensional, this representation cannot be balanced ($2 \cdot |\mathcal{O}(S)| = 8$) but there exists the admissible unitary $U = \sigma_y \otimes \sigma_x$. Doubling the dimension once more allows for the admissible and gapped unitary $U = 1/\sqrt{2}(\sigma_y \otimes \sigma_x \otimes \sigma_x + i(\mathbb{1} \otimes \sigma_y \otimes \sigma_y))$, wherefore we get

$$\mathbf{I}(\mathsf{S}_{43}) = 4\mathbb{Z}_2\,, \qquad \mathrm{si}(\rho) = d \bmod 8. \tag{2.77}$$

Groups 13,14,15, and 16 are the images of the groups 3,6,10, and 11 under φ from Lemma 2.2.11, respectively. The index groups of their corresponding types are therefore isomorphic. Note that while the groups 3,6, and 10 impose vertical eigenvalue orbits on admissible operators, the corresponding orbits for the groups 13, 14, and 15 are horizontal. The symmetry index therefore corresponds to unitaries that are gapped at $\pm i$ instead of ± 1. Group 16 on the other hand imposes a box-orbit on admissible unitaries, which is invariant under φ. The index formulas are the same, with γ replaced by $\varphi(\gamma) = \sigma_\gamma$ if present.

2.3.2 Index table

Table 2.1 lists all symmetry types without redundant symmetries and collects the results of the preceding and some subsequent sections. Let us go thought the content and describe the content in the columns:

- The defining properties of the symmetry types are shown in the central two columns. In phase convention II a type is uniquely determined by the signs of the squares of the representing operators ρ_g^2 (see Lemma 2.1.7).
- The symmetry types S are numbered in the second column and are organized in the respective symmetry groups G, shown in the first column, where also the respective action on the spectrum of admissible operators is indicated (via $\swarrow, \downarrow, \square, \leftarrow$). If applicable, the corresponding names in the Cartan classification are given in the fifth column.
- The third column contains the images $\varphi(\mathsf{S})$ under the isomorphism induced by $U \mapsto iU$ (see Lemma 2.2.11), where a blank entry stands for $\varphi(\mathsf{S}) = \mathsf{S}$. In case of $\varphi(\mathsf{S}) \neq \mathsf{S}$, the isomorphic partner which appears second is greyed out to indicate the redundancy.
- The fourth column contains the corresponding perturbation symmetry type, again with $\widetilde{\mathsf{S}} = \mathsf{S}$ for the missing entries (see Section 3.2).

G	S	φ(S)	$\widetilde{\text{S}}$		$u(g)$ $r(g)$ $s(g)$	1 1 -1	1 -1 1	1 -1 -1	-1 1 1	-1 1 -1	-1 -1 1	-1 -1 -1	**I**(S)	si	Decoupling condition
						σ	γ	σ_γ	τ	σ_τ	η	σ_η			
1	1			A											
2: ↙	2					+									$d_{10}^{\pm} = d_{01}^{\pm}$
3: ↓	3	44		AIII			+						$\mathbb{Z}$	$\operatorname{tr}\gamma$	
4	4			AI					+						
	5			AII					-						$d_{10} = 0 \bmod 2$
5: ↙	6		7							+					
	7		6							-					$d_{10} = 0 \bmod 2$
6: ↓	8	45		D							+		$\mathbb{Z}_2$	$d \bmod 2$	
	9	46		C							-		0		
7: □	10		11			+	+	+					$2\mathbb{Z} \times 2\mathbb{Z}$	$(\operatorname{tr}\gamma, \operatorname{tr}\sigma_\gamma)$	
	11		10			+	+	-					$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10}^{\pm} = d_{01}^{\pm}$
8: ↙	12		14			+			+	+					
	13		15			+			-	-					$d_{10}^{\pm} = 0 \bmod 2$
	14		12			+			+	-					$d_{10}^{\pm} = d_{01}^{\pm}$
	15		13			+			-	+					$d_{10}^{\pm} = d_{01}^{\pm}$
9: □	16					+					+	+	$2\mathbb{Z}_2{}^{*}$	$d \bmod 4$	$d_{10}^{\pm} = d_{01}^{\pm}$
	17					+					-	-	$0^{\dagger}$		$d_{10}^{\pm} = d_{01}^{\pm}$
	18	19				+					+	-	$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10}^{\pm} = d_{01}^{\pm}$
	19	18				+					-	+	$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10}^{\pm} = d_{01}^{\pm}$
10: ↓	20	47		BDI			+		+		+		$\mathbb{Z}$	$\operatorname{tr}\gamma$	
	21	48		CII			+		-		-		$2\mathbb{Z}$	$\operatorname{tr}\gamma$	
	22	49		CI			+		+		-		0		
	23	50		DIII			+		-		+		$2\mathbb{Z}_2$	$d \bmod 4$	
11: □	24	51	27				+			+		+	$2\mathbb{Z} \times \mathbb{Z}_2{}^{**}$	$(\operatorname{tr}\gamma, d_\gamma^+ \bmod 2)$	
	25	52	26				+			-		-	$2\mathbb{Z}$	$\operatorname{tr}\gamma$	
	26	53	25				+			+		-	$2\mathbb{Z}_2$	$d \bmod 4$	
	27	54	24				+			-		+	$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10} = 0 \bmod 2$
12: □	28		40			+	+	+	+	+	+	+	$2\mathbb{Z} \times 2\mathbb{Z}$	$(\operatorname{tr}\gamma, \operatorname{tr}\sigma_\gamma)$	
	29		41			+	+	+	-	-	-	-	$4\mathbb{Z} \times 4\mathbb{Z}$	$(\operatorname{tr}\gamma, \operatorname{tr}\sigma_\gamma)$	
	30		42			+	+	+	+	+	-	-	$0^{\dagger}$		
	31		43			+	+	+	-	-	+	+	$4\mathbb{Z}_2{}^{\dagger}$	$d \bmod 8$	$d_{10}^{\pm} = 0 \bmod 2$
	32	34	36			+	+	+	+	-	+	-	$2\mathbb{Z}$	$\operatorname{tr}\gamma$	
	33	35	37			+	+	+	-	+	-	+	$4\mathbb{Z} \times 2\mathbb{Z}_2{}^{\ddagger}$	$(\operatorname{tr}\gamma, d_\gamma^+ \bmod 4)$	
	34	32	38			+	+	+	+	-	-	+	$2\mathbb{Z}$	$\operatorname{tr}\sigma_\gamma$	
	35	33	39			+	+	+	-	+	+	-	$4\mathbb{Z} \times 2\mathbb{Z}_2{}^{\ddagger}$	$(\operatorname{tr}\sigma_\gamma, d_{\sigma_\gamma}^+ \bmod 4)$	
	36	38	32			+	+	-	+	+	+	-	$2\mathbb{Z}_2$	$d \bmod 4$	
	37	39	33			+	+	-	-	-	-	+	$4\mathbb{Z}_2$	$d \bmod 8$	$d_{10}^{\pm} = 0 \bmod 2$
	38	36	34			+	+	-	+	+	-	+	$2\mathbb{Z}_2$	$d \bmod 4$	
	39	37	35			+	+	-	-	-	+	-	$4\mathbb{Z}_2$	$d \bmod 8$	$d_{10}^{\pm} = 0 \bmod 2$
	40		28			+	+	-	+	-	+	+	$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10}^{\pm} = d_{01}^{\pm}$
	41		29			+	+	-	-	+	-	-	$4\mathbb{Z}_2$	$d \bmod 8$	$d_{10}^{\pm} = d_{01}^{\pm}$
	42		30			+	+	-	+	-	-	-	0		$d_{10}^{\pm} = d_{01}^{\pm}$
	43		31			+	+	-	-	+	+	+	$4\mathbb{Z}_2{}^{\ddagger}$	$d \bmod 8$	$d_{10}^{\pm} = d_{01}^{\pm}$
13: ←	44	3						+					$\mathbb{Z}$	$\operatorname{tr}\sigma_\gamma$	
14: ←	45	8										+	$\mathbb{Z}_2$	$d \bmod 2$	
	46	9										-	0		
15: ←	47	20						+	+			+	$\mathbb{Z}$	$\operatorname{tr}\sigma_\gamma$	
	48	21						+	-			-	$2\mathbb{Z}$	$\operatorname{tr}\sigma_\gamma$	
	49	22						+	+			-	0		
	50	23						+	-			+	$2\mathbb{Z}_2$	$d \bmod 4$	
16: □	51	24	54					+		+	+		$2\mathbb{Z} \times \mathbb{Z}_2{}^{**}$	$(\operatorname{tr}\sigma_\gamma, d_{\sigma_\gamma}^+ \bmod 2)$	
	52	25	53					+		-	-		$2\mathbb{Z}$	$\operatorname{tr}\sigma_\gamma$	
	53	26	52					+		+	-		$2\mathbb{Z}_2$	$d \bmod 4$	
	54	27	51					+		-	+		$2\mathbb{Z}_2$	$d \bmod 4$	$d_{10} = 0 \bmod 2$

Table 2.1: List of all non-redundant symmetry types for unitary operators. The list collects the results from the previous sections (in particular Section 2.3.1) and also some results of Section 3.2 and Section 3.5. The contents of the table are described in detail in Section 2.3.2.

- The third column from the right contains the index groups for each symmetry type (see Section 2.3.1). Thereby, the index group is computed with respect to the gap condition, which fits the action of the respective group $(\swarrow, \downarrow, \square, \leftarrow)$. The groups which do not single out symmetry protected parts of the spectrum and therefore do not allow for an index group in our sense are left blank.

  In consequence of Assumption 2.3.9 the index groups are for representations which allow for admissible unitaries. If we drop this assumption and also consider representations as building blocks, for which this is not true, some index groups change. For the types which are affected, the index group changes are

$$\begin{aligned} * &: \mathbf{I}(\mathsf{S}) \mapsto \mathbb{Z} \times \mathbf{I}(\mathsf{S}) & \dagger &: \mathbf{I}(\mathsf{S}) \mapsto 2\mathbb{Z} \times \mathbf{I}(\mathsf{S}) \\ ** &: 2\mathbb{Z} \times \mathbb{Z}_2 \mapsto \mathbb{Z} \times \mathbb{Z}_2 & \ddagger &: \mathbf{I}(\mathsf{S}) \mapsto 2\mathbb{Z}_2 \times \mathbf{I}(\mathsf{S}). \end{aligned} \tag{2.78}$$

- The corresponding symmetry index formula is given in the second column from the right. Thereby $d^{\pm}_{\rho_g}$ refers to the dimension of the ± 1 eigenspace of ρ_g, whereas d denotes the overall dimension of the representation.

- The last column contains the decoupling condition one needs on top of $\vec{\mathrm{ind}}\,(U) = 0$, in order to decouple an admissible walk U (see Section 3.5). Thereby d_{ij} denotes $\dim \mathcal{H}_{ij}$ (see (3.70) in Section 3.3 and Section 3.5) and $d^{\pm}_{ij}$ refers to the dimension of the ± 1 eigenspace of σ on $\mathcal{H}_{ij}$. Empty cells denote that $\vec{\mathrm{ind}}\,(U) = 0$ is already sufficient for a decoupling to exist.

  Note that for decoupling a system of type S, the decoupling condition for the corresponding perturbation type S has to be met. E.g. type 10 has perturbation symmetry type 11, which needs an extra decoupling condition. Hence, for walks of type 10, there does not always exist a decoupling.

3 Topological classification of symmetric quantum walks

Topological classification in physics is driven by the desire to reduce a given physical system to its most fundamental characteristics. Framing the arena with a set of physical and mathematical assumptions, such as the underlying spatial structure and the locality properties imprinted by it, a symmetry type, and a class of possible deformations of a system, the task is to pin down the differences in such systems and to find unique labels for the different classes emerging from the set of assumptions. Besides mathematical curiosity, there are also physical and even practical motivations. Choosing the set of assumptions in the right way allows for describing and predicting phenomena such as topologically protected edge states in samples of specific materials or artificially engineered systems. The fact that such phenomena arise in consequence of a topological classification based on minimal physical assumptions, such as locality and symmetries, results in remarkable stability properties under the classes of allowed deformations entering the theory, including local perturbations of a large sample or continuously driven global deformations as well as global disorder of the system.

The archetypical example of a topological phenomenon in condensed-matter physics, which opened up the whole field of of topological insulators and superconductors, was the **integer quantum Hall effect**, first observed by von Klitzing et al. in 1980 [KDP80]. In the experiment, Klitzinger et al. placed an effectively two-dimensional semiconductor (more specifically a MOSFET [1]) into a strong transverse magnetic field at low temperature. They observed that the conductivity perpendicular to the gate field and the magnetic field is quantized as a function of the magnetic field strength. Remarkably, the conductivity does not depend on the exact geometry of the sample but solely on the magnetic field strength. Alongside the quantized values of the conductivity, precisely this property singles out a topological phenomenon. Soon after the first observation, theoretical explanations for the integer quantum Hall effect followed [Lau81, AA81, Hal82, TKNdN82].

The quantization of the Hall conductance was explained in two fundamentally different ways. On the one hand, the conductance can be expressed via the (integer-valued) Chern number of the energy bands in an infinite system, i.e. via a bulk-invariant [TKNdN82]. On the other hand, based on an argument by Laughlin [Lau81], it can be expressed by the winding of the edge-state energy in a system exhibiting a one-

[1] Metal-oxide-semiconductor field effect transistor.

dimensional edge [Hal82, Hat93b]. The fact that these two ways of describing the phenomenon coincide [Hat93a, Hat97] became one of the core principles in the topological description of matter: **Bulk-boundary correspondence**. Turning around the line of reasoning, bulk-boundary correspondence has a remarkable consequence: the boundary of a topologically non-trivial sample exhibits topologically protected edge states.

The systems exhibiting the integer quantum Hall effect fall under symmetry type A in the tenfold way[2], i.e. the corresponding Hamiltonian has no non-redundant involutive symmetries in the sense of Chapter 2. In particular, the external magnetic field breaks time-reversal symmetry. In the 2000s, Kane and Mele predicted a $\mathbb{Z}_2$ valued invariant in two-dimensional systems without an external magnetic field and therefore with restored time-reversal symmetry [KM05b, KM05a]. These systems fall under class AII in the tenfold way, which, in two dimensions, indeed exhibits the index group $\mathbb{Z}_2$. These so-called **quantum spin Hall systems** were experimentally observed soon after their prediction by König et al. [KWB$^+$07], and also transferred to three-dimensional settings [Roy09]. For two-dimensional systems, bulk-boundary correspondence also holds and was rigorously analysed and proven in [GP13] for quantum spin Hall systems and for Floquet topological insulators in [GT18].

Driven by the discoveries recapped above, the search for topologically non-trivial phases of matter became an essential task in the condensed matter community (see, e.g. the reviews [HK10, QZ11] and references therein). In particular, the search was extended to all symmetry types of the tenfold way [SRFL08]. This finally lead to the discovery of the well-known **periodic table of topological insulators and superconductors** by Kitaev [Kit09] (see also [SRFL09, RSFL10, KZ15]), which unveiled the deep connection between the topological phases of matter and the tenfold way. The periodic table lists all symmetry types and assigns the respective index groups in all spatial dimensions, where $0 \leq d \leq 7$ are enough, due to Bott periodicity [Kit09]. The table contains the respective index group for each symmetry type, labelling the different possible phases of matter.

Usually, the invariants like Chern- and edge-energy winding numbers are defined over the Brillouin zone of the system, i.e. they are only well defined in case of translation invariance. On this footing, it is problematic to rigorously prove, e.g. invariance of the topological phenomena under disorder or generally any perturbation braking translation invariance. Beginning with work by Bellissard et al. [BvES94], more and more advanced techniques such as non-commutative geometry, e.g. K-theory, entered the discussion [BvES94, FM13, Thi16, SB16, GSB16]. Kitaevs work on the periodic table is also built on K-theoretic arguments. For an overview of K-theoretic methods for topological insulators and superconductors, we recommend the book by Prodan and Schulz-Baldes [PSB16].

In recent years **quantum walks** and **periodically driven systems** sparked interest in the community of topological phases of matter for simulation and model building and as topologically non-trivial systems in their own right. The topological classification of quantum walks originates in [GNVW12], where the authors completely classify discrete-time quantum walks on the one-dimensional lattice, i.e. unitaries with finite

[2]Note that the integer quantum Hall effect occurs in two-dimensional systems, for which A has a non-trivial index group (see, e.g. [RSFL10]).

interaction length. They show that the connected components with respect to norm-continuous deformations in the set of such finite interaction length unitaries are labelled by a $\mathbb{Z}$-valued index, measuring the net information flow across any possible splitting of the one-dimensional line [Kit06]. They also show the converse, i.e. that two such unitaries with the same index can always be deformed into each other on a norm-continuous path. However, no further assumptions beyond the finite interaction length, such as discrete symmetries or a protocol like structure, enter the discussion in [GNVW12].

The first steps into the direction of the topological classification of symmetric quantum walks from the perspective of topological insulators were done by Kitagawa et al. [KRBD10, KBF$^+$12], who showed that quantum walks provide a versatile platform for topologically non-trivial models for all symmetry types of the tenfold way. In [KRBD10], the authors consider different quantum walk models, such as the simple coined quantum walk $U(\theta)$ or the split-step quantum walk $U_{ss}(\theta_1, \theta_2)$, both defined on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ via

$$U_{ss}(\theta_1, \theta_2) = S_\downarrow R(\theta_2) S_\uparrow R(\theta_1) \qquad \text{and} \qquad U(\theta) = U_{ss}(\theta, 0), \tag{3.1}$$

where $S_\uparrow$ ($S_\downarrow$) shifts the $(1,0)^T$ ($(0,1)^T$) component at each $x \in \mathbb{Z}$ one cell to the right (left), and $R(\theta) = \mathbb{1} \otimes \exp(-i\theta\sigma_y)$ denotes the cell-wise σ_y-rotation by θ (see also Example 1.4.6). The walks are particle-hole symmetric with η being the complex conjugation with respect to the standard positional basis, and chiral symmetric with the (θ_1 dependent[3]) chiral symmetry γ with $\gamma^2 = \mathbb{1}$. This renders the walks to be admissible for symmetry type BDI. The walk unitaries are then analysed via their effective Hamiltonians, i.e. a Hermitian operator H_{eff} fulfilling the relation

$$U_{ss}(\theta_1, \theta_2) = e^{-iH_{eff}(\theta_1, \theta_2)}, \tag{3.2}$$

where we set $\Delta t = 1$. Fourier transformation on the first tensor factor ($\mathcal{F}\colon \ell^2(\mathbb{Z}) \to \mathcal{L}(\mathbb{T})$) yields

$$H_{eff}(\theta_1, \theta_2) = \int_{-\pi}^{\pi} dk |k\rangle\langle k| \otimes \left[E_{\theta_1\theta_2}(k) \boldsymbol{\sigma} \cdot \mathbf{n}_{\theta_1\theta_2}(k) \right], \tag{3.3}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ denotes the vector of Pauli-matrices, $E_{\theta_1\theta_2}(k)$ denotes the quasi-energy, and $\mathbf{n}_{\theta_1\theta_2}(k)$ "defines the quantization axis for the spinor eigenstates at each momentum k" [KRBD10]. H_{eff} inherits the symmetry conditions from U_{ss}, which implies that $\mathbf{n}_{\theta_1\theta_2}(k)$ always rotates on a θ_1 dependent great circle on the unit sphere, perpendicular to the quantization axis of the spinor eigenstate of the chiral symmetry. Kitagawa et al. identify the winding of $\mathbf{n}_{\theta_1\theta_2}(k)$ around this great circle as a classifying integer-valued invariant for the split-step quantum walk[4]. In analogy to Hamiltonian systems and confirmed by numerical simulations of finite systems, the authors predict topologically protected edge states at the boundary between bulks of different topological phases in the sense of this winding number.

[3] This θ_1 dependence of the chiral symmetry can be eliminated via a simple base-change by $\{\psi\} \mapsto \{R(\theta_1/2)\psi\}$ in each cell.

[4] Note that Kitagawa et al. only consider the absolute value of the winding number, without taking into account the sign.

Soon after the first publications in this direction, further techniques were developed, which unveiled the rich topological structure of symmetric quantum walks and its effects on the behaviour of such systems [Kit12, Asb12, AO13, ATD14, OANK15, CMM+16]. As discussed in the previous chapter, the symmetries single out two points in the spectrum of admissible unitaries, opposed to only one in case of Hermitian operators. These give room for a finer structure of symmetry protected eigenstates of admissible operators [Kit12, Asb12]. Moreover, Asbóth et al. found that there is an important difference between quantum walks, considered as a single time-step unitary without "remembering" the protocol between time-steps, and driven systems, driven either discretely or continuously in time, as they are often considered in the literature [AO13, ATD14]. In particular, for the split-step walk, they took both **timeframes** into account

$$U_{ss}(\theta_1,\theta_2) = \big[S_\downarrow R(\theta_2)\big]\big[S_\uparrow R(\theta_1)\big] \qquad \text{and} \qquad \widetilde{U}_{ss}(\theta_1,\theta_2) = \big[S_\uparrow R(\theta_1)\big]\big[S_\downarrow R(\theta_2)\big], \quad (3.4)$$

which unveiled more details about the topological properties of the protocol itself and not just the one-step unitary[5].

Topological aspects of symmetric quantum walks also lead to numerous experiments and experimental proposals, exhibiting the effects of the topological nature of the effective system underlying the experimental realization. These realizations and proposals include photonic quantum walks, where the state is represented by single photons in optical waveguides [KBF+12, ZXB+17, XZB+17], single-atom implementations, where actual atoms in an optical lattice represent the quantum state [GBA+16, MCM+16, RAA17, SAM+19], implementations via superconducting qubits [RFR+17, FRHG+17, BCS18], and time-multiplexed setups, where the state of the quantum walk on the lattice is represented by a chain of laser pulses in an optical fibre loop [BNE+17, BLN+18, CDQ+18, NGS+19].

We stress, however, that the works mentioned above do not aim for a topological classification in the spirit of [GNVW12], i.e. of a whole class of systems falling under some given set of assumptions. Most works concentrate on finding the existing topological classes of matter from common knowledge in quantum walk models or on unveiling topological invariants of a specific model at hand. The major distinguishing aspect of our work [CGS+16, CGG+18, CGS+18, CGG+21, CGWW21] is that we follow the general ansatz of [GNVW12] in order to provide a fundamental classification of a large class of models, with as few assumptions as possible.

Quite recently, various works on the topological classification of non-Hermitian systems subject to the Bernard-LeClair symmetry classes have been published [KSUS19, ZL19, LC19]. While being of much interest in their own right, the considerations there are not applicable for our goal of a topological classification of quantum walk, i.e. symmetric unitaries.

Besides the fact that we here consider unitary or at least essentially unitary operators, the main difference to the work mentioned above lies in the the gap condition. As discussed in Section 2.3, the gap condition plays a crucial role in our definition of the equivalence classes of finite-dimensional representations of the symmetry types.

[5] See Chapter 5 for a detailed discussion of such systems.

Following the considerations there, our goal is to characterize the symmetry protected subspaces of operators on possibly infinite-dimensional space. For this, we assume an essential gap at the symmetry protected eigenspaces, i.e. at $+1$ and -1 or ± 1 and $\pm i$ together, respectively. As we will deduce, an eigenspace carries a symmetry protected subspace, if and only if the eigenspace carries a non-trivial representation of the symmetry type in the sense of the previous chapter.

In [KSUS19, ZL19, LC19] the authors take a different route concerning the gaps. While dealing with non-Hermitian systems, the techniques are chosen in the spirit of the classification of Hamiltonians. The classification is performed via reducing the systems to Hermitian operators either by continuous deformations or by doubling the system size. These Hermitian operators are then classified using known techniques. For this, the operators under consideration are assumed to exhibit a point gap at zero (as for Hamiltonians) or a line gap along the real or imaginary axis individually (but not simultaneously). In case of a point gap, the dimension is doubled to create a Hermitian operator. In case of a line gap, the spectrum is contracted to the axis perpendicular to the gap line, which results in either a Hermitian or anti-Hermitian operator. For both gap types, however, the classification has little to say about possible deformations of symmetric unitaries, which stay unitary and symmetric on the continuous path (see the gap discussion at the beginning of Section 2.3).

Before we give an overview of the content of this chapter, let us lay out the tasks we are going to address:

- With a few exceptions, the literature on topological properties of quantum walks is model-driven. The topological features and their influence on possible detectable properties of a system are usually only discussed for a rather restricted class of models, e.g. the split-step walk. Of course, most of the findings and techniques are easily transferred to other models at hand. However, to provide a fundamental topological classification of quantum walks, one must not restrict considerations to certain types of models.

  On the other end of the spectrum lies a classification of quantum walks via K-theoretic methods [SSB17, KKT20a, KKT20b]. While K-theory is a powerful tool for general structural statements, it is, however, often not very helpful for specific models or even specific time evolution operators at hand. In particular, a K-theoretic formulation requires stabilising the underlying algebra $\mathcal{A}$ under consideration, i.e. one has to move from $\mathcal{A}$ to the matrix algebras $\mathbb{M}_n(\mathcal{A})$ over $\mathcal{A}$. This stabilisation step makes it generally hard to decide whether, e.g. a homotopy between two specific operators with the same invariants exists without enlarging the system.

  Our work aims to fill the gap between the model-driven analysis and the abstract treatment via purely K-theoretic arguments, thereby combining both sides' advantages. On the one hand, the generality and rigour of an abstract K-theoretic treatment, and, on the other, the better digestibility of a model-driven ansatz, from a physicists point of view.

- One of the most prominent features of topologically non-trivial quantum walks with symmetries is the so-called **bulk-boundary correspondence**. That is, the

appearance of symmetry protected eigenstates at the boundary between topologically different halves (bulks) of the system. In the literature on the topological classification of quantum walks, this effect is often assumed as a standing concept, which only has to be found in a given model system, or it is even raised to the level of an argument in derivations. However, a statement as the guaranteed existence of certain bound states is nothing that can be taken for granted but has to be proven. Our setting enables us to precisely formulate and prove a general version of bulk-boundary correspondence for symmetric quantum walks without relying on scientific folklore or analogy to other known systems.

Moreover, most work is done for translation-invariant systems or restricted types of disorder, limited to specific model systems. Mostly, the invariants are expressed in terms of winding numbers on the eigenbundles of the given operator over the Brillouin zone, which need translation invariance to be well defined. Joining two topologically different systems gives rise to a per se non-translation invariant setting, wherefore we here aim for a theory without translation invariance in the first place.

- While classifying quantum walks via their effective Hamiltonians certainly allows for non-trivial conclusions, one often misses properties, which are unique to unitary systems as opposed to Hermitian ones. On the one hand, this ansatz limits the considerations to the symmetry types of the tenfold way. On the other, different from Hermitian operators, unitaries subject to some symmetry types of the tenfold way exhibit **non-gentle perturbations**. These are local (resp. compact) perturbations of a given unitary, which respect the same symmetry condition but cannot be undone on a norm-continuous path of admissible unitaries. In addition to the usual prediction of localised edge-states due to bulk-boundary correspondence, these non-gentle perturbations give rise to further localised symmetry protected eigenstates of a system under consideration. The main reason for non-gentle perturbations is the aforementioned additional symmetry protected eigenspace of symmetric unitaries. While these have been addressed in the literature, non-gentle perturbations did, to our knowledge, not enter the discussion before we gave a complete classification for quantum walks with symmetries from the tenfold way [CGG$^+$18].

- Last but not least, there is a subtle difference between a stroboscopic view onto a continuously driven process and a purely time-discrete setting. This difference becomes especially relevant in the presence of symmetries that reverse the time-direction as, e.g., time-reversal or chiral symmetry. As mentioned, the effect of a protocol vs a single time-step unitary have been addressed before [AO13, ATD14, MBSO20], but the considerations in the literature are not up to the level of generality we are aiming for. However, for this chapter, we restrict ourselves to single unitaries, i.e. a purely time-discrete setting, and address the properties of driven systems in Chapter 4 and Chapter 5.

The results in this chapter have been obtained in collaboration with Christopher Cedzich, Albertro Grünbaum, Christoph Stahl, Luis Velázquez, Albert Werner and Rein-

hard Werner. The main concepts have been published in [CGS$^+$16, CGG$^+$18, CGS$^+$18, CGWW21], where the symmetry types of the tenfold way are considered. Here, we generalize our work there to the symmetry types beyond the tenfold way.

Following our ansatz in [CGS$^+$16, CGG$^+$18, CGS$^+$18, CGWW21], we start with as little assumptions as possible and work our way up to quantum walks on the one-dimensional lattice, by adding further assumptions on our way. Thereby, we evaluate the effects of each additional assumption on the classification in each step. On the one hand, this allows for a thorough analysis of the effect each assumption has on the systems under consideration. On the other, we can collect intermediate results, which are then applicable to a wide class of systems due to the "minimal set of assumptions" approach. In fact, we provide a complete classification of compact perturbations of admissible unitaries on any discrete spatial structure with respect to norm-continuous deformations, before we even introduce a locality condition. Hence, this classification applies to walks on lattices in any dimension and also on arbitrary graphs.

The main ingredient of our classification is the **symmetry index** we already defined for finite-dimensional symmetry representations in Proposition 2.3.8. We lift the definition to infinite-dimensional systems via reasonable gap assumptions on the unitary operators under consideration. This index assigns each admissible unitary an element of an abelian group and is defined separately for the symmetry protected eigenspaces of an essentially gapped system under consideration. We prove the homotopy invariance of the symmetry index and, as already broached above, use it to completely classify **compact perturbations** preserving the symmetries.

We proceed by adding **locality** on the one-dimensional lattice to our setting. This typically enters via a strict upper bound on the jump-length during one time step. However, there are several reasons why such bound might be to strict for the task of a topological classification. First, it does not get along with a standard time evolution operator originating from an exponentiated time independent local Hamiltonian, or, more general, the solution to the time dependent Schrödinger equation (see Section 1.3), which exhibits exponentially decaying interaction terms. On the other, for many statements it is convenient to work within a C^*-algebra, i.e. the norm-closure of a certain set of operators, which is already closed under multiplication. This also needs a broader definition of locality. We will discuss two different generalizations of strict locality in increasing order of generality and compare them, respectively. Along the way we will revisit a complete homotopy invariant for local unitaries on the one-dimensional lattice [Kit06, GNVW12], the so-called **information flow index**, or just **index**. We will generalize this index to the broader definitions of locality, thereby connecting it to the Fredholm index of a pair of projections [ASS94a, GNVW12, CGG$^+$18, CGWW21], and also show that it coincides with yet another index quantity in the literature [RRR04, Wil09]. We call this generalized index the **right Fredholm index** for **essentially local** unitary operators on the line and prove its completeness for unitaries subject to essential locality. Moreover, we show that this index allows to distinguish between time-discrete unitaries, that emerge from a continuous driving via an essentially local Hamiltonian and those quantum walks for which this is not possible.

In a third step, we combine the symmetry indices with the locality assumption and define the so-called **left and right symmetry indices**, which serve as the bulk indices in

the classification of symmetric quantum walks from a solid state physics point of view. We formulate the bulk-boundary correspondence for symmetric quantum walks on the basis of these indices. In order to split a one-dimensional system into two parts, while keeping unitarity, we take up an idea from [GNVW12] and discuss the possibility to gently decouple a given walk while keeping the symmetry constraints. As also shown in [CGG$^+$18], this is always possible for the symmetry types of the tenfold way. Beyond the tenfold way, however, there are further restrictions, wherefore we only get a weakened form of bulk-boundary correspondence in this case. The robustness of the left and right symmetry indices in case of the tenfold way originates from an alternative definition of the symmetry index, which also allows for a valid index definition in case of merely essentially unitary walks. This renders the aforementioned indices to be robust with respect to arbitrary continuous deformations of the underlying operator as well as all compact perturbations (even those which break unitarity), as long as the symmetry constraints are respected. Using this additional robustness in case of the tenfold way, the classification in terms of the different symmetry indices turns out to be complete, which is the main result of our work in [CGG$^+$18]. The proof for the completeness, however, will only be sketched here and the interested reader is referred to [CGG$^+$18, Ced18].

3.1 The symmetry index for unitary operators

Having outlined our program, let us start by defining the basic concepts and structures needed for our classification. That is, before we turn our attention to actual one-dimensional quantum walks, i.e. unitary operators on a one-dimensional lattice with a locality condition, we first apply and generalize the concepts we encountered so far to gapped unitaries on possibly infinite-dimensional separable Hilbert spaces. The first part of this chapter is independent of any locality condition and therefore works for every underlying discrete spatial structure. A concept motivated by later considerations involving a one-dimensional lattice structure is compact perturbations, which do not break the symmetry assumptions. The main result of this first part is the complete classification of said compact perturbations.

Let $\mathcal{H}$ be some separable Hilbert space carrying a representation of some symmetry type. In contrast to the previous chapter, this representation is no longer finite-dimensional. However, we will base our classification on finite-dimensional subspaces: the symmetry protected eigenspaces of operators under consideration, which we will assume do be finite. Although we do not take the underlying spatial structure into account, for now, we still have a single particle lattice system in mind. That is, the Hilbert space has the form

$$\mathcal{H} = \bigoplus_{x\in\Lambda} \mathcal{H}_x, \tag{3.5}$$

for some countable set Λ and finite-dimensional **cells** $\mathcal{H}_x$, such that each of these cells carries a well defined finite-dimensional representation of the symmetry type:

Assumption 3.1.1. *Let ρ be a representation of some symmetry type on $\mathcal{H}$. We assume it to split into balanced[6] finite-dimensional direct summands ρ_x with respect to the direct sum* (3.5).

[6] See Definition 2.3.4.

Note that when no spatial structure is imposed on a system in the first place, the direct sum decomposition part of the assumption is still reasonable since we could reduce a given representation ρ and define Λ as the labelling set for the irreducible representations contained in ρ. In this case, the non-trivial part of the assumption is the balancedness of each summand, which generally requires to combine multiple irreducible representations into one summand. While balanced cells are not indispensable for all considerations below, this assumption sets the trivial reference for the classification. In the context of a K-theoretic classification of topological phases of matter, it has been argued in [Thi16] (also referring to [ASS90, ASS94b][7]) that any topological phase classification of physical systems has to be relative, i.e. a classifying index should always "measure" the difference between a system and some fixed reference. Hence, choosing such a reference can be an integral part of any topological classification of physical systems. Assuming the individual cells to carry balanced representations ρ_x guarantees the existence of a gapped unitary on the whole Hilbert space and, hence, a trivial reference system. Any finite number of unbalanced cells could also serve as such reference, simply shifting all indices by some finite value. However, this would not be possible for an infinite number of unbalanced cells, and further care had to be taken.

In order to apply the structures we defined in the previous chapter, we break down the infinite representation to finite ones in yet another way. The classification is based on the symmetry protected eigenspaces of operators under consideration. For this, we assume these to be finite-dimensional, which is guaranteed by the following property:

Definition 3.1.2. *Let U be a unitary operator, which is admissible for one of the symmetry types with symmetry protected eigenspaces. We call U* ***essentially gapped*** *if its essential spectrum is gapped at all symmetry protected points. That is, at ± 1 for symmetry types with a vertical eigenvalue-orbits, and at ± 1 and $\pm i$ for those with rectangular orbits.*

For the definition and some properties of the essential spectrum of an operator see Section 1.2 (in particular Definition 1.2.8 and Lemma 1.2.9). The assumption of an essential gap is crucial for all following considerations involving admissible unitaries. Therefore, we include the property in the assumptions for the concept of admissibility:

Definition 3.1.3. *We call a unitary operator* ***admissible*** *for a symmetry representation ρ if it fulfils the symmetry conditions and is essentially gapped at the symmetry invariant points of the spectrum.*

In Section 2.1 we defined the symmetry index for finite-dimensional representations and calculated the corresponding index groups for all non-redundant symmetry types. The assumption of an essential gap for every admissible unitary allows us to apply this symmetry index to its finite-dimensional symmetry invariant eigenspaces. Note that by Definition 3.1.3, each symmetry representation induces finite-dimensional representations with well-defined symmetry indices on the symmetry invariant eigenspaces ± 1, resp. ± 1 and $\pm i$ of admissible unitaries. Hence, the following indices are well defined:

[7] In fact, the relative index used in [ASS90, ASS94b] and further developed in [ASS94a] can be identified with the information flow index of a quantum walk [GNVW12, CGG$^+$18], which we will make heavy use of for the classification of protocols and Floquet systems [CGWW21].

Definition 3.1.4. *Let U be an admissible unitary for a representation ρ of a symmetry type* S *with either vertical ($s = \mathrm{id}, r \neq \mathrm{id}$) or rectangular ($r \neq \mathrm{id}, s \neq \mathrm{id}$) eigenvalue orbit. The* ***symmetry indices*** *of U are then defined as the symmetry indices[8] of the finite-dimensional representations on the symmetry protected eigenspaces. Denote by $\mathcal{H}_\lambda$ the respective finite-dimensional eigenspaces of U and by $\mathrm{si}(\mathcal{H}_k) = \mathrm{si}(\rho|_{\mathcal{H}_k})$ the symmetry index of the finite-dimensional restriction of ρ to $\mathcal{H}_k$. Then:*

- *For symmetry types with* ***vertical orbits*** *we define*

$$\mathrm{si}_+(U) = \mathrm{si}\,(\mathcal{H}_{+1}) \quad \textit{and} \quad \mathrm{si}_-(U) = \mathrm{si}\,(\mathcal{H}_{-1})\,. \tag{3.6}$$

- *For symmetry types with* ***rectangular orbits*** *we define*

$$\mathrm{si}_{\leftrightarrow}(U) = \mathrm{si}\,(\mathcal{H}_{+1} \oplus \mathcal{H}_{-1}) \quad \textit{and} \quad \mathrm{si}_{\updownarrow}(U) = \mathrm{si}\,(\mathcal{H}_{+i} \oplus \mathcal{H}_{-i})\,. \tag{3.7}$$

In both cases we denote by $\mathrm{si}(U)$ the sum of the two individual indices, i.e.

$$\mathrm{si}(U) = \mathrm{si}_+(U) + \mathrm{si}_-(U) \quad \textit{or} \quad \mathrm{si}(U) = \mathrm{si}_{\leftrightarrow}(U) + \mathrm{si}_{\updownarrow}(U). \tag{3.8}$$

For finite-dimensional Hilbert spaces the further condition in Definition 3.1.3 becomes void and we always have $\mathrm{si}(U) = \mathrm{si}(\rho)$ for any representation. On the one hand, the representation is reduced by the projections onto the symmetry invariant eigenspaces of U, and on the other, it is balanced by definition on the complement of their union because U itself is gapped on the complement of these spaces ($\mathcal{H}_{+1} \oplus \mathcal{H}_{-1}$ for vertical- and $\mathcal{H}_{+1} \oplus \mathcal{H}_{-1} \oplus \mathcal{H}_{+i} \oplus \mathcal{H}_{-i}$ for box-orbits).

Corollary 3.1.5. *For finite-dimensional Hilbert spaces the symmetry indices of Proposition 2.3.8 and Definition 3.1.4 coincide and we have*

$$\mathrm{si}(U) = \mathrm{si}(\rho). \tag{3.9}$$

Note that assuming each cell to be balanced implies $\mathrm{si}(U) = 0$ in any finite-dimensional setting. However, for infinite-dimensional Hilbert spaces this conclusion is not true in general.

3.1.1 Homotopy invariance

In defining the symmetry indices for symmetry types, we aimed for the topological classification of quantum walks. We now come to their key property: Homotopy invariance. That is, whenever we have a continuous path $[0,1] \ni t \mapsto U_t$ between two unitaries U_0 and U_1, such that U_t is essentially gapped and admissible for all t, we get $\mathrm{si}_\star(U_0) = \mathrm{si}_\star(U_1) = \mathrm{si}_\star(U_t)$ for all t and $\star \in \{+,-\}$ or $\star \in \{\leftrightarrow, \updownarrow\}$, depending on the symmetry type under consideration. The homotopy invariance follows from the following proposition.

[8] See Proposition 2.3.8.

Proposition 3.1.6. *Let U be admissible for a representation of some symmetry type. Then there is an $\varepsilon > 0$, such that any $\widetilde{U}$ with $\|U - \widetilde{U}\| < \varepsilon$, which is admissible for the same representation, has the same symmetry indices. I.e.*

$$\mathrm{si}_\star(\widetilde{U}) = \mathrm{si}_\star(U),$$

with $\star \in \{+, -\}$ or $\star \in \{\leftrightarrow, \updownarrow\}$, depending on the type.

The first half of the proof is pretty standard in perturbation theory in terms of resolvents (see for example [Kat84, Ch. 2] or [RS78, Ch. XII]). However, we spell out the details anyhow in order to give a self-contained picture here.

Proof. Let $\lambda \in \{\pm 1\}$ for $\star = \pm$ and $\lambda \in \{\pm 1, \pm i\}$ for $\star \in \{\leftrightarrow, \updownarrow\}$ be a part of a minimal eigenvalue orbit in the spectrum of U under the action of the symmetry representation. By assumption, U is essentially gapped at each λ. Therefore, around each of these points, there exists a circle of radius δ_λ, which separates λ from all other parts of the spectrum of U. Let δ be the maximal common radius for all such separating circles, and denote by Γ_λ the circle around λ, with radius $\delta/2$. Then, $\forall \lambda$ the norm of the resolvent $R(z) = (z - U)^{-1}$ is bounded by $2/\delta$ for $z \in \Gamma_\lambda$. From the resolvent equation

$$\widetilde{R}(z) - R(z) = \widetilde{R}(z)(\widetilde{U} - U)R(z),$$

where $\widetilde{R}(z)$ denotes the resolvent of $\widetilde{U}$, we conclude that

$$\widetilde{R}(z) = R(z)\left(\mathbb{1} - (\widetilde{U} - U)R(z)\right)^{-1} = \sum_{n=0}^{\infty} R(z)\left((\widetilde{U} - U)R(z)\right)^n \tag{3.10}$$

exists and is bounded by

$$\frac{2}{\delta}\left(1 - \frac{2\|\widetilde{U} - U\|}{\delta}\right)^{-1},$$

given that $\|\widetilde{U} - U\| < \delta/2$. Indeed, in that case, the right hand side of (3.10) is $R(z)$ times a convergent series $\sum_n A^n$ with $\|A\| = \|((\widetilde{U} - U)R(z))\| < \delta/2 \cdot 2/\delta = 1$.

Let now P_λ be the spectral projection of U onto λ, which can be expressed as

$$P_\lambda = \int_{\Gamma_\lambda} \frac{\mathrm{d}z}{2\pi i} R(z)$$

[Kat84, III.6]. Moreover, let

$$Q_\lambda = \int_{\Gamma_\lambda} \frac{\mathrm{d}z}{2\pi i} \widetilde{R}(z), \tag{3.11}$$

which is a well defined projection, since $\widetilde{R}(z)$ is bounded on and inside Γ_λ. Now, for

$\|\widetilde{U} - U\| < \delta/4$ we get

$$\begin{aligned} \|Q_\lambda - P_\lambda\| &= \left\| \int_{\Gamma_\lambda} \frac{\mathrm{d}z}{2\pi i} \left(\widetilde{R}(z) - R(z) \right) \right\| \\ &= \left\| \int_{\Gamma_\lambda} \frac{\mathrm{d}z}{2\pi i} \sum_{n=1}^{\infty} R(z) \left((\widetilde{U} - U) R(z) \right)^n \right\| \\ &\leq \frac{\delta}{2} \sum_{n=1}^{\infty} \left\| R(z) \left((\widetilde{U} - U) R(z) \right)^n \right\| \\ &\leq \frac{2 \left\| \widetilde{U} - U \right\|}{\delta - 2 \left\| \widetilde{U} - U \right\|} < 1, \end{aligned} \tag{3.12}$$

where we inserted (3.10) in the first step, bounded the integral by the length of Γ_λ times the norm on the integrand in the second step, also using $\|A + B\| \leq \|A\| + \|B\|$, and evaluated the geometric series using $\|AB\| \leq \|A\|\|B\|$ in the last step. Finally, from $\|Q_\lambda - P_\lambda\| < 1$ we conclude, that $\dim Q_\lambda \mathcal{H} = \dim P_\lambda \mathcal{H}$.

Let $P_\star$ and $\widetilde{P}_\star$ be be the projections onto the symmetry invariant eigenspaces for U and $\widetilde{U}$. Moreover, given $P_\star$ let $Q_\star$ be defined similar to the considerations above. Then the finite-dimensional representations $\widetilde{P}_\star \rho \widetilde{P}_\star$ and $Q_\star \rho Q_\star$ have to differ by a balanced representation. Indeed, by construction $(Q_\star - \widetilde{P}_\star)\widetilde{U}(Q_\star - \widetilde{P}_\star)$ is a unitary, with gaps at ± 1 or $\pm 1 \cup \pm i$, respectively. Therefore we get

$$\mathrm{si}(\widetilde{P}_\star \rho \widetilde{P}_\star) = \mathrm{si}(Q_\star \rho Q_\star). \tag{3.13}$$

For symmetry types with symmetry indices given by the dimension of the representation[9], this already proves the proposition. In all other cases, the (respective part of the) symmetry index is $\mathbb{Z}$-valued and can be expressed via a trace on the respective subspace. si either equals the trace of one of the symmetries or the dimension of one of its eigenspaces. However, by $V_g^2 = \pm \mathbb{1}$ for any symmetry operator, such dimension can be computed via $\mathrm{tr}(V_g \pm \mathbb{1})/2$ or $\mathrm{tr}(V_g \pm i\mathbb{1})/2$. In both situations,with α being the placeholder for either V_g or a combination $(V_g \pm \lambda)/2$, we get

$$\begin{aligned} |\,\mathrm{si}_\star(\widetilde{U}) - \mathrm{si}_\star(U)| &= |\,\mathrm{si}(Q_\star \rho Q_\star) - \mathrm{si}(P_\star \rho P_\star)| \\ &= |\,\mathrm{tr}(Q_\star \alpha Q_\star) - \mathrm{tr}(P_\star \alpha P_\star)| \\ &\leq |\,\mathrm{tr}(Q_\star \alpha Q_\star) - \mathrm{tr}(P_\star \alpha Q_\star)| + |\,\mathrm{tr}(P_\star \alpha Q_\star) - \mathrm{tr}(P_\star \alpha P_\star)| \\ &\leq \|Q_\star - P_\star\|(\|\alpha Q_\star\|_1 + \|\alpha P_\star\|_1) \\ &\leq 2d \|Q_\star - P_\star\|, \end{aligned} \tag{3.14}$$

where $\|\cdot\|_1$ denotes the tracenorm, which fulfils $|\,\mathrm{tr}(A_1 BC) - \mathrm{tr}(A_2 BC)| \leq \|A_1 - A_2\|\|BC\|_1$. In the last step we used $\|\alpha P_\star\|_1 \leq \|\alpha\|\|P_\star\|_1 \leq \dim P_\star \mathcal{H} =: d$. Since si is $\mathbb{Z}$-valued, the difference has to be zero, whenever (3.14) is smaller than one, i.e. if $\|Q_\star - P_\star\| < 1/(2d)$.

[9] Respectively its parity or similar.

Combining this with (3.12) we get $\mathrm{si}_\star(U) = \mathrm{si}_\star(\widetilde{U})$ for $\|\widetilde{U} - U\| < \varepsilon$ with

$$\varepsilon = \frac{\delta}{2}\frac{1}{2d+1}. \tag{3.15}$$

□

For every continuous path $[0,1] \ni t \mapsto U_t$ and any $\varepsilon > 0$ we then find a sequence $0 < t_1 < \ldots < t_n < 1$, such that $\|U_{t_{i+1}} - U_{t_i}\| < \epsilon$ for all $i = 1, \ldots, n$. Hence, we get $\mathrm{si}_\star(U_0) = \mathrm{si}_\star(U_1) = \mathrm{si}_\star(U_t)$ for all t. This renders $\mathrm{si}_\star$ to be homotopy invariants on the set of admissible unitaries with a discrete underlying spatial structure. Note that we did not infer any locality condition so far, such that these invariants are valid for any underlying discrete structure, such as lattices or graphs.

In case of the tenfold way, the same statement holds for admissible essentially gapped Hamiltonians with $\mathrm{si}_\star = \mathrm{si}_0$. For a proof that is written explicitly in terms of Hamiltonians, see [CGG$^+$18, Prop. II.6].

Corollary 3.1.7. *For the symmetry types of the tenfold way, the same holds for Hamiltonians, with* $\mathrm{si}_\star = \mathrm{si}_0$.

Having established homotopy invariance of the symmetry index on the set of admissible unitaries, we find ourselves in a good position to take a step back and elaborate on the motivation behind the definitions and structures so far: Firstly, $\mathrm{si}_\star$ and $\mathrm{si} = \sum_\star \mathrm{si}_\star$ are homotopy invariants and therefore contribute to the topological classification of the set of objects they are defined on. We will later discuss that in case of the tenfold way, si_+ and si_- already provide a complete classification for the set of admissible and essentially gapped unitaries, with respect to norm-continuous deformations (see Section 3.6). Additionally, they are two in a set of three indices that completely classify the set of essentially gapped and admissible quantum walks with respect to norm-continuous deformations and compact perturbations.

Moreover, the symmetry index serves as a lower bound on the number of symmetry protected eigenstates. In particular, by homotopy invariance of $\mathrm{si}_\star$, this lower bound is stable under continuous deformations in the set of admissible unitaries. As we will discuss later, in many systems the sum of the respective indices $\mathrm{si}_{\leftrightarrow} + \mathrm{si}_{\updownarrow}$ and $\mathrm{si}_+ + \mathrm{si}_-$ is also stable under local, respectively compact, admissible perturbations. This fact gives rise to an instance of a well-known concept, namely bulk-boundary correspondence. The instance in our case typically refers to the occurrence of symmetry protected, localized states at the boundary of a symmetric lattice system with "non-trivial topology" or at the crossover between "topologically different" halves of the system. We will equip these rather vague statements with the necessary rigour later in Section 3.5.4.

3.2 Complete classification of compact perturbations

As already laid out in the introduction, we are not only interested in continuous deformations of the unitary operators under consideration but also local or, more general, compact perturbations respecting the symmetries. Thereby, compact perturbations are the natural generalization of strictly local ones, which act only on a finite spatial region.

In anticipation of the discussion of different locality conditions, let us define the versions of perturbations we consider here.

Definition 3.2.1. *Let U be unitary with an underlying spatial structure Λ (see (3.5) and the discussion thereafter), which is admissible for a representation of one of the 38 symmetry types. A perturbation U' of U is another unitary, which is admissible for the same representation. We call a perturbation*

i) ***gentle**, if there exists a norm-continuous path $t \mapsto U_t$, $t \in [0,1]$ with $U_0 = U$ and $U_1 = U'$, such that U_t is admissible for every t.*

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

iii) ***finite rank**, if $U' - U$ has finite rank.*

iv) ***compact**, if $U' - U$ is compact.*

Note, that by definition we have $ii) \subset iii) \subset iv)$, whereas each of these can either be gentle or not. In the latter case we call the perturbation **non-gentle**. For Hamiltonians, the distinction between $i)$ and the other three types of perturbations, respectively, becomes void. In this case, any compact (finite rank or local) perturbation can be reached via an admissible homotopy. Indeed, consider two admissible Hamiltonians H_0 and H_1, such that $H_1 - H_0$ is non-zero only on finitely many cells, of finite rank, or compact. Then

$$H_t = (1-t)H_0 + tH_1 = H_0 + t(H_1 - H_0), \quad t \in [0,1] \tag{3.16}$$

is a continuous deformation of H_0 into H_1, respecting the symmetries for all t[10]. The crucial part is the compactness of $H_1 - H_0$, since it guarantees, that the essential gap of H_t stays open for all t (see Lemma 1.2.9). But in principle, any perturbation (being compact or not), which has this property results in a gentle one. Hence, the existence of non-gentle perturbations is only possible for unitary operators and, as we will see below, the "non-gentleness" of a perturbation can be classified by the symmetry indices.

While for Hamiltonians any perturbation can be written additively as in (3.16), the most convenient way in a unitary setting is to write a perturbation multiplicatively:

$$U' = VU, \qquad \text{with} \qquad V = U'U^*, \tag{3.17}$$

Properties $ii) - v)$ in Definition 3.2.1 of such perturbations then translate to $V - \mathbb{1}$ being strictly local, finite rank or compact, and the task of continuously connecting U and U' boils down to contracting V to the identity, keeping the symmetry for $U_t = V_t U$ on the way. Let us discuss such multiplicative perturbations V in detail. In preparation for this, given a representation ρ of a symmetry type, consider the following induced representation $\widetilde{\rho}$ of the so-called perturbation symmetry type, the name of which will become clear later on.

[10] Moreover, H_t heirs the weaker of the two locality conditions of H_0 and H_1 (see Section 3.3).

Lemma 3.2.2. *Let $[\rho]$ be a one of the 38 symmetry types, ρ an explicit representation, and G the corresponding symmetry group. Moreover, let U be an admissible unitary. We define the* ***perturbation symmetry type*** *to be the type $[\widetilde{\rho}]$ of the representation*

$$\widetilde{\rho}\colon \quad g \mapsto \widetilde{\rho}_g = U^{\frac{1}{2}(1-ur(g))}\rho_g = \begin{cases} U\rho_g & ur(g) = -1 \\ \rho_g & ur(g) = 1 \end{cases} . \tag{3.18}$$

$\widetilde{\rho}$ respects phase convention II from Lemma 2.1.7 and its multiplication function is given by

$$\widetilde{m}(g,h) = s(g)^{\frac{1}{2}(1-ur(h))}m(g,h). \tag{3.19}$$

Proof. First, note that the (anti-) unitarity of the group elements is not changed by (3.18). Second, let us check that $\widetilde{\rho}$ is indeed a projective representation of G. We have

$$\begin{aligned} \widetilde{\rho}_g\widetilde{\rho}_h &= \left(U^{\frac{1}{2}(1-ur(g))}\rho_g\right)\left(U^{\frac{1}{2}(1-ur(h))}\rho_h\right) \\ &= U^{\frac{1}{2}(1-ur(g))}\left(s(g)U^{ur(g)}\right)^{\frac{1}{2}(1-ur(h))}\rho_g\rho_h \\ &= s(g)^{\frac{1}{2}(1-ur(h))}m(g,h)\left(U^{\frac{1}{2}(1-ur(gh))}\rho_{gh}\right) \\ &= s(g)^{\frac{1}{2}(1-ur(h))}m(g,h)\widetilde{\rho}_{gh}, \end{aligned}$$

where we used $ur(g)ur(h) = ur(gh)$ in the third step. This also proves (3.19). Since $\widetilde{m} = \pm m$, we are still in the setting of Proposition 2.1.4 and Lemma 2.1.6. Moreover, for the 38-fold way, we can always choose σ and/or γ as the unitary generators of G, since the groups containing only σ_γ and the identity as unitary elements are ruled out by Lemma 2.2.11 and the discussion thereafter. But evaluating $\widetilde{m}(\widetilde{\rho}_g, \widetilde{\rho}_g)$ for these two symmetries we get $\widetilde{\sigma}^2 = \sigma^2$ and $\widetilde{\gamma} = \gamma^2$. Therefore, the phase convention of Lemma 2.1.7 is respected by $\widetilde{\rho}$. □

Note that the only property distinguishing between the types $[\rho]$ and $[\widetilde{\rho}]$ is the alternating character s. Hence, for the symmetry types of the tenfold way, which correspond to groups with $s \equiv 1$, the two representation ρ and $\widetilde{\rho}$ are actually of the same type. This observation will be important later on for the characterization of local perturbations of unitaries in case of the tenfold way. To begin with this characterization, the following Lemma first settles the conditions for a perturbed unitary $U' = VU$ to be admissible for the same type as U, which also justifies the name **perturbation symmetry type** for $[\widetilde{\rho}]$ above.

Lemma 3.2.3. *Let U be a unitary, which is admissible for a representation ρ of one of the 38 symmetry types. Moreover let $U' = VU$ be a perturbation of U. Then:*

- *U' is admissible for ρ if and only if V is admissible for the symmetry representation $\widetilde{\rho}$ from Lemma 3.2.2 in the following sense:*

$$\widetilde{\rho}_g V \widetilde{\rho}_g^* = V^{ur(g)}. \tag{3.20}$$

- *The subspace*

$$\mathcal{H}_V = P_V\mathcal{H} := (V - \mathbb{1})\mathcal{H} = (V^* - \mathbb{1})\mathcal{H} = (VU - U)\mathcal{H} \tag{3.21}$$

*is invariant under V, V^* and also under the action of $\widetilde{\rho}$. We call $\mathcal{H}_V$ the **perturbation subspace**. If V is a compact perturbation, the spectrum of $P_V V P_V$, considered on $\mathcal{H}_V$, consists only of finitely degenerated eigenvalues, with $+1$ being the only possible limit point. In particular, the -1 eigenspace $\mathcal{H}_V^- \subset \mathcal{H}_V$ of V is finite-dimensional and also invariant under $\widetilde{\rho}$.*

Proof. On the one hand, assuming $ur(g) = 1$, admissibility of U' translates to

$$\rho_g VU\rho_g^* = sVU \quad \Leftrightarrow \quad s\rho_g V\rho_g^* U = sVU \quad \Leftrightarrow \quad \rho_g V\rho_g^* = V.$$

For $ur(g) = -1$, on the other hand, we get

$$\rho_g VU\rho_g^* = sU^*V^* \quad \Leftrightarrow \quad s\rho_g V\rho_g^* U^* = sU^*V^* \quad \Leftrightarrow \quad (U\rho_g)V(U\rho_g)^* = V^*.$$

In both cases the character s drops out of the condition for V, and we get $\widetilde{\rho}$ from Lemma 3.2.2 together with (3.20) as the necessary and sufficient symmetry condition for V. The equalities in (3.21) are a consequence of $(V - \mathbb{1}) = (V^* - \mathbb{1})(-V)$ and $\mathcal{H} = V\mathcal{H} = U\mathcal{H}$. Moreover, the invariance of $\mathcal{H}_V$ under V, V^* and the action of $\widetilde{\rho}$ follows directly from this equation.

The last part of the Lemma is a direct consequence of $V - \mathbb{1}$ being compact, the definition of a compact perturbation and the invariance of $\mathcal{H}_V^-$ under $\widetilde{\rho}$ is a consequence of the action on V (see, e.g., the discussion in Section 2.3). □

While $\widetilde{\rho}$ remains a representation of the same abstract group of involutive symmetries for unitary operators, its action on V will in general not be given by one of the symmetry types of the 38-fold way, without redundancies. Indeed, the alternating character drops out of the symmetry condition. Hence, if we started with a symmetry group containing $\sigma \equiv (1, 1, -1)$, this symmetry becomes redundant for V. Therefore, for $\widetilde{\rho}$ considered as the representation of a symmetry group for V, the elements might no longer be uniquely labelled by the character triplet (u, r, s). In other cases, however, $\widetilde{\rho}$ might still be part of the 38-fold way. In particular, if we started with a symmetry type from the tenfold way, we get $[\widetilde{\rho}] = [\rho]$.

Nevertheless, we can use the perturbation symmetry type and an adapted index (defined below) for a topological classification of compact perturbations, which do not break the symmetry (see Theorem 3.2.6 below). For the tenfold way, due to $[\widetilde{\rho}] = [\rho]$, this classification of perturbations turns out to be already determined by the indices $\mathrm{si}_\pm$ (see Proposition 3.2.8).

Definition 3.2.4. *Let U be an admissible unitary and V be a compact perturbation, such that $U' = VU$ is also admissible. We define the **perturbation index** of U' with respect to U as*

$$\mathrm{si}(U' : U) = \widetilde{\mathrm{si}}_-(V) := \mathrm{si}\left(P_V^-\widetilde{\rho}P_V^-\right), \tag{3.22}$$

with $P_V^-\mathcal{H} = \mathcal{H}_V^-$.

Let us briefly check that $\widetilde{\mathrm{si}}_-(V)$ is indeed well defined: By Lemma 3.2.3, the -1 eigenspace of V is finite-dimensional for a compact perturbation and also invariant under $\widetilde{\rho}$. Hence, $P_V^-\widetilde{\rho}P_V^-$ defines a finite-dimensional representation of the symmetry type $[\widetilde{\rho}]$. The action of $\widetilde{\rho}$ on V imposes a vertical orbit on eigenvalues, or the orbit is trivial. Hence, by Definition 2.3.4, balanced refers to the existence of an admissible unitary, which is gapped at ± 1. One has to be a bit careful concerning the fact that $\widetilde{\rho}$ is not necessarily part of the 38-fold way. In particular, we cannot just read off the corresponding index groups in Table 2.1. However, the considerations in Section 3.1 and, in particular, the definition of the symmetry index do not require the underlying symmetry group to be free of redundant symmetries. Therefore, $\mathrm{si}(VU : U) = \widetilde{\mathrm{si}}_-(V)$ is defined equally well also in this situation. We do not compute all the perturbation index groups here but only discuss some examples below. The computations are similar to the index group computations in Section 2.3, with the difference that the character s drops out of the symmetry condition.

Corollary 3.2.5. *Let U be an admissible unitary for some symmetry type and $t \mapsto U_t = V_t U$ be a continuous family of admissible compact perturbations of U. Then $t \mapsto \mathrm{si}(U_t : U)$ is constant.*

Proof. The perturbation index is defined as a symmetry index in the sense of Definition 3.1.4. Therefore it is constant for a continuous family of compact perturbations, by Proposition 3.1.6. □

The perturbation index allows us to classify compact admissible perturbations of admissible unitary operators up to gentle perturbations.

Theorem 3.2.6. *Let U and $U' = VU$ admissible for a representation ρ, with a compact perturbation V. Then the following are equivalent:*

i) $\mathrm{si}(U' : U) = 0$

ii) There is a continuous path $t \mapsto V_t$ of $\widetilde{\rho}$ admissible unitaries on $\mathcal{H}_V$, connecting V with $\mathbb{1}$ and hence, a continuous path $U_t = V_t U$ of ρ admissible unitaries, connecting U and VU.

Proof. The direction $ii) \Rightarrow i)$ follows from the homotopy invariance of $\widetilde{\mathrm{si}}_-(V)$ and $\widetilde{\mathrm{si}}_-(\mathbb{1}) = 0$. For the other direction, consider V restricted to $\mathcal{H}_V$. First note that (3.20) either imposes a trivial or a vertical orbit on the eigenvalues of V. In the first case, we can move every eigenvalue of V to 1 without touching the eigenvectors, which provides the admissible path.

If the orbits are non-trivial, V is gapped on the complement of $\mathcal{H}_V^-$ in $\mathcal{H}_V$, wherefore, on this subspace, we can deform the eigenvalues pairwise to $+1$, again without touching the eigenvectors. This leaves us with $V = \mathbb{1}_{\mathcal{H}_V} - 2P_V^-$. Now, by $\mathrm{si}(U' : U) = \widetilde{\mathrm{si}}_-(V) = \mathrm{si}\left(P_V^-\widetilde{\rho}P_V^-\right) = 0$, there exists an admissible unitary on $\mathcal{H}_V^-$, which is gapped at ± 1. Performing the same trick on this unitary, we can deform it to $-\mathbb{1}$ and $+\mathbb{1}$, which finally provides a continuous admissible path between V and $\mathbb{1}$ on $\mathcal{H}_V$. □

Theorem 3.2.6 is the first completeness result involving the symmetry index si. The perturbation index provides a complete classification of compact symmetric perturbations for unitaries of all 38 symmetry types.

Since all index groups are additive under direct sums, it implies that non-gentle perturbations with orthogonal perturbation subspaces add up in the perturbation index. While in the setting of the following corollary we always get $\mathrm{si}(U'' : U) = \mathrm{si}(U'' : U') + \mathrm{si}(U' : U)$, orthogonal perturbations subspaces simplify this relation in the following way:

Corollary 3.2.7. *Let U be admissible for one of the 38 symmetry types, and $U' = V_1U$ and $U'' = V_2U' = V_2V_1U$ be compact admissible perturbations of U, such that $\mathcal{H}_{V_2V_1} = \mathcal{H}_{V_1} \oplus \mathcal{H}_{V_2}$. Then*

$$\mathrm{si}(U'' : U) = \mathrm{si}(V_1U : U) + \mathrm{si}(V_2U : U). \tag{3.23}$$

In particular, two non-gentle perturbations can cancel out each other, when their individual perturbation indices have opposite values.

Since the perturbation index is purely relative, the question arises, how the perturbation index connects to the absolute homotopy invariants[11] $\mathrm{si}_\star(U)$ and $\mathrm{si}_\star(U')$, ($\star \in \{\pm, \dotplus\}$), defined in Definition 3.1.4. As we will see later, for the tenfold way, the combined index $\mathrm{si} = \mathrm{si}_+ + \mathrm{si}_-$ is invariant under every compact perturbation, which respects the symmetries. The individual terms $\mathrm{si}_\star$ on the other hand can be changed under such perturbations. We already saw this in Example 2.3.2 for type 8 (D) and in Example 2.3.3 for type 16 (which is not part of the tenfold way)[12].

It is clear by homotopy invariance that a compact perturbation, which changes $\mathrm{si}_\star$ cannot be gentle. This raises the question, whether every non-gentle perturbation can be **detected** by the $\mathrm{si}_\star$-indices. Indeed, this is the case for the symmetry types of the tenfold way: In this case, a perturbation is non-gentle if and only if it changes $\mathrm{si}_\pm$. Furthermore, the fact that the perturbation symmetry type for V is the same as the original symmetry type for U allows us to directly express the perturbation index in terms of the indices $\mathrm{si}_\pm$:

Proposition 3.2.8. *Let U be admissible for a symmetry type of the tenfold way and let $U' = VU$ be an admissible compact perturbation of U. Then*

$$\mathrm{si}(U' : U) = \mathrm{si}_-(U') - \mathrm{si}_-(U) = -\big(\mathrm{si}_+(U') - \mathrm{si}_+(U)\big). \tag{3.24}$$

Proof. We first give a sketch of the proof, which makes clear the line of argument, and fill in the details (D1-D4) below. The main concept is depicted in Figure 3.1. The second equality in (3.24) follows from $\mathrm{si} = \mathrm{si}_+ + \mathrm{si}_-$ and the invariance of si under compact perturbations (which will be shown later in Section 3.5.1). Hence, we focus on the first equality. In a preparatory step, we continuously deform V into $\mathbb{1} - 2P$, where P is the projection onto the -1-eigenspace of V, as described in the proof of Theorem 3.2.6. Hence, for the rest of the proof we can assume $V = \mathbb{1} - 2P$. Again, by the same arguments as above, $\widetilde{\rho}$ commutes with P and we denote by $\widetilde{\rho}_P$ the finite-dimensional symmetry representation $P\widetilde{\rho}P$ on $P\mathcal{H}$. Further denoting by N and N' the -1-eigenspace

[11] Note that the "absolute" indices are absolute only for the set of operators we consider here (essentially gapped unitaries with symmetry). In a broader sense, they are still relative (see [Thi16] and the discussion after Assumption 3.1.1) since we assumed the underlying Hilbert space to consist of balanced cells, ensuring a gapped reference unitary.

[12] For a finite-dimensional representation of any symmetry type, all admissible unitaries are compact perturbations of each other.

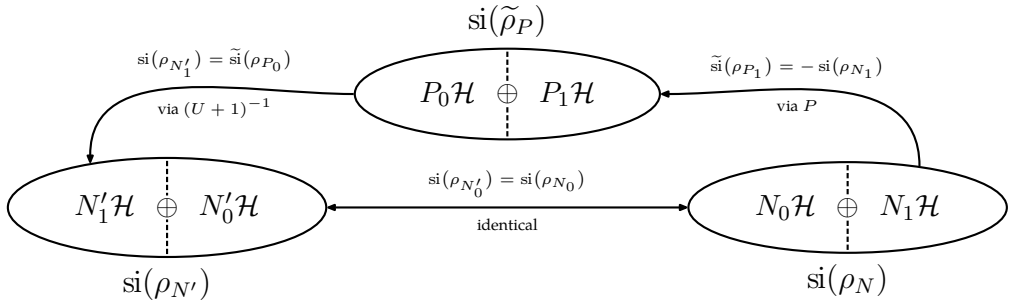


Figure 3.1: Mappings between the relevant subspaces for a compact perturbation $U' = (\mathbb{1} - 2P)U$ (from the proof of Proposition 3.2.8). The mapping operators between the spaces are shown below the arrows. The resulting equations for the symmetry indices of the respective representations restricted to the subspaces are denoted above the arrows. See also [CGG+18, Fig. 6].

projections of U and U', respectively, (3.24) is equivalent to

$$\text{si}(\widetilde{\rho}_P) = \text{si}(\rho_{N'}) - \text{si}(\rho_N). \tag{3.25}$$

We split each subspace $X\mathcal{H}$ ($X = N, N', P$) into $X\mathcal{H} = X_0\mathcal{H} \oplus X_1\mathcal{H}$, where the X_0s are defined as

$$\begin{aligned} N_0\mathcal{H} &= N\mathcal{H} \cap P^\perp\mathcal{H} \\ N_0'\mathcal{H} &= N'\mathcal{H} \cap P^\perp\mathcal{H} \\ P_0\mathcal{H} &= P\mathcal{H} \cap N^\perp\mathcal{H} \end{aligned} \tag{3.26}$$

and $X_1\mathcal{H} = (X - X_0)\mathcal{H}$ denotes their complement, respectively. Then N_i and N_i' ($i = 1, 2$) commute with ρ and P_i commutes with $\widetilde{\rho}$, which induces the symmetry representations $\rho_{N_i}, \rho_{N_i'}$ and $\widetilde{\rho}_{P_i}$ (D1). Hence, we can rewrite (3.25) as

$$\text{si}(\widetilde{\rho}_{P_0}) + \text{si}(\widetilde{\rho}_{P_1}) = \text{si}(\rho_{N_0'}) + \text{si}(\rho_{N_1'}) - \text{si}(\rho_{N_0}) - \text{si}(\rho_{N_1}). \tag{3.27}$$

The statement now follows from by the following three identifications (D2-D4):

$$\text{si}(\rho_{N_0'}) = \text{si}(\rho_{N_0}), \qquad \text{si}(\widetilde{\rho}_{P_1}) = -\text{si}(\rho_{N_1}) \qquad \text{and} \qquad \text{si}(\widetilde{\rho}_{P_0}) = \text{si}(\rho_{N_1'}). \tag{3.28}$$

Details:

(D1) Symmetry invariance of N_i, N_i' and P_i:
Let us start with $N_0\mathcal{H}$. Invariance of $N_0\mathcal{H}$ under ρ also implies invariance of $N_1\mathcal{H}$, because their direct sum $N\mathcal{H}$ is the -1-eigenspace of U, which is also invariant. Let $\varphi \in N_0\mathcal{H}$, then we get

$$P\rho_g\varphi = P\rho_g U^{\frac{1}{2}(ur(g)-1)}U^{\frac{1}{2}(1-ur(g))}\varphi = ur(g)P\widetilde{\rho}_g\varphi = ur(g)\widetilde{\rho}_g P\varphi = 0 \tag{3.29}$$

where we used the definition of the perturbation symmetries[13], $[P, \widetilde{\rho}_g] = 0$, which follows by admissibility of V for $\widetilde{\rho}$, and $U^{\frac{1}{2}(1-ur(g))}\varphi = ur(g)\varphi$, due to $\varphi \in N\mathcal{H}$. Hence,

[13] $U^{\frac{1}{2}(1-ur(g))}\rho_g = s(g)\rho_g U^{\frac{1}{2}(ur(g)-1)} = \widetilde{\rho}_g$

$\rho_g\varphi \in N_0\mathcal{H}$ for every g, wherefore N_0 and therefore also N_1 are invariant under ρ. The same arguments apply for N_i'. For P_i, note that P commutes with the symmetries of $\widetilde{\rho}$. Moreover, since N commutes with U and also with ρ, it also commutes with $\widetilde{\rho}$, wherefore $P_0\mathcal{H}$ and $P_1\mathcal{H}$ are invariant under $\widetilde{\rho}$.

(D2) $\mathrm{si}(\rho_{N_0'}) = \mathrm{si}(\rho_{N_0})$:
This is trivially true due to $N_0 = N_0'$: On $\ker P$, U is not affected by V, and therefore this part of the -1 eigenspace is not changed by the perturbation. Consider the eigenvalue equation $U'\psi = -\psi$, which, inserting $V = \mathbb{1} - 2P$, reads

$$(U + \mathbb{1})\psi = 2PU\psi. \tag{3.30}$$

The solutions $\psi \in N_0'\mathcal{H}$ correspond to the case where both sides are identically zero.

(D3) $\mathrm{si}(\widetilde{\rho}_{P_1}) = -\mathrm{si}(\rho_{N_1})$:
Note that on $N\mathcal{H}$, the kernel of P is given by $N_0\mathcal{H}$. Hence, considered as a map $P\colon N_1\mathcal{H} \to P_1\mathcal{H}$, P is a bijection. Moreover, as already seen in (3.29) and the discussion thereafter, P intertwines ρ on $N_1\mathcal{H}$ with $\widetilde{\rho}' = ur\widetilde{\rho}_g$ on $P_1\mathcal{H}$. Taking the polar isometry of this intertwining map, we get a unitary equivalence between ρ_{N_1} and $\widetilde{\rho}'_{P_1}$, wherefore we conclude $\mathrm{si}(\widetilde{\rho}'_{P_1}) = \mathrm{si}(\rho_{N_1})$. The modification for $\widetilde{\rho}' = ur\widetilde{\rho}$, however, is exactly the one, which leads to the inverse element of the index group (see Lemma 2.3.7). Hence, we get $\mathrm{si}(\rho_{N_1}) = \mathrm{si}(\widetilde{\rho}'_{P_1}) = -\mathrm{si}(\widetilde{\rho}_{P_1})$.

(D4) $\mathrm{si}(\widetilde{\rho}_{P_0}) = \mathrm{si}(\rho_{N_1'})$:
In order to tackle this last equality, we need to investigate the solutions to the eigenvalue equation (3.30) in detail. We already discussed those solutions, where both sides are identically zero in (D2), since these span $N_0'\mathcal{H} = N_0\mathcal{H}$. $N_1'\mathcal{H}$ on the other hand is spanned by the non-zero solutions. Let $\varphi \neq 0$ be a vector, which is equal to both sides in (3.30). Then, by the right hand side of (3.30), we get $\varphi \in P\mathcal{H}$ and by the left hand side we get $\varphi \in N^\perp\mathcal{H}$. Hence, $\varphi \in P_0\mathcal{H}$. Moreover, by $\varphi = (U + \mathbb{1})\psi \neq 0$, we also have $\psi \in N^\perp\mathcal{H}$. Restricted to $N^\perp\mathcal{H}$, the inverse of $(U+\mathbb{1})$ exists[14], wherefore we can compute ψ form φ via $\psi = (U + \mathbb{1})^{-1}\varphi$. Inserting this back into (3.30), multiplying everything with P_0 from the left and using $\varphi = P_0\varphi$, we get the consistency condition

$$-iH\varphi := P_0(\mathbb{1} - U)(U + \mathbb{1})^{-1}P_0\varphi = 0, \tag{3.31}$$

which defines a $\widetilde{\rho}_{P_0}$ admissible Hamiltonian H on $P_0\mathcal{H}$. Indeed, inserting $\mathbb{1} = U^*U$, we get

$$\begin{aligned} P_0(\mathbb{1} - U)U^*U(U + \mathbb{1})^{-1}P_0 &= P_0(U^* - \mathbb{1})(\mathbb{1} + U^*)^{-1}P_0 \\ &= -\left[P_0(\mathbb{1} - U)(U + \mathbb{1})^{-1}P_0\right]^*, \end{aligned} \tag{3.32}$$

[14]Such a restricted inverse is also called a **pseudo inverse**. It is bounded due to the essential gap condition. For simplicity, we simply denote it by $(U+\mathbb{1})^{-1}$, given, that we restrict considerations to $\ker(U+\mathbb{1})^\perp$ here.

which shows self-adjointness of H. Moreover, we have

$$\begin{aligned}\widetilde{\rho}_g H \widetilde{\rho}_g^* &= \widetilde{\rho}_g \left[iP_0(\mathbb{1}-U)(U+\mathbb{1})^{-1}P_0\right]\widetilde{\rho}_g^* \\ &= u(g)\left[iP_0\widetilde{\rho}_g(\mathbb{1}-U)(U+\mathbb{1})^{-1}\widetilde{\rho}_g^* P_0\right] \\ &= u(g)\left[iP_0(\mathbb{1}-U^{ur(g)})(U^{ur(g)}+\mathbb{1})^{-1}P_0\right] \\ &= u(g)ur(g)\left[iP_0(\mathbb{1}-U)(U+\mathbb{1})^{-1}P_0\right] \\ &= r(g)H,\end{aligned} \tag{3.33}$$

where we used $\widetilde{\rho}_g U \widetilde{\rho}_g^* = \rho_g U \rho_g^* = U^{ur(g)}$ ($s \equiv 1$ here) in the third step, and (3.32) in the fourth step. Hence, H is admissible for $\widetilde{\rho}$. Now, since there obviously exists a gapped Hamiltonian on $P_0\mathcal{H} \ominus \ker H$ (H itself), by Lemma 2.3.5, we conclude that

$$\mathrm{si}(\widetilde{\rho}_{P_0}) = \mathrm{si}(\widetilde{\rho}_{\ker H}). \tag{3.34}$$

Finally, we relate the symmetry representations $\widetilde{\rho}_{\ker H}$ and ρ_{N_1} with each other. Every φ, which is a non-zero realization of (3.30), fulfils the consistency condition (3.31) and, moreover, the vectors ψ solving (3.30) span $N_1'\mathcal{H}$. Therefore, multiplying $\varphi = (U+\mathbb{1})\psi$ with $(U+\mathbb{1})^{-1}$ from the left, we conclude that $(U+\mathbb{1})^{-1}$ bijectively maps $\ker H$ onto $N_1'\mathcal{H}$. Moreover, by

$$\begin{aligned}(U+\mathbb{1})^{-1}\widetilde{\rho}_g\varphi &= (U+\mathbb{1})^{-1}U^{\frac{1}{2}(1-ur(g))}\rho_g\varphi \\ &= \rho_g(U^{ur(g)}+\mathbb{1})^{-1}U^{\frac{1}{2}(ur(g)-1)}\varphi \\ &= \rho_g\left(U^{\frac{1}{2}(1+ur(g))}+U^{\frac{1}{2}(1-ur(g))}\right)^{-1}\varphi \\ &= \rho_g(U+\mathbb{1})^{-1}\varphi,\end{aligned} \tag{3.35}$$

$(U+\mathbb{1})^{-1}$ intertwines the symmetry representations $\widetilde{\rho}_{P_0}$ and $\rho_{N_1'}$. Note that we used $s(g)=1$ for all g, which is valid for all symmetries from the tenfold way. Similar as in (D3), the polar isometry of $(U+\mathbb{1})^{-1}$ defines a unitary equivalence of these representations, wherefore we get

$$\mathrm{si}(\widetilde{\rho}_{\ker H}) = \mathrm{si}(\rho_{N_1'}), \tag{3.36}$$

which together with (3.34) finishes the proof. □

For symmetry types that are not part of the tenfold way, a formula as (3.24) would have the fundamental problem that the two sides of the equation were no longer part of the same algebraic structure since the index group for U and U' is in general different from the perturbation index group. It might still be possible to detect the gentleness of a compact perturbation by changes of the indices $\mathrm{si}_\star$ without having an explicit formula. However, this is not possible in general. We conclude the section with three finite-dimensional examples, which show that beyond the tenfold way, any possible relation between the gentleness of a perturbation and the symmetry indices $\mathrm{si}_\leftrightarrow$ and $\mathrm{si}_\updownarrow$ can occur:

- Types with non-trivial index groups that do not allow for non-gentle perturbations at all.

- Non-gentle perturbations that do not affect $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$.
- Non-gentle perturbations that are detectable by $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$.

First, we take a closer look at unitaries of symmetry type 10, which has a non-trivial index group but a trivial perturbation index group, i.e. every compact perturbation turns out to be gentle. Second, we discuss an explicit example of symmetry type 27, exhibiting non-gentle perturbations with $\mathrm{si}(U' : U) \neq 0$, which do not change the symmetry indices, i.e. $\mathrm{si}_{\leftrightarrow}(U') = \mathrm{si}_{\leftrightarrow}(U)$ and similarly for $\mathrm{si}_{\updownarrow}$. Finally, we give an example of a non-gentle perturbation of symmetry type 11, which changes the symmetry indices $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$.

Example 3.2.9 (Symmetry type 10)**.** *Type 10 consists of the three unitary symmetries σ, γ and σ_γ, which commute pairwise and therefore all square to $+\mathbb{1}$ in phase convention II. The perturbation symmetry type is defined by*

$$\widetilde{\sigma} = \sigma, \qquad \widetilde{\gamma} = U\gamma, \qquad \text{and} \qquad \widetilde{\sigma}_\gamma = U\sigma_\gamma. \tag{3.37}$$

According to Lemma 3.2.2 it is equivalent to type 11, apart from the action on a perturbation V. As discussed in the proof of Lemma 3.2.2, the squares of the generators $\widetilde{\sigma}$ and $\widetilde{\gamma}$ remain unchanged but we get $\widetilde{\sigma}_\gamma^2 = -\mathbb{1}$ and the symmetry operators now anti-commute pairwise.

Considering the appropriate symmetry action (3.20) *for a perturbation now already renders each representation of $\widetilde{\rho}$ to be balanced. Indeed, setting*

$$\widetilde{V} = i\widetilde{\sigma}, \tag{3.38}$$

we find, that $\widetilde{V}$ is admissible with respect to (3.20)*, and by $\widetilde{V}^2 = -\mathbb{1}$ also gapped at ± 1. In particular, for any admissible perturbation $U' = VU$ of a type 10 admissible unitary U, the representation $\widetilde{\rho}$ leaves invariant $\mathcal{H}_V^-$, wherefore the perturbation subspace always hosts the gapped admissible unitary $i\widetilde{\sigma}_{\mathcal{H}_V^-}$. Hence, we get*

$$\mathrm{si}(U' : U) = 0 \tag{3.39}$$

for every compact perturbation, which by Theorem 3.2.6 implies that every compact perturbation is gentle.

At first sight, the considerations above seem to imply that there are no finite-dimensional unitaries of symmetry type 10 with non-trivial symmetry indices $\mathrm{si}_\star$ because any finite-dimensional unitary is just a compact perturbation of the identity. Hence, if there are no non-gentle compact perturbations, there can also not be a non-trivial unitary. However, this reasoning is based on the implicit assumption that the identity is admissible, which is wrong. The identity cannot be admissible for any type involving a symmetry with $s = -1$, e.g. type 10.

Example 3.2.10 (Symmetry type 27)**.** *Symmetry type 27 consists of the three symmetries γ, σ_τ and σ_η, the latter two of which are antiunitary. It is characterized by $\sigma_\eta^2 = -\sigma_\tau^2 = \mathbb{1}$*

and imposes a rectangular eigenvalues-orbit on admissible unitaries. On $\mathcal{H} = \mathbb{C}^4$, consider the explicit representation ρ given by

$$\gamma = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}, \qquad \sigma_\tau = \begin{pmatrix} -i\sigma_y & 0 \\ 0 & -i\sigma_y \end{pmatrix} K, \qquad \textit{and} \qquad \sigma_\eta = \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} K. \quad (3.40)$$

This representation exhibits the admissible unitary

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \sigma_z & -i\sigma_x \\ -i\sigma_x & -\sigma_z \end{pmatrix}, \quad (3.41)$$

with $\mathrm{spec}(U) = \{\pm e^{\pm i\pi/4}\}$. *Hence, ρ is balanced and we have* $\mathrm{si}_\star(U) = 0$, *for* $\star \in \{\updownarrow, \leftrightarrow\}$. *The corresponding perturbation symmetry type according to Lemma 3.2.2 is type 24. However, considering the action on multiplicative perturbation operators* (3.20), *type 24 becomes equivalent to type 20 (i.e.* BDI), *which is part of the tenfold way. The corresponding perturbation representation $\widetilde{\rho}$ is given by*

$$\widetilde{\gamma} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & -\sigma_y \\ -\sigma_y & -\mathbb{1} \end{pmatrix}, \qquad \widetilde{\sigma}_\tau = \frac{1}{\sqrt{2}} \begin{pmatrix} -\sigma_x & -i\sigma_z \\ -i\sigma_z & \sigma_x \end{pmatrix} K, \qquad \textit{and} \qquad \widetilde{\sigma}_\eta = \sigma_\eta \quad (3.42)$$

For finite-dimensional representations $\widetilde{\rho}$ of type BDI *the symmetry index $\widetilde{\mathrm{si}}_-(V)$ of an admissible unitary V can be calculated via $\widetilde{\mathrm{si}}_-(V) = 1/2\,\mathrm{tr}\,(\widetilde{\gamma}(\mathbb{1} - V))$ ([CGG+18], see also Section 2.3.1). Hence, the admissible perturbation*

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathbb{1} & \sigma_y \\ \sigma_y & \mathbb{1} \end{pmatrix}, \qquad \textit{with} \qquad \widetilde{\mathrm{si}}_-(V) = \frac{\mathrm{tr}\big(\widetilde{\gamma}(\mathbb{1} - V)\big)}{2} = 2 \quad (3.43)$$

has a non-trivial perturbation index. The resulting perturbed unitary $U' = VU$ evaluates to

$$U' = \begin{pmatrix} -\sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}. \quad (3.44)$$

U' is already in diagonal form, such that we can simply read of the eigenvalues, which are contained in $\{\pm 1\}$, wherefore we trivially get $\mathrm{si}_\updownarrow(U') = 0$. Moreover, since the real eigenvalues span the whole space and we started with a balanced representation we also get $\mathrm{si}_\leftrightarrow(U') = 0$. Hence, to conclude, we constructed an example of a non-gentle perturbation $U' = VU$, with $\mathrm{si}(U' : U) = 2$, of a type 27-admissible unitary, which leaves invariant the symmetry indices $\mathrm{si}_\star$. This certainly rules out a general version of Proposition 3.2.8 beyond the tenfold way.

In both examples above, the symmetry indices were invariant under the non-gentle perturbations under consideration. Let us close the discussion with an example of a non-gentle perturbation of type 11, which changes $\mathrm{si}_\leftrightarrow$ and $\mathrm{si}_\updownarrow$.

Example 3.2.11 (Symmetry type 11)**.** *Type 11 corresponds to the same group as type 10, i.e. it contains σ, γ and σ_γ, with the difference, that σ and γ anti-commute. For this example it suffices to consider only one irreducible representation, which is given by a copy of the Pauli-matrices (up to a factor of i for the third symmetry). Without loss of generality, we chose*

$$\sigma = \sigma_z \qquad \gamma = \sigma_x \qquad \sigma_\gamma = i\sigma_y. \quad (3.45)$$

Being two-dimensional, this representation is certainly not balanced, since the eigenvalue-orbits are rectangular (see Section 2.3.1). It is easy to see, that

$$U = \gamma \quad \textit{and} \quad U' = \sigma_\gamma \tag{3.46}$$

serve as admissible unitaries. Since U has eigenvalues ± 1 and U' has eigenvalues $\pm i$, they certainly have different values of $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$, namely

$$\mathrm{si}_{\leftrightarrow}(U) = \mathrm{si}_{\updownarrow}(U') = 2 \ \ (\in 2\mathbb{Z}_2) \quad \textit{and} \quad \mathrm{si}_{\updownarrow}(U) = \mathrm{si}_{\leftrightarrow}(U') = 0. \tag{3.47}$$

Consequently, since $\mathrm{si}_\star$ are homotopy invariants, the corresponding perturbation between U and U'

$$V = U'U^* = \sigma_\gamma \gamma = \sigma \tag{3.48}$$

is non-gentle.

3.3 Locality and index

One of the key ingredients for the definition of quantum walks, or rather any physical system, is locality, that is, some kind of bound on the spreading of information through a lattice per unit of time. The usual standing assumption for locality in discrete-time quantum walks is a strict upper bound on the jump-length in every time step (compare Section 1.4), but for many use cases, this assumption is too rigid. Given, e.g. a time-independent Hamiltonian H with interaction terms that only affect neighbouring cites on a lattice, respectively, the time evolution operator $U_t = \exp(iHt)$ generically does not end up being strictly local, but exhibits interaction between far away cites with exponentially decaying strength [LR72].

Starting with strict locality, we first generalise this concept to band dominated operators, which are norm-limits of strictly local ones. After a second generalisation step, our standing assumption will be **essential locality**. Being a rather weak locality assumption, essential locality still allows for a complete topological classification of unitary operators on the one-dimensional lattice via an integer valued index. We go on and discuss a classifying index for local operators. Starting with the information flow index [Kit06, GNVW12] for strictly local walks on the one-dimensional lattice, we arrive at the **right Fredholm index** for band dominated and essentially local operators. [RRR04, Wil09, CGG$^+$18, CGWW21]. This index is complete for the set of essentially local operators and precisely distinguishes the unitaries that allow for a Floquet type driving from those for which no such drivings exist [GNVW12, CGWW21]. Thereby we also discuss the concept of **decoupling** an essentially local unitary with respect to a splitting of the one-dimensional lattice into two half-chains. This decoupling will be the basis for later definitions of topological invariants with additional symmetries in Section 3.5. Moreover, the decoupling construction is one of the main ingredients in Chapter 4, where we prove that any strictly local unitary on the one-dimensional lattice can be factorised into a sequence of shift and coin operations [CGW21].

3.3.1 Locality conditions

Let us start by recalling the framework from Section 1.4, i.e. the underlying Hilbert space for single particles on the one-dimensional lattice with inner degrees of freedom. Similarly to (3.5), let

$$\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x, \tag{3.49}$$

where the cell dimensions $d_x = \dim \mathcal{H}_x$ are uniformly bounded from above, i.e. there exists a $d \in \mathbb{N}$, such that $d_x < d$ for all $x \in \mathbb{Z}$. We address parts of the system, e.g. a single cell, a collection of cells, or a whole half-chain via the projections

$$P_x\mathcal{H} = \mathcal{H}_x, \qquad P_X = \bigoplus_{x\in X\subset\mathbb{Z}} \mathcal{H}_x, \qquad P_{\geq x} = P_{[x,\infty)}. \tag{3.50}$$

Typically, if not specified otherwise, we will abbreviate $P = P_{\geq 0}$.

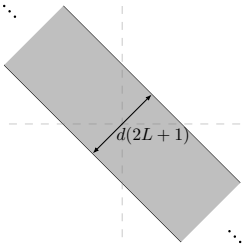
Definition 3.3.1. *An operator A on $\mathcal{H}$ as in* (3.49) *is called* ***strictly local*** *or* ***banded****, if there exists an $L \in \mathbb{N}$, such that*

$$\langle \psi_m, A\psi_n\rangle = 0, \quad \forall\, \psi_x \in \mathcal{H}_x, \text{ such that } |n-m| > L. \tag{3.51}$$

We call the minimal L, for which this is valid, the jump length or interaction length of A.

If not specified otherwise, we will choose a basis, which respects the order of the underlying spacial structure, i.e. the basis elements of the individual cells $\mathcal{H}_x$ are labelled right after another, following those of $\mathcal{H}_{x-1}$, and to be followed by those of $\mathcal{H}_{x+1}$ and so on in both directions $(-\infty \leftarrow x \rightarrow \infty)$. This leads to a straight forward identification of any Hilbert space of the form (3.49) with $\ell^2(\mathbb{Z})$ equipped with the standard basis, by regrouping $\mathbb{Z}$ into the cells $\mathcal{H}_x$. Considered as a doubly infinite matrix with respect to this basis, the non-zero matrix elements of a strictly local operator A all lie on the $(\max(\dim \mathcal{H}_x)) \cdot (2L+1) = d_{max}(2L+1)$ diagonals around the main diagonal, i.e.

$$A = \begin{pmatrix} \ddots & & & \\ & & & \\ & & & \\ & & & \ddots \end{pmatrix}.$$



Hence, the term **banded**.

Observation 3.3.2. *As long as the local cell Hilbert spaces are uniformly bounded from above, a strictly local operator with respect to some one-dimensional local structure is strictly local with respect to any other one-dimensional local structure. This fails if we allow the cell dimensions to diverge.*

The identification allows us to think of the decomposition into local cells more as an additional "graining" of $\ell^2(\mathbb{Z})$, which does not affect the locality with respect to $\ell^2(\mathbb{Z})$. Hence, we will mostly speak about banded operators and their generalisations on $\mathcal{H} = \ell^2(\mathbb{Z})$ in the following, keeping in mind that everything also applies to the "grained" versions $\mathcal{H} = \bigoplus \mathcal{H}_x$.

Given two banded operators A and B, it is obvious that their sum, their product, and their adjoints are again banded, with jump lengths

$$L_{A^*} = L_A, \qquad L_{A+B} = \max\{L_A, L_B\}, \qquad \text{and} \qquad L_{AB} \leq L_A + L_B. \tag{3.52}$$

In other words, the set of banded operators on $\mathcal{H}$ forms a $*$-algebra. The first generalisation step for the locality condition is to close this algebra in operator norm and to consider the resulting C^* algebra as the new set of "local" operators.

Definition 3.3.3. *An operator A on $\mathcal{H}$ is called **band-dominated** if there is a norm-convergent sequence of strictly local operators A_n, such that*

$$\lim_{n\to\infty} A_n = A. \tag{3.53}$$

We denote the C^*-algebra of band-dominated operators on $\mathcal{H}$ by $\mathcal{A}_{bd}$.

We will not discuss the algebra of band-dominated operators here in detail. The interested reader is referred to [RRS98, RRR04, Wil09] and further references therein. Instead, let us introduce our standing assumption for a "local" operator: **essential locality**. It is a weaker notion of locality than band-dominatedness and is motivated by two observations: The more fundamental one is the fact that essential locality is the most general form of locality, for which the **right Fredholm index** (or sometimes just called the **index**) of an operator with a locality condition makes sense and is complete. However, while this was the driving force for us to come up with the definition, we will content ourselves with this bit of outlook here since we discuss the index in great detail a little later. For the second observation, consider the commutator of a strictly local operator with a half-space projection $P_{\geq x}$. By definition, its rank is upper bounded by $2L$. Hence, every strictly local operator has a finite rank commutator with every half-space projection. Note, however, that this is insufficient, as the following example of a band-dominated but not a strictly local operator shows.

Example 3.3.4. *Let*

$$\psi = \sum_{x=1}^{\infty} 1/\sqrt{2}^x \psi_x \qquad \text{and} \qquad \varphi = \sum_{x=-1}^{-\infty} 1/\sqrt{2}^{|x|} \varphi_x \tag{3.54}$$

for some normalized $\psi_x, \varphi_x \in \mathcal{H}_x$, and set $A = |\varphi\rangle\langle\psi| + |\psi\rangle\langle\varphi|$. Then $[A, P_{\geq 0}]$ has rank 2, but we get

$$\langle \varphi_{-x}, A\psi_x\rangle = 1/2^x \neq 0 \quad \forall x > 0, \tag{3.55}$$

and hence, there is no L, such that (3.51) is fulfilled.

It would not be too unreasonable to lift the finite rank of $[A, P_{\geq x}]$ to the strict locality assumption, replacing strictly finite jump length, but this would not include all band-dominated operators. A similar lift of assumptions happens in the generalisation step to essentially local operators. The approximation property of band dominated operators transfers to the commutator with a given half-space projection. Hence, the commutator of a band-dominated operator with the $P_{\geq x}$ is the norm limit of finite rank operators, and therefore compact (see Section 1.2). While every band dominated operator has a compact commutator with any half-space projection, the opposite is not necessarily true (see Example 3.3.10). Raising the compactness of the commutator to the defining property results in essential locality:

Definition 3.3.5. *An operator A on $\mathcal{H}$ is called **essentially local**, if its commutator with the halfspace projection $P_{\geq 0}$ is compact. An essentially local unitary is called a **quantum walk**.*

Essential locality will be the standing assumption for quantum walks for the remainder of this thesis, and we will particularly specify strict locality when strictly local walks are under consideration (e.g. in Chapter 4).

At first sight, essential locality seems to be ill-defined because the definition depends on the choice of the specific half-space projection $P_{\geq 0}$. Nevertheless, as the following lemma show, the definition is, in fact, independent of the cut point:

Lemma 3.3.6. *The commutator of an operator A with a half-space projection $P_{\geq x}$ is compact for every $x \in \mathbb{Z}$ if and only if A is essentially local in the sense above. In particular, an operator of the form $A = A_L \oplus A_R$, with $A_{L/R}$ acting only on the half-spaces $P_{<x}\mathcal{H}$ and $P_{\geq x}\mathcal{H}$, respectively, is essentially local.*

Proof. For the non-trivial direction, let A be essentially local, i.e., let $[A, P_{\geq 0}]$ be compact. Then, for every $x \in \mathbb{Z}$, $Q := P_{\geq x} - P_{\geq 0}$ is of finite rank. Therefore

$$[A, P_{\geq x}] = [A, P_{\geq 0} + Q] = [A, P_{\geq 0}] + [A, Q], \tag{3.56}$$

differs from $[A, P_{\geq 0}]$ by a finite rank operator, and hence, is also compact.

For $A = A_L \oplus A_R$ we have $[A, P] = 0$. □

Similar to band-dominated operators, the set of essentially local operators forms a C^* algebra:

Lemma 3.3.7. *Let $\mathcal{H}$ as above. Then the set of essentially local operators $\mathcal{A}_{el} \subset \mathcal{B}(\mathcal{H})$ forms a C^*-algebra.*

Proof. A^* is essentially local if and only if A is. Moreover, by $[P, AB] = A[P, B] + [P, A]B$ and $[P, A+B] = [P, A]+[P, B]$, the product and the sum of two essentially local operators A, B are again essentially local. Hence, $\mathcal{A}_{el}$ is a $*$-subalgebra of $\mathcal{B}(\mathcal{H})$ and we only need to check that it is norm-closed: Let $\{A_n \in \mathcal{A}_{el}\}_n$ be a norm-convergent series of essentially local operators with limit A. Then, $\|[P, A] - [P, A_n]\| = \|[P, A - A_n]\| \leq 2\|A - A_n\|$ implies that $[P, A]$ is the limit of a norm convergent series of compact operators. Since the compact operators are a norm-closed ideal in $\mathcal{B}(\mathcal{H})$, $[P, A]$ must be compact and hence, A is essentially local. □

The fact that $\mathcal{A}_{el}$ is a C^*-algebra is not just an interesting observation but enables us to apply the machinery of C^*-algebras. In particular, we get the following corollary of Theorem 1.3.1 in Section 1.3.

Corollary 3.3.8. *Let $\partial_t U(t) = -iH(t)U(t)$ be a Hamiltonian driving with a piecewise continuous function $[0,1] \ni t \mapsto H(t) \in \mathcal{A}_{el}$ of essentially local Hamiltonians with $U(0) \in \mathcal{A}_{el}$. Then the solution*

$$U(t) = \mathcal{T} \exp\left(-i \int_0^t H(s)ds\right) \in \mathcal{A}_{el}. \tag{3.57}$$

*is essentially local, and therefore an essentially local **quantum walk**, for all $t \in [0,1]$.*

This allows us to treat Hamiltonians and quantum walks on the same footing regarding the locality conditions. The more restricting strict locality would leave a discrepancy between the two pictures: Hamiltonian time evolution on the one hand and discrete-time quantum walks on the other. In particular, the Floquet operator of any periodically driven system with an essentially local Hamiltonian driving $H(t)$ is a quantum walk. Note that all we needed was the fact that the essentially local operators form a C^* algebra, wherefore the same statement holds for band dominated operators.

Another property of essentially local operators, which will turn out to be helpful later on, is the following:

Lemma 3.3.9. *Let $A \in \mathcal{A}_{el}$ be a Fredholm operator[15]. Then its absolute value $|A| = \sqrt{A^*A}$ and its polar isometry U_A are essentially local.*

Proof. The statement about the absolute value already follows from the continuous functional calculus for C^*-algebras (see Section 1.2). For the polar isometry, however, this is not generally true. But for $A \in \mathcal{A}_{el}$ we get

$$[P, A] = [P, U_A|A|] = U_A[P, |A|] + [P, U_A]|A|, \tag{3.58}$$

wherefore $[P, U_A]|A|$ is the difference of compact operators. Since A is Fredholm, the only way for $[P, U_A]|A|$ to be compact is compactness of $[P, U_A]$ or, equivalently, essential locality of U_A. □

Above, we provided an example of an operator, which is band-dominated but not strictly local. Let us also give an example of an essentially local operator that is not band-dominated, thereby showing that the inclusion $\mathcal{A}_{bd} \subset \mathcal{A}_{el}$ is proper.

Example 3.3.10. *Let $\mathcal{H} = \ell^2(\mathbb{Z})$ and $\{e_x\}_{x\in\mathbb{Z}}$ be the standard positional basis for $\mathcal{H}$. We define an operator A as a permutation of basis elements via a bijective mapping between the sets $\{e_{3x}\}_{x\in\mathbb{Z}}$ and $\{e_{3x+1}, e_{3x+2}\}_{x\in\mathbb{Z}}$. In particular we set*

$$Ae_x = \begin{cases} e_{\lfloor x/2 \rfloor + 1} & x \equiv 0 \bmod 3 \\ e_{2x-2} & x \equiv 1 \bmod 3 \\ e_{2x-1} & x \equiv 2 \bmod 3. \end{cases} \tag{3.59}$$

It can easily be checked that this is indeed a bijection on $\mathbb{Z}$. Figure 3.2 shows a matrix plot of a section of A around zero. From this, it becomes apparent that A has matrix elements of value 1,

[15] See Section 1.2.

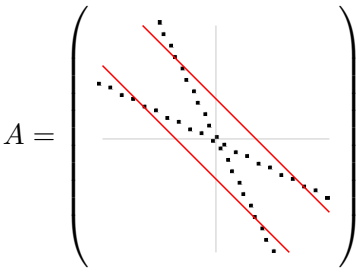


Figure 3.2: Matrixplot of a section of A, for $x \in [-30, 30]$. Black squares represent matrix elements $A_{nm} = 1$ and all others are 0. The red lines depict a possible banded operator, from which it becomes clear that A has matrix elements of value 1 outside of any possible banded region.

whose distance to the main diagonal increases linearly in x. This implies that A has at least norm-distance 1 to every banded operator. Therefore, there cannot exist a norm-convergent sequence of banded operators converging to A, and hence, A is not band dominated. On the other hand, by definition, for $x \geq 0$ and $e_y = Ae_x$ we also get $y \geq 0$. Hence, A commutes with the half-space projection $P_{\geq 0}$ and is therefore essentially local.

Interlude: Locality for translation invariant operators. A translation invariant operator A on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ acts as a multiplication operator $\widehat{A}(k)$ in momentum space, i.e. after Fourier transformation (see Section 1.4.2) we get

$$\widehat{(A\psi)}(k) = \widehat{A}(k)\widehat{\psi}(k), \quad \widehat{\psi} \in \mathcal{L}^2(\mathbb{T}) \otimes \mathbb{C}^d,\ \widehat{A}(k) \in \mathcal{B}(\mathbb{C}^d). \tag{3.60}$$

For these, the different locality conditions can be expressed via continuity conditions on the multiplication operator $\widehat{A}(k)$ [CGS$^+$18]. We already discussed this for strictly local operators, for which $\widehat{A}(k)$ turns out to be a Laurent polynomial in e^{ik}. The following theorem collects the results for band dominated and essentially local operators from [CGS$^+$18, Propositions 2.1 and 2.2].

Theorem 3.3.11. *Let A be a translation invariant operator on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ and $\widehat{A}(k),\ k \in [-\pi, \pi]$ the corresponding multiplication operator. Then A is*

i) strictly local, if and only if $\widehat{A}(k)$ is a Laurent polynomial of finite degree in e^{ik}.

ii) band-dominated, if and only if $\widehat{A}(k)$ is continuous with periodic boundary conditions.

iii) essentially local, if and only if $\widehat{A}(k)$ is quasi-continuous with periodic boundary conditions.

The notion of quasi-continuity [Pel03, BS06] is defined as follows: Let L^∞ be the Banach space of essentially bounded measurable (possibly matrix-valued) functions on the unit circle with periodic boundary conditions and denote by C the subalgebra of continuous functions. Moreover, let $H^\infty \subset L^\infty$ be the subalgebra of functions with vanishing Fourier coefficients for negative powers. A function f is called quasi continuous

if it lies in $(C + H^\infty) \cap (C + \overline{H^\infty})$, i.e. it can be written as $f = g + h$ with $g \in C$ and $h \in H^\infty$ and a similar decomposition exists for f^*.

The continuity properties of the multiplication operators of local operators allow for the definition of winding numbers of, e.g. their determinant as indices for translation invariant walks [CGS$^+$18, GNVW12, Pel03]. In this thesis, however, we do not discuss the details of the classification when translation invariance is assumed but concentrate our considerations to the general case.

3.3.2 Indices for local operators

We now come to the definition of one of the most important quantities for the topological classification of quantum walks: the **right Fredholm index** or **information flow index**. To our knowledge, it was first introduced as the **flow of a unitary operator** by Kitaev [Kit06] and further developed as a complete index for strictly local quantum walks by Gross et al. [GNVW12], where also a corresponding version for quantum cellular automata was defined. In [Kit06] it was also connected to the index of a pair of projections, defined in [ASS94a]. Inspired by [ASS94a], we further generalised the index to essentially local unitaries in [CGG$^+$18], where its connection to another known index quantity, namely the right Fredholm index [RRR04, Wil09] (there, for band dominated operators) was established. The generalised index is a complete homotopy invariant for the set of essentially local unitaries on $\ell^2(\mathbb{Z})$ [CGWW21]. In this subsection, we will first define the index on the different levels of generality and discuss its properties. We then close the section with the completeness of the right Fredholm index for essentially local unitaries, a decoupling construction for essentially local unitaries with trivial index, and a characterisation of continuously driven one-dimensional lattice systems. The latter will serve as the motivating result for Chapter 5, where we focus on driven systems with chiral symmetry.

The information flow index

We start by introducing the flow of a unitary matrix for strictly local unitaries as it is defined in [Kit06].

Definition 3.3.12. *Let U be a banded unitary on $\mathcal{H}$ according to* (3.49)*. Then its **information flow index** is defined as* [16]

$$\operatorname{ind}(U) = \sum_{x<0\leq y} \operatorname{tr}(P_x U P_y U^*) - \operatorname{tr}(P_y U P_x U^*). \tag{3.61}$$

The map $U \mapsto \operatorname{ind}(U)$ is continuous and, as we will see later, $\operatorname{ind}(U)$ is integer-valued. Therefore, it must be constant on norm-continuous paths of banded operators. Actually, U does not have to be strictly local for the expression (3.61) to be well defined

[16] Note that in [Kit06] and [GNVW12] the index is defined the other way around, resulting in $\operatorname{ind} \to -\operatorname{ind}$. We chose this definition here, because it aligns better with later considerations and is also in line with our work in [CGG$^+$18, CGS$^+$18, CGWW21].

and integer valued. By [Kit06, Theorem C.1] it suffices to assume a weaker form of locality, namely algebraic decay of matrix blocks:

$$\|U_{yx}\|_{HS}^2 = \mathrm{tr}(U^* P_y U P_x) \leq c|x-y|^{-2\alpha}, \quad \forall x, y \in \mathbb{Z} \tag{3.62}$$

with constants $\alpha > 1, c > 0$ and $\|\cdot\|_{HS}^2$ denoting the Hilbert-Schmidt norm. This condition guarantees $[U, P]$, $(P = P_{\geq 0})$, to be a Hilbert-Schmidt operator and is therefore also sufficient for U to be essentially local (since every Hilbert-Schmidt operator is compact). Indeed, we have $[P, U] = PUP^\perp - P^\perp UP$, with $P^\perp = \mathbb{1} - P$. Considering the individual terms gives

$$\begin{aligned} \|PUP^\perp\|_{HS}^2 = \mathrm{tr}\left(U^* PUP^\perp\right) &= \sum_{x<0\leq y} \mathrm{tr}\left(U^* P_y U P_x\right) \\ &\leq \sum_{x<0\leq y} c|x-y|^{-2\alpha} = c\sum_{n=1}^{\infty} n \cdot n^{-2\alpha} = c\sum_{n=1}^{\infty} n^{-\alpha}, \end{aligned} \tag{3.63}$$

which converges if and only if $\alpha > 1$, and similarly for the other term. In [CGS$^+$18] (3.62) was given for the matrix norm instead of the Hilbert-Schmidt norm, but since $\|A\|_{HS}^2 \leq d\|A\|^2$, for a complex $d \times d$-matrix, (3.63) remains true after replacing c by dc.

Instead of directly proving that the expression in (3.61) is integer valued, we give an alternative definition, which was also introduced in [Kit06], and further elaborated on in [GNVW12]. This will in the end also lead to the general form of the index as the right Fredholm index of U, i.e. the Fredholm index of the right half-chain restriction PUP of U, which is integer-valued by definition and coincides with the definitions given before. Assuming for the moment strict locality of U, consider the commutator of U and P. For $\psi_x \in \mathcal{H}_x$, $\psi_y \in \mathcal{H}_y$ we get the matrix elements

$$\langle \psi_x, [U, P]\psi_y \rangle = \begin{cases} \langle \psi_x, U_{xy}\psi_y \rangle - \langle \psi_y, U_{yx}\psi_x \rangle & x < 0 \leq y \\ 0 & \text{else.} \end{cases} \tag{3.64}$$

Comparing (3.64) with (3.61), we find that the index is given by

$$\mathrm{ind}\, U = \mathrm{tr}\left(UPU^* - P\right) = \mathrm{tr}\left(Q - P\right). \tag{3.65}$$

Note that the necessary condition for this to be well defined is that $Q - P = UPU^* - P$ is a trace class operator, which is also in line with the condition (3.62) given in [Kit06]. Expressing the index as the trace of the difference of two projections makes the connection between the information flow index and the index of a pair of projections, defined in [ASS94a], which finally leads to the right Fredholm index of U.

The right Fredholm index

The right Fredholm index [RRR04, Wil09][17] is a straight forward generalization of the information flow index above to weaker locality conditions. Let us first define the index for essentially local operators and prove its equivalence to the information flow index for strictly local unitaries afterwards.

[17] In [RRR04, Wil09] it is called the **plus-index**.

Lemma 3.3.13. *Let U be an essentially local unitary on $\mathcal{H}$ and P a half-space projection. Then its projection to the half-line PUP is a Fredholm operator on $P\mathcal{H}$. Its Fredholm index*

$$\vec{\mathrm{ind}}\,(U) = \dim\ker{}_{P\mathcal{H}}(PUP) - \dim\ker{}_{P\mathcal{H}}(PU^*P) \tag{3.66}$$

*is called the **right Fredholm index** of U. Moreover, $\vec{\mathrm{ind}}$ is additive under products of essentially local unitaries U, V, i.e.*

$$\vec{\mathrm{ind}}\,(UV) = \vec{\mathrm{ind}}\,(U) + \vec{\mathrm{ind}}\,(V). \tag{3.67}$$

Proof. We can write U as

$$\begin{aligned} U &= (\mathbb{1}-P)U(\mathbb{1}-P) + PUP + P[P,U] + [U,P]P \\ &= U_L \oplus U_R + K, \end{aligned} \tag{3.68}$$

with $U_R = PUP|_{P\mathcal{H}}$ and similarly for U_L and $(\mathbb{1}-P)$. Thereby, K is compact by essential locality of U. Therefore, $U_L \oplus U_R$ is unitary up to a compact operator and hence, Fredholm. But since it is given by a direct sum, also the individual summands have to be Fredholm on their respective subspaces.

For equation (3.67) note, that

$$PUVP - PUPVP = PU(\mathbb{1}-P)VP = [P,U](\mathbb{1}-P)VP \tag{3.69}$$

is compact, by essential unitarity of U. Hence, $PUVP$ and $(PUP)(PVP)$ have the same Fredholm index. But the latter is the product of the two Fredholm operators PUP and PVP, since both, U and V are assumed to be essentially local. The statement in (3.67) then follows by additivity of the Fredholm index under products of Fredholm operators (Lemma 1.2.7). □

In [ASS94a] the index of a **Fredholm pair of projections** is introduced, which consists of two projections Q and P, such that the operator QP, considered as a map $QP\colon \operatorname{ran} P \to \operatorname{ran} Q$ is Fredholm. Their index is defined as the Fredholm index of QP with the appropriate restrictions to $\operatorname{ran} P$, and $\operatorname{ran} Q$ from the right and the left. Setting $Q = UPU^*$ for an essentially local unitary, this index coincides with the index defined above. In order to show this equality, as well as the equivalence to the flow index in case of a banded unitary U defined in (3.65), we introduce the following subspaces (compare [Hal69]):

$$\begin{aligned} \mathcal{H}_{00} &= \{\varphi\in\mathcal{H} \;\big|\; P\varphi = Q\varphi = 0\} &&= \ker P \cap \ker Q \\ \mathcal{H}_{11} &= \{\varphi\in\mathcal{H} \;\big|\; P\varphi = Q\varphi = \varphi\} &&= \operatorname{img} P \cap \operatorname{img} Q \\ \mathcal{H}_{10} &= \{\varphi\in\mathcal{H} \;\big|\; P\varphi = \varphi \wedge Q\varphi = 0\} &&= \operatorname{img} P \cap \ker Q \\ \mathcal{H}_{01} &= \{\varphi\in\mathcal{H} \;\big|\; P\varphi = 0 \wedge Q\varphi = \varphi\} &&= \ker P \cap \operatorname{img} Q \\ \mathcal{H}_{\perp} &= \bigcap_{pq} \mathcal{H}_{pq}^{\perp}. \end{aligned} \tag{3.70}$$

This decomposition of the Hilbert space with respect to P and Q will also turn out to be helpful later on for the decoupling of essentially (or strictly) local unitaries with $\vec{\mathrm{ind}} = 0$.

Inspired by [ASS94a], let us introduce the two self-adjoint operators

$$A = P - Q \qquad \text{and} \qquad B = \mathbb{1} - P - Q. \tag{3.71}$$

The following lemma describes how A relates to the subspaces introduced above and the connection of these to the index (compare [ASS94a, Proposition 3.1]):

Lemma 3.3.14. *Let P be a half-space projection and $Q = UPU^*$ be related to P via an essentially local unitary U. Moreover, let A be defined as above. Then:*

(1.) *The spectrum of A consists of finitely degenerated isolated eigenvalues and 0 is the only limit point. Moreover:*

$$\begin{aligned} H_{00} \oplus \mathcal{H}_{11} &= \ker A \\ \mathcal{H}_{10} &= \ker(A - \mathbb{1}) \\ \mathcal{H}_{01} &= \ker(A + \mathbb{1}) \\ \mathcal{H}_{\perp} &= \bigoplus_{\substack{\lambda \in \sigma(A) \\ 0<\lambda<1}} \ker(A - \lambda) \oplus \ker(A + \lambda). \end{aligned} \tag{3.72}$$

In particular, on $\mathcal{H}_{\perp}$, the eigenvalues of A come in pairs $\pm\lambda$, with $0 < \lambda < 1$.

(2.) *We have*

$$\overrightarrow{\mathrm{ind}}\,(U) = \dim \mathcal{H}_{01} - \dim \mathcal{H}_{10}. \tag{3.73}$$

(3.) *When A is trace class we get $\overrightarrow{\mathrm{ind}}\,(U) = -\operatorname{tr}(A)$.*

Note, that by [ASS94a, Proposition 3.1], (2.) connects the right Fredholm index to the Fredholm index of $QP\colon \operatorname{ran} P \to \operatorname{ran} Q$ defined therein.

Proof. (1.): By $P - Q = [P, U]U^*$ and essential locality of U, A is compact, which implies the stated spectral properties (Lemma 1.2.4). For the relations to the spaces $\mathcal{H}_{pq}$ and $\mathcal{H}_{\perp}$ note, that A and B from (3.71) fulfil the two equations

$$AB + BA = 0 \tag{3.74}$$

$$A^2 + B^2 = \mathbb{1}, \tag{3.75}$$

which both follow from straight forward algebra. The inclusion "$\subseteq$" in the first equation in (3.72) is trivial. So let $\varphi \in \ker A$. From (3.75) it follows, that $\ker A = \ker A^2 = \ker(\mathbb{1} - B^2)$. Hence, we either get $B\varphi = \varphi$ or $B\varphi = -\varphi$, which by $P\varphi = Q\varphi$ (on $\ker A$) implies $P\varphi = Q\varphi = 0$ in the first case and $P\varphi = Q\varphi = \varphi$ in the second, proving the inclusion "$\supseteq$". The equalities for $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$ follow by similar reasoning, using that for $\varphi \in \ker(A - \mathbb{1}) \oplus \ker(A + \mathbb{1})$ (3.75) implies $B^2\varphi = B\varphi = 0$.

On $\mathcal{H}_{\perp}$ it follows from (3.75) and the equalities we established so far, that $0 < A^2 < \mathbb{1}$ and therefore also $0 < B^2 < \mathbb{1}$. Hence we also get $\ker B \perp \mathcal{H}_{\perp}$. Now let $\varphi \in \mathcal{H}_{\perp}$ be an eigenvector of A, with eigenvalue λ (i.e. $A\varphi = \lambda\varphi$ with $0 < |\lambda| < 1$). Then, by (3.74), $A(B\varphi) = -\lambda(B\varphi)$, which yields a second eigenvector $B\varphi$ of A in $\mathcal{H}_{\perp}$, corresponding to the eigenvalue $-\lambda$.

(2.): Using $Q = UPU^*$, we get

$$\begin{aligned} \mathcal{H}_{10} &= \{\varphi \in P\mathcal{H} | UPU^*\varphi = 0\} = \{\varphi \in P\mathcal{H} | PU^*P\varphi = 0\} \\ &= \ker_{P\mathcal{H}}(PU^*P) \end{aligned}$$

and similarly also

$$\mathcal{H}_{01} = \{\varphi \in Q\mathcal{H} | QUQ\varphi = 0\} = \ker_{Q\mathcal{H}}(QUQ).$$

Now, by $\varphi \in Q\mathcal{H} \Rightarrow U^*\varphi \in P\mathcal{H}$, this gives

$$\begin{aligned} U^*\mathcal{H}_{01} &= \{U^*\varphi = \psi \in P\mathcal{H} | UPUP\psi = 0\} = \{\psi \in P\mathcal{H} | PUP\psi = 0\} \\ &= \ker_{P\mathcal{H}}(PUP). \end{aligned}$$

In particular $\dim \mathcal{H}_{01} = \dim \ker_{Q\mathcal{H}}(QUQ) = \dim \ker_{P\mathcal{H}}(PUP)$, which proves the statement.

$(3.)$ is a direct consequence of $(1.)$ and $(2.)$. □

Of course, the definition of $\vec{\mathrm{ind}}$ via a Fredholm index also applies to strictly local operators and by item $(3.)$ in the Lemma above, we know that this definition coincides with Definition 3.3.12, i.e. $\mathrm{ind}\,(U) \equiv \vec{\mathrm{ind}}\,(U)$. This finally also proves the integer valuedness of the former. We take the right Fredholm index as the standing definition in all cases from now on.

Example 3.3.15. *The prototypical example of a local unitary on $\ell^2(\mathbb{Z})$ with non-trivial index is the bilateral shift from Definition 1.4.4:*

$$Se_x = e_{x+1}, \tag{3.76}$$

where $\{e_x\}_{x\in\mathbb{Z}}$ denotes the standard positional basis for $\ell^2(\mathbb{Z})$.

PSP, considered on $P\mathcal{H}$, is the unilateral shift, the standard example of a Fredholm operator with a non-trivial Fredholm index. The kernel of PSP is trivial on $P\mathcal{H}$, whereas the kernel of PS^*P on $P\mathcal{H}$ is spanned by the basis element e_0. Therefore

$$\vec{\mathrm{ind}}\,(S) = 0 - 1 = -1. \tag{3.77}$$

Beside being a good standard example, the powers of the shift can also be used, to reach every index value, which proves that the map $\vec{\mathrm{ind}} : \mathcal{A}_{sl} \subset \mathcal{A}_{el} \to \mathbb{Z}$ is onto. By Lemma 3.3.13 we get

$$\vec{\mathrm{ind}}\,(S^n) = -n, \quad \forall n \in \mathbb{Z}. \tag{3.78}$$

Note, that this allows us to achieve a trivial index for any unitary, by simply multiplying with the appropriate shift.

$$\vec{\mathrm{ind}}\,(US^{\vec{\mathrm{ind}}\,(U)}) = \vec{\mathrm{ind}}\,(U) - \vec{\mathrm{ind}}\,(U) = 0, \quad \forall U \in \mathcal{A}_{el}. \tag{3.79}$$

If $\dim \mathcal{H}_x > 1$, the partial shift S_ϕ from Definition 1.4.4 can be considered as the standard example. All considerations above apply similarly.

Properties of the index

Having established the index for the types of locality we consider in this thesis, let us continue with its properties. The most fundamental one is its invariance under norm-continuous deformations.

Lemma 3.3.16. *Let $[0,1] \ni t \mapsto U_t$ be a norm-continuous family of essentially local unitaries. Then*

$$\overrightarrow{\mathrm{ind}}\,(U_t) = \overrightarrow{\mathrm{ind}}\,(U_0) \quad \forall t \in [0,1]. \tag{3.80}$$

Proof. Since U_t is a norm-continuous path of essentially local operators, PU_tP defines a norm-continuous path of Fredholm operators on $P\mathcal{H}$, the statement follows from norm-continuity of the Fredholm index (Lemma 1.2.7). □

This, of course, also establishes norm-continuity in the sets of strictly local and band-dominated operators. The Fredholm index is not only constant on norm-continuous paths of Fredholm operators but also under additive compact perturbations, which gives rise to a further invariance property of the index.

Lemma 3.3.17. *Let U, U' be essentially local unitaries, such that $U - U'$ is compact. Then*

$$\overrightarrow{\mathrm{ind}}\,(U) = \overrightarrow{\mathrm{ind}}\,(U'). \tag{3.81}$$

Proof. Again, the invariance follows directly from properties of the Fredholm index, since any compact perturbation U' of U gives rise to a compact perturbation $PU'P$ of PUP. Since the Fredholm index is invariant under the addition of compact operators (see Lemma 1.2.7), the statement follows. □

This property allows us to define the index also for **essentially unitary** operators, which are defined es as follows (see, e.g. [Lan84] for a detailed discussion on essentially unitary operators):

Definition 3.3.18. *An operator U is called to be **essentially unitary**, if $U^*U - \mathbb{1}$ and $UU^* - \mathbb{1}$ are compact.*

Since the right Fredholm index only needs Fredholmness of PUP, the index from Lemma 3.3.13 is well defined and stable under continuous as well as compact perturbations also on the set of essentially unitary operators.

So far, we have discussed the basic properties and invariances of the index for quantum walks. We collect the main results for this section in the following theorem, which we will often use in the remaining chapters. For strictly local unitaries, the statements were already proven in [GNVW12], but in order to provide a complete picture, we will give the full proof also here. For essentially local unitaries, we established item (*1.*) in [CGG$^+$18] and items (*2.*) and (*3.*) in [CGWW21].

Theorem 3.3.19. *Let U, U' be essentially (strictly) local unitaries on a Hilbert space $\mathcal{H}$ with a one-dimensional spatial structure as in* (3.49)*. Then*

(1.) ***Decoupling:*** *There exists is a compact (local) perturbation $\widetilde{U} = VU$ of U, such that $\widetilde{U} = U_L \oplus U_R$, if and only if $\overrightarrow{\mathrm{ind}}(U) = 0$. Thereby, the direct sum is with respect to a splitting of the Hilbert space into half-spaces $\mathcal{H} = \mathcal{H}_L \oplus \mathcal{H}_R = (1-P)\mathcal{H} \oplus P\mathcal{H}$, and U_L and U_R are unitary.*

(2.) ***Completeness:*** *There is a norm continuous path $t \mapsto U_t$ of essentially (strictly) local unitaries with $U_0 = U$ and $U_1 = U'$, if and only if $\overrightarrow{\mathrm{ind}}(U) = \overrightarrow{\mathrm{ind}}(U')$.*

(3.) ***Floquet type:*** *U is a Floquet unitary if and only if $\overrightarrow{\mathrm{ind}}(U) = 0$.*

This means there exists an essentially (or strictly) local Hamiltonian driving $[0,1] \ni t \mapsto H(t) = H(t)^*$, such that

$$U = U(1) = \mathcal{T} \exp\left(-i \int_0^1 H(t)dt\right) \tag{3.82}$$

is the endpoint of the solution to $\partial_t U(t) = -iH(t)U(t)$, $U(0) = \mathbb{1}$, where $\|H(t)\|$ is bounded for all $t \in [0,1]$ and piecewise constant.

We split the proof into three parts, proving each statement separately and discuss some of their implications and corollaries in between.

Proof of Theorem 3.3.19 (1.) ***Decoupling****:* Since a decoupled unitary $\widetilde{U}$ implies that $U_R = P\widetilde{U}P|_{P\mathcal{H}}$ is unitary, it follows that a decoupling is only possible if $\overrightarrow{\mathrm{ind}}(U) = \mathrm{ind}_F(U_R) = 0$. Conversely, we need to construct a decoupling for any U with $\overrightarrow{\mathrm{ind}}(U) = 0$. A unitary is decoupled if and only if it commutes with P. Hence, by $PVU = VUP \Leftrightarrow PV = VQ$, the decoupling unitary V needs to be another intertwining unitary for P and Q, with the additional assumption that $V - \mathbb{1}$ is compact (local).

We prove the existence of V in two steps, separately on the spaces $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$ and $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$. Starting with $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$, a first candidate, which is also discussed in [ASS94a], is B from (3.71). It fulfils $PB = BQ = -PQ$, but equals $-\mathbb{1}$ on $\mathcal{H}_{11}$, which is infinite-dimensional in general. Therefore $\mathbb{1} - B$ is not guaranteed to be compact. This can be fixed by flipping the sign on half of the chain, e.g. by multiplying B with $(\mathbb{1} - 2P)$, leading to an operator that was also considered in [Kat84] (in a different context):

$$X = (\mathbb{1} - 2P)B = \mathbb{1} - P - Q + 2PQ = \mathbb{1} + AQ - PA. \tag{3.83}$$

X still intertwines P and Q, and it is straight forward to check, that X is normal:

$$X^*X = XX^* = B^2 = (X + X^*)/2. \tag{3.84}$$

By this it also follows that the spectrum of X lies on a the circle $(a-1/2)^2 + b^2 = 1/4$ (for $z = a + ib \in \mathbb{C}$), i.e. a circle of radius $1/2$ around $1/2$ (see Figure 3.3). Moreover, we see that the kernel of X is precisely given by $\mathcal{H}_{10} \oplus \mathcal{H}_{01} = \ker(A^2 - 1)$. The last expression in (3.83) also makes clear that $\mathbb{1} - X$ is indeed compact since A is compact for an essentially local U. Clearly, X is not unitary. However, by the compactness of $\mathbb{1} - X$, the only limit point in the spectrum of X is 1, and the remaining spectrum consists of finitely degenerated isolated eigenvalues. This allows us to project every eigenvalue different

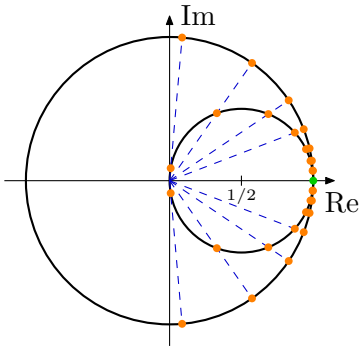


Figure 3.3: Visualisation of the spectra of X (inner circle) and V_X (outer circle). Orange points denote isolated eigenvalues, and the green point denotes the only limit point in the spectrum of both operators. The dashed lines depict the correspondence between the respective eigenvalues. Figure taken from [CGG+18].

from 1 onto the unit circle as depicted in Figure 3.3. The resulting operator V_X is unitary on the complement of its kernel and inherits from X the properties of intertwining P and Q and being a compact perturbation of the identity. Put differently: instead of X, we consider its polar isometry

$$V_X = (X^*X)^{-1/2}X, \tag{3.85}$$

which is unitary on the complement of $\ker X$.

Intertwining P and Q on the remaining subspace $\ker X = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$ is equivalent to swapping the direct summands. By $\overrightarrow{\mathrm{ind}}\,(U) = 0$ in combination with Lemma 3.3.14, the two summands are of the same finite dimension. Hence we can choose any swapping unitary $V_{\ker X}$, such that $V_{\ker X}\mathcal{H}_{10} = \mathcal{H}_{01}$ and vice versa. The overall decoupling is then given by

$$V = V_X \oplus V_{\ker X}. \tag{3.86}$$

Since $V_{\ker X}$ is a finite-dimensional unitary, $\mathbb{1} - V$ is compact whenever $\mathbb{1} - V_X$ is. Hence, we are done for essentially local unitaries. Moreover, note that the constructed V acts trivially on $\mathcal{H}_{00} \oplus \mathcal{H}_{11}$. For strictly local unitaries, the complement of these space, namely $\mathcal{H}_\perp \oplus \mathcal{H}_{10} \oplus \mathcal{H}_{01}$, is contained in a finite collection of cells $\mathcal{H}_{-L} \oplus \ldots \oplus \mathcal{H}_L$. Therefore, $\mathbb{1} - V$ acts non-trivially only on this finite number of cells and hence, the decoupling is local. □

Corollary 3.3.20. *The decoupling in (1.) of Theorem 3.3.19 can be chosen gentle. I.e. there is a continuous path of compact perturbations $[0,1] \ni t \mapsto U_t = V_t U$, such that U_1 is decoupled.*

Proof. V is a compact perturbation of the identity, i.e. $V - \mathbb{1}$ is compact. Therefore, 1 is the only limit point in spectrum of V and all other parts are isolated eigenvalues. Hence, we can continuously move every eigenvalue of V to 1, without changing the eigenspaces. This way, the resulting V_t remains a compact perturbation of the identity for all t. □

Proof of Theorem 3.3.19 (2.) ***Completeness*** *(and (3.) for strict locality):*
The only if part is already clear by invariance of $\vec{\mathrm{ind}}\,(\cdot)$ under norm-continuous deformations of the argument. This applies to both types of locality. It remains to construct a continuous path between any two unitaries with the same index. We do this by showing that any local unitary on $\mathcal{H} = \bigoplus \mathcal{H}_x$ with index $\vec{\mathrm{ind}}\,(U) = n$ can be deformed into S^{-n}, where S denotes a standard reference shift, which shifts a one-dimensional subspace of each $\mathcal{H}_x$ to the right. As a first step, note that $U = S^{-n}(S^n U)$ and $\vec{\mathrm{ind}}\,(S^n U) = \vec{\mathrm{ind}}\,(S^n) + \vec{\mathrm{ind}}\,(U) = 0$. Hence, it suffices to show that every local unitary with index zero can be deformed into the identity without breaking the respective locality condition on the way. We will do this separately for the two locality conditions:

Strict locality:[18] In case of a strictly local unitary U with interaction length L, the decoupling constructed above acts on $\mathcal{H}_{x-L} \oplus \ldots \oplus \mathcal{H}_{x+L-1}$ in order to decouple the walk with respect to $P_{<x}\mathcal{H} \oplus P_{\geq x}\mathcal{H}$. Hence, we can decouple the unitary simultaneously between every multiple of $2L$ cells without worrying about the decouplings interfering with each other. The resulting unitary $\widetilde{U} = VU = \bigoplus_n \widetilde{U}_n$ will be block diagonal with every block consisting of $2L$ cells. Moreover, the decoupling unitary $V = \bigoplus_m V_m$ is also block diagonal, with the same block size, but shifted by L blocks with respect to the decomposition of $\widetilde{U}$. Hence,

$$U = V^* \widetilde{U} = \left(\begin{array}{c} \ddots \\ \square \\ \square\square \\ \square \\ \ddots \end{array} \right) \left(\begin{array}{c} \square \\ \square\square \\ \square\square \\ \square \end{array} \right) \tag{3.87}$$

is the product of two block-diagonal unitaries[19]. Being block-diagonal, both operators are certainly strictly local, with an interaction length smaller or equal to $2L$. We can now deform each finite-dimensional block to the identity in the following way: consider the spectral decomposition of each block

$$\widetilde{U}_n = \sum_i e^{i\alpha_{n,i}} |\varphi_{n,i}\rangle\langle\varphi_{n,i}| \qquad \text{and} \qquad V_m^* = \sum_i e^{-i\beta_{m,i}} |\psi_{m,i}\rangle\langle\psi_{m,i}|, \tag{3.88}$$

and set

$$H_{\widetilde{U},n} = \sum_i -2\alpha_{n,i} |\varphi_{n,i}\rangle\langle\varphi_{n,i}| \qquad \text{and} \qquad H_{V^*,m} = \sum_i 2\beta_{m,i} |\psi_{m,i}\rangle\langle\psi_{m,i}|. \tag{3.89}$$

Finally, we combine these into a single time depend, but piecewise constant Hamiltonian on the full space via

$$H(t) = \begin{cases} \bigoplus_n H_{\widetilde{U},n} & \text{if } 0 \leq t \leq 1/2 \\ \bigoplus_m H_{V^*,m} & \text{if } 1/2 < t \leq 1 \end{cases}, \tag{3.90}$$

[18] There is an alternative proof, which uses the result from Chapter 4. By Theorem 4.2.2 every strictly local unitary can be written as a shift coin sequence. Decomposing U and U' with respect to the same shift-register, we just deform each coin to the identity in each cell. We are then left with a product of shift operations, which multiplies to $S^{\vec{\mathrm{ind}}\,(U)} = S^{\vec{\mathrm{ind}}\,(U')}$.

[19] Note that, although depicted all the same for better illustration, the individual blocks might be of different sizes due to $\dim \mathcal{H}_x \neq \dim \mathcal{H}_y$.

for $t \in [0,1]$. We get a continuous path

$$[0,1] \ni t \mapsto U(t) = \mathcal{T} \exp\left(-i \int_0^t H(s) ds\right), \tag{3.91}$$

which connects $U = U(1)$ with the identity $\mathbb{1} = U(0)$. Since we kept the block structure during the process, $U(t)$ is strictly local for all t. This also proves the "if"-part of item $(3.)$ for strictly local unitaries.

Essential locality: Let $VU = U_L \oplus U_R$ be a gentle decoupling for U, the existence of which we have already established. Since every decoupled unitary commutes with the half-space projection with respect to the point of decoupling, VU stays essentially local for every deformation of U_L and U_R. Since the unitary groups on $(\mathbb{1} - P)\mathcal{H}$ and $P\mathcal{H}$ are path-connected, respectively, we can deform U_L and U_R to the identities on the respective half-spaces, providing us with the desired deformation of U to $\mathbb{1}$ on the whole space. □

While the classification via the right Fredholm index is complete for strictly and essentially local unitary operators, respectively, it is, to our knowledge, not known whether the same holds for band dominated operators.

Open question: *Does Theorem 3.3.19 $(2.)$ also hold for band-dominated unitaries? Or, equivalently: Is the unitary group in the C*-algebra of band dominated operators on $\ell^2(\mathbb{Z}_+)$ path connected?*

The proof techniques for strict and essential locality above are both not applicable for band dominated operators. On the one hand, for band dominated operators, the decoupling space $\mathcal{H}_{10} \oplus \mathcal{H}_{01} \oplus \mathcal{H}_\perp$ for a single decoupling is not contained in a finite number of cells, such that we cannot perform an infinite number of decouplings simultaneously in order to break down the operator into a product of block-diagonal ones, with finite-dimensional blocks. On the other, it is not known whether the unitary group of the algebra of band-dominated operators on a half-line $\ell^2(\mathbb{Z}_+)$ is path-connected. The latter question is also mentioned in [RRR04], where the authors report having tried to prove this fact without succeeding. Moreover, the index is conjectured to be complete for band-dominated operators in a more recent work [KKT20a][20], where the authors find the same way of generalising the flow index via the right Fredholm index [RRR04][21], as can be found in our work [CGG$^+$18, CGS$^+$18, CGWW21] (and as detailed above).

It remains to prove item $(3.)$ for essentially local untiaries:

Proof of Theorem 3.3.19 $(3.)$ ***Floquet type*** *(for essential locality):* The "only if" part follows again from the invariance of the index under norm-continuous deformations. Every continuously driven process is continuously connected to the identity $(t \to 0)$. Since we already did the strictly local case in the proof of $(2.)$, let U be essentially local.

[20] The conjecture (Conjecture 6.3 in combination with the comment following Corollary 6.5) is contained in the first version of the arXiv publication. In an updated version [KKT20b] the authors removed the part containing it and instead refer to future work.

[21] In [RRR04] the authors discuss the right (and left) Fredholm index in its own right, without the context of the information flow index.

Differently from the strictly local case, the essentially local operators on $\mathcal{H}$ form a C^*-algebra $\mathcal{A}_{el}$. This allows us to solve the task of constructing a Hamiltonian driving by using the continuous functional calculus. The existence of a continuous path of essentially local unitaries $[0,1] \ni t \mapsto U_t$, connecting U with the identity is guaranteed by (2.). Moreover, there certainly exists a set of finitely many intermediate points $0 = t_0 < t_1 < t_2 < \ldots < t_n = 1$, with $\|U_{t_k} - U_{t_{k-1}}\| < 2$. I.e., setting $V_k = U_{t_k} U_{t_{k-1}}^*$, $k = 1, \ldots n$, we get

$$U = V_n V_{n-1} \ldots V_1, \tag{3.92}$$

with $\|V_k - \mathbb{1}\| < 2$. Now, in every C^*-algebra $\mathcal{A}$, a unitary V with $\|V - \mathbb{1}\| < 2$ can be written as $V = \exp(-iH)$, with a self-adjoint element $H \in \mathcal{A}$. Indeed, if $\|V - \mathbb{1}\| < 2$, V must be gapped at -1. Hence, we can set $H = i\log(V)$, where the branch cut of the logarithm is set to the negative real axis and therefore, $\log(\cdot)$ is continuous on the spectrum of V, which guarantees $\log(V) \in \mathcal{A}$. Hence, for each V_k we find an H_k, such that $V_k = \exp(-iH_k) = \exp\left(-i\int_{t_{k-1}}^{t_k} H_k/(t_k - t_{k-1})dt\right)$. The concatenation of the V_k can then be expressed as

$$U = \mathcal{T}\exp\left(-i\int_0^1 H(t)dt\right), \qquad \text{with} \qquad H(t) = \begin{cases} H_1/t_1, & \text{if } 0 < t < t_1 \\ \vdots & \vdots \\ H_k/(t_k - t_{k-1}), & \text{if } t_{k-1} < t < t_k \\ \vdots & \vdots \end{cases}, \tag{3.93}$$

i.e. $H(t)$ is a piecewise constant Floquet driving for U. □

The right Fredholm index decides whether a given discrete time evolution can be realised by some continuous driving process or not. One could now argue that this immediately rules out all discrete-time evolutions with non-trivial indices since, in the end, every process has to be driven continuously. We would not go so far as to question this last statement, but instead emphasise another aspect: The physical implementation for a designed system often only exploits part of the degrees of freedom of the underlying physical system (say, an arrangement of atoms in an optical lattice [KFC+09], or a sequence of laser pulses [SCP+10]). Consequently, the subsystem under consideration (be it the only one, one has control over, or simply the one one is interested in) might well exhibit index-wise non-trivial discrete-time evolutions, although the overall driving process was continuous. A particularly simple example for this is the bi-directional shift operation, which is often used for the definition of a quantum walk (see Section 1.4):

$$\begin{pmatrix} S & 0 \\ 0 & S^* \end{pmatrix} \in \mathcal{B}\left(\mathbb{C}^2 \otimes \ell^2(\mathbb{Z})\right), \qquad \begin{pmatrix} \varphi_x \\ \psi_x \end{pmatrix} \mapsto \begin{pmatrix} \varphi_{x+1} \\ \psi_{x-1} \end{pmatrix}. \tag{3.94}$$

The direct summands S and S^* have a non-trivial index, whereas the overall unitary is in the connected component of the identity. Hence, there exists a driving process for the whole unitary, but not for its individual components. In fact, by doubling the system, any non-trivial evolution can be trivialised via $U \mapsto U \oplus U^*$ [GNVW12]. However, the setting one deals with might restrict the access to the system to only one of the blocks

at full-time periods, which results in a non-trivial discrete time evolution. Precisely this non-triviality of a subsystem will be a cornerstone for the classification of chiral symmetric driven systems we will discuss later in Chapter 5. There, similar to the example above, the chiral symmetry imprints a 2×2 substructure onto the Hilbert space, with respect to which the operators can be considered as 2×2 block-matrices.

3.4 Decoupling under symmetry

We turn our focus back to symmetric unitaries, now equipped with a locality condition, i.e. quantum walks. So far, we discussed the symmetry index for admissible, that is, symmetric and essentially gapped unitaries, independently of the underlying lattice structure. In this section, we combine these general considerations with the concept of splitting the one-dimensional system into two half-chains, i.e. decoupling. This gives rise to another index quantity, the **left and right symmetry indices**, which serve as the bulk indices for the bulk-boundary correspondence of one-dimensional quantum walks. Moreover, in the case of the tenfold way, the right symmetry index becomes one of a set of three homotopy invariants $(\mathrm{si}, \mathrm{si}_+, \vec{\mathrm{si}})$, which provides a complete classification of symmetric quantum walks [CGG$^+$18]. Beyond the tenfold way, the situation is more complicated, and we were not able to generalize this result to all symmetry types. However, a weakened form of bulk-boundary correspondence also holds for the symmetry types beyond the tenfold way.

In this section, we first add the symmetry conditions to the decoupling construction from the last section. That is, we discuss the possibility of (gently) decoupling a given walk while keeping the symmetries of any symmetry type under consideration. For the symmetry types of the tenfold way with non-trivial index group, this is always possible. Beyond those, we will meet decoupling conditions, which must be fulfilled for a decoupling to exist. The necessary condition $\vec{\mathrm{ind}}\,(U) = 0$, on the other hand, is always fulfilled for admissible walks. Whenever the symmetry type contains a symmetry with $ur(g) = -1$, we get

$$\vec{\mathrm{ind}}\,(U) = \vec{\mathrm{ind}}\,(\rho_g U \rho_g^*)^{22} = \vec{\mathrm{ind}}\,(s(g)U^{ur(g)}) = ur(g)\,\vec{\mathrm{ind}}\,(U) = -\,\vec{\mathrm{ind}}\,(U). \tag{3.95}$$

Hence, $\vec{\mathrm{ind}} = 0$ holds for admissible unitaries of those types. However, the gap assumption we made earlier already implies $\vec{\mathrm{ind}} = 0$ for every unitary under consideration, independent of the symmetry type. As the following result from [CGG$^+$18, Proposition VII.1] shows, the essential spectrum of any unitary operator with non-trivial index is the full unit circle (see also [Lan84, Corolary 2] and [BDF73, Theorem 3.1]). Conversely, this means that any gapped unitary must have trivial index.

Lemma 3.4.1. *Let U be an essentially local unitary operator with $\vec{\mathrm{ind}}\,(U) \neq 0$. Then the essential spectrum of U is the full unit circle.*

The proof relies on the so-called Wold-von Neumann decomposition ([vN29, Sect. X], [NFBK10, Sect. I, Theorem 1.1]), which states that every isometry V can be decomposed

[22] ρ_g commutes with the half-space projection P and $\dim\ker(A) = \dim\ker(\rho_g A \rho_g^*)$ for all $A \in \mathcal{B}(\mathcal{H})$ with a unitary or antiunitary ρ_g.

into a direct sum $\widetilde{S} \oplus \widetilde{V}$, of a unilateral shift $\widetilde{S}$ and a unitary $\widetilde{V}$. Let us briefly sketch the idea behind this: Consider an isometry V, i.e. $V^*V = \mathbb{1}$ and $VV^* = \mathbb{1} - P_V$ for some projection P_V. Define $\widetilde{\mathcal{H}}_0 = P_V\mathcal{H}$ and successively build a "cell structure" via $\widetilde{\mathcal{H}}_n = V^n\widetilde{\mathcal{H}}_0$. By construction V now acts as a unilateral shift $\widetilde{S}$ on $\bigoplus_n \widetilde{\mathcal{H}}_n$[23]. Moreover, V leaves invariant the complement, i.e. $V\left(\mathcal{H} \ominus \left(\bigoplus_n \widetilde{\mathcal{H}}_n\right)\right) = \left(\mathcal{H} \ominus \left(\bigoplus_n \widetilde{\mathcal{H}}_n\right)\right)$, and is therefore a surjective isometry on that space, which defines the unitary $\widetilde{V}$.

Proof. We use the Wold-von Neumann decomposition to show that every essentially local unitary with non-trivial index is a compact perturbation of a direct sum that contains at least one unilateral shift as a direct summand. Since the essential spectrum of the unilateral shift is equal to the unit circle[24], the essential spectrum of U also has to contain the full unit circle.Note that the unilateral shift $\widetilde{S}$ not necessarily shifts with respect to the cell structure underlying the locality condition of U, which, however, is not relevant for the conclusion about the spectrum of U.

Without loss of generality, let $\overrightarrow{\mathrm{ind}}\,(U) = n < 0$ (otherwise consider U^* instead) and S be a bilateral shift with $\overrightarrow{\mathrm{ind}}\,(S) = n$. We can write $U = S(S^*U)$ and since $\overrightarrow{\mathrm{ind}}\,(S^*U) = n - n = 0$, the right factor of U can be decoupled into $W(S^*U) = U_L \oplus U_R$ via a compact perturbation W by Theorem 3.3.19. The resulting $U' = S(U_L \oplus U_R) = SWS^*U$ is a compact perturbation of U. We further manipulate U' into $U'' = (\mathbb{1} - P)U'(\mathbb{1} - P) + PU'P$, where P is the half-space projection matching the splitting of $U_L \oplus U_R$. By essential locality, U'' is still a compact perturbation of U and hence, they have the same essential spectrum. We now set

$$V_R = PU'P|_{P\mathcal{H}} = (PSP|_{P\mathcal{H}})U_R = S_RU_R, \tag{3.96}$$

where S_R is a unilateral shift on $P\mathcal{H}$ with Fredholm index $n < 0$ (i.e. $S_R^*S_R = \mathbb{1}_R$ and $S_RS_R^* = \mathbb{1} - K_n$ for some a rank n projection K_n) and similarly for V_L. Note, that by construction, V_R is an isometry on $P\mathcal{H}$:

$$V_R^*V_R = U_R^*S_R^*S_RU_R = \mathbb{1}_R \qquad \text{and} \qquad V_RV_R^* = S_RS_R^* = \mathbb{1}_R - K_n. \tag{3.97}$$

Therefore, we can apply the Wold-von Neumann decomposition, which yields $V_R = \widetilde{S} \oplus \widetilde{V}_R$ with a unilateral shift $\widetilde{S}$ and a unitary $\widetilde{V}$ [25]. The result is a direct sum decomposition $U'' = V_L \oplus V_R = V_L \oplus (\widetilde{S} \oplus \widetilde{V})$, which contains a unilateral shift as a direct summand. Hence, the essential spectrum of U'' and U must be the full unit circle. □

By the preceding lemma, every essentially local and essentially gapped unitary can be decoupled via the method presented in the proof of Theorem 3.3.19. Note that the essential gap assumption always also guarantees a strict gap somewhere around ± 1 or $\pm i$, since otherwise these eigenspaces could not be finitely degenerate.

Let us now add symmetries to the decoupling construction. It turns out that the part V_X on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$ of the decoupling we constructed in the proof of Theorem 3.3.19 is already admissible.

[23] Of course, one has to show that the $\widetilde{\mathcal{H}}_n$ are orthogonal subspaces of $\mathcal{H}$, but we skip this here.

[24] The spectrum of the unilateral shift is the closed unit disk $\mathbb{D}$, with the essential spectrum sitting on the boundary $\partial\mathbb{D} = S^1$ (see also Example 1.2.10).

[25] We stress again, that $\widetilde{S} \neq S_R$ and $\widetilde{V} \neq U_R$.

3.4.1 Admissibility of the partial decoupling V_X on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$

For the decoupling construction we used the decomposition of the Hilbert space with respect to the two projections P and $Q = UPU^*$, where $P = P_{\geq x}$ is a half-space projection, and the decoupling splits the unitary between x and $x-1$. Hence, to investigate the possibility of a symmetric decoupling, let us study the action of the symmetries of a given type $[\rho]$ on these projections. In order to archive an admissible multiplicative decoupling, we need to consider the respective perturbation symmetry type $[\widetilde{\rho}]$ instead of $[\rho]$ itself (see Lemma 3.2.2).

Lemma 3.4.2. *Let U be admissible for a representation ρ of a symmetry type $[\rho]$, P a half-space projection and $Q = UPU^*$. Moreover, let $[\widetilde{\rho}]$ be the corresponding perturbation symmetry type according to Lemma 3.2.2. Then*

$$\widetilde{\rho}_g P \widetilde{\rho}_g^* = \begin{cases} P, & \text{if } ur(g) = 1 \\ Q, & \text{if } ur(g) = -1 \end{cases} \quad \text{and} \quad \widetilde{\rho}_g Q \widetilde{\rho}_g^* = \begin{cases} Q, & \text{if } ur(g) = 1 \\ P, & \text{if } ur(g) = -1. \end{cases} \tag{3.98}$$

Proof. This follows from straight forward algebra, using the definition of the perturbation symmetry representation $\widetilde{\rho} = U^{\frac{1}{2}(1-ur(g))}\rho_g$ (see (3.18)). For $ur(g) = 1$ we have $\widetilde{\rho}_g = \rho_g$ and since we assume the symmetries to act cell wise[26], every half-space projection P naturally commutes with all symmetries. Moreover, by $\rho_g U = U\rho_g$ due to $ur(g) = 1$, the same is true for Q. For $ur(g) = -1$ on the other hand, we get

$$\begin{aligned} \widetilde{\rho}_g P &= U\rho_g P = UPU^*U\rho_g = Q\widetilde{\rho}_g \\ \widetilde{\rho}_g Q &= U\rho_g UPU^* = UU^*PU\rho_g = P\widetilde{\rho}_g. \end{aligned} \tag{3.99}$$

□

The observation above allows us to prove admissibility for the partial decoupling V_X on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$ from the proof of Theorem 3.3.19. Moreover, we can show that the partial decoupling $V_X \oplus \mathbb{1}_{\ker X}$ is gentle.

Lemma 3.4.3. *Let U be admissible for a representation of any symmetry type $[\rho]$. Then the partial decoupling operator V_X on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$ is admissible for the corresponding perturbation symmetry type $[\widetilde{\rho}]$, and $U' = (V_X \oplus \mathbb{1}_{\ker X})U$ is a gentle perturbation of U.*

Proof. This is easily seen for the operator $X = \mathbb{1} - P - Q + 2PQ$ from the proof of Theorem 3.3.19:

$$\widetilde{\rho}_g X \widetilde{\rho}_g^* = \begin{cases} X, & \text{if } ur(g) = 1 \\ X^*, & \text{if } ur(g) = -1 \end{cases}.$$

The polar isometry V_X of X inherits these relations with the symmetries and hence we get

$$\widetilde{\rho}_g V_X \widetilde{\rho}_g^* = V_X^{ur(g)}.$$

Gentleness of $V_X \oplus \mathbb{1}_{\ker X}$ follows from Theorem 3.2.6 and the fact that, by construction, V_X has only eigenvalues with positive real part, wherefore $\widetilde{\mathrm{si}}_-(V_X \oplus \mathbb{1}_{\ker X}) = \mathrm{si}(U' : U) = 0$. □

[26] See Assumption 3.1.1

To decouple a symmetric walk without breaking the symmetry, we are hence left with the task of constructing an admissible gentle decoupling $V_{\ker X}$ on the finite dimension space $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$. As we will see below, this is not possible in general for all symmetry types. However, for most of the symmetry types of the tenfold way (excluding AII), the situation turns out to be a bit easier and we can indeed construct a gentle decoupling [CGG$^+$18]. We first discuss the gentle decoupling for the symmetry types of the tenfold way and turn to the obstructions for the types beyond afterwards.

3.4.2 Gentle decoupling for the tenfold way

A necessary condition for a gentle decoupling $V_{\ker X}$ on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ is that $\widetilde{\rho}$ doesn't force $V_{\ker X}$ to have a symmetry protected eigenspace at -1. We can use Proposition 3.2.8 to verify that this is indeed not the case for the symmetry types of the tenfold way.

Lemma 3.4.4. *Let U be essentially local and admissible for a representation ρ of a symmetry type from the tenfold way. Then the representation $\widetilde{\rho}$, restricted to $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ is balanced.*

Proof. Given U and a half-space projection P, consider the unitary $U' = (\mathbb{1} - 2P)U(\mathbb{1} - 2P) =: VU$. By essential locality of U, VU is a compact perturbation of U. Because $\mathbb{1} - 2P$ commutes with the symmetries of ρ, U' is also admissible for ρ. Hence, $V = (\mathbb{1} - 2P)(\mathbb{1} - 2Q)$ is admissible for $\widetilde{\rho}$. Moreover, U and U' are unitarily equivalent, by a symmetry commuting unitary. Therefore, they must have the same symmetry indices $\mathrm{si}_-(U) = \mathrm{si}_-(U')$. Applying Proposition 3.2.8 to U and U', we find, that $\widetilde{\mathrm{si}}_-(V) = 0$, i.e. the symmetry representation of $\widetilde{\rho}$, restricted to the -1-eigenspace of V is balanced. Moreover, the -1 eigenspace of V is equal to $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$. Indeed, $V\varphi = -\varphi$ is equivalent to $(P + Q)\varphi = \varphi = (\mathbb{1} - B)\varphi$, with B from (3.71), and, as discussed in the proof of Lemma 3.3.14, $\ker B = \ker(A - \mathbb{1}) \oplus \ker(A + \mathbb{1}) = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$. □

With this, we can construct a gentle decoupling also on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ for the symmetry types of the tenfold way. Thereby type 5 (resp. AII) is the only symmetry type, for which an additional assumption, namely $\dim \mathcal{H}_{10} \equiv 0 \bmod 2$ is needed.

Lemma 3.4.5. *Let $\mathcal{K} = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$, with $\mathcal{H}_{ij}$ according to* (3.70)*, corresponding to a quantum walk U, that is essentially gapped and admissible for a symmetry representation ρ of the tenfold way. Moreover, for type 5 in Table 2.1 (resp.* AII*) let $\dim \mathcal{H}_{10} \equiv 0 \bmod 2$. Then there exist a $\widetilde{\rho}$ admissible unitary V on $\mathcal{K}$ with $V^2 = -\mathbb{1}$ and $V\mathcal{H}_{ij} = \mathcal{H}_{ji}$.*

Proof. First note that by Lemma 3.4.1 and Lemma 3.3.14 we have $\dim \mathcal{H}_{10} = \dim \mathcal{H}_{01}$, which is necessary for a swapping unitary to exist.

The proof will be case by case. We start with the symmetry types including a chiral symmetry $\widetilde{\gamma}$ (AIII, BDI, CI, CII and DIII), where we distinguish between the commuting types (AIII, BDI and CII) and the two remaining ones (CI and DIII)[27]. Afterwards, we tackle the remaining types (A, D, C, AI and AII), by mostly reusing the constructions of the cases earlier. If needed, we construct V specifically, by choosing a basis. Thereby, we

[27]The term "commuting types" refers to the phase convention of Lemma 2.1.7, which we chose as the standing assumption here, since we also assumed this convention in the discussion of perturbations (see Section 3.2). In the phase convention of Lemma 2.1.5 these would be the types with $\gamma^2 = \mathbb{1}$, as in [CGG$^+$18].

always choose the basis, such that it respects the splitting $\mathcal{K} = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$ and denote it by $\{\chi_n^{ij}\}_n$, with $i \neq j \in \{0, 1\}$.

- For AIII, BDI and CII, consider $A = P - Q$, which, restricted to $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$, acts as $+\mathbb{1}$ on the first summand and as $-\mathbb{1}$ on the second. Moreover, since $\widetilde{\gamma}$ intertwines P and Q, we get $\widetilde{\gamma}A = -A\widetilde{\gamma}$. Now, let $V = A\widetilde{\gamma}$. By the phase convention of Lemma 2.1.7, which we chose as the standing assumption here, we always have $\gamma^2 = \mathbb{1}$ and therefore, by Lemma 3.2.2, also $\widetilde{\gamma}^2 = \mathbb{1}$. Hence, $\widetilde{\gamma}$ is self-adjoint, which implies $V^* = -V \Rightarrow V^2 = -\mathbb{1}$. Moreover, since the symmetry representations for the present cases are commutative, V is automatically admissible by $\widetilde{\rho}_g A = ur(g)A\widetilde{\rho}_g$, which follows from Lemma 3.4.2.

- For CI, $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$ are even-dimensional, because they are left invariant by $\widetilde{\eta}$, with $\widetilde{\eta}^2 = -\mathbb{1}$. We choose a basis $\{\chi_n^{10}\}_n$ for $\mathcal{H}_{10}$, which fulfils $\chi_{2k}^{10} = \widetilde{\eta}\chi_{2k-1}^{10}$ and extend it to $\mathcal{H}_{01}$ via $\chi_n^{01} = \widetilde{\tau}\chi_n^{10}$. Setting $V\chi_n^{10} = -\chi_n^{01}$ and $V\chi_n^{01} = \chi_n^{10}$ then defines the admissible V with $V^2 = -\mathbb{1}$[28].

- In case of DIII we have $\widetilde{\eta}^2 = \mathbb{1}$, wherefore we can choose an $\widetilde{\eta}$-invariant basis $\{\chi_n^{10}\}_n$ for $\mathcal{H}_{10}$ and again set $\chi_n^{01} = \widetilde{\tau}\chi_n^{10}$. Since $\widetilde{\rho}$ is balanced on $\mathcal{K}$, its dimension is a multiple of four, and therefore each subspace $\mathcal{H}_{ij}$ is again even-dimensional. Hence, we can define an admissible V via $V\chi_{2k-1}^{ij} = \chi_{2k}^{ji}$ and $V\chi_{2k}^{ij} = -\chi_{2k-1}^{ji}$, with $V^2 = -\mathbb{1}$[28].

- In case of A, D, C and AI we are free to choose the basis arbitrarily for A, $\widetilde{\eta}$-invariant for D, similar to type CI for C (without having to relate the two basis sets via $\widetilde{\tau}$), and related via $\widetilde{\tau}$ for AI. In all cases V can then be chosen as for type CI.

- For type AII, we can use the construction for type DIII without having to worry about the basis being $\widetilde{\eta}$-invariant. Thereby, the extra assumption of $\dim \mathcal{H}_{10} = 0 \bmod 2$ guarantees that we can choose the basis pairwise, as needed.

□

So far we only saw, that $\dim \mathcal{H}_{10} = 0 \bmod 2$ is sufficient for the existence of V in case of AII. But it is also necessary, as the following observation shows: Let V be a swapping unitary on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ that is admissible for $\widetilde{\tau}$ with $\widetilde{\tau}^2 = -\mathbb{1}$. Moreover, choose a basis as in case AI and AII above. Then, by $\widetilde{\tau}V\widetilde{\tau}^* = V^*$, the off diagonal blocks V_i of V fulfil $V_i^T = -V_i$. Since V swaps $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$, these blocks are unitary, which is only possible in even dimensions. Note that this applies to all types involving $\widetilde{\tau} \equiv (-1, 1, 1)$ with $\widetilde{\tau}^2 = -\mathbb{1}$, but only AII needs the extra assumption because it is automatically fulfilled in the other cases.

Assembling the different steps, we can now formulate the gentle decoupling theorem for the symmetry types of the tenfold way (compare [CGG+18, Theorem VII.4]).

[28] By construction, V is admissible for $\widetilde{\eta}$ and $\widetilde{\tau}$. The admissibility for $\widetilde{\gamma}$ follows automatically and is independent of the phase convention.

Theorem 3.4.6 (Gentle decoupling theorem for the tenfold way)**.** *Let U be an essentially local essentially gapped unitary, which is admissible for one of the symmetry types of the tenfold way, such that $\dim \mathcal{H}_{10} = 0 \bmod 2$ for type* AII*. Then there exists an admissible, compact, and gentle perturbation $VU = U_L \oplus U_R$, which decouples U into two unitaries on the two half-spaces, respectively.*

Proof. Let $V = V_X \oplus V_{\ker X}$ be as in the proof of Theorem 3.3.19. Thereby V_X is admissible by Lemma 3.4.3, and we set $V_{\ker X}$ equal to the V constructed in Lemma 3.4.5. □

3.4.3 Additional invariants beyond the tenfold way

We already saw that the partial decoupling on $\mathcal{H}_{00} \oplus \mathcal{H}_{11} \oplus \mathcal{H}_\perp$ is admissible for all 38 types. On $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$, on the other hand, we had to construct specific unitaries for each type of the tenfold way. Thereby we used the balancedness of the perturbation symmetry representation $\widetilde{\rho}$ on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ (which, for the tenfold way, is of the same symmetry type as ρ). In order to show that this representation is indeed balanced, we used Proposition 3.2.8, which is not applicable for the types beyond the tenfold way. Beside this, there is another fundamental restriction: The **alternating symmetry** σ (with $\sigma U \sigma^* = -U$) gives rise to a second decoupling invariant $U \mapsto \operatorname{dec}(U) \in \mathbb{Z}$ in addition to $\overrightarrow{\operatorname{ind}}(U)$. We will first discuss this invariant in general and particularise its influence on the structure of $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ afterwards.

Let σ be an alternating symmetry with $\operatorname{tr} \sigma = 0$ in each cell[29], and let U be admissible for σ. Then, in the σ-eigenbasis, U is of the form

$$U = \begin{pmatrix} 0 & A \\ B & 0 \end{pmatrix}, \tag{3.100}$$

with unitary operators A and B and we get $\ker(U) = \ker(A) \oplus \ker(B)$, as well as $\ker(U^*) = \ker(B^*) \oplus \ker(A^*)$. Since the same applies to the projected versions PXP, $X \in \{U, A, B\}$, we also get $\overrightarrow{\operatorname{ind}}(U) = \overrightarrow{\operatorname{ind}}(A) + \overrightarrow{\operatorname{ind}}(B)$.

Now, let $U' = VU$ be a gentle decoupling for U (assuming its existence for a moment). Then U' is admissible for σ if and only if $\sigma V = V \sigma$. This enforces V to be block diagonal with respect to the σ eigenbasis:

$$V = \begin{pmatrix} V_A & 0 \\ 0 & V_B \end{pmatrix}, \qquad \text{i.e.} \qquad U' = \begin{pmatrix} 0 & V_A A \\ V_B B & 0 \end{pmatrix}. \tag{3.101}$$

That is, to decouple U while obeying the σ symmetry, we need to decouple A and B separately. Denoting by $\operatorname{dec}(U) := \overrightarrow{\operatorname{ind}}(A)$ the right Fredholm index of the upper right corner in (3.100), we get:

Lemma 3.4.7. *Let U a quantum walk, which is admissible for an alternating symmetry σ. Then there exists a gentle σ-symmetric decoupling for U, if and only if $\overrightarrow{\operatorname{ind}}(U) = 0$ and $\operatorname{dec}(U) = \overrightarrow{\operatorname{ind}}(A) = 0$.*

Proof. We already saw that there is a σ-symmetric gentle decoupling for U, if and only if there is one for A and B, respectively. I.e., if and only if $\overrightarrow{\operatorname{ind}}(A) = \operatorname{dec}(U) = 0$ and $\overrightarrow{\operatorname{ind}}(B) = \overrightarrow{\operatorname{ind}}(U) - \operatorname{dec}(U) = 0$. □

[29] Otherwise there are no admissible local unitaries in the individual cells, i.e. no trivial local reference.

Note that differently from $\overrightarrow{\mathrm{ind}}(U) = 0$, $\mathrm{dec}(U) = 0$ is not enforced by the gap condition on U, because the spectral properties of U do not transfer to the off-diagonal blocks A and B as it would be the case for a direct sum. Let us provide two examples, which are admissible for the same representation of type 10 and are both maximally gapped[30]. One of the two examples can be decoupled, while the other one cannot:

Example 3.4.8. *Consider the Hilbert space $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^4$. In each cell, let the generators of type 10 be defined by $\sigma_x = \left(\begin{smallmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{smallmatrix}\right)$ and $\gamma_x = \left(\begin{smallmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{smallmatrix}\right)$. On $\mathcal{H}$, we consider the two walks*

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} & & S & S \\ & & -S & S \\ S^* & S^* & & \\ -S^* & S^* & & \end{pmatrix} \qquad \text{and} \qquad U_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} & & 1 & S \\ & & -S^* & 1 \\ 1 & S & & \\ -S^* & 1 & & \end{pmatrix} \tag{3.102}$$

where, as usual, S denotes the bilateral right-shift on $\ell^2(\mathbb{Z})$. It is straight forward to check that U_1 and U_2 are admissible for the given symmetry representation and that they are also both gapped at ± 1 and $\pm i$ ($U_i^4 = -\mathbb{1} \Rightarrow \sigma(U_i) \subset \{\pm e^{\pm i\pi/4}\}$).

Since the representation is already given in σ-eigenbasis, we can simply read off the upper right blocks A_i entering the decoupling invariant $\mathrm{dec}(U)$. The decoupling indices evaluate to $\mathrm{dec}(U_1) = \overrightarrow{\mathrm{ind}}(A_1) = -2$ and $\mathrm{dec}(U_2) = \overrightarrow{\mathrm{ind}}(A_2) = 0$. Hence, we can find an admissible decoupling for U_2, but no decoupling exists for U_1.

By Lemma 3.4.3 the partial decoupling V_X can always be chosen admissible. Hence, the decoupling condition has to manifest itself on $\ker X = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$. Let us investigate this in detail. Since σ leaves the spaces $\mathcal{H}_{ij}$ invariant, we can arrange its eigenbasis, such that

$$\sigma = \begin{pmatrix} \mathbb{1}_{d_{10}^+} & & & \\ & -\mathbb{1}_{d_{10}^-} & & \\ & & \mathbb{1}_{d_{01}^+} & \\ & & & -\mathbb{1}_{d_{01}^-} \end{pmatrix}, \tag{3.103}$$

where $d_{ij}^{\pm} = \frac{1}{2}\left|\mathrm{tr}\left((\sigma \mp \mathbb{1})P_{\mathcal{H}_{ij}}\right)\right|$ denotes the dimension of the overlap of the ± 1 eigenspace of σ with $\mathcal{H}_{ij}$. Since a decoupling V has to swap the $\mathcal{H}_{ij}$, while leaving the eigenspaces of σ invariant it must be of the form

$$V = \begin{pmatrix} & & V_{10}^+ & \\ & & & V_{10}^- \\ V_{01}^+ & & & \\ & V_{01}^- & & \end{pmatrix}, \tag{3.104}$$

where we labelled the blocks $V_{ij}^{\pm}$ with the pair $\{ij\}$ of the respective target space, i.e. $V_{ij}^{\pm} \colon \mathcal{H}_{ji} \to \mathcal{H}_{ij}$. The block-structure of V now enforces

$$d_{10}^{\pm} = d_{01}^{\pm}, \tag{3.105}$$

[30] In the sense that the spectrum is contained in $\{\pm e^{\pm i\pi/4}\}$.

additionally to $d_{10} = d_{01}$. In other words, the index condition has to be fulfilled in each σ-eigenspace separately, which is equivalent to $\overrightarrow{\mathrm{ind}}(A) = \overrightarrow{\mathrm{ind}}(B) = 0$, i.e. $\mathrm{dec}(U) = 0$. From this consideration we also see that for some symmetry types the presence of additional symmetries ρ_g with $c(\sigma, \rho_g) = -ur(g) = 1$ already guarantees $\mathrm{dec}(U) = 0$ for any admissible unitary. In this case $ur(g) = -1$ forces ρ_g to swap $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$, while leaving invariant the σ-eigenspaces due to $c(\sigma, \rho_g) = 1$, which results in $d_{10}^{\pm} = d_{01}^{\pm}$. For other types, the condition needs to be assumed for a decoupling to exist.

So far we met the necessary and sufficient decoupling conditions $d_{10} = 0 \bmod 2$ for symmetry type 5 (AII: only τ, with $\tau^2 = -\mathbb{1}$) and $d_{10}^{\pm} = d_{01}^{\pm}$ for symmetry type 2 (only σ). For some symmetry types, e.g. type 13, yet another condition needs to be fulfilled. Type 13 is generated by σ and τ, with $c(\sigma, \tau) = 1$ and $\tau^2 = -\mathbb{1}$. Since τ swaps the spaces $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$, but leaves invariant the σ-eigenspaces, $d_{10}^{\pm} = d_{01}^{\pm}$ is automatically fulfilled. Moreover, each block of V in (3.104) has to fulfil $(V_{ij}^{\pm})^T = -V_{ij}^{\pm}$, similar to the condition for type AII in the proof of Lemma 3.4.5. This is only possible for matrices in even dimension, and therefore

$$d_{10}^{\pm} = 0 \bmod 2 \tag{3.106}$$

is a necessary condition.

Concluding the discussion with the following lemma, we state that there are no further decoupling conditions. That is, each type of the 38-fold way can either be decoupled from the outset or if and only if one of the three conditions above is fulfilled. We also listed the decoupling condition for each type in Table 2.1.

Lemma 3.4.9. *Let $\mathcal{K} = \mathcal{H}_{10} \oplus \mathcal{H}_{01}$, with $\mathcal{H}_{ij}$ according to* (3.70)*, correspond to an essentially gapped and admissible quantum walk for a symmetry representation ρ of one of the 38 symmetry types. Then there exists a $\widetilde{\rho}$-admissible unitary V on $\mathcal{K}$ with $V^2 = -\mathbb{1}$ and $V\mathcal{H}_{ij} = \mathcal{H}_{ji}$ if and only if $\widetilde{\rho}$ fulfils the corresponding decoupling condition in the following table:*

Condition	*Types*
None	*1, 3, 4, 6, 8-10, 12, 20-26, 28-30, 32, 33, and 36*
$d_{10} = 0 \bmod 2$	*5, 7, and 27*
$d_{10}^{\pm} = d_{01}^{\pm}$	*2, 11, 14-18, and 40-43*
$d_{10}^{\pm} = 0 \bmod 2$	*13, 31, and 37*

Proof. Similar to the proof of Lemma 3.4.5, we have to construct V separately case by case. This makes the proof rather tedious, wherefore we do not present it here. The computations for the types beyond the tenfold way are given in Appendix A. □

3.5 The left and right symmetry index

The gentle decoupling allows us to split a given quantum walk into two independent half-line unitaries without changing the symmetry index. This allows us to attribute symmetry indices to the left and right half-system, respectively, which have to add up to the total symmetry index defined via the symmetry protected eigenspaces of the whole underlying walk:

$$\mathrm{si}(U_L \oplus U_R) = \mathrm{si}(U_L) + \mathrm{si}(U_R) \tag{3.107}$$

For this section, we will first assume the decoupling condition (see Table 2.1) to be met for any walk under consideration and address possible applications to walks that cannot be decoupled later. For systems subject to the symmetry types of the tenfold way, the left and right symmetry indices serve as proper homotopy invariants not only in the formulation of bulk-boundary correspondence for quantum walks, but also for the complete topological classification. Beyond the tenfold way, we still get a similar correspondence but were not able to prove the invariance of the bulk-indices under arbitrary deformations of the whole system[31] for all symmetry types. The left and right symmetry indices are invariant under local, respectively compact perturbations, and in particular, they do not depend on the decoupling position. This last fact has the consequence that the indices can be computed arbitrarily far to the right (left). Hence, they do only depend on the infinite tail of the half-chain. For example, given a crossover scenario of two bulks joined into one system, the left and right symmetry indices only depend on the two bulk systems individually and not on how the crossover is engineered.

Let us begin with the formal definition of the left and right symmetry index:

Definition 3.5.1. *Let U be a **strictly local walk**, which is admissible for a representation of a symmetry type from the 38-fold way. Moreover, let the corresponding decoupling condition be fulfilled and $VU = U_L \oplus U_R$ be a gentle decoupling of U at some x. We define the **left and right symmetry index** as*

$$\overleftarrow{\mathrm{si}}(U) = \mathrm{si}(U_L) \qquad \text{and} \qquad \overrightarrow{\mathrm{si}}(U) = \mathrm{si}(U_R), \tag{3.108}$$

where the symmetry indices $\mathrm{si}(U_L)$ and $\mathrm{si}(U_R)$ are defined on the half-spaces $\mathcal{H}_L$ and $\mathcal{H}_R$, respectively.

Per se, the left and right symmetry indices are not well defined, because they might depend on the specific decoupling V one chooses in order to archive $VU = U_L \oplus U_R$ or on the cut position. However, this is not the case (compare [CGS$^+$16], where this technique was used for the symmetry types of the tenfold way).

Theorem 3.5.2. *Let U be as in Definition 3.5.1. Then we have*

$$\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U) \tag{3.109}$$

and $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ are

i) independent of the cut-position.

ii) invariant under local admissible perturbations.

Note that by item $ii)$ the left and right symmetry indices also become independent of the way we decouple U in order to get $U_L \oplus U_R$. Every decoupling of a strictly local walk, be it gentle or not, is a local perturbation of a gently decoupled walk defining $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$. Moreover, this also shows the invariance of si under local perturbations, whenever a decoupling is applicable.

[31] Defined as symmetry indices of the half-space unitaries, the left and right indices are invariant under the deformations of these, but not necessarily under deformations of the underlying full chain walk prior to the decoupling.

Proof. By assumption, we can always choose a gentle decoupling. Since the symmetry index is a homotopy invariant (see Proposition 3.1.6), we get

$$\mathrm{si}(U) = \mathrm{si}(VU) = \mathrm{si}(U_L \oplus U_R) = \mathrm{si}(U_L) + \mathrm{si}(U_R) = \overleftarrow{\mathrm{si}}\,(U) + \overrightarrow{\mathrm{si}}\,(U). \tag{3.110}$$

i): Let $VU = U_L \oplus U_R$ be decoupled at some point n and $\overleftarrow{\mathrm{si}}\,(U), \overrightarrow{\mathrm{si}}\,(U)$ be the corresponding left and right indices. Moreover, let $V'VU = U_L \oplus U_M \oplus U'_R$ be further decoupled additionally at $m > n$. We get

$$\mathrm{si}(U) = \mathrm{si}(U_L) + \mathrm{si}(U_M) + \mathrm{si}(U'_R) = \overleftarrow{\mathrm{si}}\,(U) + \mathrm{si}(U_M) + \overrightarrow{\mathrm{si}}\,'(U). \tag{3.111}$$

Now, since U_M is a unitary on a finite number of cells $n \leq x < m$ we have $\mathrm{si}(U_M) = 0$ by Assumption 3.1.1 in combination with Corollary 3.1.5. Hence,

$$\overrightarrow{\mathrm{si}}\,(U) = \overrightarrow{\mathrm{si}}\,'(U), \tag{3.112}$$

independently of the cut position m. The same follows for $\overleftarrow{\mathrm{si}}$ with $m < n$.

ii): Let VU be a local admissible perturbation of U and $M \subset \mathbb{Z}$ the labelling set of the supporting cells of $V - \mathbb{1}$. We can decouple U twice, such that

$$U = U_L \oplus U_M \oplus U_R \qquad \text{and} \qquad VU = U_L \oplus U'_M \oplus U_R. \tag{3.113}$$

Thereby, we enlarge M until $|M| > 2L$, where L is the interaction length of the strictly local walk, which guarantees that the decouplings do not interfere with each other. This way, we "cut out" the local perturbation. By the same argument as before we get $\mathrm{si}(U_M) = \mathrm{si}(U'_M) = 0$, i.e. $\overrightarrow{\mathrm{si}}\,(U) = \overrightarrow{\mathrm{si}}\,(VU)$ and the same for $\overleftarrow{\mathrm{si}}$.

□

Note that Theorem 3.5.2 does not claim homotopy invariance of $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$. One might argue that these indices are defined via the symmetry index si of the half-space systems after gently decoupling the system, and therefore naturally have to be invariant under continuous admissible perturbations. Surely, this reasoning implies that, e.g., $\overrightarrow{\mathrm{si}}$ is a homotopy invariant for the set of half-space unitaries U_R. However, taken as quantities for the full system U, such a conclusion is not possible at this point. Although being gentle, the decoupling is not continuous with respect to deformations of the underlying walk U, i.e. a continuous path of admissible walks $t \mapsto U$ does not necessarily lead to a continuous path of admissible half-space walks $U_R(t)$. Let us illustrate this via an example:

Example 3.5.3. *Let U be a strictly local walk, which is admissible for a symmetry type that exhibits non-gentle perturbations (see Section 3.2). Moreover, let $U_1 = V_1 U$ and $U_2 = V_2 U$ be local non-gentle perturbations of U, such that $\mathcal{H}_{V_1} \subset (\mathbb{1} - P)\mathcal{H}$ and $\mathcal{H}_{V_2} \subset P\mathcal{H}$, where the regions have a distance of at least $2L$ to the cut point, and $\mathrm{si}(U_1 : U) = \mathrm{si}(U_2 : U) \neq 0$. In other words, V_1 is located on the left half-chain and V_2 on the right, whereas both are "non-gentle in the same way".*

Then, $W = V_2 V_1^*$ is a gentle perturbation of U_1 with $WU_1 = U_2$. Indeed, by $V_1^* U_1 = U$, we have $\mathrm{si}(V_1^* U_1 : U_1) = \mathrm{si}(U : U_1) = -\mathrm{si}(U_1 : U)$, and therefore we get

$$\begin{aligned} \mathrm{si}(WU_1 : U_1) &= \mathrm{si}(V_2 U_1 : U_1) + \mathrm{si}(V_1^* U_1 : U_1) \\ &= \mathrm{si}(V_2 U : U) - \mathrm{si}(V_1 U : U) \\ &= 0, \end{aligned} \tag{3.114}$$

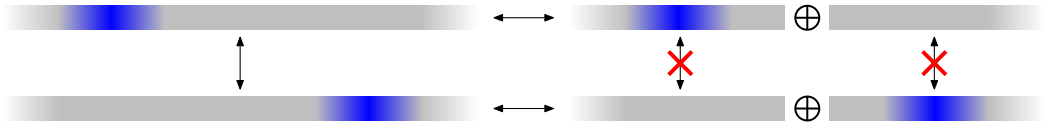


Figure 3.4: Visualisation of the construction in Example 3.5.3. Top: U_1 (left) and its decoupled version (right). Bottom: U_2 and its decoupled version. The non-gentle perturbations V_1, V_2 are depicted in blue and arrows indicate the existence of a homotopy.

where we used Corollary 3.2.7 in the first step and the fact that V_1 and V_2 do not spatially interfere with each other in the second. This shows that moving a local perturbation to a disjoint set of cells can be archived on a continuous path of walks, i.e. is a gentle deformation.

Hence, by Theorem 3.2.6, there is a norm-continuous admissible path between U_1 and U_2. However, decoupling both walks, we find that the corresponding half-chain walks on the right $U_{2,R} = V_2 U_{1,R}$ are non-gentle perturbations of each other, which excludes a norm-continuous admissible path between $U_{1,R}$ and $U_{2,R}$ on $P\mathcal{H}$. See Figure 3.4 for an illustration.

By invariance of $\overleftarrow{\mathfrak{si}}$ and $\overrightarrow{\mathfrak{si}}$ under local perturbations, the continuous deformation of the example above does not change these indices, indicating that they might still be proper homotopy invariants. However, the example demonstrates that we cannot rely on the gentleness of the decoupling to conclude such property since there might be other, non-local deformations with similar effects. Moreover, the example shows that the individual components of $\overleftarrow{\mathfrak{si}}$ and $\overrightarrow{\mathfrak{si}}$, namely $\overleftarrow{\mathfrak{si}}_\star$ and $\overrightarrow{\mathfrak{si}}_\star$, with $\star \in \{\pm, \dotplus\}$, are certainly not homotopy invariants of U in general. In particular in case of the tenfold way, where $\mathfrak{si}_\pm$ directly measure the gentleness of a perturbation (see Proposition 3.2.8), $\overleftarrow{\mathfrak{si}}_\pm$ and $\overrightarrow{\mathfrak{si}}_\pm$ have to change in the example above. Hence:

Corollary 3.5.4. *The quantities $\overleftarrow{\mathfrak{si}}_\star(U)$ and $\overrightarrow{\mathfrak{si}}_\star(U)$, with $\star \in \{\pm, \dotplus\}$, are in general neither invariant under continuous deformations of U, nor under compact (local) perturbations.*

While not provably invariant under continuous deformations, $\overleftarrow{\mathfrak{si}}$ and $\overrightarrow{\mathfrak{si}}$ still add up to the invariant quantity $\mathfrak{si}$, which, by the discussion following Corollary 3.1.7 in Section 3.1.1, serves as a lower bound on the number of symmetry protected eigenspaces of U. Moreover, the argument in the proof for invariance of $\overleftarrow{\mathfrak{si}}$ and $\overrightarrow{\mathfrak{si}}$ under local perturbations also shows that these indices can be computed arbitrarily far to the left and to the right, respectively. Hence, they only depend on the infinite tails to the left and the right, i.e. the behaviour of a walk at infinity. This fact allows us to call them **bulk-indices**, i.e. quantities which depend only on the idealized infinite chunks of a system that can be treated as a homogeneous **bulk**[32]. In this sense, Theorem 3.5.2 may be understood as the bulk-boundary correspondence for symmetric quantum walks, which is one of the main motivating concepts behind the topological classification of lattice systems. Before we detail the bulk-boundary correspondence, however, let us introduce more robust invariants for the symmetry types of the tenfold way and discuss where the generalization fails beyond it.

[32] Wee will elaborate on the term **bulk** in Section 3.5.4.

3.5.1 Robust symmetry indices for the tenfold way

For the symmetry types of the tenfold, we can define the symmetry indices, in particular $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$, in a more robust way [CGG+18]. Recall Lemma 2.3.5, where we showed that for the symmetry types of the tenfold way, there exists an admissible gapped unitary for a finite-dimensional representation, if and only if there exists a gapped Hamiltonian. This makes the index groups from Table 2.1 valid in both settings: walks and Hamiltonians. We can now use this correspondence to redefine left and right symmetry indices.

In doing so, we extend the definition of the symmetry index si (not the individual ones $\mathrm{si}_\pm$) to the set of merely essentially unitary operators similar to the considerations for right Fredholm index $\overrightarrow{\mathrm{ind}}$ (see Definition 3.3.18). Moreover, we will see later that we can express all symmetry indices for chiral symmetric protocols in terms of Fredholm indices, which will allow us to completely classify such protocols (see Chapter 5).

Definition 3.5.5. *Let U be an essentially unitary essentially gapped operator[33], which is admissible for a representation of a symmetry type of the tenfold way. Then*

$$\mathrm{Im}(U) := \frac{U - U^*}{2i} \tag{3.115}$$

is an admissible and essentially gapped Hamiltonian for the same representation. Moreover, we can define the symmetry index $\mathrm{si}(U)$ via

$$\mathrm{si}(U) := \mathrm{si}\left(\mathrm{Im}(U)\right) = \mathrm{si}\left(\rho_{\ker \mathrm{Im}(U)}\right). \tag{3.116}$$

Let us briefly check the claims made in the definition above. $\mathrm{Im}(U)$ is self-adjoint by definition, and its admissibility follows via

$$\rho_g \,\mathrm{Im}(U)\rho_g^* = \frac{u(g)}{2i}\rho_g(U - U^*)\rho_g^* = \frac{u(g)ur(g)}{2i}(U - U^*) = r(g)\,\mathrm{Im}(U). \tag{3.117}$$

Moreover, the essential gaps of U at ± 1 directly transfer to the essential gap of $\mathrm{Im}(U)$ at 0. For unitary operators the two definitions for $\mathrm{si}(U)$ (Definition 3.1.4 and Definition 3.5.5) coincide, because in this case the combined eigenspaces of U at ± 1 directly translate to the kernel of $\mathrm{Im}(U)$. Therefore, we make Definition 3.5.5 the standing definition for the symmetry index of unitaries, which are admissible for a symmetry type of the tenfold way. It is important to note that via this method, we lose the possibility of distinguishing the two essential gaps for unitary operators, wherefore we cannot define the individual indices $\mathrm{si}_\pm$ via $\mathrm{Im}(U)$. However, these rely on symmetry protected eigenspaces of the operator and are therefore not applicable for essentially unitary operators anyhow.

Similar to the right Fredholm index in Lemma 3.3.13 we can now define the symmetry index also for walks projected down to a half-line. The essential locality condition guarantees that the projected version PUP of any (essential) unitary walk is essentially unitary on the half-space $P\mathcal{H}$, wherefore we can define the right symmetry index $\overrightarrow{\mathrm{si}}(U)$ as the symmetry index $\mathrm{si}(PUP)$ on $P\mathcal{H}$.

[33] Note, that an essentially unitary operator is not necessarily normal, such that we cannot think of "essentially gapped" as being gapped up to finite-dimensional eigenspaces. However, it is still well defined via gaps the essential spectrum.

Definition 3.5.6. *Let U be an admissible walk (possibly only essentially unitary) for one of the symmetry types of the tenfold way. We define its left and right symmetry indices via*

$$\overrightarrow{\mathrm{si}}(U) := \mathrm{si}\left(PUP|_{P\mathcal{H}}\right) \qquad \text{and} \qquad \overleftarrow{\mathrm{si}}(U) := \mathrm{si}\left(P^{\perp}UP^{\perp}|_{P^{\perp}\mathcal{H}}\right). \tag{3.118}$$

Defined this way, $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$ have much stronger invariance properties:

Theorem 3.5.7. *Let $U, \mathrm{si}, \overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$ be defined as above. Then*

$$\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U), \tag{3.119}$$

and $\overleftarrow{\mathrm{si}}, \overrightarrow{\mathrm{si}}$ are

i) independent of the cut-position.

ii) invariant under compact admissible perturbations.

iii) invariant under continuous deformations of U in the set of admissible essentially unitary operators.

For exactly unitary strictly local walks, $\overrightarrow{\mathrm{si}}, \overleftarrow{\mathrm{si}}$ coincide with the quantities defined in Definition 3.5.1.

Proof. We prove this for $\overrightarrow{\mathrm{si}}$. For $\overleftarrow{\mathrm{si}}$ the proof is completely analogous.

Invariance under continuous and compact perturbations: Any norm-continuous path $t \mapsto U_t$ in the set of essentially unitary admissible unitaries gives a norm-continuous path of admissible self-adjoint imaginary parts $\mathrm{Im}(PU_tP)$. Hence, invariance under norm-continuous perturbations simply follows form the invariance of si on the set of self-adjoint operators (Corollary 3.1.7). Now, as already mentioned in Section 3.2, any compact perturbation H' of an admissible Hamiltonian H can be archived via a continuous path of admissible Hamiltonians by "turning on" the perturbation using the convex combination

$$t \mapsto H_t = H + t(H' - H), \quad t \in [0, 1]. \tag{3.120}$$

Hence, invariance under compact perturbations follows automatically. From this we also get

$$\mathrm{si}(U) = \mathrm{si}(P^{\perp}UP^{\perp} \oplus PUP) = \overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U), \tag{3.121}$$

because U and $P^{\perp}UP^{\perp} \oplus PUP$ are compact perturbations of each other.

Equivalence to the decoupling method: Any decoupling $U' = U_L \oplus U_R$ of an essentially unitary operator U is a compact perturbation of U. Hence, $\overrightarrow{\mathrm{si}}(U) = \overrightarrow{\mathrm{si}}(U')$. Now, since $PU'P|_{P\mathcal{H}} = U_R$ and $\ker(U' - \mathbb{1}) \oplus \ker(U' + \mathbb{1}) = \ker\left(\mathrm{Im}(PU'P)|_{P\mathcal{H}}\right)$, we get

$$\begin{aligned} \overrightarrow{\mathrm{si}}(U) = \overrightarrow{\mathrm{si}}(U') &= \mathrm{si}\left(\rho_{\ker(U_R+\mathbb{1})} \oplus \rho_{\ker(U_R-\mathbb{1})}\right) \\ &= \mathrm{si}\left(\rho_{\ker(\mathrm{Im}(PU'P)|_{P\mathcal{H}})}\right) \\ &= \mathrm{si}\left(PU'P|_{P\mathcal{H}}\right), \end{aligned} \tag{3.122}$$

where in the second and third last line the symmetry indices are considered as usual for finite-dimensional representations (Proposition 2.3.8), whereas in the last line it refers to Definition 3.5.5.

Independence of the cut position: Choosing a different cut position is just a compact perturbation and therefore follows from the point above. To be more precise: Let $P_{\geq a}$ and $P_{\geq b}$ be half-space projections with $b > a$ and $P_M = P_{\geq a}P_{<b}$, i.e. $P_M\mathcal{H} = \mathcal{H}_a \oplus \ldots \oplus \mathcal{H}_{b-1}$. Then

$$P_{\geq a}UP_{\geq a} = (P_M + P_{\geq b})U(P_M + P_{\geq b}) = P_{\geq b}UP_{\geq b} + K, \tag{3.123}$$

with $K = P_MUP_M + P_MUP_{\geq b} + P_{\geq b}UP_M$ compact, because P_M has finite rank. Hence,

$$\vec{\mathrm{si}}\,(U) = \mathrm{si}(P_{\geq a}UP_{\geq a}) = \mathrm{si}(P_{\geq b}UP_{\geq b}). \tag{3.124}$$

□

The similarity to the right Fredholm index mentioned before Definition 3.5.6 becomes explicit for the particular example of symmetry type 3 (AIII), which contains only the chiral symmetry γ. We will discuss walks of this type in great detail in Chapter 5. However, let us give a brief preview, demonstrating the robustness of the symmetry indices when they are defined as above.

Example: Chiral symmetric walks

In every representation of symmetry type 3 we can choose the chiral symmetry γ to square to the identity. Switching to its eigenbasis, we get

$$\gamma = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \qquad \text{and} \qquad U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \delta \end{pmatrix}, \tag{3.125}$$

with $\alpha^* = \alpha$ and $\delta^* = \delta$, for each admissible unitary U, due to $\gamma U\gamma^* = U^*$. Note that by Assumption 3.1.1, each cell carries a balanced representation (i.e. $\mathrm{tr}\,\gamma_x = 0$). Hence, the eigenspaces of γ are both infinite-dimensional. Moreover, the matrix blocks of an admissible U are essentially local if and only if U is. In the chiral eigenbasis we get

$$2i\,\mathrm{Im}(U) = \begin{pmatrix} 0 & \beta \\ -\beta^* & 0 \end{pmatrix}. \tag{3.126}$$

In this form, the essential gap condition is equivalent to Fredholmness of β [34]. In particular, evaluating $\mathrm{tr}\,\gamma$ on $\ker\left(\mathrm{Im}(U)\right)$ yields

$$\mathrm{si}(U) = \mathrm{tr}\left(\gamma|_{\ker(\mathrm{Im}(U))}\right) = \ker(\beta^*) - \ker(\beta) = -\mathrm{ind}\,(\beta), \tag{3.127}$$

i.e. the Fredholm index of the off-diagonal block β. By essential locality of β, also $P\beta P$ from PUP is Fredholm, and therefore the right symmetry index evaluates to

$$\vec{\mathrm{si}}\,(U) = -\,\vec{\mathrm{ind}}\,(\beta). \tag{3.128}$$

The connection of the symmetry indices to the Fredholm-type indices once again proves the robustness of the former ones. We will heavily use these correspondences later when we discuss the complete set of indices for chiral symmetric protocols in Chapter 5.

[34] See Chapter 5 for a more details.

For translation invariant systems with chiral symmetry, $\vec{\mathrm{si}}$ can be expressed in yet another form. By the Gohberg-Krein theorem [GGK93, XXIII.5, Thm. 5.1], the right Fredholm index of β is equal to the negative winding number of $\det(\widehat{\beta}(k))$ [CGS$^+$18], i.e.

$$\vec{\mathrm{si}}\,(U) = -\,\vec{\mathrm{ind}}\,(\beta) = \mathrm{wind}\left(k \mapsto \det(\widehat{\beta}(k))\right) \tag{3.129}$$

where $\widehat{\beta}(k)$ denotes the Fourier transformation of β. This correspondence connects the right symmetry index to the ad hoc definitions of topological invariants in earlier works, e.g. [AO13]. In [CGS$^+$18] we discuss similar correspondences of the right symmetry indices to winding numbers for the remaining non-trivial symmetry types of the tenfold way (see also [Sta18]).

3.5.2 No robust indices beyond the tenfold way

For the symmetry types beyond the tenfold way, we do not know equally robust invariants from the symmetry indices. The reason for this lies in the more complex balancedness condition, namely the fact that a balanced finite-dimensional representation has to admit unitaries with four instead of two gaps in the spectrum. While it remains possible to transfer the problem to a Hamiltonian and define left- and right symmetry indices this way, we cannot rely on the homotopy stability of these simpler systems as for the tenfold way.

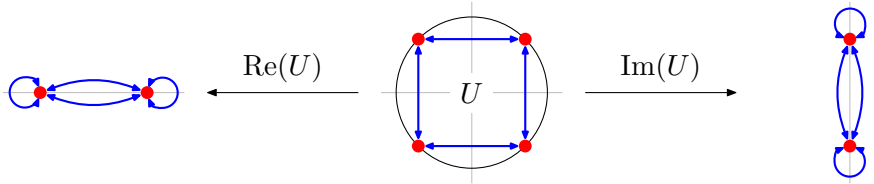
For all non-trivial symmetry types beyond the tenfold way we are concerned with box-eigenvalue orbits (see Lemma 2.3.1). Consequently, the eigenspaces at ± 1 and $\pm i$ have to be combined in order to be invariant under the symmetries. This suggests to transfer the idea of Definition 3.5.5 to the individual indices $\mathrm{si}_\star$ instead of their sum $\sum_\star \mathrm{si}_\star$, using $\mathrm{Im}(U)$ for $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{Re}(U)$ for $\mathrm{si}_{\updownarrow}$. We get

$$\ker\left(\mathrm{Im}(U)\right) = \mathcal{H}_{+1} \oplus \mathcal{H}_{-1} \qquad \text{and} \qquad \ker\left(\mathrm{Re}(U)\right) = \mathcal{H}_{+i} \oplus \mathcal{H}_{-i} \tag{3.130}$$

and therefore also

$$\mathrm{si}_{\leftrightarrow}(U) = \mathrm{si}\left(\rho_{\ker \mathrm{Im}(U)}\right) \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(U) = \mathrm{si}\left(\rho_{\ker \mathrm{Re}(U)}\right). \tag{3.131}$$

One is attempted to conclude that due to (3.131) we can define $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$ also for essentially unitary admissible operators, and therefore also for PUP, which would provide a method to define left and right-sided symmetry indices without the need of a gentle decoupling. For this, we needed a correspondence between unitaries and Hamiltonians similar to Lemma 2.3.5, which enabled us to rephrase the task in terms of Hamiltonians in Definition 3.5.5 and use the topological stability for the symmetry index of those. However, we do not have such a direct correspondence beyond the tenfold way. Instead, each eigenspace of $\mathrm{Im}(U)$ and $\mathrm{Re}(U)$ has to be evenly degenerate, such that the symmetry that maps the respective spaces from the corresponding unitary box orbit onto each other acts as a swapping operator inside these degenerated spaces:



(3.132)

That is, for a finite-dimensional representation of a symmetry type with box orbit, there exists a gapped admissible unitary, if and only if there exist a gapped admissible Hamiltonian with evenly degenerate eigenspaces[35]. Adding this degeneracy as an assumption on the set of admissible Hamiltonians, we could go on and define the symmetry indices on this set. Being just a reformulation, these naturally inherited the homotopy invariance from the unitary formulation, similar to the tenfold way.

However, the extra condition is not automatically fulfilled for essentially unitary operators. In that case, the admissibility of an essentially unitary operator A does not necessarily lead to appropriately degenerate null spaces of $\mathrm{Im}(A)$ and $\mathrm{Re}(A)$. In particular, the degeneracy condition does not survive the projection of a unitary U onto a half-line. We will readily discuss an example walk of symmetry type 10, which exhibits non-degenerate null spaces of $\mathrm{Im}(PUP)$. Hence, the expression of the symmetry indices in terms of $\mathrm{Im}(U)$ and $\mathrm{Re}(U)$ does not unveil further stability properties as it was the case for the symmetry types of the tenfold way.

Nevertheless, (3.131) can still be helpful for computing the symmetry indices in specific cases (see the examples below).

3.5.3 Spatial invariants via forgetting symmetries

If a walk is admissible for a symmetry type beyond the tenfold way containing a chiral, particle-hole and/or time-reversal symmetry, it can also be considered a tenfold way admissible walk by keeping only a subgroup of symmetries. While in some cases, the forgotten additional symmetries trivialize the tenfold- left and right symmetry indices, there are symmetry types where this forgetting method enables us to obtain robust invariants beyond the tenfold way. We will not discuss the subtleties of classifying symmetry types via forgetting symmetries in full detail here but restrict ourselves to three specific types, namely 10, 11 and 24. For type 10, we can restore the complete symmetry index out of the more robust symmetry indices of tenfold subtypes, whereas no index information can be inferred from the tenfold subtypes in the case of type 11. Type 24 lies in between those two examples. That is, the tenfold subtype carries part of the index information of the whole type.

We close this discussion with a detailed analysis of an example walk of symmetry type 10 and a brief discussion of an example walk of symmetry type 11. A variant of the type 10 symmetric walk has already been realized in the lab by Barkhofen et al. in a "time-multiplexing optical fibre-loop"-setup [BLN$^+$18].

Type 10

Type 10 consists of the symmetries σ, γ and σ_γ, commuting with each other (see also Example 3.2.9), and

$$\sigma U \sigma^* = -U, \qquad \gamma U \gamma^* = U^*, \qquad \text{and} \qquad \sigma_\gamma U \sigma_\gamma^* = -U^*. \tag{3.133}$$

For any U we have

$$\mathrm{si}_{\leftrightarrow}(U) = (\mathrm{tr}\,\gamma, \mathrm{tr}\,\sigma_\gamma)\,|_{\ker \mathrm{Im}(U)} \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(U) = (\mathrm{tr}\,\gamma, \mathrm{tr}\,\sigma_\gamma)\,|_{\ker \mathrm{Re}(U)}. \tag{3.134}$$

[35] For this statement, it does not matter whether one chooses $\mathrm{Im}(U)$ or $\mathrm{Re}(U)$.

It turns out that two of the four components can be reduced to tenfold type symmetry indices by simply forgetting some of the symmetries of type 10, while the two other components are trivial for any admissible unitary, anyhow. Let us start with the trivial components: the second component of $\mathrm{si}_{\leftrightarrow}$ is given by $\mathrm{tr}\,\sigma_\gamma$, evaluated on the combined ± 1 eigenspace of U. On this space, however, σ_γ acts as a swapping unitary, mapping $\mathcal{H}_{+1}$ to $\mathcal{H}_{-1}$ and vice versa. Consequently, its trace on this space is always trivial. A similar reasoning applies to the first component of $\mathrm{si}_{\updownarrow}$, i.e. $\mathrm{tr}\,\gamma$ on the combined $\pm i$ eigenspace. We get

$$\mathrm{si}_{\leftrightarrow}(U) = \left(\mathrm{tr}\,\gamma|_{\ker \mathrm{Im}(U)}\,,\,0\right) \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(U) = \left(0\,,\,\mathrm{tr}\,\sigma_\gamma|_{\ker \mathrm{Re}(U)}\right). \tag{3.135}$$

Considering now the first component of $\mathrm{si}_{\leftrightarrow}$, note that this precisely matches the symmetry index of U, considered as a walk of type AIII, i.e. with only the chiral symmetry γ. Hence,

$$\mathrm{si}_{\leftrightarrow}(U) = \left(\mathrm{si}^{\gamma}_{\mathsf{AIII}}(U)\,,\,0\right), \tag{3.136}$$

where the subscript AIII refers to the reduced type and the superscript γ to the symmetry constituting that type (specifying both seems redundant, but will important just a thought ahead).

An equally simple reduction can be archived for the second component of $\mathrm{si}_{\updownarrow}$. On the one hand, note that σ_γ acts as a normal chiral symmetry for iU. On the other, the factor of i moves the eigenspaces at $\pm i$ to ± 1. Hence, we can express the second component of $\mathrm{si}_{\updownarrow}$ as the symmetry index of iU, considered as a walk of type AIII with chiral symmetry σ_γ:

$$\mathrm{si}_{\updownarrow}(U) = \left(0\,,\,\mathrm{si}^{\sigma_\gamma}_{\mathsf{AIII}}(iU)\right). \tag{3.137}$$

In both cases, the individual components are either directly expressed as tenfold-type indices or as isomorphic pictures of such. Hence, they exhibit well defined left and right symmetry indices, i.e.

$$\mathrm{si}_{\leftrightarrow}(U) = \overleftarrow{\mathrm{si}}_{\leftrightarrow}(U) + \overrightarrow{\mathrm{si}}_{\leftrightarrow}(U) \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(U) = \overleftarrow{\mathrm{si}}_{\updownarrow}(U) + \overrightarrow{\mathrm{si}}_{\updownarrow}(U). \tag{3.138}$$

In particular, we get a bulk-boundary correspondence for each symmetry protected eigenspace individually. However, note that we needed to express the symmetry indices in terms of tenfold-type indices, which was possible due to the special formula for the symmetry index for type 10 ($\mathrm{si}(\rho) = (\mathrm{tr}\,\gamma, \mathrm{tr}\,\sigma_\gamma)$). This direct correspondence to some type of the tenfold way is generally not be possible for all types.

Type 11

Similar to type 10, type 11 consists of the symmetries σ, γ and σ_γ, but with anti-commuting generators σ and γ. Hence, all irreducible representations are isomorphic to a copy of the Pauli-matrices (see also Example 3.2.11). The symmetry index is given by $\mathrm{si}(\rho) = d \bmod 4$ and for admissible U we get

$$\mathrm{si}_{\leftrightarrow}(U) = \dim\left(\ker \mathrm{Im}(U)\right) \bmod 4 \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(U) = \dim\left(\ker \mathrm{Re}(U)\right) \bmod 4. \tag{3.139}$$

Forgetting two of the symmetries, while keeping γ or σ_γ, similarly to type 10 before, does not reveal any invariants from the subtype AIII for U, respectively iU. Since γ and σ_γ anti-commute, they have to swap their respective eigenspaces. Hence, in any representation $tr\gamma = \operatorname{tr}\sigma_\gamma = 0$, and we always get $\mathrm{si}^{\gamma}_{\mathsf{AIII}}(U) = \vec{\mathrm{si}}^{\gamma}_{\mathsf{AIII}}(U) = 0$ and $\mathrm{si}^{\sigma_\gamma}_{\mathsf{AIII}}(iU) = \vec{\mathrm{si}}^{\sigma_\gamma}_{\mathsf{AIII}}(iU) = 0$.

On the other hand, type 11 always allows for a gentle decoupling, which enables us to define left and right symmetry indices properly, and, as the example below shows, these can take non-trivial values.

Type 24

Type 24 consists of the symmetries γ, σ_τ and σ_η, with commuting generators and $\sigma_\tau^2 = \sigma_\eta^2 = \mathbb{1}$. In this case, in contrast to type 11, forgetting symmetries provides part of the index information, but not all of it as it was the case for type 10. The index group is given by $\mathbf{I}(\mathsf{S}) = 2\mathbb{Z} \times \mathbb{Z}_2$ and the symmetry index of a finite-dimensional representation is computed via

$$\mathrm{si}(\rho) = \left(\operatorname{tr}\gamma, d_\gamma^+ \bmod 2\right), \tag{3.140}$$

where $d_\gamma^+ = \dim\ker(\gamma - \mathbb{1})$ denotes the dimension of the $+1$-eigenspace of γ. Hence, the first component of $\mathrm{si}(\rho)$ can be inferred from the subtype AIII, by only considering γ. The second component, however, carries no non-trivial index-value when only γ is considered. Indeed, it can be changed e.g., by adding the balanced AIII-representation $\gamma = \sigma_z$[36].

Example: A walk of symmetry type 10

Let us discuss an example of symmetry type 10 in detail. Consider the following walk on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^4$, inspired by [BLN$^+$18]:

$$U = \begin{pmatrix} 0 & S_\downarrow^* R(\theta) \\ \sigma_x R(-\theta) S_\downarrow \sigma_x & 0 \end{pmatrix} = \begin{pmatrix} & & c_\theta & -s_\theta \\ & & Ss_\theta & Sc_\theta \\ c_\theta S^* & -s_\theta & & \\ s_\theta S^* & c_\theta & & \end{pmatrix}, \tag{3.141}$$

where $R(\theta) = \exp(-i\sigma_y\theta)$ denotes the standard rotation around the σ_y-axis in a two-dimensional subspace in each cell (with $(c_\theta, s_\theta) = (\cos(\theta), \sin(\theta))$ and

$$S_\downarrow = \begin{pmatrix} 1 & 0 \\ 0 & S^* \end{pmatrix} \tag{3.142}$$

is the shift down operation from Example 1.4.6. Note that while being irrelevant in the translation invariant case, the order of operations (e.g. Ss_θ v.s. $s_\theta S$) becomes important when position dependent coin angles θ_x are chosen. The walk is admissible for a representation of symmetry type 10, generated by

$$\sigma = \mathbb{1} \otimes \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \qquad \text{and} \qquad \gamma = \mathbb{1} \otimes \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}. \tag{3.143}$$

Moreover, U is translation invariant and, therefore, has only essential spectrum

[36] Note that this representation is not balanced for type 24.

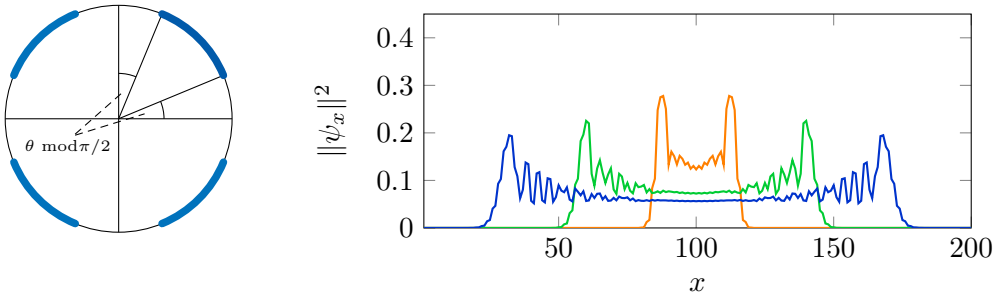


Figure 3.5: Spectrum and position distribution for U with $\theta = \pi/8$, for the initial state $\psi = (1, i, 1, i)/2$ at $x = 100$ after $n = 20, 110$ and 200 steps.

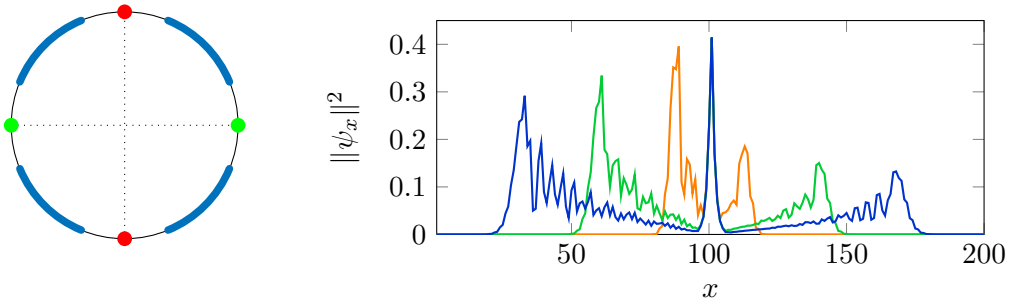


Figure 3.6: Spectrum and position distribution for $\widetilde{U}$ with $\theta_{x\geq 100} = \pi/8$ and $\theta_{x<100} = -\pi/8$, for the initial state $\psi = (1, i, 1, i)/2$ at $x = 100$ after $n = 20, 110$ and 200 steps.

[CGS+18]. The spectrum is absolutely continuous and contained in four intervals on the unit circle specified by $\pm e^{\pm i\lambda}$ with $\lambda \in [\theta \pmod{\pi/2}, -\theta \pmod{\pi/2}]$ and the full unit circle at the endpoints $\theta = n\pi/2$, $n \in \mathbb{Z}$. In particular, U is gapped at ± 1 and $\pm i$ for $\theta \neq n\pi/2$, $n \in \mathbb{Z}$, and for $\theta = (n + 1/2)\pi/2$ the spectrum is contained in $\pm\exp(\pm i\pi/4)$, i.e. U has flat bands. Choosing e.g. $\theta = \pi/8$ we get the spectrum and propagation behaviour shown in Figure 3.5.

The decoupling index of U is determined by $\mathrm{dec}\,(U) = \vec{\mathrm{ind}}\,(S^*_{\downarrow}) = -1$. Hence, U cannot be decoupled and we cannot define the left and right symmetry indices directly. Moreover, as we will see below, $\mathrm{Im}(PUP)$ and $\mathrm{Re}(PUP)$ exhibit one-dimensional null spaces, which rules out a definition of $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$ in terms of these operators. However, as also reported in [BLN+18] we can still observe symmetry protected edge states for certain choices of θ in U. If we choose $\theta \in (0, \pi/2)$ for $x \geq 0$ and $\theta \in (-\pi/2, 0)$ for $x < 0$, the resulting operator $\widetilde{U}$ hosts a pair of symmetry protected edge states at the boundary (see Figure 3.6). This can be seen most easily for the flatband case, i.e. $\theta_{x\geq 0} = \pi/4$ and $\theta_{x<0} = -\pi/4$, which give

$$\widetilde{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} & & \mathbb{1} & \mathbb{1} - 2P \\ & & S(2P - \mathbb{1}) & S \\ S^* & \mathbb{1} - 2P & & \\ (2P - \mathbb{1})S^* & \mathbb{1} & & \end{pmatrix}, \tag{3.144}$$

with $P = P_{\geq 0}$, as usual. In this case we can directly determine the eigenspaces at ± 1

and $\pm i$ and compute $\mathrm{si}_{\leftrightarrow}$ and $\mathrm{si}_{\updownarrow}$. By homotopy invariance of $\mathrm{si}_\star$, these must have the same value also for other choices of $0 < \theta_{x\geq 0} < \pi/2$ and $-\pi/2 < \theta_{x<0} < 0$. For (3.144) the ± 1 and $\pm i$ eigenspaces of $\widetilde{U}$ are each one-dimensional and spanned by

$$\begin{aligned}
\psi_{+1} &= \frac{1}{2}\left[e_{-1}\otimes\left(0,0,-1/\sqrt{2},1/\sqrt{2}\right)+e_0\otimes\left(-1,1,-1/\sqrt{2},1/\sqrt{2}\right)\right]\\
\psi_{-1} &= \frac{1}{2}\left[e_{-1}\otimes\left(0,0,-1/\sqrt{2},1/\sqrt{2}\right)+e_0\otimes\left(1,-1,-1/\sqrt{2},1/\sqrt{2}\right)\right]\\
\psi_{+i} &= \frac{1}{2}\left[e_{-1}\otimes\left(0,0,-1/\sqrt{2},1/\sqrt{2}\right)+e_0\otimes\left(-i,-i,1/\sqrt{2},-1/\sqrt{2}\right)\right]\\
\psi_{-i} &= \frac{1}{2}\left[e_{-1}\otimes\left(0,0,-1/\sqrt{2},1/\sqrt{2}\right)+e_0\otimes\left(i,i,1/\sqrt{2},-1/\sqrt{2}\right)\right],
\end{aligned} \tag{3.145}$$

where e_n denotes the basis element in $\ell^2(\mathbb{Z})$ corresponding to the n'th cell. Evaluating $(\mathrm{tr}(\gamma),\mathrm{tr}(\sigma_\gamma))$ on the combined eigenspaces $\mathcal{H}_{+1}\oplus\mathcal{H}_{-1}$ and $\mathcal{H}_{+i}\oplus\mathcal{H}_{-i}$ according to Table 2.1 and Definition 3.1.4 we get

$$\mathrm{si}_{\leftrightarrow}(\widetilde{U}) = (-2,0) \qquad \text{and} \qquad \mathrm{si}_{\updownarrow}(\widetilde{U}) = (0,2)\,. \tag{3.146}$$

The non-trivial values of the symmetry indices guarantee that the eigenspaces are indeed symmetry protected and cannot change under homotopies, which keep the symmetries and the essential gap. In particular, they are stable for the ranges of θ described above.

Although we cannot decouple the model without breaking the σ-symmetry, we are able to retrieve left and right symmetry indices from the AIII-subtypes, according to the discussion above. This underlines the topological stability and allows to predict the edge states via bulk-boundary correspondence (see Section 3.5.4). We again choose the flatband case, i.e. $\theta = \pi/4$ for the right half of the system and $\theta = -\pi/4$ for the left half. The relevant operators are $\mathrm{Im}(P\widetilde{U}P)$ and $\mathrm{Im}(P^\perp\widetilde{U}P^\perp)$ for the subtype containing only γ, and $\mathrm{Re}(P\widetilde{U}P)$ and $\mathrm{Re}(P^\perp\widetilde{U}P^\perp)$ for the subtype containing only σ_γ. In the first case, the nullspaces are given by

$$\begin{aligned}
\ker\left(\mathrm{Im}(P\widetilde{U}P)|_{P\mathcal{H}}\right) &= \mathrm{span}\left\{e_0\otimes(1,-1,0,0)/\sqrt{2}\right\}\\
\ker\left(\mathrm{Im}(P^\perp\widetilde{U}P^\perp)|_{P^\perp\mathcal{H}}\right) &= \mathrm{span}\left\{e_{-1}\otimes(0,0,1,-1)/\sqrt{2}\right\},
\end{aligned} \tag{3.147}$$

and evaluating $\mathrm{tr}\,\gamma$ on these spaces yields $\overrightarrow{\mathrm{si}}^{\gamma}_{\mathsf{AIII}}(\widetilde{U}) = \overleftarrow{\mathrm{si}}^{\gamma}_{\mathsf{AIII}}(\widetilde{U}) = -1$ for the symmetry indices with respect to only the chiral symmetry. Similarly, for the σ_γ-subtype, the nullspaces of $\mathrm{Re}(P\widetilde{U}P)$ and $\mathrm{Re}(P^\perp\widetilde{U}P^\perp)$ are given by

$$\begin{aligned}
\ker\left(\mathrm{Re}(P\widetilde{U}P)|_{P\mathcal{H}}\right) &= \mathrm{span}\left\{e_0\otimes(1,1,0,0)/\sqrt{2}\right\}\\
\ker\left(\mathrm{Re}(P^\perp\widetilde{U}P^\perp)|_{P^\perp\mathcal{H}}\right) &= \mathrm{span}\left\{e_{-1}\otimes(0,0,1,-1)/\sqrt{2}\right\}
\end{aligned} \tag{3.148}$$

which yield $\overrightarrow{\mathrm{si}}^{\sigma_\gamma}_{\mathsf{AIII}}(i\widetilde{U}) = \overleftarrow{\mathrm{si}}^{\sigma_\gamma}_{\mathsf{AIII}}(i\widetilde{U}) = 1$.

The left and right symmetry indices for the whole symmetry type are then individually stable for each symmetry protected eigenspace $\mathcal{H}_{\leftrightarrow}$ and $\mathcal{H}_{\updownarrow}$. According to the discussion on type 10 above, we get the four components

$$\begin{aligned} \overleftarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) &= (-1,0) & \overrightarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) &= (-1,0) \\ \overleftarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) &= (0,1) & \overrightarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) &= (0,1). \end{aligned} \tag{3.149}$$

These may be combined in two different ways, which on the one hand defines the overall left and right symmetry indices

$$\begin{aligned} \overrightarrow{\mathrm{si}}(\widetilde{U}) &= \overrightarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) + \overrightarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) = (-1,1) \\ \overleftarrow{\mathrm{si}}(\widetilde{U}) &= \overleftarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) + \overleftarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) = (-1,1), \end{aligned} \tag{3.150}$$

and on the other yields the eigenspace indices

$$\begin{aligned} \mathrm{si}_{\leftrightarrow}(\widetilde{U}) &= \overrightarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) + \overleftarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}) = (-2,0) \\ \mathrm{si}_{\updownarrow}(\widetilde{U}) &= \overleftarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) + \overrightarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}) = (0,2). \end{aligned} \tag{3.151}$$

Note that (3.150) seems to be in contradiction with (3.135), since both components of the indices are non-zero. However, (3.135) only holds for the symmetry indices associated to unitaries that are admissible for type 10. Since the present example does not allow for a decoupling, $\overrightarrow{\mathrm{si}}_{\star}(\widetilde{U})$ is not defined as such, but obtained from the AIII-subtype symmetry index.

Example: A walk of symmetry type 11

For this example, we consider the symmetry representation of type 11 generated by

$$\sigma = \mathbb{1} \otimes \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \qquad \text{and} \qquad \gamma = \mathbb{1} \otimes \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}. \tag{3.152}$$

Note the difference in γ to the previous example, resulting in anti-commuting generators $\sigma\gamma = -\gamma\sigma$. Moreover, let

$$U(\theta_1,\theta_2,\theta_3,\theta_4) = \begin{pmatrix} 0 & S_\uparrow R(\theta_2) S_\downarrow R(\theta_1) \\ S_\uparrow R(\theta_4) S_\downarrow R(\theta_3) & 0 \end{pmatrix}, \tag{3.153}$$

which is admissible for the symmetry representation above. U is an off-diagonally doubled version of the split-step walk, which we already briefly mentioned in Section 1.4 and which we will study in detail in Section 5.4. Therefore, let us here only mention the bare necessities to underline our point above, i.e. that there exist walks of type 11, which exhibit non-trivial values of $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$.

The walk $U(\theta_1,\theta_2,\theta_3,\theta_4)$ can be decoupled between $x = 0$ and $x = -1$ by setting $\theta_2 = \theta_4 = \pi/2$, locally at $x = -1$, while leaving the choice for the remaining angles completely free. Because the decoupling is realised by choosing certain coin angles, which can be reached on a continuous path of angles, it is clearly gentle.

Let us particularly consider the two different translation invariant scenarios

$$U_I = U(\pi/2, 0, \pi/2, \pi/2) \qquad \text{and} \qquad U_{II} = U(\pi/2, 0, -\pi/2, \pi/2). \tag{3.154}$$

Without the decoupling coin at $x = -1$, both choices are gapped walks with flat bands in the sense that the spectra are contained in $\{\pm e^{\pm i\pi/4}\}$. After adding the decoupling coin at $x = -1$, the resulting walks $\widetilde{U}_I$ and $\widetilde{U}_{II}$ each exhibit 4 eigenvalues differing from $\{\pm e^{\pm i\pi/4}\}$.

For $\widetilde{U}_I$ we get two eigenvalues at ± 1. The corresponding eigenspaces are spanned by

$$\begin{aligned} \psi_{\pm,R} &= e_0 \otimes (\mp 1, 0, 1, 0)/\sqrt{2} \\ \psi_{\pm,L} &= e_{-1} \otimes (0, \mp 1, 0, 1)/\sqrt{2}, \end{aligned} \tag{3.155}$$

i.e. on each side of the cut, we get one eigenspace for each eigenvalue ± 1. Consequently, the left and right symmetry index components evaluate to

$$\overrightarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}_I) = \overleftarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}_I) = 2 \bmod 4 \qquad \text{and} \qquad \overrightarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}_I) = \overleftarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}_I) = 0 \bmod 4, \tag{3.156}$$

which gives

$$\overrightarrow{\mathrm{si}}(U_I) = \overleftarrow{\mathrm{si}}(U_I) = 2 \bmod 4. \tag{3.157}$$

For $\widetilde{U}_{II}$, on the other hand, we get two eigenvalues at $\pm i$, with the eigenspaces

$$\begin{aligned} \varphi_{\pm,R} &= e_0 \otimes (\pm i, 0, 1, 0)/\sqrt{2} \\ \varphi_{\pm,L} &= e_{-1} \otimes (0, \pm i, 0, 1)/\sqrt{2}. \end{aligned} \tag{3.158}$$

Again, each half-space hosts two eigenspaces for each eigenvalue $\pm i$, resulting in

$$\overrightarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}_{II}) = \overleftarrow{\mathrm{si}}_{\leftrightarrow}(\widetilde{U}_{II}) = 0 \bmod 4 \qquad \text{and} \qquad \overrightarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}_{II}) = \overleftarrow{\mathrm{si}}_{\updownarrow}(\widetilde{U}_{II}) = 2 \bmod 4, \tag{3.159}$$

i.e. we again get

$$\overrightarrow{\mathrm{si}}_{\updownarrow}(U_{II}) = \overleftarrow{\mathrm{si}}_{\updownarrow}(U_{II}) = 2 \bmod 4 \tag{3.160}$$

Note that the left and right symmetry indices have the same values in both scenarios, but are composited in different ways. While the non-trivial values for $\widetilde{U}_I$ originate in the real symmetry protected eigenspaces at ± 1, those for $\widetilde{U}_{II}$ have their origin in the imaginary symmetry protected eigenspaces at $\pm i$. Hence, combining the two scenario into a single walk $\widetilde{U}$, e.g., with U_{II} on the left and U_I on the right half chain, we get the non-trivial indices

$$\mathrm{si}_{\leftrightarrow}(\widetilde{U}) = \mathrm{si}_{\updownarrow}(\widetilde{U}) = 2 \bmod 4. \tag{3.161}$$

These are homotopy invariants and, in particular, stable under continuous deformations of the angles $(\theta_1, \theta_2, \theta_3, \theta_4)$, as long as the essential gaps are not closed. Hence, a crossover like $\widetilde{U}$ produces topologically protected eigenstates at the symmetry protected parts of the spectrum.

3.5.4 Bulk-boundary correspondence

Since $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$ are independent of the cut-position, they can be calculated arbitrarily far to the right and to the left, respectively. Therefore, we can justifiably call them **bulk-invariants**, i.e. invariants, which do not depend on how crossover regions are designed, but only on the **bulk** of a system. A bulk is the standing concept of a system that is "large enough". Usually, this means that, although finite, a system can be treated as infinite for all practical purposes. Therefore, one allows oneself to apply the techniques and findings for infinite systems, such as spectral bands and corresponding winding numbers. However, often this term lacks a precise definition but is assumed to be common knowledge, and the necessary properties are often only vaguely sketched. To avoid this, we here define a **bulk** to be a half-infinite system. This means that a bulk-unitary/walk is an essentially local (possibly essentially unitary) operator on $P\mathcal{H} = \bigoplus_{x\geq 0} \mathcal{H}_x$. It might emerge from a unitary/walk U on the whole Hilbert space by decoupling ($U \mapsto U' = U_L \oplus U_R$) as suggested by Section 3.5 or simply by projecting down to the half-line (PUP and $P^\perp U P^\perp$) as in Section 3.5.1.

For physical applications, where no system is infinite, this definition of a bulk requires an idealization step [CGG$^+$18]. Whenever a system is large in the sense that its spatial extent is much bigger than the localization length of the system, we treat it as practically infinite. This can be done by periodically extending the system to infinity, or, if a specific model with disorder stemming from a known (or guessed) distribution is under consideration, extending the disordered system, while drawing from the same distribution. We stress that this idealization step is crucial in order to define bulk invariants. On the one hand, in our theory, every finite piece is trivial with respect to $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$. On the other, the classifying indices in the literature often rely on winding numbers in the bundles defined by the band structures of a translation-invariant system. These are not defined if the system is not infinite in at least one direction. Moreover, also more sophisticated techniques, e.g., a classification using K-theoretic methods, need properly infinite systems to be applicable.

An interesting property of the topological classification of lattice systems, be it continuously driven time evolutions by a Hamiltonians or quantum walks in discrete time, is the so-called **bulk-boundary correspondence**. It asserts the equality of two different kinds of invariants: On the one hand, bulk invariants like winding numbers for translation-invariant systems and on the other, boundary-invariants depending on the eigenspace at the boundary of a system. In the case of the symmetry types of the tenfold way, bulk-boundary correspondence manifests itself in the equation

$$\mathrm{si}_+ + \mathrm{si}_- = \overleftarrow{\mathrm{si}} + \overrightarrow{\mathrm{si}}. \tag{3.162}$$

The left side is the sum of the symmetry indices corresponding to the finite-dimensional eigenspaces of a walk operator under consideration, which, in an appropriately homogeneous (e.g., translation invariant) system, are always associated with the boundary or with spatially finite perturbations [CGS$^+$18]. The right side consists of the left- and right symmetry indices, which are proper homotopy invariants in the tenfold way, and only depend on the half infinite systems to the left and to the right.

For the symmetry types beyond the tenfold way, we have the similar formula

$$\mathrm{si}_{\leftrightarrow} + \mathrm{si}_{\updownarrow} = \overleftarrow{\mathrm{si}} + \overrightarrow{\mathrm{si}}. \tag{3.163}$$

It is important to stress, however, that this is in general no bulk-boundary correspondence in the typical sense. The left and right symmetry indices are not provably homotopy invariant, and it might well be that in this case, the proper bulk invariants do not coincide with $\overleftarrow{\mathrm{si}}$ and $\overrightarrow{\mathrm{si}}$.

The physical implication of bulk-boundary correspondence in our one-dimensional setting is that every system in which two bulks of different topological classes are joined possesses symmetry protected bound states near the boundary. Thereby, one system could be the vacuum, i.e. a half-line system in a non-trivial topological class always hosts bound states at the edge. This implication is true in both scenarios, as the following corollary shows. According to the different levels of the robustness of $\overrightarrow{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}$ for the different sets of symmetry types in Section 3.5 and Section 3.5.1, we distinguish two different levels of generality. In both cases, we consider walks, which are crossovers between two bulks:

(1) Exactly unitary strictly local walks U, which are admissible for a symmetry type beyond the tenfold way and exhibit well defined left- and right symmetry indices according to Definition 3.5.1. Moreover, U is assumed to equal two admissible strictly local walks U_L and U_R on the left, respectively the right half-chain in the sense that there exist $a < b \in \mathbb{Z}$, such that

$$P_{<a}(U - U_L)P_{<a} = P_{\geq b}(U - U_R)P_{\geq b} = 0. \tag{3.164}$$

(2) Exactly unitary essentially local walks U, which are admissible for a symmetry type of the tenfold way, with left and right symmetry indices according to Definition 3.5.6. Moreover, U is assumed to equal admissible essentially local walks U_L and U_R in the limits far to the left and far to the right, i.e. U fulfils

$$\lim_{x\to-\infty} \|P_{<x}(U - U_L)P_{<x}\| = \lim_{x\to\infty} \|P_{\geq x}(U - U_R)P_{\geq x}\| = 0. \tag{3.165}$$

Corollary 3.5.8. *Let U be as in one of the scenarios above, and* si, $\overrightarrow{\mathrm{si}}$ *and* $\overleftarrow{\mathrm{si}}$ *be defined accordingly. Then*

$$\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U_L) + \overrightarrow{\mathrm{si}}(U_R) \tag{3.166}$$

defines a lower bound on the number of symmetry protected eigenstates via $|\mathrm{si}(U)|$ *if* $\mathbf{I}(\mathsf{S}) \cong n\mathbb{Z}$ *or* $m\mathbb{Z}_2$ *and* $\max(|a|, |b|)$ *for* $\mathbf{I}(\mathsf{S}) \cong A \times B$, $a \in A, b \in B$ *and* $A, B \in \{n\mathbb{Z}, m\mathbb{Z}_2\}$.

Proof. **Scenario (1):** U coincides with U_L on the left half-chain and with U_R on the right half-chain, with a finite crossover region in between. Hence, (3.166) is a direct consequence of Theorem 3.5.2.

Scenario (2): Any unitary crossover between U_L and U_R according to (3.165) is a compact perturbation of U. In particular, by (3.165), $P_{\geq x}UP_{\geq x} - P_{\geq x}U_RP_{\geq x}$ is the norm limit of finite rank operators and therefore compact. Hence, we get $\overrightarrow{\mathrm{si}}(U) = \overrightarrow{\mathrm{si}}(U_R)$, and similarly also $\overleftarrow{\mathrm{si}}(U) = \overleftarrow{\mathrm{si}}(U_L)$.

In both scenarios, we have

$$\mathrm{si}(U) = \sum_{\star} \mathrm{si}_{\star}(U) \tag{3.167}$$

and, as discussed at the end of Section 3.1.1, $\mathrm{si}_{\star}$ is a lower bound on the dimension of the respective symmetry protected eigenspaces of U. □

While the symmetry index si provides a lower bound on the total number of protected eigenstates corresponding to real eigenvalues $\pm 1/\pm i$, we cannot distinguish between these eigenvalues in general. In fact, as Example 3.5.3 shows, the distribution of eigenstates between the eigenvalues $\pm 1/\pm i$ depends on how the crossover is manufactured and can therefore not be determined by quantities that are invariant under local (compact) perturbations. This is only the case for single-timestep unitaries, i.e. the scenario of a quantum walk we are concerned with here. In Chapter 5 we discuss another kind of quantum walk definition, which relies on a (possibly discrete) protocol in contrast to a single time-step. Protocols bridge between purely discrete quantum walks and continuously driven Floquet systems. We will focus exclusively on chiral symmetric systems and investigate the influence of such symmetry on the whole driving process. Thereby, we find that the chiral symmetry stabilizes the predicted edge states in a protocol and enables us to distinguish between the eigenvalues ± 1 in the bulk-boundary correspondence, which then predicts the protected edge states for each eigenvalue separately (see Section 5.5.2).

3.6 Completeness for the tenfold way

A remarkable property of the symmetry indices, and also the main result of our work in [CGG$^+$18], is that in case of the tenfold way, they provide a complete classification with respect to continuous and/or compact deformations in the set of admissible walks. The result holds for almost all symmetry types of the tenfold way (all but $1, 4$ and 5 in Table 2.1)[37], but we will also comment on completeness for these outliers. We state the completeness results here and also sketch the proofs. However, the remaining main topic of this thesis will be the complete classification of chiral protocols and Floquet systems in Chapter 5. Therefore, we do not provide the full proofs here, but refer the interested reader to [CGG$^+$18, Ced18] for the detailed version.

The completeness result covers three different scenarios, each equipped with a set of allowed deformations. In each scenario there is a subset of the indices $(\mathrm{si}, \overleftarrow{\mathrm{si}}, \overrightarrow{\mathrm{si}}, \mathrm{si}_{\pm})$, which labels the connected components up to the allowed deformations. That is, two objects can be obtained from each other via these deformations if and only if their values of the respective subset of indices coincide. The scenarios are the following:

(I) Admissible quantum walks up to continuous deformations with the indices

$$(\mathrm{si}, \overrightarrow{\mathrm{si}}, \mathrm{si}_{+})\,. \tag{3.168}$$

[37] A, AI and AII

(II) Admissible quantum walks up to continuous deformations as well as compact perturbations, with the indices

$$(\mathrm{si}, \vec{\mathrm{si}}) \,. \tag{3.169}$$

(III) Admissible unitaries (without a locality assumption) up to continuous deformations, with the indices

$$(\mathrm{si}, \mathrm{si}_+) \,. \tag{3.170}$$

Before we state the completeness theorem, let us comment on why we have to restrict ourselves to the tenfold way here. We already saw, that the indices in each scenario cannot be directly generalized to complete index sets for the remaining symmetry types of the 38-fold way. On the one hand, concerning scenarios I and II, as discussed in Section 3.5.2, we were not able to come up with a definition of the right symmetry index $\vec{\mathrm{si}}$, which is robust against continuous deformations in the set of essentially unitary essentially local unitaries. On the other, in Example 3.2.10, we discussed a non-gentle perturbation of a walk of symmetry type 27, which could not be detected by the spectral-dependent indices $\mathrm{si}_\star$, ruling out a direct generalization of the index pair $(\mathrm{si}, \mathrm{si}_+)$ to $(\mathrm{si}, \mathrm{si}_\star)$ $(\star \in \{\leftrightarrow, \updownarrow\})$ in scenario III.

Theorem 3.6.1. *For the symmetry types* $3, 8, 9, 20, 21, 22$ *and* 23[38] *in Table 2.1, and each Scenario above, the corresponding set of indices is complete. Moreover, each index combination can be realized by joining two strictly local translation invariant walks with a finite crossover region.*

We sketch the proof strategy and state the needed intermediate results, without proving all of them. We already discussed the invariance properties of the indices under consideration in detail in earlier sections an chapters. Hence, we are left with constructing actual deformations between two given walks/unitaries with the same indices. One of the mayor steps for this task is the so called flattening construction, a version of which will also be important in Chapter 5. Therefore, we discuss our proof from [CGG$^+$18] here, which shows the existence of a flattening path, without explicitly constructing one. Later in Chapter 5, when we specialize on driven systems with chiral symmetry, we also provide an explicit construction for walks of this type.

Lemma 3.6.2. *In all three scenarios above and for all symmetry types in Theorem 3.6.1 every walk/unitary* U *can be continuously deformed, without breaking the assumptions of the scenario, into a* ***flatband*** *walk/unitary* $U^\flat$*, such that*

- *the* ± 1 *eigenspaces of* $U^\flat$ *are finite-dimensional and do not contain any balanced representations of the symmetry type, respectively.*
- *the spectrum of* $U^\flat$ *is contained in* $\{\pm 1, \pm i\}$.

See Figure 3.7 for an illustration.

Proof. The proof is split into two steps: By the admissibility condition, the eigenspaces of U are finite-dimensional and isolated from the rest of the spectrum. Let ρ_+ be any balanced subrepresentation of the $+1$ eigenspace of U. Then there exists a gapped unitary

[38] AIII, D, C, BDI, CII, CI and DIII

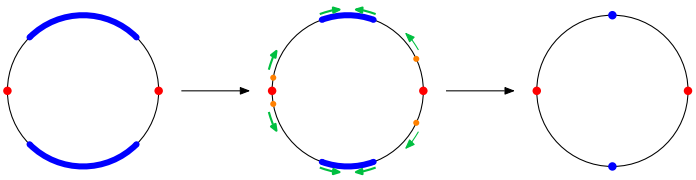


Figure 3.7: Flattening the band structure.

V, which is admissible for ρ_+. Moreover, let $H = -i \log V$ be a corresponding Hamiltonian, where we chose the branch cut of the logarithm at -1. Then $t \mapsto V_t = \exp(iHt)$, $t \in [0, 1]$ provides a continuous path, which removes the respective part of the $+1$ eigenspace of U. A similar construction works for -1. This can be done until the ± 1 eigenspaces of U no longer contain balanced representations. Since these changes on U are of finite rank, they do not harm essential locality.

In the second step we deform the non-real parts of the spectrum to $\pm i$. This can be done in the continuous functional calculus of the C^* algebra of essentially local operators. Note that the admissibility conditions for U are valid also for any Laurent polynomial in U, with real coefficients. Moreover, by the Weierstraß Theorem, we conclude that any continuous function f on the unit circle, with $\big(f(z)\big)^* = f(z^*)$, applied to U in the functional calculus also fulfils the admissibility conditions[39]. Hence, we certainly find a continuous path between the functions $f_0(z) = z$ and $f_1(z) = \mathrm{sign}(\mathrm{Im}(z))i$ for $|\mathrm{Im}(z)| > \varepsilon$, where ϵ is determined by the gap size of U.

□

Sketch of proof for Theorem 3.6.1. First note, that we already established completeness of si_+ (or equivalently si_-) for compact admissible perturbations. I.e., proving completeness of si and $\overrightarrow{\mathrm{si}}$ for scenario (II) also establishes completeness of si, $\overrightarrow{\mathrm{si}}$ and si_+ for scenario (I)[40]. Hence, we only focus on scenario (II) and (III). The proof is done in several steps:

- In the first step one reduces the scenarios (II) to the third one (III). This is done by first decoupling a given walk U via a gentle decoupling. Since any decoupled walk is essentially local (see Lemma 3.3.6) we can then freely deform U_L and U_R separately, without having to deal with any locality condition. Note that for this we have to employ the full potential of essential locality, and this reduction is clearly not possible for strictly local or band dominated walks (compare Example 3.3.10).

  As already discussed, the individual invariants $\overleftarrow{\mathrm{si}}_\pm$ and $\overrightarrow{\mathrm{si}}_\pm$ of U_L and U_R are not invariant with respect to homotopies of the full unitary U. Hence, given two walks U and U', it is not guaranteed, that we end up with $\mathrm{si}_\pm(U_{L/R}) = \mathrm{si}_\pm(U'_{L/R})$. However, one can show, that this can always be archived via a compact perturbation[41].

[39] This only works for symmetries, with $s = 1$ (i.e. the tenfold way). Since for $s = -1$ only odd powers of U are admissible in the same way as U itself.

[40] There are some subtleties to respect for this argument to hold throughout the whole following construction. However, for this sketch of a proof, we will generously omit those and invite the interested reader to study the full proof in [CGG+18] or [Ced18].

[41] Or even a gentle one, see [40].

- In the second and third step one shows completeness for scenario (III). Given two admissible unitaries U_1 and U_2 for the same representation of a symmetry type and with the same symmetry indices $\mathrm{si}_\pm$, we apply Lemma 3.6.2 to both of them. This provides us with two admissible unitaries with the same spectrum and, moreover, with the same multiplicities of the finite-dimensional eigenspaces. Hence, they are unitarily equivalent with a symmetry commuting unitary V, i.e. $U_2 = VU_1V^*$ (see [CGG$^+$18, discussion below Lem. VIII.2]).
- The last step is to show that the set of symmetry commuting unitaries has only one connected component with respect to continuous deformations (see [CGG$^+$18, Lem. VIII.3]), which finishes the proof.

□

We excluded three types of the tenfold way in Theorem 3.6.1, namely $1, 4$ and 5[42]. This is due to their lack of a spectral orbit, that singles out invariant points of the spectrum. For all three types, each spectral projection commutes with the symmetries. Hence, the symmetry indices $\mathrm{si}_\pm$ are always trivial, because we can always move away any finite-dimensional eigenspace from ± 1. However, the essential gap condition prevents us from also doing so with essential parts of the spectrum. I.e. a unitary with essential spectrum below and above the real line is topologically different from one, where only the upper part of the unit circle carries essential spectrum. This observation already results in a complete classification: Denoting by $n_\pm$ the rank of the spectral projection onto the part of the spectrum with positive/negative imaginary part we get:

Proposition 3.6.3. *For the symmetry types $1, 4$ and 5 there are three connected components of admissible unitaries with respect to continuous deformations and/or compact perturbations: Either $n_+ < \infty$, $n_- < \infty$ or both are infinite. The same is true for essentially local unitaries, i.e. walks.*

For the proof see the discussion below Thm. VIII.1 in [CGG$^+$18].

With this, we end the general discussion about the topological classification of single time-step quantum walks with involutive symmetries and turn our focus to driven systems with or without chiral symmetry. In Chapter 5 we pick up the results we archived so far in the discussion of chiral protocols. On the one hand, we completely classify such protocols and relate the findings to the complete classification of single time-step unitaries presented above. This includes a stronger version of bulk-boundary correspondence, which allows us to distinguish between the two symmetry protected eigenspaces in chiral protocols. The classification will be completely in terms of Fredholm type indices. That is we use the results from Section 3.3 and apply it to the new setting. On the other hand, we discuss the possibility of non-gentle perturbations in discretely driven systems, picking up the discussion from Section 3.2.

[42] A, AI and AII

4 Shift-coin decomposition for strictly local quantum walks

In the preliminary Section 1.4 we discussed different possibilities of defining strictly local walks. On the one hand, we presented the axiomatic definition, in which a quantum walk is just a unitary with finite interaction length (Definition 1.4.1). On the other, quantum walks are often defined constructively as a sequence of shift and coin operations (Definition 1.4.5). Of course, a finite sequence of shifts and coins results in a strictly local walk in the sense of the axiomatic approach, but the converse is not clear from the outset. In this chapter, we show that the two approaches are equivalent. That is, any banded unitary can be factorised into a sequence of shift and coin operations with respect to an almost arbitrary[1] but fixed one-dimensional cell structure. The results presented in this chapter were obtained in collaboration with Christopher Cedzich and Reinhard Werner and have been published in part in [CGW21].

Both approaches to quantum walks have their benefits, depending on the underlying setting or task. From a mathematical point of view, it is generally more convenient to define a quantum walk axiomatically. As we discussed in the previous chapter, this definition provides a straightforward lift to different C^*-algebras of band-dominated or essentially local operators, suitable for the earlier discussions. However, the constructive approach for quantum walks via a shift-coin sequence is favourable for many applications and experimental realisations. This includes the construction of explicit models as analogues of condensed matter systems [KRBD10, SK10, FOZ17, SAM+19, CFGW20, PFM20] (see also the introductions to Section 1.4 and Chapter 3), as well as the design of algorithms based on quantum walks [Kem03, AKR05, VA12] (see also the introduction to Section 1.4).

Moreover, as we already discussed in Section 3.3, there is a significant difference between quantum walks as single time step unitaries, and those which arise from a continuous driving process. The latter are always trivial with respect to the right Fredholm index, whereas a simple shift already provides an $\overrightarrow{\mathrm{ind}}$-wise non-trivial example of a single time-step unitary. A protocol like a shift-coin sequence fills a gap between these two pictures. On the one hand, it emphasises the underlying driving process, in contrast to just the full time-step unitary. On the other, it allows for non-trivial index values and is still discrete.

In the translation-invariant case, where quantum walks may be represented as Lau-

[1] For the precise conditions, see below.

rent polynomials in e^{ik}, where k denotes the Fourier-parameter, such a factorisation already exists [Vog09]. The shift coin sequence is obtained by factorising the corresponding matrix-valued Laurent polynomial, building on techniques from the theory of filter banks [VD89, BJ02, GNS01]. In [Vog09] the factorisation is then used to embed any translation-invariant one-dimensional quantum walk into an interacting many-particle system, as the one-particle sector of particle-number conserving Quantum cellular automaton (QCA) [SW04, Arr19, Far20]. Establishing a shift-coin protocol for any banded unitary generalises this method to non-translation invariant quantum walks.

Another task requiring shift-coin protocols is to couple quantum walks to external electromagnetic fields, which are implemented via commutation phases of the shift operators [CRW$^+$13, GAS$^+$13, CGWW19, SAM$^+$19].

Last but not least, the possibility of factorising a banded unitary with respect to any given cell structure is a desirable technique also from an experimenters point of view. Many experimental realisations of quantum walks rely on a sequence of shifts and coins. Moreover, in most implementations, the underlying physical system heavily restricts the dimension of the local coin spaces, which restricts the set of possibly implementable protocols. However, our factorisation method provides a shift-coin sequence for any banded unitary for any cell structure. In particular, the desired protocol on some cell structure that does not fit the physical implementation at hand can always be interpreted as a banded unitary without any cells and then be re-factorised with respect to the structure fitting the experimenters needs. This re-coining procedure might also help implement quantum walk based algorithms in physical implementations, thereby acting as a compiling step for the implementation.

4.1 Translation invariant quantum walks

We begin with a summary of the result from [Vog09] for translation-invariant quantum walks. These can be considered as matrix-valued Laurent polynomials in e^{ik} via the Fourier transformation, where k is the Fourier parameter (see Section 1.4.2):

$$U(k) = \sum_{n=-L_-}^{L_+} e^{ikn} U_n. \tag{4.1}$$

Note that, in slight deviation from our earlier conventions, we here distinguish the interaction lengths to the left (L_-) and to the right (L_+) in order to match the considerations in [Vog09]. The L given earlier would then be defined as $L = \max\{L_+, L_-\}$. A coin is given by a unitary $d \times d$ matrix, where d is the dimension of the single cell Hilbert space and a partial shift with respect to $\varphi \in \mathcal{H}_x$ takes the form

$$S_\varphi = \mathbb{1}_d + (e^{ik} - 1)P_\varphi, \tag{4.2}$$

with P_φ being the projection onto the subspace spanned by φ. Setting $\varphi \equiv (1, 0, \ldots, 0)$ for a standard reference shift, this becomes

$$S = \mathrm{diag}(e^{ik}, 1, \ldots, 1). \tag{4.3}$$

Building on techniques from the theory of filter banks [GNS01, Mey96], Vogts proves in [Vog09] that up to a global factor of e^{ikL_-}, every translation invariant walk with finite jump length can be decomposed into a finite sequence of coin operations and powers of the reference shift in (4.3). We will not repeat the proof of the following result here, but refer the reader to [Vog09, Prop. 6.3].

Lemma 4.1.1. *Let $U(k)$ be a unitary $d \times d$ matrix over Laurent polynomials in e^{ik} with index n. Then there exist coins $C_0, C_1, \ldots, C_{n+dL_-}$, such that*

$$U(k) = e^{-ikL_-} C_0 S C_1 S \ldots C_{n+dL_- -1} S C_{n+dL_-}. \tag{4.4}$$

Of course, the global factor $e^{ikL_-} \cdot \mathbb{1}$ can also be decomposed into a sequence of coins and the reference shift S as follows:

$$e^{-ikL_-} \cdot \mathbb{1} = S^{L_-} \left(C_{\pi(12)} S^{L_-} C_{\pi(12)}\right) \ldots \left(C_{\pi(1d)} S^{L_-} C_{\pi(1d)}\right),$$

where $C_{\pi(ij)}$ denotes the permutation-unitary, which swaps the i'th and j'th basis vector and leaves invariant the remaining ones. In total, since the absolute value of the index $|n|$ is bounded from above by $d \cdot \max\{L_+, L_-\}$, the number of shifts and coins needed for this decomposition (counting monomials in S as a single factor) is of order $\mathcal{O}(dL)$. We will see that in the generalised version for arbitrary banded unitaries on homogeneous cell structures, the number of factors will be of order $\mathcal{O}(d^2 L^2)$. However, this might well be an artefact of the proof technique. We will not tackle the optimisation of the length of the shift coin sequence but focus solely on proving the existence of a finite sequence.

4.2 Banded unitary operators on the line

We now come to the general case: strictly local quantum walks or banded unitaries without assuming translation invariance. The setting will be that of Definition 1.4.1, with an additional condition on the local cell dimensions $d_x = \dim \mathcal{H}_x$. We do not assume the cells $\mathcal{H}_x$ to be of the same dimension. However, as discussed in Section 3.3, we generally assume a uniform upper bound on d_x. We have to add a further assumption for this section, namely a lower bound for the dimension of at least some of the cells. Let us begin with a no-go example when the cells are too small:

Example 4.2.1. *Consider the simplest possible cell structure, with only one-dimensional cells $\mathcal{H}_x = \mathbb{C}$, i.e. $\mathcal{H} = \ell^2(\mathbb{Z})$. By Observation 3.3.2 the specific underlying structure does not restrict the set of possible banded unitaries, as long as no further assumptions as translation invariance are met. Hence, every banded unitary on every one-dimensional spatial structure with bounded cell dimensions can be considered a banded unitary on $\ell^2(\mathbb{Z})$ by relabelling the basis.*

However, the set of banded unitaries, which shifts and coins can realise, is very restricted on $\ell^2(\mathbb{Z})$. With $\mathcal{H}_x = \mathbb{C}$, the coin operations are confined to diagonal unitaries, i.e. multiplication with phases $C\phi_x = \lambda_x \phi_x$ locally. Such building blocks do not leave enough freedom to generate all banded unitaries. In fact, any sequence $U = C_{n+1} S^{k_n} \ldots C_2 S^{k_1} C_1$ of shifts and coins of this kind has non-trivial matrix elements only on the $-\overrightarrow{\mathrm{ind}}(U)$'s diagonal, where $\overrightarrow{\mathrm{ind}}(U) = -\sum_i k_i$. Clearly, not every banded unitary is of this form.

If we assume the cells to be at least two-dimensional, on the other hand, the situation drastically changes, as the following theorem shows. We do not need to assume $d_x > 1$ for every x, but only for "sufficiently many" ones:

Theorem 4.2.2. *Let U be a unitary on $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$, such that there exist positive integers $d, r \in \mathbb{N}$ with*

$$\dim \mathcal{H}_x < d \qquad \textit{and} \qquad r < \dim\left(\mathcal{H}_x \oplus \ldots \oplus \mathcal{H}_{x+r-1}\right), \quad \forall x. \tag{4.5}$$

Then the following are equivalent:

1) U is strictly local, i.e. banded.

2) U can be written as a finite product of partial shifts S_{φ^i}:

$$U = S_{\varphi^n}^{n_k} \ldots S_{\varphi^2}^{n_k} S_{\varphi^1}^{n_1} \tag{4.6}$$

3) U can be written as a finite product of coin operations C_i and powers of a fixed reference shift S:

$$U = C_{k+1} S^{n_k} C_k \ldots S^{n_1} C_1 \tag{4.7}$$

Let us first comment on the conditions on the cell dimensions. We already discussed the upper bound d in Section 3.3 as a physical assumption. Here it will become necessary for the proofs of *1)* $\Rightarrow$ *3)* and *3)* $\Rightarrow$ *2)*. The lower bound, on the other hand, is new here and guarantees that each consecutive set of r cells contains at least one cell of dimension $d_x > 1$, i.e. it bounds the maximal length of consecutive one-dimensional cells, which turned out to be problematic in the example above. The bound is necessary for the proof of Lemma 4.2.3, which contains the main ingredient for the proof of *1)* $\Rightarrow$ *3)*. The equivalence *2)* $\Leftrightarrow$ *3)* also holds without this lower bound. We first prove *2)* $\Leftrightarrow$ *3)* and address *1)* $\Rightarrow$ *3)* afterwards. The implications *3)* $\Rightarrow$ *1)* and *2)* $\Rightarrow$ *1)* are trivial.

2) $\Rightarrow$ 3): Let $S \equiv S_\chi$ be the reference shift for *3)*. Then, for any partial shift S_φ we define the coin

$$C_\varphi = \bigoplus_x \left(\mathbb{1}_x - |\chi_x\rangle\langle\chi_x| - |\varphi_x\rangle\langle\varphi_x| + |\chi_x\rangle\langle\varphi_x| + |\varphi_x\rangle\langle\chi_x|\right). \tag{4.8}$$

With this, we get $S_\varphi = C_\varphi S_\chi C_\varphi^* \equiv C_\varphi S C_\varphi^*$, i.e. any partial shift can be written as a sequence of coins and the reference shift S.

3) $\Rightarrow$ 2): We need to realize the coin operations as products of partial shifts. Consider the shifts S_φ and $S_{\widetilde{\varphi}}$ with respect to $\{\varphi\} \equiv \{\ldots, \varphi_{x-1}, \varphi_x, \varphi_{x+1}, \ldots\}$ and $\{\widetilde{\varphi}\}$, such that $\widetilde{\varphi}_x = \lambda_x \varphi_x$, with phases $\lambda_x \in \mathbb{T}$. For these, we get

$$S_\varphi^* S_{\widetilde{\varphi}} \varphi_x = \frac{\lambda_{x+1}}{\lambda_x} \varphi_x = \mu_x \varphi_x \qquad \text{and} \qquad S_\varphi^* S_{\widetilde{\varphi}} \psi_x = \psi_x \tag{4.9}$$

for $\varphi_x \perp \psi_x \in \mathcal{H}_x$. Hence, by choosing some initial value $\lambda_0 = 1$, we can iteratively pick phases λ_x in order to realize any set of phases $\{\mu_x\}$ via (4.9). This way, for every choice of local vectors $\{\varphi_x\}$ and phases $\{\mu_x\}$, we get the operator

$$S_\varphi^* S_{\widetilde{\varphi}} = \bigoplus_{x\in\mathbb{Z}} \Big((\mathbb{1}_x - P_{\varphi_x}) + \mu_x P_{\varphi_x} \Big). \tag{4.10}$$

which acts as the identity everywhere except on a one-dimensional subspace $P_{\varphi_x}\mathcal{H}_x$ in each cell, where it multiplies with μ_x. This already suffices to realize every coin, since we can diagonalize $C_i|_{\mathcal{H}_x}$ locally in each cell and write C_i as a product of at most d pairs $S^*_{\varphi^i}S_{\widetilde{\varphi}^i}$, where $d = \max d_x$ is the maximal cell dimension[2].

In order to prove the remaining non-trivial implication *3) ⇒ 1)*, we make use of the decoupling construction in Theorem 3.3.19, which allows us to write any banded unitary as the product of two block-unitaries with overlapping blockings into groups of $2L$ cells (see (3.87) in Section 3.3.2 or (4.22) below). Before we prove the general case, let us consider a simpler one with only one factor where only one of the blocks differs from the identity. The proof for this simpler case already contains the key element for the general statement.

Lemma 4.2.3. *Let U_1 be a unitary on $\mathcal{H} = \bigoplus_x \mathcal{H}_x$, such that U_1 differs from the identity only on a subspace $\mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_r$ with $r < \dim(\mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_r)$. Then U_1 can be written as a sequence of coin operations and a fixed reference shift.*

Proof. Choose a basis $\{\phi_{x,i}\}_{x=1}^{d_x}$ in each cell $\mathcal{H}_x$, such that the reference shift S is the partial shift $S_{\phi_{x,1}}$, which maps the first basis element $\phi_{x,1} \in \mathcal{H}_x$ of each cell to the first basis element $\phi_{x+1,1} \in \mathcal{H}_{x+1}$ in the neighbouring cell to the right. We will occasionally call the set of one-dimensional subspaces spanned by these $\{\phi_{x,1}\}_x$ the shift-register.

Denote by D the finite-dimensional part of U_1, which acts on $\bigoplus_{x=1}^r \mathcal{H}_x$. D is an $N \times N$-dimensional unitary, with $N = \sum_{x=1}^r d_x$. Every $N \times N$-dimensional unitary can be factorized into a product of $N(N-1)/2$ elementary unitary operations of the form

$$M^{nm} = \begin{pmatrix} \mathbb{1} & & & & \\ & (M^{nm})_{11} & & (M^{nm})_{12} & \\ & & \mathbb{1} & & \\ & (M^{nm})_{21} & & (M^{nm})_{22} & \\ & & & & \mathbb{1} \end{pmatrix} \equiv \begin{pmatrix} \ddots & & & & \\ & \square & & \square & \\ & & \ddots & & \\ & \square & & \square & \\ & & & & \ddots \end{pmatrix}, \tag{4.11}$$

[Mur62, RZBB94, SHH10]. Thereby, M^{nm} differs from the identity only in the 4 matrix elements at $(n,n), (n,m), (m,n)$ and (m,m), which are replaced by the entries of a 2×2 unitary $(M^{nm})_{ij}$. The factorisation is of the form

$$D = \prod_{n=1}^{N-1} \left(\prod_{m=n+1}^{N} M^{nm} \right) \equiv \begin{pmatrix} \boxplus & & \\ & \ddots & \end{pmatrix} \ldots \begin{pmatrix} \ddots & & \\ & \square & \square \\ & \square & \end{pmatrix} \begin{pmatrix} \boxplus & & \\ & \ddots & \end{pmatrix} \ldots \begin{pmatrix} \ddots & & \\ & \square & \square \\ & \square & \end{pmatrix} \ldots\ldots \begin{pmatrix} \ddots & \\ & \boxplus \end{pmatrix}. \tag{4.12}$$

Note that in [SHH10] the decomposition is finer: There, D is decomposed into rotations, structured as the M^{nm} above, multiplied with additional phase shifts, i.e. diagonal unitaries. However, for this proof, we can absorb these phases into the elementary unitaries M^{nm}. Of course, this factorisation remains true when we embed everything back into the full Hilbert space by padding all finite-dimensional matrix blocks with identities on the two semi-infinite half-chains.

[2]Note, that for cells with $d_x < d$, we need to realize more factors then eigenvectors. But in this case, we can choose any vector $\varphi_x^{i>d_x} \in \mathcal{H}_x$ and adjust phases, such that $\mu_x^{i>d_x} = 1$. This way, for $i > d_x$, each factor $S^*_{\varphi^i}S_{\widetilde{\varphi}^i}$ just acts as the identity on $\mathcal{H}_x$.

The key step is now, to show that any such embedded elementary unitary can be written as a product

$$M^{nm} = C_3^* S^{-k_2} C_2^* S^{-k_1} C_1 S^{k_1} C_2 S^{k_2} C_3, \tag{4.13}$$

where S is the shift with respect to the shift-register as described above and C_i are coin operations acting non-trivially only on the non-trivial domain of D. Replacing every M^{nm} in the factorisation above then provides a shift-coin decomposition for U_1.

Consider the following two labellings of the basis for $\mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_r$: On the one hand, there are the local basis vectors $\phi_{x,i}$ of the cells $\mathcal{H}_x$ and on the other, we denote by $\{\psi_i\}_{i=1}^N$ a consecutive labelling, which is related to the former as

$$\{\psi_1, \ldots \psi_{d_1}, \psi_{d_1+1}, \ldots\ldots, \psi_N\} = \{\phi_{1,1}, \ldots, \phi_{1,d_1}, \phi_{2,1}, \ldots\ldots, \phi_{r,d_r}\}. \tag{4.14}$$

With these we can address the non-trivial matrix elements of M^{nm} via

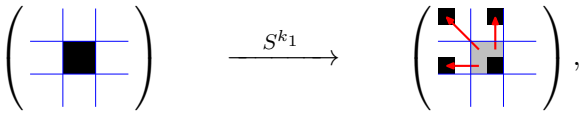
$$\begin{aligned} M^{nm} =& (M^{nm})_{11}|\psi_n\rangle\langle\psi_n| + (M^{nm})_{12}|\psi_n\rangle\langle\psi_m| \\ &+ (M^{nm})_{21}|\psi_m\rangle\langle\psi_n| + (M^{nm})_{22}|\psi_m\rangle\langle\psi_m|. \end{aligned} \tag{4.15}$$

If ψ_n and ψ_m belong to the same cell, M^{nm} is a coin operation itself and we set $C_1 = M^{nm}$, $k_i = 0$, and $C_2 = C_3 = \mathbb{1}$.

Otherwise, let $\psi_n \in \mathcal{H}_a$, $\psi_m \in \mathcal{H}_b$ and $\mathcal{H}_c$ be a cell with $\dim \mathcal{H}_c > 1$. Moreover, let $k_1 = c - a$ and $k_2 = c - b$. We then set $C_1 = \mathbb{1}_L \oplus C_c \oplus \mathbb{1}_R$, where C_c acts on $\mathcal{H}_c$ and is given by

$$C_c = \begin{pmatrix} (M^{nm})_{11} & (M^{nm})_{12} & \\ (M^{nm})_{21} & (M^{nm})_{22} & \\ & & \mathbb{1} \end{pmatrix}. \tag{4.16}$$

This way, in $S^{-k_1} C_1 S^{k_1}$, the matrix element $(M^{nm})_{11}$ ends up acting in $\mathcal{H}_a$ and $(M^{nm})_{12}$, resp. $(M^{nm})_{21}$ map from $\mathcal{H}_c$ to $\mathcal{H}_a$ or vice versa, while $(M^{nm})_{22}$ remains untouched. Let us accompany the proof with a specific example that is suitable for visualisation, while keeping the written proof steps completely general. For this, consider $r = 3$ with qubit cells, i.e. $\mathcal{H}_a \oplus \mathcal{H}_c \oplus \mathcal{H}_b = \mathbb{C}^6$, in which we want to realise some M^{26}. Choosing $\mathcal{H}_c$ as the middle cell, the first step can be depicted as



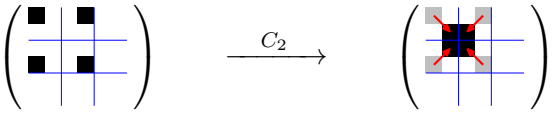
where the black squares denote the (not furhter specified) matrix elements of the M^{26} we want to realise, and the blue lines illustrate the decomposition of $\mathbb{C}^6$ into the three cells $\mathcal{H}_a \bigoplus \mathcal{H}_c \oplus \mathcal{H}_b$. We then move $(M^{nm})_{22}$ into the shift register in $\mathcal{H}_c$ and $(M^{nm})_{11}$ away from the shift register by conjugating with

$$C_2 = \Gamma(\phi_{c,1}, \phi_{c,2})\Gamma(\phi_{a,1}, \phi_{a,2}), \tag{4.17}$$

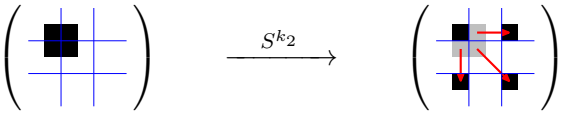
where

$$\Gamma(\varphi, \chi) = \mathbb{1} - \big(|\varphi\rangle\langle\varphi| + |\chi\rangle\langle\chi|\big) + |\chi\rangle\langle\varphi| + |\varphi\rangle\langle\chi|\big) \tag{4.18}$$

swaps the respective vectors in the argument and leaves invariant their complement.

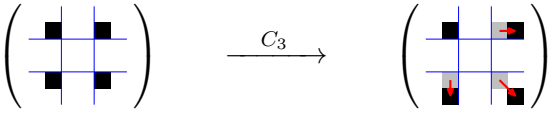


After conjugating with another shift S^{k_2}, we get $S^{-k_2}C_2^*S^{-k_1}C_1S^{k_1}C_2S^{k_2}$, in which $(M^{nm})_{11}$ and $(M^{nm})_{22}$ end up in $\mathcal{H}_a$ and $\mathcal{H}_b$, respectively, and the off-diagonal elements map between these spaces.



In a final step, we move these matrix elements to the correct positions inside each cell via conjugation with

$$C_3 = \Gamma(\phi_{a,2}, \psi_n)\Gamma(\phi_{b,1}, \psi_m). \tag{4.19}$$



With this, every matrix element ends up where it belongs, and we get

$$M^{nm} = C_3^*S^{-k_2}C_2^*S^{-k_1}C_1S^{k_1}C_2S^{k_2}C_3, \tag{4.20}$$

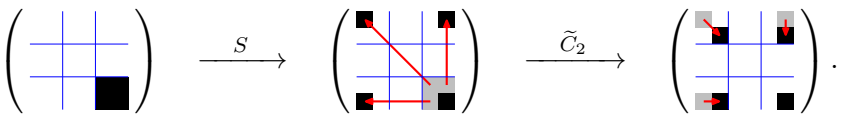
as wanted. Replacing every factor in (4.12) finally provides us with a shift-coin decomposition for U_1.

□

Note that if $\dim \mathcal{H}_b > 1$, as it is the case for standard examples with $d_x > 1\,\forall x$, we can set $\mathcal{H}_c = \mathcal{H}_b$. With this we may choose $k_2 = 0$ and the decomposition simplifies to

$$M^{nm} = \widetilde{C}_2^*S^{-k}C_1S^k\widetilde{C}_2, \tag{4.21}$$

with $k = k_1$ and $\widetilde{C}_2 = \Gamma(\phi_{a,1}, \psi_n)\Gamma(\phi_{b,2}, \psi_m)$. In our visualisation example this simplified version corresponds to

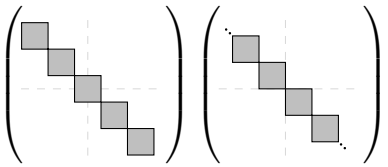


With this at hand, we are now able to assemble the remaining proof-direction for Theorem 4.2.2:

Proof of Theorem 4.2.2, 1) ⇒ 3). For the construction we will assume $\overrightarrow{\text{ind}}\, U = 0$. If this is not the case, we construct the shift-coin sequence for $U' = S^nU$, with $n = \overrightarrow{\text{ind}}\,(U)$. Then U' has trivial index and the factorisation for U follows from that of U' by multiplying with an additional shift-factor: $U = S^{-n}U'$.

$\vec{\mathrm{ind}}\,(U) = 0$ allows us to decouple the walk between every $\mathrm{lcd}(2L, r)$ cells, as in the proof of Theorem 3.3.19 (2.). Thereby lcd denotes the lowest common denominator, L the interaction length of U and r the integer entering the bound on the cell dimension. Choosing $\mathrm{lcd}(2L, r)$ as the block size guarantees that on the one hand, the decouplings do not interfere with each other, such that U is given as the product of two block-diagonal unitaries

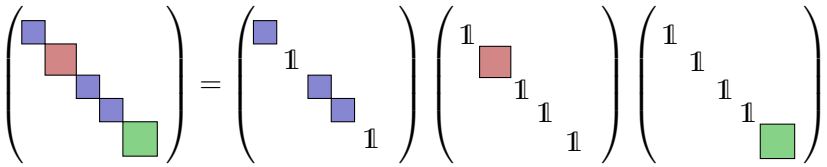
$$U = \left(\right) \left(\right) . \tag{4.22}$$



On the other hand, each block contains at least one cell with dimension $\dim \mathcal{H}_x > 1$ as in Lemma 4.2.3.

If the cells are all of equal size, we also end up with equally sized blocks in each of the two factors above. We can then directly apply the factorisation (4.12) in parallel to each block, with the same number of factors, respectively (also keeping possibly trivial factors $M^{nm} = \mathbb{1}$). For the shift-coin decompositions, the blocks can then share the same "shift-skeleton" globally, and we only have to choose the appropriate coin operations for each block locally. This way, the factors M^{nm} can be realised for all blocks simultaneously, which yields a shift-coin decomposition with $5(2(dL)^2 - dL) = \mathcal{O}((dL)^2)$ factors[3].

Otherwise, we utilise the uniform upper bound on the cell dimensions. There is only a finite number of possible configurations $\mathcal{H}_x \oplus \ldots \oplus \mathcal{H}_{x+\mathrm{lcd}(2L,r)}$ with $1 \leq \dim(\mathcal{H}_x) < d$, $\forall x$. Hence, we can further factorise (4.22), collecting all blocks with the same configuration in each factor, respectively. This leads to a finite product of block-diagonal unitaries, with possibly only sparsely distributed blocks of the same size and cell structure, respectively:



We can then apply the shift-coin decomposition of Lemma 4.2.3 for each factor separately, using a global shift-skeleton each time. The result will still be a finite sequence of shift and coin operations, which finishes the proof. □

In the proof above, we focus on the existence of a shift-coin decomposition and therefore, we took the most straightforward route to keep it as simple as possible. Thereby, we accepted a very long sequence of shift and coin operations. The number of factors can surely be improved, which raises the question of how to find a sequence of minimal length for a given strictly local unitary. However, we will content ourselves with the existence statement in this work and leave the optimisation question open.

Let us comment on where the assumptions on the cell dimensions were crucial: The upper bound entered the discussion at two points of the proof. In both situations, it

[3]Note that for equally sized cells, we must have $r = 1$ and all cells are at least two-dimensional.

guaranteed that the constructed sequences of the respective building turn out to be finite. On the one hand, in the last step of *1)* $\Rightarrow$ *3)*, it guarantees the existence of a common shift skeleton for the realisation of the different elementary unitaries in each block. On the other, in *3)* $\Rightarrow$ *2)* it guarantees the existence of $d = \max_x d_x$. The lower bound is necessary for the proof of Lemma 4.2.3, which we used for $1) \Rightarrow 3)$. There, we defined the coin $C_1 = \mathbb{1}_L \oplus C_c \oplus \mathbb{1}_R$, where C_c contains a non-trivial 2×2 unitary. Of course this is only possible for $d_c > 1$.

As already described in the proofs, the factorisation becomes considerably simpler in case of $\mathcal{H}_x = \mathcal{H}_0$ for all x. This is for example the case, when a given translation-invariant walk is "re-coined" to a different local cell size. Note that such a re-coining of translation-invariant walks is not captured by the technique described in Section 4.1, since the cell dimension stays fixed in that case. Indeed, the result of such a process is not necessary translation-invariant with respect to the new cells. We invite the reader to study the example we provided in [CGW21], where a quantum walk with three-dimensional coins is re-coined for a cell structure with two-dimensional cells, i.e. qubits.

5 Topological classification of chiral symmetric protocols

In this chapter, we consider chiral symmetric quantum walks, protocols and periodically driven systems, i.e. Floquet systems, at half-period. The underlying question motivating the following discussion is: "What is a chiral symmetric quantum walk"? There are several possible answers to this question: A quantum walk can be understood as the Floquet operator of a periodically driven system, a single time-step unitary without a Floquet history or a protocol with a fixed sequence of single operations, e.g., shifts and coins as in the previous chapter. These scenarios are fundamentally different in how a chiral symmetry acts. For a single time-step unitary U, the symmetry action is imposed on U itself, i.e. mapping it to its adjoint. For periodically driven systems, it is natural to assume the symmetry to act at any point in time on the driving Hamiltonian $H(t)$, $t \in [0, T]$ and not only at the endpoint of the evolution, namely on the Floquet operator $U(T)$. These conceptually different notions of chiral symmetric quantum walks result in similar but, nevertheless, slightly different topological classifications.

We already gave an overview on the literature on the topological aspects of discrete-time quantum walks and quantum walk protocols in the introduction of Chapter 3. Let us also give a brief overview of the literature on the topological aspects of symmetric Floquet systems, which have also been studied in a wide range of different contexts. The development started roughly simultaneously with that of topological phases in quantum walks [KBRD10], and it was soon found that Floquet systems host additional "anomalous edge-states" [RLBL13] that are not present in static systems. Different symmetries from the tenfold way were examined [ATD14, OANK15, CDFG15, Fru16, RH16, RH17a], leading to a periodic table of Floquet topological insulators [RH17b]. Beside that, topological phases in Floquet systems where studied in different contexts, including interacting systems [PMV16], systems with an additional time-glide symmetry [MPV17, MBSO20], using K-theory [SSB17], and two-dimensional systems with disorder [GT18]. Of particular interest for our considerations is the influence of chiral symmetry on Floquet systems in one dimension [ATD14, OANK15, LHR18, MBSO20]. In these publications, the authors observe that a chiral symmetry singles out the time evolution operator at half period $U(T/2)$, which will also be the main structural element for our theory. In particular, in [MBSO20], the effect of the chiral symmetry on a Floquet setting is analysed. Moreover, the authors additionally consider a time-glide symmetry [MPV17], which imposes a structure on the Floquet driving that is similar to the chiral symmetric setting. The ansatz in [MBSO20] is also centred around the half-step oper-

ator. However, the authors restrict their consideration to translation-invariant systems, i.e. they work with winding numbers in Fourier space as invariants. Besides that, the processes under consideration are assumed to originate from a time-continuous Floquet driving, which we explicitly do not assume.

The project presented in this chapter grew out of an apparent contradiction between the results in [AO13] and our classification in Section 3.6 and [CGG$^+$18]. Our classification in terms of three symmetry indices $(\mathrm{si}, \vec{\mathrm{si}}, \mathrm{si}_+)$ is complete, i.e. there cannot be a finer structure on the set of chiral symmetric quantum walks than imposed by these three indices, without further constraints. Nevertheless, in [AO13] such a finer structure is found for the split-step example. The difference leading to this is the assumed underlying scenario. Both works are on quantum walks, but while [AO13] considers the whole protocol, we worked with single-timestep unitaries. The essential structure, which captures both points of view lies somewhat in between these two settings. Each chiral symmetric quantum walk exhibits a half-step operator F, which is singled out by the chiral symmetry and constitutes two different timeframes of the process [AO13, ATD14, LHR18]. That is, in continuous time, two different Floquet operators for the same process, distinguished by different choices for the origin of the period. Working directly with the half-step operator, we can treat Floquet drivings, protocols and single time-step walks on a common footing.

We provide a complete topological classification of half-step operators via a set of five integer-valued indices, thereby resolving the apparent discrepancy between [AO13] and [CGG$^+$18]. The idea of considering different timeframes of a walk process originates from [AO13]. Building on this idea, we further enhance the roll of the half-step operator and combine it with our theory [CGG$^+$18, CGS$^+$18]. We also show that even without an underlying protocol or continuous driving process, there always exists a half-step operator for any chiral symmetric walk. This allows us to use the half-step operator as the constituting element for any of the three scenarios sketched above, and therefore, to unify the different ansatzes for the topological classification of chiral symmetric one-dimensional quantum walks. The results presented in this chapter were obtained in collaboration with Christopher Cedzich, Albert Werner and Reinhard Werner and have been published in [CGWW21].

We begin with fixing the setting. That is, we investigate the influence of chiral symmetry on driven systems and lay down the assumptions, as well as the classification task. From this, we identify the half-step operator as the structural ingredient to study. We proceed with analysing the basic properties and index relations for the half-step operator in Section 5.2, where we also establish its existence for any chiral symmetric walk. The main result of this chapter is presented in Section 5.3, where we derive a set of five independent integer-valued indices for the classification of chiral half-step walks, prove its completeness, and show that there are no empty classes with respect to this index set by providing a generating example. In Section 5.5 we analyse the relations and differences between the classification of single time-step walks from Section 3.6 and the classification in terms of the half-step operator presented in this chapter. We end the chapter with a discussion of compact perturbations in the current setting and some thoughts on half-step operators on finite systems, e.g. quantum walks on a ring of N cells.

5.1 Setting

As usual, we work on a Hilbert space with a one-dimensional structure according to (3.49). On this, we want to pin down the differences between the scenarios for chiral symmetric quantum walks from the point of view of a topological classification. On the level of a single time-step quantum walk U, the chiral symmetry relation is $\gamma U \gamma^* = U^*$. In the Floquet setting, i.e. in a continuously driven system with a time-periodic driving Hamiltonian $H(t)$ (see Section 1.3), the action of the chiral symmetry on $H(t)$ is best understood by considering it as the combination of the physically more intuitive time-reversal and particle-hole symmetry, even when these two are not part of the setting. A particle-hole symmetry η acts as $\eta H(t)\eta^* = -H(t)$, mapping positive to negative energies and vice versa, and a time-reversal symmetry τ as $\tau H(t)\tau^* = H(-t)$, reversing the direction of time. Combining the two gives the action of the chiral symmetry

$$\gamma H(t)\gamma^* = -H(-t), \tag{5.1}$$

which we study in the following. Combining this symmetry condition with periodicity in time, i.e. $H(t) = H(t+1)$, where, without loss of generality, we fixed the period to $T = 1$, gives

$$H(1-t) = -\gamma H(t)\gamma^*. \tag{5.2}$$

Hence, the first half of the driving period $t \in [0, 1/2]$ already determines the full period. This condition transfers to the time-ordered exponentials according to (1.23) as

$$\begin{aligned}
\gamma U(t)\gamma^* &= \gamma \mathcal{T} e^{-i\int_0^t H(s)ds}\gamma^* \\
&= \sum_{n=0}^{\infty}\left(\frac{1}{i}\right)^n \int_0^t ds_n \int_0^{s_n} ds_{n-1}\cdots\int_0^{s_2} ds_1 \gamma H(s_n)\gamma^*\cdots\gamma H(s_1)\gamma^* \\
&= \sum_{n=0}^{\infty}\left(\frac{-1}{i}\right)^n \int_0^t ds_n \int_0^{s_n} ds_{n-1}\cdots\int_0^{s_2} ds_1 H(-s_n)\cdots H(-s_1) \\
&= \sum_{n=0}^{\infty}\left(\frac{1}{i}\right)^n \int_1^{1-t} ds_n \int_1^{1-s_n} ds_{n-1}\cdots\int_1^{1-s_2} ds_1 H(s_n)\cdots H(s_1) \\
&= \mathcal{T} e^{-i\int_1^{1-t} H(s)ds} \\
&= U(1-t)U(1)^*,
\end{aligned} \tag{5.3}$$

where we substituted variables according to $s_i \to 1 - s_i$ and used the time-periodicity in the third step (compare [RH17b, Appendix A]). The last expression describes the time evolution operator from 1 to t, backwards in time.

For $t = 1/2$ we find

$$U(1) = \gamma U(1/2)^*\gamma^* U(1/2), \tag{5.4}$$

i.e. the Floquet-operator $U(1)$ can be expressed in terms of the operator at half period $U(1/2)$. Hence, in presence of chiral symmetry, the long time behaviour of the Floquet evolution is already determined by the **half-step operator**

$$F = \mathcal{T} e^{-i\int_0^{1/2} H(s)ds}. \tag{5.5}$$

Emphasizing the half-step operator F instead of only the Floquet operator gives rise to two **timeframes** U and U' of the driving process:

$$U = \gamma F^* \gamma^* F \qquad \text{and} \qquad U' = F \gamma F^* \gamma. \tag{5.6}$$

Both operators represent stroboscopic snapshots of the continuous time evolution, but with shifted origin in time, one starting at $t = 0$ and the other at $t = 1/2$. Both expressions are chiral symmetric, without further conditions on F. Indeed, the first half period $[0, 1/2] \ni t \mapsto H(t)$ of the driving can be arbitrary, as long as the second period is related to the first one according to (5.2).

The close relationship between general quantum walks and Floquet systems raises the question, whether a timeframe decomposition as in (5.6) exist for any single time-step quantum walk or quantum walk protocol, like, e.g. shift-coin sequences. For our theory, we take the half-step operator as a setting in its own, without assuming it to originate from a Floquet driving. Hence, we distinguish the following three scenarios:

(H) **Floquet scenario:** A quantum walk is the Floquet operator of a periodically driven process in continuous time, i.e. via a periodic family of bounded time dependent (local) Hamiltonians $H(t)$ with $H(t+1) = H(t)$.

(F) **Half-step scenario:** A quantum walk is defined by a unitary (local) half-step operator F via (5.6).

(U) **One-step scenario:** A quantum walk is a (local) unitary operator U.

Note that we added the locality condition only in brackets, indicating that each of these scenarios might be considered with or without it. As in Chapter 3, we start without assuming a locality condition and add it to the discussion later. Considering scenario (F) as a setting in its own right allows us to include **discrete protocols** into the classification that cannot be realized via a Floquet driving process[1], that is, protocols of the form $U = U_{2n} \dots U_1$, where the chiral symmetry is imposed via $\gamma U_i \gamma^* = U_{2n-i+1}^*$. This fits into the half-step scenario with the half-step operator $F = U_n \dots U_1$. The individual steps U_i might be any ($\vec{\text{ind}}$-wise non-trivial) unitaries without an underlying continuous driving.

The three scenarios are listed in increasing order of generality, i.e. a Floquet driving always defines a half-step operator F and a corresponding walk U, but not necessarily vice versa. These relations are expressed in the diagram

$$H(t) \xrightarrow{(5.5)} F \xrightarrow{(5.6)} \begin{matrix} U \\ U' \end{matrix}, \tag{5.7}$$

[1]The full walk operator of, e.g., the split-step walk (see Example 1.4.6 and Section 5.4), can always be considered as the Floquet operator of a continuously driven system, due to the chiral symmetry and the essential gap (see Section 3.4 and Theorem 3.3.19). However, the protocol structure with the partial shifts separated from each other cannot.

where each arrow represents a norm-continuous map from the left scenario to the corresponding one on the right, respectively. Hence, any norm continuous deformation turns out to be norm-continuous also in the more general scenario. Therefore, a topological classification of one-step unitaries U and U' also provides a classification of half-step operators F (at least partly) and Floquet drivings $H(t)$. We impose three constraints, which differ slightly in each scenario:

Chiral symmetry: On the level of one-step walks, chiral symmetry is imposed as usual, via $\gamma U \gamma^* = U^*$. For Floquet systems, we assume (5.2) to hold. There is no chiral symmetry condition on the level of half-step walks since it is imposed implicitly in how timeframes U and U' are built from F.

Gap condition: A gap condition is imposed for all scenarios implicitly via U and U'. We only consider processes with essentially gapped timeframes U and U'. Note that by the unitary equivalence of the two, they share the same spectrum.

Essential locality: Essential locality is assumed on each level separately. Since the mappings between the scenarios are continuous, an essentially local Hamiltonian driving $H(t)$ always results in an essentially local half-step walk F, which always defines essentially local timeframes U and U'.

The question about differences between the scenarios is now a question about the inversion of the arrows, i.e. given a walk U or a pair of timeframes (U, U'), can we find a half-step operator F, and given an F, can we find a bounded driving process $H(t)$? We already answered the latter question in Theorem 3.3.19, where we showed that an essentially local unitary F exhibits a Floquet driving if and only if $\vec{\mathrm{ind}}\,(F) = 0$. Let us collect the questions we demand our theory to answer:

- Inversion of arrows: Does any chiral symmetric walk U exhibit a half-step operator F? Moreover, what are the conditions on a pair of walks (U, U') to originate from the same F?
- Complete topological classification: Here, we focus on scenario (F), i.e. half-step walks, under the assumptions listed above. This includes showing that there are no empty classes, which we do by providing a generating example.
- Connection to the symmetry indices: Chiral symmetric walks are completely classified by the symmetry indices (see Section 3.6). Given two timeframes U and U' with a common half-step walk F, to what extend do their topological classes determine the topological class of F?

We answer the question about the existence of F in Section 5.2 (see Theorem 5.2.9 and Corollary 5.2.11), provide a complete classification of half-step walks in Section 5.3 (see Theorem 5.3.1), and discuss the connection of the F-indices to the walk indices in Section 5.5 (see Corollary 5.5.1).

5.2 The half-step operator

We now turn our focus to the half-step operator as the object of interest. First, we collect its essential properties and index relations, which we later use for the classification. For this, we first omit the essential locality assumption, keeping in mind that results that are valid for essentially unitary operators are readily applicable to the half-space compressions of any unitary operators under consideration, similar to the definition of $\vec{\mathrm{ind}}$ in Section 3.3.2 and $\vec{\mathrm{si}}$ in Section 3.5.1. This way, the indices requiring essential locality are automatically also covered. Whenever essential locality becomes a non-trivial or crucial assumption, we will state it as such. From Section 5.3 on, essential locality will again be fixed in the set of assumptions.

5.2.1 General properties and indices

Before diving into the classification, let us pick a standard basis and fix the notation we will use during this chapter. We are concerned with driven time evolutions that exhibit chiral symmetric full-period unitary operators. This allows us to express everything in the chiral eigenbasis, which will be the basic structure in the following. As usual, we assume each cell to be balanced, wherefore $\mathrm{tr}\,\gamma_x = 0$ for every x. Hence, in its eigenbasis, each γ_x is of the form $\gamma_x = \sigma_z \otimes \mathbb{1}_{d_x/2}$ and rearranging the basis appropriately allows us to decompose the full Hilbert space in the same way. I.e.

$$\mathcal{H} = \mathbb{C}^2 \otimes \widetilde{\mathcal{H}}, \qquad \text{with} \qquad \gamma = \sigma_z \otimes \mathbb{1} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} = \Gamma_+ - \Gamma_-. \tag{5.8}$$

where $\Gamma_\pm$ denote the eigenprojections of γ. With respect to this decomposition, every operator becomes a 2×2-block matrix and the chiral blocks of the two timeframes U and U'[2] and the half-step operator F will be denoted by

$$U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \delta \end{pmatrix}, \qquad U' = \begin{pmatrix} \alpha' & \beta' \\ -\beta'^* & \delta' \end{pmatrix}, \qquad \text{and} \qquad F = \begin{pmatrix} A & B \\ C & D \end{pmatrix}. \tag{5.9}$$

By construction the one-dimensional structure of the underlying Hilbert space transfers to $\widetilde{\mathcal{H}}$ and therefore, each block in the decompositions above inherits possibly present locality properties of the full operator with respect to the same cell structure, with halved cells. The chiral blocks of U and U' are determined from F via the timeframe equations $U = \gamma F^* \gamma F$ and $U' = F \gamma F^* \gamma$:

$$\begin{aligned} \alpha &= A^*A - C^*C & \alpha' &= AA^* - BB^* \\ \beta &= A^*B - C^*D & \beta' &= BD^* - AC^* \\ \delta &= D^*D - B^*B & \delta' &= DD^* - CC^*. \end{aligned} \tag{5.10}$$

Thus, α, δ, α' and δ' are self-adjoint. Note, however, that this extra condition on α, δ, as well as the relation between the off-diagonal blocks $\beta, -\beta^*$ is not only a speciality of unitaries with a timeframe structure but holds in general for any chiral symmetric

[2] See also (3.125) in Section 3.5.1.

unitary in the chiral eigenbasis[2]. The relations between the chiral blocks of U and U' and, in particular, their relations to the chiral blocks of the half-step operator F allow us to express the defining properties and the symmetry indices for U and U' in terms of these blocks. We start with the essential gap condition[3]

Lemma 5.2.1. *Let F be an **essentially unitary half-step operator** for an essential unitary U with chiral symmetry. Then the following are equivalent*

i) U and U' are essentially gapped at ± 1.

ii) The off-diagonal chiral blocks β and β' of U and U' are Fredholm.

iii) The chiral blocks A, B, C and D of F are Fredholm.

This remains true if we drop the "essentials", i.e. for a strictly unitary half-step operator F, the corresponding unitaries U, U' are gapped if and only if the chiral blocks of F, resp. β and β', are invertible.

Proof. We will prove this for strictly unitary operators F and U, U' and exactly gapped U, U'. For essentially unitary and essentially gapped operators, it then automatically follows by considering the images of the involved operators in the Calkin algebra (see Definition 1.2.5).

i)⇔iii): Since U and U' are unitarily equivalent, it suffices to consider only U. So let F and U be exactly unitary. U is gapped if and only if $U \mp \mathbb{1} = \gamma F^* \gamma F \mp \mathbb{1} = \gamma F^* \gamma \left(F \mp \gamma F \gamma\right)$ are invertible. Since $\gamma F^* \gamma$ is unitary, it follows that

$$F - \gamma F \gamma = 2 \begin{pmatrix} 0 & B \\ C & 0 \end{pmatrix} \qquad \text{and} \qquad F + \gamma F \gamma = 2 \begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} \tag{5.11}$$

have to be invertible. Clearly this is the case if and only if the blocks A, B, C and D themselves are invertible.

i)⇔ii): U is gapped at ± 1 if and only if

$$2i \operatorname{Im}(U) = U - U^* = 2 \begin{pmatrix} 0 & \beta \\ -\beta^* & 0 \end{pmatrix} \tag{5.12}$$

is gapped at 0, i.e. invertible. Clearly this is the case if and only if β is invertible. The same holds for U' and β'. □

Remark 5.2.2. *Using the proof of Lemma 5.2.1 $i) \Leftrightarrow ii)$ we can express the ± 1 eigenspaces of U and U' in terms of its matrix blocks in a simple way, which will turn out to be useful later on. As already mentioned in the proof, the combined ± 1 eigenspace of U is equal to the null space of $\operatorname{Im}(U)$, which equals $\ker \beta^* \oplus \ker \beta$. Using this, we can directly evaluate $U(\varphi, \psi) = \pm(\varphi, \psi)$, with $\beta^* \varphi = \beta \psi = 0$, which yields*

$$\ker(U \pm \mathbb{1}) = \ker(\alpha \pm \mathbb{1}) \oplus \ker(\delta \pm \mathbb{1}). \tag{5.13}$$

[3]Note that the equivalence *i)* ⇔ *ii)* was already established in [CGS+18].

The essential gap is the standing assumption for the topological classification of chiral symmetric unitaries. We will therefore also adopt it here.

Assumption 5.2.3. *All half-step operators F are assumed to constitute essentially gapped (essentially) unitary operators as their timeframes. I.e. their chiral blocks A, B, C and D are assumed to be Fredholm.*

In particular, the chiral blocks have well defined Fredholm indices, which raises the question to what extent these can be used as classifying topological invariants for half-step walks F. The first thing that comes to mind in this direction is to express the Fredholm index of F itself in terms of the indices of its chiral blocks.

Lemma 5.2.4. *Let F be an essentially unitary half-step operator. Then its Fredholm index is given by*

$$\operatorname{ind}(F) = \operatorname{ind}(B) + \operatorname{ind}(C) = \operatorname{ind}(A) + \operatorname{ind}(D). \tag{5.14}$$

Proof. Using the essential unitarity of F on the level of the chiral blocks, we get that $A^*B + C^*D$ is compact. Hence, since $\beta = A^*B - C^*D$ is Fredholm for essentially gapped U and U' we get $\operatorname{ind}(\beta) = \operatorname{ind}(2A^*B) = \operatorname{ind}(-2C^*D)$. In particular this implies $\operatorname{ind}(B) - \operatorname{ind}(A) = \operatorname{ind}(D) - \operatorname{ind}(C)$, which proves the second equality in (5.14).

Now, since $X \in \{A, B, C, D\}$ is Fredholm, we find another Fredholm operator X^I, such that $XX^I - \mathbb{1}$ and $X^IX - \mathbb{1}$ are compact (see Lemma 1.2.7). Hence, starting with $A^*B + C^*D$ we can write

$$D = -C^{*I}A^*B + K = -CC^IC^{*I}A^*B + K = CMA^*B + K, \tag{5.15}$$

with K compact[4] and $M := C^IC^{*I}$ positive. With this we can factorize F into

$$F = \begin{pmatrix} A & B \\ C & -CMA^*B + K \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & C \end{pmatrix} \begin{pmatrix} A & \mathbb{1} \\ \mathbb{1} & -MA^* \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & B \end{pmatrix} + K. \tag{5.16}$$

Clearly, the first and last factor are Fredholm operators with indices $\operatorname{ind}(C)$ and $\operatorname{ind}(B)$. The middle factor is invertible, as we will show separately after this proof and, in particular, Fredholm with trivial index. Hence, we get

$$\operatorname{ind}(F) = \operatorname{ind}(F + K) = \operatorname{ind}(C) + \operatorname{ind}(B). \tag{5.17}$$

□

Lemma 5.2.5. *Let M be a positive and A be an arbitrary operator. Then*

$$X = \begin{pmatrix} A & \mathbb{1} \\ \mathbb{1} & -MA^* \end{pmatrix} \tag{5.18}$$

is invertible.

[4] K is to be understood as a placeholder for any compact operator here and does not have to be the same in every expression.

Proof. Evaluating $X(\varphi,\psi)=0$ and $X^*(\varphi,\psi)=0$ we find that the kernels of X and X^* are given by

$$\begin{aligned}\ker(X) &= \{(MA^*\psi,\psi) \mid (\mathbb{1}+AMA^*)\psi=0\}\\ \ker(X^*) &= \{(\varphi,-A^*\varphi) \mid (\mathbb{1}+AMA^*)\varphi=0\}\,.\end{aligned} \tag{5.19}$$

Since M is positive, $(\mathbb{1}+AMA^*)$ is strictly positive and has a trivial kernel, wherefore $\ker(X)=\ker(X^*)=0$. □

The next invariants that come to mind are the symmetry indices $\mathrm{si}, \vec{\mathrm{si}}$ and $\mathrm{si}_\pm$ of the timeframes U and U'. We start with si and $\mathrm{si}_\pm$, which are well defined also without locality assumptions and discuss $\vec{\mathrm{si}}$, which require locality on the one-dimensional lattice, later. However, as already mentioned, formulating everything for merely essentially unitary operators whenever possible allows us to apply the results to the half-space projections of essentially local operators later.

Lemma 5.2.6. *In both settings of Lemma 5.2.1 (essentially and exactly unitary), we get*

$$\begin{aligned}\mathrm{si}(U) = \mathrm{ind}\,(A) - \mathrm{ind}\,(B) &= \mathrm{ind}\,(C) - \mathrm{ind}\,(D)\\ \mathrm{si}(U') = \mathrm{ind}\,(C) - \mathrm{ind}\,(A) &= \mathrm{ind}\,(D) - \mathrm{ind}\,(B).\end{aligned} \tag{5.20}$$

Proof. Using Definition 3.5.5 and the formula for the symmetry index for type 3 ($\equiv$ AIII) in Table 2.1, we can express the symmetry index of U as the trace of γ, restricted to the kernel of

$$\mathrm{Im}(U) = \frac{U-U^*}{2i} = \frac{1}{i}\begin{pmatrix} 0 & A^*B - C^*D \\ D^*C - B^*A & 0\end{pmatrix} = i\begin{pmatrix} 0 & \beta \\ -\beta^* & 0\end{pmatrix}, \tag{5.21}$$

with

$$\ker \mathrm{Im}(U) = \{(\varphi_+,\varphi_-) \mid \varphi_+ \in \ker(\beta^*) \text{ and } \varphi_- \in \ker(\beta)\}\,. \tag{5.22}$$

Evaluating the trace of γ on this subspace, we find $\mathrm{si}(U) = \dim\ker(\beta^*) - \dim\ker(\beta) = \mathrm{ind}\,(\beta^*)$. By essential unitarity of F, $A^*B + C^*D$ is compact, such that $2iB^*A$ and $-2iD^*C$ are compact perturbations of β^*. Hence, we get

$$\mathrm{si}(U) = \mathrm{ind}\,(\beta^*) = \mathrm{ind}\,(B^*A) = \mathrm{ind}\,(D^*C), \tag{5.23}$$

which proves the claimed formula for $\mathrm{si}(U)$ via the product property of the Fredholm index. By the same line of reasoning, with $\beta' = BD^* - AC^*$, we get

$$\mathrm{si}(U') = \mathrm{ind}\,(\beta'^*) = \mathrm{ind}\,(CA^*) = \mathrm{ind}\,(DB^*). \tag{5.24}$$

□

The results so far are valid for essentially unitary operators F, U and U'. We proceed with the indices that require the spectral decomposition of U and U', i.e. $\mathrm{si}_\pm$. In order to say something about these, exact unitary is needed. Hence, before we relate those invariants to the indices of the chiral blocks, let us discuss some general properties of exactly unitary 2×2 block-operators with Fredholm blocks. These will lead to a standard form for any F, which we will use in several situations. So let F any 2×2-block unitary

with Fredholm blocks A, B, C and D. We will repeatedly make use of the unitarity conditions on the level of the blocks, so let us state them here:

$$\underline{F^*F = \mathbb{1}}: \qquad\qquad \underline{FF^* = \mathbb{1}}:$$

$$A^*A + C^*C = \mathbb{1} \quad (5.25) \qquad AA^* + BB^* = \mathbb{1} \quad (5.28)$$

$$B^*B + D^*D = \mathbb{1} \quad (5.26) \qquad CC^* + DD^* = \mathbb{1} \quad (5.29)$$

$$B^*A + D^*C = 0 \quad (5.27) \qquad AC^* + BD^* = 0 \quad (5.30)$$

Let $\psi \in \ker A$. Then, by (5.27), we get $D^*C\psi = 0$, i.e. $C\psi \in \ker D^*$ and therefore $C \ker A \subset \ker D^*$. This is an isometric embedding, because C is isometric on $\ker A$ by (5.25). Moreover, let $\varphi \in \ker D^*$. Then, by (5.30), we get $C^* \ker D^* \subset \ker A$. Again, this embedding is isometric by (5.29). Hence, we conclude that $\ker A$ and $\ker D^*$ are unitarily equivalent, with C restricted to those spaces being the unitary relating the two. With similar arguing we find the following four unitary equivalences

$$\begin{aligned} C \ker A &= \ker D^* & \qquad B \ker D &= \ker A^* \\ D \ker B &= \ker C^* & \qquad A \ker C &= \ker B^*. \end{aligned} \tag{5.31}$$

In particular, the respective kernels have the same dimension, wherefore we get

$$\mathrm{ind}\,(A) = -\mathrm{ind}\,(D) \qquad \text{and} \qquad \mathrm{ind}\,(B) = -\mathrm{ind}\,(C). \tag{5.32}$$

Note, that these relations simplify the expression for $\mathrm{ind}\,(F)$ in Lemma 5.2.4. However, this only holds for exactly unitary F and therefore does not apply, e.g., to the corresponding right Fredholm index equation.

We can further relate the kernels of the chiral blocks of F to the ± 1 eigenspaces of the two corresponding unitaries U and U'. As already mentioned in the proof of Lemma 5.2.6, the ± 1-eigenspaces $\mathcal{H}_\pm = \ker(U \pm \mathbb{1})$ of U are given by the kernels of $(F \mp \gamma F \gamma)$. This yields $\mathcal{H}_+ = \ker C \oplus \ker B$ and $\mathcal{H}_- = \ker A \oplus \ker D$. Via a similar calculation as in the proof of Lemma 5.2.6, we find that the ± 1-eigenspaces $\mathcal{H}'_\pm$ of U' are equal to the kernels of $(\gamma F^* \gamma \mp F^*)$, which gives $\mathcal{H}'_+ = \ker B^* \oplus \ker C^*$ and $\mathcal{H}_- = \ker A^* \oplus \ker D^*$.

In summary, using also Remark 5.2.2, we get

$$\begin{aligned} \mathcal{H}_+ &= \ker(\alpha - \mathbb{1}) \oplus \ker(\delta - \mathbb{1}) = \ker C \oplus \ker B \\ \mathcal{H}_- &= \ker(\alpha + \mathbb{1}) \oplus \ker(\delta + \mathbb{1}) = \ker A \oplus \ker D \end{aligned} \tag{5.33}$$

and

$$\begin{aligned} \mathcal{H}'_+ &= \ker(\alpha' - \mathbb{1}) \oplus \ker(\delta' - \mathbb{1}) = \ker B^* \oplus \ker C^* \\ \mathcal{H}'_- &= \ker(\alpha' + \mathbb{1}) \oplus \ker(\delta' + \mathbb{1}) = \ker A^* \oplus \ker D^*. \end{aligned} \tag{5.34}$$

Let us extract the relevant index information from the discussion above, before we go on and discuss the standard form for half-step unitaries F.

Lemma 5.2.7. *Let F be an **exactly unitary half-step operator** for essentially gapped unitaries U, U'. Then the ± 1 eigenspaces and the corresponding indices $\mathrm{si}_\pm$ are well defined and we get*

$$\mathrm{si}_+(U) = \mathrm{ind}\,(C) = -\mathrm{ind}\,(B) \quad \textit{and} \quad \mathrm{si}_-(U) = \mathrm{ind}\,(A) = -\mathrm{ind}\,(D) \tag{5.35}$$

and

$$\mathrm{si}_\pm(U') = \pm\,\mathrm{si}_\pm(U). \tag{5.36}$$

Proof. The direct sums in (5.33) already respect the splitting $\Gamma_+\mathcal{H} \oplus \Gamma_-\mathcal{H}$ of the Hilbert space into the eigenspaces of γ. Hence, we can subtract the dimensions of the involved kernels of A, B, C and D to evaluate the trace of γ on $\mathcal{H}_\pm$ and $\mathcal{H}'_\pm$. Together with (5.31) and (5.32) this gives the claimed formulas. □

We can now use the findings of the discussion above in order to define a standard form for any half-step unitary F for essentially gapped unitaries U and U'. From (5.33), we know that the chiral blocks of F considered as mappings between the complements of the ±1-eigenspaces $\mathcal{H}_\pm$ and $\mathcal{H}_\mp$ of U and U',respectively, are invertible. Denote these spaces by

$$\mathcal{K} = (\mathcal{H}_+ \oplus \mathcal{H}_-)^\perp \qquad \text{and} \qquad \mathcal{K}' = (\mathcal{H}'_+ \oplus \mathcal{H}'_-)^\perp. \tag{5.37}$$

With respect to these spaces, together with appropriately rearranged direct summands in (5.31) we can decompose the Hilbert space in two different ways:

$$\begin{aligned} \mathcal{H} &= (\ker C \ \oplus \ker B\ ) \oplus (\ker A\ \oplus \ker D\ ) \oplus \mathcal{K} \\ &= (\ker B^* \oplus \ker C^*) \oplus (\ker A^* \oplus \ker D^*) \oplus \mathcal{K}'. \end{aligned} \tag{5.38}$$

The direct sum pairs inside the parentheses are with respect to the eigenspace decomposition of γ and the first two summands of the outer sums correspond to $\mathcal{H}_+ \oplus \mathcal{H}_-$ and $\mathcal{H}'_+ \oplus \mathcal{H}'_-$, respectively. In these decompositions, we then consider F as a mapping between the timeframes U and U'.

Definition 5.2.8 (Standard form for F)**.** *Let F be an exactly unitary half-step operator for essentially gapped unitaries U and U'. We define the **standard form** for F considered as a mapping between the two decompositions of the Hilbert space in* (5.38) *as*

$$F = \begin{pmatrix} A_+ & 0 \\ 0 & D_+ \end{pmatrix} \oplus \begin{pmatrix} 0 & B_- \\ C_- & 0 \end{pmatrix} \oplus \begin{pmatrix} A_\mathcal{K} & B_\mathcal{K} \\ C_\mathcal{K} & D_\mathcal{K} \end{pmatrix}. \tag{5.39}$$

Here, $A_+ : \ker C \to \ker B^*$, $B_- : \ker D \to \ker A$, $C_- : \ker A \to \ker D^*$ and $D_+ : \ker B \to \ker C^*$ are the finite-dimensional unitary restrictions of the operators operators from (5.31) *and $A_\mathcal{K}, B_\mathcal{K}, C_\mathcal{K}$ and $D_\mathcal{K}$ are invertible operators between $(\Gamma_+ \oplus \Gamma_-)\mathcal{K}$ and $(\Gamma_+ \oplus \Gamma_-)\mathcal{K}'$. For exactly gapped unitaries U and U', the (co-) kernels of A, B, C and D vanish and we get $\mathcal{H} = \mathcal{K} = \mathcal{K}'$.*

It is important to note that the finite-dimensional unitaries A_+, B_-, C_- and D_+ are not necessarily of the same size. In fact, by Lemma 5.2.7 and (5.31) the dimension difference of A_+ and D_+ determines $\operatorname{ind}(B) = -\operatorname{si}_+(U) = -\operatorname{si}_+(U')$, whereas that of C_- and B_- determines $\operatorname{ind}(A) = \operatorname{si}_-(U) = -\operatorname{si}_-(U')$. As we will see later, any combination of $(\operatorname{si}_+, \operatorname{si}_-) \in \mathbb{Z}^2$ can be realized not only abstractly but also with strictly local half-step operators F constituting strictly local quantum walks U and U'.

5.2.2 Existence of the half-step operator

From the point of view of chiral symmetric quantum walks U and U', the question arises, under which conditions there exists a half-step operator F. In this section, we discuss the necessary conditions on U and U' to admit a common half-step operator F, and explicitly construct this F. In the case where only one timeframe U is kept fixed, the

situation simplifies. We will show that then there always exists and F producing this U. The construction will naturally respect essential locality but is not exclusively applicable to essentially local unitaries, i.e. walks, but also to general chiral symmetric unitaries without any locality assumption.

We already came across one of the necessary conditions, namely the index equation (5.36) in Lemma 5.2.7, which also fixes the relation between $\mathrm{si}(U)$ and $\mathrm{si}(U')$.

Theorem 5.2.9. *Let U and U' a pair of chiral symmetric unitaries, with essential gaps at ± 1. Then the following are equivalent:*

i) There exists a half-step operator F, such that

$$U = \gamma F^* \gamma F \qquad \text{and} \qquad U' = F \gamma F^* \gamma. \tag{5.40}$$

ii) The symmetry indices of U and U' fulfil the necessary condition

$$\mathrm{si}_{\pm}(U) = \pm \mathrm{si}_{\pm}(U'), \tag{5.41}$$

and U and U' are unitarily equivalent with a unitary V that intertwines $\gamma_{\mathcal{K}}$ and $\gamma_{\mathcal{K}'}$:

$$U' = VUV^* \qquad \text{and} \qquad \gamma_{\mathcal{K}'} V_{\mathcal{K}} = V_{\mathcal{K}} \gamma_{\mathcal{K}}. \tag{5.42}$$

If U and U' are essentially local, the statement holds with essentially local F and V.

In (5.42), $V_{\mathcal{K}}$, $\gamma_{\mathcal{K}}$, and $\gamma_{\mathcal{K}'}$ denote the restriction of V and γ to $\mathcal{K}$ and $\mathcal{K}'$ respectively. Since V is the unitary equivalence operator for U and U', its restriction is a unitary $V_{\mathcal{K}} : \mathcal{K} \to \mathcal{K}'$. The intertwining property then guarantees that this unitary additionally maps the γ eigenspaces restricted to $\mathcal{K}$ and $\mathcal{K}'$ onto each other. Note that U and U' are chiral symmetric for the same γ, but $\gamma_{\mathcal{K}}$ and $\gamma_{\mathcal{K}'}$ refer to the possibly different complements of the $\pm$-eigenspaces of U and U', respectively.

Proof. $i) \Rightarrow ii)$: We already established the index condition in Lemma 5.2.7. Unitary equivalence alone is guaranteed by F itself, since $U' = FUF^*$. However, to show the extra condition involving $\gamma_{\mathcal{K}}$ and $\gamma'_{\mathcal{K}}$ we need to invest some work. We construct the unitary V in the same standard form decomposition as in Definition 5.2.8. Since the extra condition on V only involves $\mathcal{K}$ and $\mathcal{K}'$, we can use the first two summands F_+ and F_- in (5.39) as a mapping between U and U' restricted to $\mathcal{H}_+ \oplus \mathcal{H}_-$ and $\mathcal{H}'_+ \oplus \mathcal{H}'_-$, respectively. Hence, we set

$$V = F_+ \oplus F_- \oplus V_{\mathcal{K}}, \tag{5.43}$$

and are left with the construction of $V_{\mathcal{K}} : \mathcal{K} \to \mathcal{K}'$ with $V_{\mathcal{K}} \gamma_{\mathcal{K}} = \gamma_{\mathcal{K}'} V_{\mathcal{K}}$. For this task we will drop the $\mathcal{K}$ subscript to lighten notation, keeping in mind the following mapping directions for the upcoming operators

$$U, \gamma, \widetilde{F} : \mathcal{K} \to \mathcal{K}, \qquad F, V : \mathcal{K} \to \mathcal{K}' \quad \text{and} \quad U', \gamma' : \mathcal{K}' \to \mathcal{K}'. \tag{5.44}$$

Consider U and its chiral blocks $\alpha, \beta, -\beta^*$ and δ. Since, restricted to $\mathcal{K}$, U is gapped at ± 1 and unitary, β is invertible by Lemma 5.2.1. Consequently (by unitarity of U on $\mathcal{K}$)

$|\alpha| < \mathbb{1}$ and $|\delta| < \mathbb{1}$, such that $\mathbb{1} \pm \alpha$ as well as $\mathbb{1} \pm \delta$ are strictly positive operators. With this, and denoting by V_β the polar unitary of β, let

$$\widetilde{F} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\mathbb{1}+\alpha} & V_\beta \sqrt{\mathbb{1}-\delta} \\ -V_\beta^* \sqrt{\mathbb{1}-\alpha} & \sqrt{\mathbb{1}+\delta} \end{pmatrix}. \tag{5.45}$$

By the off-diagonal unitarity conditions of U we have $\alpha\beta = \beta\delta$ and $\beta^*\alpha = \delta\beta^*$, which also holds after replacing β with its polar isometry. Therefore we get $\sqrt{\mathbb{1}-\alpha}V_\beta = V_\beta\sqrt{\mathbb{1}-\delta}$. Moreover, the diagonal unitarity conditions of U yield $\beta = V_\beta\sqrt{\mathbb{1}-\delta^2} = \sqrt{\mathbb{1}-\alpha^2}V_\beta$. Using these identities, it follows by straightforward computation, that $\widetilde{F}$ is unitary and in particular, that it is a chiral symmetric square root for U. I.e. $\widetilde{F}^2 = U$, with $\gamma\widetilde{F}\gamma = \widetilde{F}^*$, which gives

$$U = \gamma\widetilde{F}^*\gamma\widetilde{F} = \gamma F^*\gamma' F. \tag{5.46}$$

Multiplying the second equality with $F\gamma$ from the left and $\widetilde{F}^*$ from the right, we get $V\gamma = \gamma' V$ with $V := F\widetilde{F}^*$,which also gives

$$\begin{aligned} U' &= F\gamma F^*\gamma' = V\widetilde{F}\gamma\widetilde{F}^*V^*\gamma' \\ &= V\widetilde{F}\gamma\widetilde{F}^*\gamma V^* = V\widetilde{F}^2V^* \\ &= VUV^*, \end{aligned} \tag{5.47}$$

as needed.

Switching back to the whole Hilbert space, we can assemble $V = F_+ \oplus F_- \oplus V_{\mathcal{K}}$, which provides us with a unitary equivalence operator for $VUV^* = U'$, with the necessary intertwining property for $\gamma_{\mathcal{K}}$ and $\gamma_{\mathcal{K}'}$. Note that since V was constructed in terms of F and U, or rather continuous functions of α and δ and the polar isometry of β, it is automatically essentially local whenever U and F are (see Section 3.3).

$ii) \Rightarrow i)$: We again use the standard form for the construction. Let us start with the finite rank summands $F_\pm$, which are supposed to map between the real eigenspaces of U and U', i.e. $F_\pm : \mathcal{H}_\pm, \to \mathcal{H}'_\pm$. By assumption, U and U' are unitarily equivalent, i.e. $\dim(\mathcal{H}_\pm) = \dim(\mathcal{H}'_\pm)$. By (5.33) and (5.34) this is equivalent to

$$\dim\ker(\alpha \pm \mathbb{1}) + \dim\ker(\delta \pm \mathbb{1}) = \dim\ker(\alpha' \pm \mathbb{1}) + \dim\ker(\delta' \pm \mathbb{1}). \tag{5.48}$$

Moreover, combining (5.33) and (5.34) with Lemma 5.2.7, the index condition $\mathrm{si}_\pm(U) = \pm\,\mathrm{si}_\pm(U')$ becomes

$$\dim\ker(\alpha \mp \mathbb{1}) - \dim\ker(\delta \mp \mathbb{1}) = \pm\left(\dim\ker(\alpha' \mp \mathbb{1}) - \dim\ker(\delta' \mp \mathbb{1})\right). \tag{5.49}$$

Together, these two dimension-conditions yield

$$\begin{aligned} &\dim\ker(\alpha - \mathbb{1}) = \dim\ker(\alpha' - \mathbb{1}) && \dim\ker(\alpha + \mathbb{1}) = \dim\ker(\delta' + \mathbb{1}) \\ &\dim\ker(\delta - \mathbb{1}) = \dim\ker(\delta' - \mathbb{1}) && \dim\ker(\delta + \mathbb{1}) = \dim\ker(\alpha' + \mathbb{1}). \end{aligned} \tag{5.50}$$

Therefore, we certainly find finite-dimensional unitaries

$$\begin{aligned} &A_+ : \ker(\alpha - \mathbb{1}) \to \ker(\alpha' - \mathbb{1}) && C_- : \ker(\alpha + \mathbb{1}) \to \ker(\delta' + \mathbb{1}) \\ &D_+ : \ker(\delta - \mathbb{1}) \to \ker(\delta' - \mathbb{1}) && B_- : \ker(\delta + \mathbb{1}) \to \ker(\alpha' + \mathbb{1}). \end{aligned} \tag{5.51}$$

Arranging these unitaries as in (5.39) provides us with F_+ and F_-. Thereby, the specific choices for these unitaries do not matter, since every choice yields

$$\gamma_\pm F_\pm^* \gamma'_\pm F_\pm = \pm P_\pm \qquad \text{and} \qquad F_\pm \gamma_\pm F_\pm^* \gamma'_\pm = \pm P'_\pm, \tag{5.52}$$

where $P_\pm, P'_\pm$ denote the projections onto $\mathcal{H}_\pm, \mathcal{H}'_\pm$, and $\gamma_\pm, \gamma'_\pm$ the corresponding restrictions of γ. Note that, due to (5.50),

$$\gamma_+ = \begin{pmatrix} \mathbb{1}_{\ker(\alpha-1)} & 0 \\ 0 & -\mathbb{1}_{\ker(\delta-1)} \end{pmatrix} \qquad \text{and} \qquad \gamma'_+ = \begin{pmatrix} \mathbb{1}_{\ker(\alpha'-1)} & 0 \\ 0 & -\mathbb{1}_{\ker(\delta'-1)} \end{pmatrix} \tag{5.53}$$

have the same matrix representation on the different but isomorphic subspaces $\mathcal{H}_+$ and $\mathcal{H}'_+$, but

$$\gamma_- = \begin{pmatrix} \mathbb{1}_{\ker(\alpha+1)} & 0 \\ 0 & -\mathbb{1}_{\ker(\delta+1)} \end{pmatrix} \qquad \text{and} \qquad \gamma'_- = \begin{pmatrix} \mathbb{1}_{\ker(\alpha'+1)} & 0 \\ 0 & -\mathbb{1}_{\ker(\delta'+1)} \end{pmatrix} \tag{5.54}$$

are actually different. This difference is necessary for $\mathrm{si}_\pm(U) = \mathrm{tr}(\gamma_\pm) = \pm\,\mathrm{tr}(\gamma'_\pm) = \pm\,\mathrm{si}_\pm(U')$. Since $F_\pm$ are of finite rank, we do not need to take essential locality into account at this point. The resulting F will be essentially local if and only if the infinite-dimensional block $F_\mathcal{K}$ is.

In order to construct $F_\mathcal{K}$, we decompose the unitary equivalence operator V into $V = V_+ \oplus V_- \oplus V_\mathcal{K}$, where $V_\mathcal{K} : \mathcal{K} \to \mathcal{K}'$ is assumed to intertwine $\gamma_\mathcal{K}$ and $\gamma'_\mathcal{K}$. We use $\widetilde{F}_\mathcal{K}$ from the first proof direction and set $F_\mathcal{K} = V_\mathcal{K}\widetilde{F}_\mathcal{K}$. By a computation similar to (5.46) and (5.47), $F_\mathcal{K}$ fulfils the timeframe equations on $\mathcal{K}$ and $\mathcal{K}'$

$$U_\mathcal{K} = \gamma_\mathcal{K} F_\mathcal{K}^* \gamma_{\mathcal{K}'} F_\mathcal{K} \qquad \text{and} \qquad U'_{\mathcal{K}'} = F_\mathcal{K} \gamma_\mathcal{K} F_\mathcal{K}^* \gamma_{\mathcal{K}'}. \tag{5.55}$$

Moreover, if U and V are essentially local, $F_\mathcal{K}$ inherits this property.

In summary, we constructed

$$F = \begin{pmatrix} A_+ & 0 \\ 0 & D_+ \end{pmatrix} \oplus \begin{pmatrix} 0 & B_- \\ C_- & 0 \end{pmatrix} \oplus \frac{V_\mathcal{K}}{\sqrt{2}} \begin{pmatrix} \sqrt{\mathbb{1}+\alpha} & V_\beta\sqrt{\mathbb{1}-\delta} \\ -V_\beta^*\sqrt{\mathbb{1}-\alpha} & \sqrt{\mathbb{1}+\delta} \end{pmatrix}, \tag{5.56}$$

where α, δ, V_β are the blocks of U, resp. its polar isometry, restricted to $\mathcal{K}$, A^+, B^-, C^-, D^+ are arbitrary unitaries of dimension $\dim\ker(\alpha \pm \mathbb{1})$ and $\dim\ker(\delta \pm \mathbb{1})$ (see (5.51)), and $V_\mathcal{K}$ is the restriction of V to $\mathcal{K}$ and $\mathcal{K}'$ from the right and from the left, respectively. □

Instead of fixing two timeframes U and U' one could also ask the question for a single U, i.e. which chiral walks U admit a half-step operator F. Or, in other words, which chiral walks U allow the assignment of a second timeframe U'. A critical condition for this is the existence of an appropriate V as in Theorem 5.2.9. V has to identify the spaces $\mathcal{K}$ and $\mathcal{K}'$, such that γ and γ' are intertwined. Moreover, it also needs to be essentially local if the setting demands it to be. Let us, therefore, squeeze in a small technical lemma before we answer the question of whether an F exists for a single timeframe without further restrictions in the affirmative.

Lemma 5.2.10. *Let Q_1 and Q_2 be two finite rank projections on a Hilbert $\mathcal{H}$ space with a one-dimensional lattice structure (see (3.49)). Then there exists an essentially local partial isometry Λ, such that*

$$\Lambda^*\Lambda = \mathbb{1} - Q_1 \qquad \textit{and} \qquad \Lambda\Lambda^* = \mathbb{1} - Q_2. \tag{5.57}$$

If $\operatorname{rank} Q_1 = \operatorname{rank} Q_2$, there exists a (unitary) finite rank perturbation V of the identity, such that $Q_1 = V^* Q_2 V$.

Proof. Let us start with the second statement, which is rather obvious and only included here for completeness. Let $\mathcal{Q} \subset \mathcal{H}$ be a finite-dimensional subspace containing $Q_1\mathcal{H}$ and $Q_2\mathcal{H}$[5]. In $\mathcal{Q}$, let $\{\varphi_1^i\}$ and $\{\varphi_2^i\}$ with $i = 1, \ldots, \dim \mathcal{Q}$ be eigenbases of Q_1 and Q_2, such that the first $\dim Q_j$ vectors correspond to the $+1$ eigenvalue of Q_j, respectively. Then

$$V = \mathbb{1}_{\mathcal{Q}^\perp} \oplus \sum_i |\varphi_2^i\rangle\langle\varphi_1^i| \tag{5.58}$$

is a finite rank perturbation of the identity. In particular V is essentially local and intertwines Q_1 and Q_2.

Turning to the first statement, we can reduce the problem to the simpler one of constructing an essentially local co-isometry I with $I^*I = \mathbb{1} - Q$ and $II^* = \mathbb{1}$, with only one finite rank projection Q. Indeed, given two such isometries I_1 and I_2 for Q_1 and Q_2, we set $\Lambda = I_2^* I_1$, which fulfils (5.57).

For the construction of I, let $\operatorname{rank} Q = n$, $P = P_{\geq 0}$ be the usual half-space projection, and S be the generalized shift, with respect to some shift register $\{\varphi_x\}_x$ (w.l.o.g. we can choose φ_x to be the first basis vector of some base choice in each cell). Sandwiching S with P defines the unilateral shift on $P\mathcal{H}$, which fulfils $(PS^{*n}P)(PS^nP) = P$ and

$$(PS^nP)(PS^{*n}P) = P - \sum_{k=0}^{n-1} |\varphi_k\rangle\langle\varphi_k| =: P - N. \tag{5.59}$$

Hence, for

$$\widetilde{I} := (\mathbb{1} - P) + PS^{*n}P \tag{5.60}$$

we get

$$\widetilde{I}\,\widetilde{I}^* = \mathbb{1} \qquad \text{and} \qquad \widetilde{I}^*\widetilde{I} = \mathbb{1} - N. \tag{5.61}$$

By construction $\widetilde{I}$ is essentially (even strictly) local. By the second statement of the lemma, there exists an essentially local unitary V with $Q = V^*NV$ because we chose $\widetilde{I}$ such that $\operatorname{rank} N = \operatorname{rank} Q$. Therefore, setting $I = \widetilde{I}V$ provides us with an essentially local co-isometry with

$$I^*I = V^*\widetilde{I}^*\widetilde{I}V = V^*(\mathbb{1} - N)V = \mathbb{1} - Q \qquad \text{and} \qquad II^* = \widetilde{I}\widetilde{I}^* = \mathbb{1}, \tag{5.62}$$

as needed. □

With this at hand, the existence of an F for a single timeframe follows straightforwardly:

[5] E.g., the minimal one, spanned by $\{\psi + \varphi \mid \psi \in Q_1\mathcal{H},\ \varphi \in Q_2\mathcal{H}\}$

Corollary 5.2.11. *Let U be a chiral symmetric essentially gapped unitary. Then there exists a half-step unitary F, such that*

$$U = \gamma F^* \gamma F. \tag{5.63}$$

If U is essentially local, this F can also be chosen essentially local.

Proof. The proof is similar to the one for Theorem 5.2.9, the only difference being that the decomposition of $\mathcal{H}$ into $\mathcal{H}'_\pm$ and $\mathcal{K}'$ is not fixed by a second timeframe. Hence, we can choose an appropriate decomposition and show, that everything just works out. So let $\ker(\alpha' \pm \mathbb{1})$ and $\ker(\delta' \pm \mathbb{1})$[6] be some finite-dimensional spaces with dimensions as fixed in (5.50). This also defines $\mathcal{K}'$ as the complement of the chosen spaces. In order to construct an appropriate V, which identifies $\mathcal{K}$ and $\mathcal{K}'$, we apply Lemma 5.2.10. Thereby, the intertwining relation for $\gamma_\mathcal{K}$ and $\gamma_{\mathcal{K}'}$, can be fulfilled by constructing V separately for each chiral eigenspace. Concretely, consider $\mathcal{K}^\pm = \Gamma^\pm \mathcal{K}$ and $\mathcal{K}'^\pm = \Gamma^\pm \mathcal{K}'$. Both are the complements of finite-dimensional subspaces of $\Gamma^\pm \mathcal{H}$, respectively. Hence we find partial isometries $V^\pm$ such that $V^{\pm *} V^\pm = \mathcal{K}^\pm$ and $V^\pm V^{\pm *} = \mathcal{K}'^\pm$. Combining them as

$$V = \begin{pmatrix} V^+ & 0 \\ 0 & V^- \end{pmatrix} \tag{5.64}$$

provides us with an appropriate partial isometry on $\mathcal{H}$, which unitarily maps $\mathcal{K}$ onto $\mathcal{K}'$, while intertwining $\gamma_\mathcal{K}$ and $\gamma_{\mathcal{K}'}$.

Applying the arguments from the $ii) \Rightarrow i)$ proof direction of Theorem 5.2.9 finishes the proof. □

Having established the existence of the half-step operator F for two given timeframes U, U' with appropriate index relations, or a single chiral unitary U it is natural to investigate whether a given F is uniquely determined by U and U'. The following lemma describes, to what extend a half-step operator for a given chiral unitary U or pair of timeframes (U, U') can vary, while producing the same timeframes.

Lemma 5.2.12. *Let F_0 be a half-step operator for an admissible unitary U, i.e. $U = \gamma F_0^* \gamma F_0$. Then:*

i) Any other F is also a half-step operator for U if and only if $F = V F_0$, with a γ commuting unitary V. In the chiral eigenbasis this means

$$F = \begin{pmatrix} V_+ & 0 \\ 0 & V_- \end{pmatrix} F_0, \tag{5.65}$$

with arbitrary unitary blocks $V_\pm$. Similarly, if $U' = F_0 \gamma F_0^* \gamma$ is kept fixed instead of U, the condition is $F = F_0 V'$, with $V'\gamma = \gamma V'$.

ii) F is a half-step operator for both timeframes U and U' if and only if $F = V F_0$ with $[\gamma, V] = [U', V] = 0$ or $F = F_0 V'$ with $[\gamma, V'] = [U, V'] = 0$.

[6]Note, that $\ker(\alpha' \pm \mathbb{1})$ and $\ker(\delta' \pm \mathbb{1})$ are to be understood only as a denotation for certain finite-dimensional subspaces here, without referring to actually existing operators α' and δ'.

Proof. i): Since any other F for U fulfils $\gamma F^*\gamma F = \gamma F_0^*\gamma F_0$, we immediately get

$$F^*\gamma F = F_0^*\gamma F_0 \qquad \Leftrightarrow \qquad FF_0^*\gamma = \gamma F F_0^*. \tag{5.66}$$

Hence $F = (FF_0^*)F_0$ is a γ-commuting unitary times F_0. For U' the computation is analogous.

ii): This also follows from straightforward computation. Let $F = VF_0$, then, by $\gamma V = V\gamma$, due to i),

$$U' = (VF_0)\gamma(F_0^*V^*)\gamma \qquad \Leftrightarrow \qquad VU'V^* = U', \tag{5.67}$$

and similarly for $F = F_0V'$ and U. □

5.3 Complete set of indices

We now come to the central part of this chapter, the topological classification of half-step walks. In Section 5.2, where we discussed the fundamental properties of F, we expressed the symmetry indices of U and U' in terms of Fredholm indices of the chiral blocks of F. Following this path, we will further characterize F in terms of Fredholm indices in this chapter, which leads to a complete classification by five integer-valued indices.

To this end, remember that we already identified five different indices directly associated with F: The Fredholm indices of the four chiral blocks A, B, C and D, as well as the index of F itself, if F is merely essentially unitary. However, the results of Section 5.2 show, that these five indices are not independent: By Lemma 5.2.4 we can drop $\mathrm{ind}\,(F)$, because it is completely determined by the indices ot the four blocks A, B, C and D. Moreover, by Lemma 5.2.7 we can also drop two of these. Doing so also resolves the dependencies imposed by Lemma 5.2.6, such that the considerations above do not introduce further restrictions. Without loss of generality we chose $\mathrm{ind}\,(A)$ and $\mathrm{ind}\,(B)$ as the remaining independent indices. We know from Corollary 5.2.11 that for every chiral symmetric gapped walk U, there exists a half-step walk F. In particular, every pair $(\mathrm{si}_+, \mathrm{si}_-)$ can be realized in this way. Combining this with Lemma 5.2.7, we find that $\mathrm{ind}\,(A)$ and $\mathrm{ind}\,(B)$ are independent since any pair in $\mathbb{Z}^2$ can be realized via an F.

However, the two indices $\mathrm{ind}\,(A)$ and $\mathrm{ind}\,(B)$ are insufficient to characterize any half-step walk completely. In particular, the considerations so far did not yet include any locality assumption. Taking locality into account leads to another set of five indices. For an essentially local F also the chiral blocks have to be essentially local because any half-space projection commutes with the chiral symmetry. Hence, compressing the blocks to a half-space via $P \cdot P$ according to Lemma 3.3.13 again provides us with Fredholm operators on $P\mathcal{H}$. These add the five right Fredholm indices $\overrightarrow{\mathrm{ind}}\,(\cdot)$ of A, B, C, D, and F itself to the list of indices.

We can again identify some of the indices as dependent ones and therefore cross them from the list. Lemma 5.2.6 and Lemma 5.2.4 are also valid for essentially unitary operators. Similarly, the half-space compressions of essentially local unitaries U and U' are essentially unitary and yield the right symmetry indices according to Definition

3.5.6. Hence, we can apply the two lemmas also to the half space compressions of F and its chiral blocks, which gives

$$\begin{aligned} \overrightarrow{\mathfrak{si}}(U) = \overrightarrow{\mathrm{ind}}(A) - \overrightarrow{\mathrm{ind}}(B) &= \overrightarrow{\mathrm{ind}}(C) - \overrightarrow{\mathrm{ind}}(D) \\ \overrightarrow{\mathfrak{si}}(U') = \overrightarrow{\mathrm{ind}}(C) - \overrightarrow{\mathrm{ind}}(A) &= \overrightarrow{\mathrm{ind}}(D) - \overrightarrow{\mathrm{ind}}(B) \end{aligned} \tag{5.68}$$

and

$$\overrightarrow{\mathrm{ind}}(F) = \overrightarrow{\mathrm{ind}}(B) + \overrightarrow{\mathrm{ind}}(C) = \overrightarrow{\mathrm{ind}}(A) + \overrightarrow{\mathrm{ind}}(D). \tag{5.69}$$

Lemma 5.2.7 on the other hand needs exact unitarity and therefore has nothing to say in this scenario. Again, by (5.69), the index of F itself is determined by those of its chiral blocks and can be dropped. Moreover, the two equivalent relations between the right Fredholm indices of the chiral blocks given by (5.68) allow us to drop one further index. Without loss of generality, we choose $\overrightarrow{\mathrm{ind}}(A), \overrightarrow{\mathrm{ind}}(B)$ and $\overrightarrow{\mathrm{ind}}(C)$ as the remaining three indices. These three indices are again independent. However, their independence is not as obvious as before for $\mathrm{ind}(A)$ and $\mathrm{ind}(B)$. We will show this, by constructing a generating example, which allows us to realize every possible index combination. But first, let us formulate the main result of this chapter. The remainder of the section is dedicated to the proof of this theorem.

Theorem 5.3.1. *Let F be a unitary essentially local half-step walk for essentially gapped chiral walks U and U'. Assign to F the quintuple*

$$\big(\mathrm{ind}(A), \mathrm{ind}(B), \overrightarrow{\mathrm{ind}}(A), \overrightarrow{\mathrm{ind}}(B), \overrightarrow{\mathrm{ind}}(C)\big) \in \mathbb{Z}^5. \tag{5.70}$$

Then these indices are invariant under continuous deformations in the set of essentially local half-step walks as well as under compact perturbations. The classification in terms of the index quintuple is complete, i.e. two half-step walks F and F' are connected via a norm continuous path of half-step walks if and only if their index quintuples coincide. Moreover, any combination in $\mathbb{Z}^5$ can be realized by suitable F.

The invariance of the five indices is straightforward. Deforming F inside the class of half-step walks with essentially gapped timeframes U and U', the chiral blocks stay Fredholm for continuous and trivially also for compact perturbations. Hence, the invariance of $\mathrm{ind}(A)$ and $\mathrm{ind}(B)$ already follows from the invariance of the Fredholm index. Moreover, as already discussed above, any half-space projection commutes with the chiral symmetry, whereas the chiral blocks of F are essentially local for every essentially local F. Hence the invariance of $\overrightarrow{\mathrm{ind}}(A), \overrightarrow{\mathrm{ind}}(B)$ and $\overrightarrow{\mathrm{ind}}(C)$ follow from Lemma 3.3.16 and Lemma 3.3.17.

5.3.1 The generating example

We will prove the independence and realisability of the five indices by constructing a generating example. For each quintuple of indices there exists a choice of parameters for the example realising the given indices.

Let $\mathcal{H} = \mathbb{C}^2 \otimes \widetilde{\mathcal{H}}$ according to (5.8) and S some partial shift with $\overrightarrow{\mathrm{ind}}\,(S) = -1$ on $\widetilde{\mathcal{H}}$. The generating example then involves the following two unitary operators:

$$f(a,b) = \frac{1}{\sqrt{2}} \begin{pmatrix} S^a & S^b \\ S^{-b} & -S^{-a} \end{pmatrix} \quad \text{and} \quad T(c) = \begin{pmatrix} S^c & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \quad a,b,c \in \mathbb{Z}. \tag{5.71}$$

As one readily checks, $f(a,b)$ is a valid half-step operator, producing exactly gapped timeframes. According to (5.69) we get $\overrightarrow{\mathrm{ind}}\,(f(a,b)) = 0$ for all $a,b \in \mathbb{Z}$. Hence, by Theorem 3.3.19, there exists a local decoupling $f(a,b) \mapsto f_L(a,b) \oplus f_R(a,b)$. Since the left and right half of the system are no longer connected, we are free to choose the parameters a and b independently on each side, i.e. $f_L(a_L,b_L) \oplus f_R(a_R,b_R)$ still provides a valid half-step operator with essentially gapped timeframes.

Definition 5.3.2. *With $\mathcal{H}$, $f_{L/R}(a_{L/R},b_{L/R})$ and $T(c)$ as above, we define the **generating example** as*

$$F(a_L,b_L,a_R,b_R,c) = T(c)\big(f_L(a_L,b_L) \oplus f_R(a_R,b_R)\big). \tag{5.72}$$

Note that we have $\mathrm{ind}\,(S^a) = 0$, $\overrightarrow{\mathrm{ind}}\,(S^a) = -a$ and $\mathrm{ind}\big(P^\perp S^{a_L} P^\perp \oplus P S^{a_R} P\big) = a_L - a_R$, where the argument in the last expression is a compact perturbation of the upper left corner of $f_L(a_L,b_L) \oplus f_R(a_R,b_R)$, which therefore has the same right Fredholm index. Using similar identities, we find that the index quintuple for the generating example F is given by

$$(a_L - a_R, b_L - b_R, -a_R - c, -b_R - c, b_R)\,. \tag{5.73}$$

I.e. the index quintuple for F is obtained by applying the integer matrix

$$M = \begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad \text{with} \qquad M^{-1} = \begin{pmatrix} 1 & 0 & -1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & -1 \end{pmatrix} \tag{5.74}$$

to the parameter vector (a_L,b_L,a_R,b_R,c). Since M is invertible and the inverse is also an integer matrix, we conclude that, conversely, every index combination in $\mathbb{Z}^5$ can be realized via this example by chosing the parameters according to

$$(a_L,b_L,a_R,b_R,c) = M^{-1}\left(\mathrm{ind}\,(A), \mathrm{ind}\,(B), \overrightarrow{\mathrm{ind}}\,(A), \overrightarrow{\mathrm{ind}}\,(B), \overrightarrow{\mathrm{ind}}\,(C)\right) \tag{5.75}$$

Moreover, since we showed that the index quintuple can reach every vector in $\mathbb{Z}^5$, we also showed their independence.

5.3.2 Completeness proof

It remains to prove the completeness statement. We do this in several steps: First, we establish the so-called flattening construction, which enables us to deform each F into a simpler form. Thereby, "flattening" refers to the spectrum of the corresponding timeframes similar to Lemma 3.6.2. We then use Theorem 3.3.19 and the standard form derived in Definition 5.2.8 to show that each F with trivial right Fredholm indices $\overrightarrow{\mathrm{ind}}\,(A)$, $\overrightarrow{\mathrm{ind}}\,(B)$, and $\overrightarrow{\mathrm{ind}}\,(C)$ can be deformed into a particularly simple reference

operator F_0. All other values of these three indices can then be reached by multiplying the reference operator with appropriate shift combinations. We finish the proof by explicitly constructing a homotopy between two Fs that share the same values for $(\mathrm{ind}\,(A), \mathrm{ind}\,(B), 0, 0, 0)$.

The flattening construction

In Section 3.6 the flat band condition referred to a walk, whose spectrum is contained in $\{\pm 1, \pm i\}$, where the finite-dimensional eigenspaces at ± 1 do not contain any balanced sub-representations. Here we relax this condition a bit and only demand finite-dimensional eigenspaces at ± 1. We will comment on the implications of this relaxation later, after the proof of Lemma 5.3.4 and start here by expressing this relaxed flatband condition on the timeframes U and U' in terms of the half-step walk.

Lemma 5.3.3. *Let F be a half-step walk for U and U' with chiral blocks A, B, C and D. Then the following are equivalent:*

i) *U and U' are essentially flatband.*

ii) *$\sqrt{2}X$, for $X \in \{A, B, C, D\}$ are essentially unitary.*

Proof. As in to the proof of Lemma 5.2.1 we formulate the proof for the exact case, i.e. for the images of the involved operators in the Calkin algebra. The "essential" versions then follow automatically.

Let U and U' be exactly flatband, with spectrum in $\{\pm i\}$. This means $U = -U^*$ and similarly for U'. By (5.10) this is equivalent to $A^*A = C^*C$, $B^*B = D^*D$, $AA^* = BB^*$ and $CC^* = DD^*$, which, using the unitarity conditions for F, is equivalent to $\sqrt{2}X$ being unitary for $X \in \{A, B, C, D\}$, as claimed.

□

Keeping in mind that (essential) flatbandedness refers to the timeframes U and U' we also call the half-step walk F (essentially) flatband whenever it has (essentially) unitary chiral blocks up to a factor of $\sqrt{2}$.

In Lemma 3.6.2 we saw that every (tenfold way) admissible walk U can be continuously deformed into an essentially flatband one, and this was used to prove the completeness result for tenfold way admissible quantum walks. As indicated, this deformation can also be done in the present scenario, directly on the level of F.

Lemma 5.3.4. *Let F be a half-step walk. Then there exists a norm-continuous path $t \mapsto F_t$, $t \in [0, 1]$, of half-step walks, such that $F_0 = F$ and F_1 is essentially flatband, i.e. constitutes essentially flatband walks U and U'.*

Proof. We again start with the exactly gapped case: Let F be the half-step walk for exactly gapped walks U and U'. Then, by Lemma 5.2.1, all blocks are invertible. Using the polar decomposition, we can express each block as $X = U_X|X| = U_X\sqrt{X^*X}$. Since all blocks are invertible, the polar isometries U_X are unitary. Moreover, using the unitarity

conditions (5.25)-(5.30) we can express the absolute values of all blocks via the absolute value $|A| = \sqrt{A^*A}$ of A and the polar isometries of the blocks:

$$\begin{aligned} A &= U_A\sqrt{A^*A} & B &= U_B\sqrt{\mathbb{1} - U_B^*U_AA^*AU_A^*U_B} \\ C &= U_C\sqrt{\mathbb{1} - A^*A} & D &= U_D\sqrt{U_B^*U_AA^*AU_A^*U_B}, \end{aligned} \tag{5.76}$$

where we used $A^*A + C^*C = \mathbb{1}$ for C, $XX^* = U_XX^*XU_X^*$ and $AA^* + BB^* = \mathbb{1}$ for B, as well as $D^*D + B^*B = \mathbb{1}$ for D. The remaining unitarity conditions are equivalent to $D = -(C^*)^{-1}A^*B = -CA^*(B^*)^{-1}$, which, inserting the identifications above, reduces to

$$U_D = -U_CU_A^*U_B. \tag{5.77}$$

Now let

$$F_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} U_A & U_B \\ U_C & U_D \end{pmatrix}, \tag{5.78}$$

which is unitary by the reduced condition on the polar isometries. Since each block of F_1 is unitary up to a factor of $\sqrt{2}$ it fulfils the flatband condition in Lemma 5.3.3. Moreover, by (5.76), it suffices to find a continuous path, which connects A^*A and $\mathbb{1}/2$ in order to construct a path between F and F_1. An especially simple one is the linear interpolation $t\mathbb{1}/2 + (1-t)A^*A$. Thereby, the unitarity condition on the polar isometries then also guarantees unitarity of F_t along the path. We did not yet take locality into account. However, by Lemma 3.3.9, the polar isometries and the absolute values are essentially local. Further, the deformation of $\sqrt{A^*A}$ stays in the C^*-algebra of essentially local operators, which follows from the continuous functional calculus. Hence, each F_t is a well defined half-step walk.

For the general case we will use the standard form established in Definition 5.2.8, i.e.

$$F = \begin{pmatrix} A_+ & 0 \\ 0 & D_+ \end{pmatrix} \oplus \begin{pmatrix} 0 & B_- \\ C_- & 0 \end{pmatrix} \oplus \begin{pmatrix} A_{\mathcal{K}} & B_{\mathcal{K}} \\ C_{\mathcal{K}} & D_{\mathcal{K}} \end{pmatrix}, \tag{5.79}$$

where the first two summands are associated with the ± 1-eigenspaces of U and U' and contain finite-dimensional unitaries A_+, D_+, B_-, C_- (of different dimension), whereas the right most block consists of invertible blocks and reproduces the gapped parts of U and U'. Consequently, we do not have to touch the first two summands, which reduces the problem to the scenario of exactly gapped walks U and U'.

Deforming the right summand according to the first half of the proof, we get the polar unitaries of each block $X_{\mathcal{K}}$. Considering these as isometries on the full space and combining them with the finite-dimensional unitary blocks $X_\pm$, we can consider these as the polar isometries of A, B, C, D. In general, these are proper partial isometries that constitute an essentially flatband half-step walk F_1. □

As already mentioned, after the flattening construction from Lemma 3.6.2 the finite-dimensional real eigenspaces of U and U' would not contain balanced sub-representations of the chiral symmetry. In the standard form this would correspond to only one of the blocks in the first two summands $F_\pm$ being present, respectively. For $\operatorname{ind}(A) > 0$ ($\operatorname{ind}(A) < 0$) the kernel of A^* (A) would have to be trivial, wherefore only B_- (C_-)

was present in the second summand, whereas $\mathrm{ind}\,(B) > 0$ ($\mathrm{ind}\,(B) < 0$) would result in only A_+ (D_-) being present in the first summand. However, reducing the first two block matrices in the standard form to single blocks makes the picture of the standard form a bit less intuitive, wherefore we leave it there and discuss the finite-dimensional spaces $\mathcal{H}_\pm$ later, without this simplification.

With the flattening construction at hand, we can proceed and assemble the completeness proof. The index quintuple contains two different kinds of indices, which require different techniques during the proof. On the one hand, there are the Fredholm indices of A and B, and on the other the right Fredholm indies of A, B and C. Similar to the completeness proof for the right Fredholm index for essentially local unitaries, it suffices to prove connectedness of the trivial component with respect to the latter three indices. Indeed, given F, let $(a, b, c) = \left(\overrightarrow{\mathrm{ind}}\,(A), \overrightarrow{\mathrm{ind}}\,(B), \overrightarrow{\mathrm{ind}}\,(C)\right)$ and consider

$$\widetilde{F} = \begin{pmatrix} \widetilde{A} & \widetilde{B} \\ \widetilde{C} & \widetilde{D} \end{pmatrix} = \begin{pmatrix} S^a & 0 \\ 0 & S^c \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S^{b-a} \end{pmatrix}. \tag{5.80}$$

For $\widetilde{F}$ the right Fredholm indices evaluate to

$$\left[\overrightarrow{\mathrm{ind}}\,(\widetilde{A}) = \overrightarrow{\mathrm{ind}}\,(S^a A)\right] = \left[\overrightarrow{\mathrm{ind}}\,(\widetilde{C}) = \overrightarrow{\mathrm{ind}}\,(S^c C)\right] = \left[\overrightarrow{\mathrm{ind}}\,(\widetilde{B}) = \overrightarrow{\mathrm{ind}}\,(S^a B S^{b-a})\right] = 0. \tag{5.81}$$

Any homotopy of $\widetilde{F}$ lifts to F by multiplying with the inverse shift-combinations from left and right, respectively. Hence, we are free to assume the right Fredholm indices to be zero for the rest of the proof.

Lemma 5.3.5. *Let F be a half-step walk in standard form, with $\overrightarrow{\mathrm{ind}}\,(A) = \overrightarrow{\mathrm{ind}}\,(B) = \overrightarrow{\mathrm{ind}}\,(C) = 0$. Then there is a continuous path of half-step walks connecting F and*

$$F_0 = \begin{pmatrix} \mathbb{1}_{d(C)} & 0 \\ 0 & \mathbb{1}_{d(B)} \end{pmatrix} \oplus \begin{pmatrix} 0 & \mathbb{1}_{d(D)} \\ \mathbb{1}_{d(A)} & 0 \end{pmatrix} \oplus \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & -\mathbb{1} \end{pmatrix}, \tag{5.82}$$

with $d(X) = \dim \ker(X)$.

Proof. We start by flattening F according to Lemma 5.3.4. Deforming the first two summands is then straightforward since we only have to connect each finite-dimensional block A_+, B_-, C_- and D_+ continuously to the identity, which is certainly possible for finite-dimensional unitaries without further restrictions. Since the blocks are of finite rank, any deformation of them stays essentially local. For the right summand, we again drop the subscript $\mathcal{K}$ for the blocks $X_\mathcal{K}$. Up to a factor of $\sqrt{2}$, we are left with the three unitary blocks U_A, U_B, U_C and the fourth one $U_D = -U_C U_A^* U_B$. The right Fredholm indices of the first three blocks are trivial, wherefore they are homotopic to the identity on an essentially local unitary path by Theorem 3.3.19. Keeping $U_D = -U_C U_A^* U_B$ during this process guarantees unitarity of the block matrix and thereby also deforms U_D to $-\mathbb{1}$, as needed. □

Now suppose, we are given two half-step walks F_1 and F_2 with $\mathrm{ind}\,(A_1) = \mathrm{ind}\,(A_2)$, $\mathrm{ind}\,(B_1) = \mathrm{ind}\,(B_2)$, and $\overrightarrow{\mathrm{ind}}\,(A_i) = \overrightarrow{\mathrm{ind}}\,(B_i) = \overrightarrow{\mathrm{ind}}\,(C_i) = 0$. According to Lemma 5.3.5

we can deform both of them into unitaries which have the structure of (5.82). However, the decompositions into $\mathcal{H}_\pm$ and $\mathcal{K}$, and $\mathcal{H}'_\pm$ and $\mathcal{K}'$ from the standard from are in general different for F_1 and F_2. Moreover, the index relations $\mathrm{ind}\,(A_1) = \mathrm{ind}\,(A_2) = d(C_i) - d(B_i)$ and $\mathrm{ind}\,(B_1) = \mathrm{ind}\,(B_2) = d(D_i) - d(A_i)$ only fix the differences $d(C_i) - d(B_i)$ and $d(A_i) - d(D_i)$, and not the individual values of the $d(X_i)$. We first concentrate on the second problem, beginning with the first summand. Without loss of generality let $n = d(C_1) - d(C_2) > 0$, which, by $\mathrm{ind}\,(A_1) = \mathrm{ind}\,(A_2)$, also implies $n = d(B_1) - d(B_2)$. We can split a $2n$-dimensional part off of the left summand of F_1, and rearrange the basis, such that

$$\begin{pmatrix} \mathbb{1}_{d(C_1)} & 0 \\ 0 & \mathbb{1}_{d(B_1)} \end{pmatrix} \equiv \begin{pmatrix} \mathbb{1}_{d(C_2)} & 0 \\ 0 & \mathbb{1}_{d(B_2)} \end{pmatrix} \oplus \begin{pmatrix} \mathbb{1}_n & 0 \\ 0 & \mathbb{1}_n \end{pmatrix}. \tag{5.83}$$

This can then be continuously deformed into

$$\begin{pmatrix} \mathbb{1}_{d(C_2)} & 0 \\ 0 & \mathbb{1}_{d(B_2)} \end{pmatrix} \oplus \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1}_n & \mathbb{1}_n \\ \mathbb{1}_n & -\mathbb{1}_n \end{pmatrix}. \tag{5.84}$$

In a final rearranging of the basis, we then include the right $2n$-dimensional summand into $F_\mathcal{K}$, which adjusts the size of the first summand of F_1 to the size of the first summand of F_2. We can treat the second summand in a similar way, splitting off $\sigma_x \otimes \mathbb{1}_n$ and deforming into

$$\begin{pmatrix} 0 & \mathbb{1}_{d(D_1)} \\ \mathbb{1}_{d(A_1)} & 0 \end{pmatrix} \sim \begin{pmatrix} 0 & \mathbb{1}_{d(D_2)} \\ \mathbb{1}_{d(A_2)} & 0 \end{pmatrix} \oplus \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1}_n & \mathbb{1}_n \\ \mathbb{1}_n & -\mathbb{1}_n \end{pmatrix} \tag{5.85}$$

as the intermediate step. Finally, we move the finite-dimensional subspaces $\mathcal{H}_{\pm,i}$ and $\mathcal{H}'_{\pm,i}$, $i = 1, 2$, i.e. the complements of $\mathcal{K}$ and $\mathcal{K}'$ for F_1 and F_2 onto each other, respectively. For this, let $V_\pm$ and $V'_\pm$ be unitaries with $V_\pm \mathcal{H}_{\pm,1} = \mathcal{H}_{\pm,2}$ and $V'_\pm \mathcal{H}'_{\pm,1} = \mathcal{H}'_{\pm,2}$ according to Lemma 5.2.10. That is, finite rank perturbations of the identity that intertwine the projections onto the respective subspaces. In particular, $V_\pm$ and $V'_\pm$ can be chosen essentially local. We can further assume them to respect the splitting into the γ-eigenspaces, by applying Lemma 5.2.10 to $\Gamma_\pm \mathcal{H}$ separately. With these we get

$$F_2 = V'_- V'_+ F_1 V_+^* V_-^*. \tag{5.86}$$

Finally, we get a continuous path between F_1 and F_2 by continuously deforming $V_\pm$ and $V'_\pm$ to the identity on paths of finite rank perturbations, which finishes the proof of Theorem 5.3.1.

□

5.4 Example: The split-step walk

Before we compare the classification of half-step walks above with the classification of the timeframes as discrete time quantum walks, let us discuss a motivating example: The well known split-step walk (see also Example 1.4.6), which was first introduced by Kitagawa et al. in [KRBD10]. This model became the workhorse among the example models for the topological classification of symmetric quantum walks [Kit12, Asb12,

AO13, ATD14, TAD14, KBF+12, CGS+16, Sta15, CGG+18, CGG+21], which makes it the good example model to apply our theory to.

The split-step walk is defined as a shift coin sequence on $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ via

$$U_{ss} = S_\downarrow C_2 S_\uparrow C_1, \tag{5.87}$$

where $S_\uparrow$ ($S_\downarrow$) denotes the partial shift S_φ from Definition 1.4.4, with $\varphi_x = (1, 0)$ (resp. S_φ with $\varphi_x = (0, 1)$), i.e.

$$S_\uparrow = \begin{pmatrix} S & 0 \\ 0 & \mathbb{1} \end{pmatrix} \qquad \text{and} \qquad S_\downarrow = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S^* \end{pmatrix}, \tag{5.88}$$

with the usual bilateral right shift S on $\ell^2(\mathbb{Z})$. C_i are possibly position dependent coin operations with $\sigma_x C_i \sigma_x = C_i^*$. In the standard split-step walk, the coins are usually defined as real rotations $C_i(x) = R(\theta_i(x)) = \exp(-i\theta_i(x)\sigma_y)$. Due to $\sigma_x S_{\uparrow/\downarrow} \sigma_x = S^*_{\downarrow/\uparrow}$ and $\sigma_x C_i \sigma_x = C_i^*$, U_{ss} is chiral symmetric with $\gamma = (\mathbb{1} \otimes \sigma_x) C_1$, which is self-adjoint and squares to the identity, rendering it a valid chiral symmetry in the context of the first part of this thesis. With C_1 also γ is position dependent, wherefore it is sometimes not considered a valid chiral symmetry [Asb12]. However, a simple base-change $R(-\pi/4)\sqrt{C_1} \cdot \sqrt{C_1}^* R(\pi/4)$ transforms U_{ss} into

$$R(-\pi/4)\sqrt{C_1} S_\downarrow C_2 S_\uparrow \sqrt{C_1} R(\pi/4) = R(\theta_1/2 - \pi/4) S_\downarrow R(\theta_2) S_\uparrow R(\theta_1/2 + \pi/4), \tag{5.89}$$

which is chiral symmetric for $\gamma = \mathbb{1} \otimes \sigma_z$. In this form the most straight forward half-step operator is

$$F = R(\theta_2/2 - \pi/4) S_\uparrow R(\theta_1/2 + \pi/4). \tag{5.90}$$

With $c_\pm = \cos((\theta_1 \pm \theta_2)/2)$ and $s_\pm = \sin((\theta_1 \pm \theta_2)/2)$ this gives

$$F = \frac{1}{2} \begin{pmatrix} (c_+ + s_-)\mathbb{1} + (c_+ - s_-)S & (c_- - s_+)\mathbb{1} - (c_- + s_+)S \\ (c_- + s_+)\mathbb{1} - (c_- - s_+)S & (c_+ - s_-)\mathbb{1} + (c_+ + s_-)S \end{pmatrix}. \tag{5.91}$$

Turning to the translation invariant standard example of the split-step walk, i.e. $\theta_i(x) = \theta_i$, let us calculate its indices for different values of θ_1 and θ_2. For this task, the following Lemma is helpful:

Lemma 5.4.1. *Let S be the bilateral right-shift on $\ell^2(\mathbb{Z})$ and $a, b \in \mathbb{C}$. Then $a\mathbb{1} + bS$ is Fredholm with trivial index if and only if $|a| \neq |b|$. Moreover, $a + bS$ is essentially local with*

$$\vec{\mathrm{ind}}\,(a\mathbb{1} + bS) = \begin{cases} -1 & \text{if } |a| < |b| \\ 0 & \text{if } |a| > |b|. \end{cases} \tag{5.92}$$

In particular, the gaps close if and only if $|a| = |b|$, which follows from Lemma 5.2.1 in combination with the result above.

Proof. S is normal and the spectrum consists of the whole unit circle, with $\sigma_e(S) = \sigma(S)$. Therefore $\sigma_e(a\mathbb{1} + bS) = \sigma(a\mathbb{1} + bS) = a + b\sigma(S) = \{a + be^{i\phi} | \phi \in [0, 2\pi)\}$, which contains 0 if and only if $|a| = |b|$. This shows the first part of the Lemma. The second statement on $\vec{\mathrm{ind}}\,(a\mathbb{1} + bS)$ follows from the fact that, by continuously changing a and b, we get continuous paths of essentially local Fredholm operators between $a\mathbb{1} + bS$ and S if $|a| < |b|$ (see Example 3.3.15), and between $a\mathbb{1} + bS$ and $\mathbb{1}$ if $|a| > |b|$. □

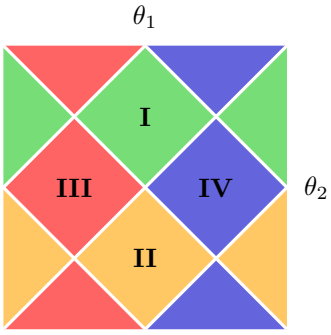
From (5.91) and Lemma 5.4.1 we can now directly compute the indices for the translation invariant split-step walk. First note that $\mathrm{ind}\,(A) = \mathrm{ind}\,(B) = 0$ for all values of θ_1 and θ_2. In fact this is true for every translation invariant walk [CGS+18]. Let us further evaluate the gap-closure condition $|a| = |b|$, which is met for at least one of the four matrix elements of F in (5.91) whenever

$$\theta_2 = \pm\theta_1 \bmod \pi. \tag{5.93}$$

These conditions correspond to the white lines in the parameter plane for (θ_1, θ_2) in Figure 5.1. Consequently, since changing the coin angles continuously is a gentle perturbation, the plaquettes between these lines correspond to parameter values with constant indices, respectively. Hence, we can evaluate these indices by picking particularly simple parameter values in each plaquette. Picking, e.g., the centers of the plaquettes I and II, which correspond to the parameter pairs $(0, \pi/2)$ and $(0, -\pi/2)$, respectively, we get

$$F_I = \frac{1}{\sqrt{2}}\begin{pmatrix} S & -S \\ \mathbb{1} & \mathbb{1} \end{pmatrix} \qquad \text{and} \qquad F_{II} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbb{1} & \mathbb{1} \\ -S & S \end{pmatrix}, \tag{5.94}$$

with the obvious index triples $(-1, -1, 0)$ and $(0, 0, -1)$ for $(\vec{\mathrm{ind}}\,(A), \vec{\mathrm{ind}}\,(B), \vec{\mathrm{ind}}\,(C))$. Evaluating F for all other plaquettes in a similar way, we get the following index regions:



	$(\vec{\mathrm{ind}}\ \mathbf{A}, \vec{\mathrm{ind}}\ \mathbf{B}, \vec{\mathrm{ind}}\ \mathbf{C})$		$(\vec{\mathrm{si}}\,(U), \vec{\mathrm{si}}\,(U'))$
I	$(-\mathbf{1}, -\mathbf{1}, \ \mathbf{0})$	◆	$(\ \mathbf{0}, \ \mathbf{1})$
II	$(\ \mathbf{0}, \ \mathbf{0}, -\mathbf{1})$	◆	$(\ \mathbf{0}, -\mathbf{1})$
III	$(-\mathbf{1}, \ \mathbf{0}, -\mathbf{1})$	◆	$(-\mathbf{1}, \ \mathbf{0})$
IV	$(\ \mathbf{0}, -\mathbf{1}, \ \mathbf{0})$	◆	$(\ \mathbf{1}, \ \mathbf{0})$

Figure 5.1: Regions corresponding to different topological phases in the (θ_1, θ_2)-parameter plane for the split-step walk. Figure taken from [CGWW21].

Note that on the level of the single timeframes (without considering the other timeframe, respectively) the patches **I** and **II** are labelled equally by $\vec{\mathrm{si}} = 0$ and similarly for the patches **III** and **IV** with $\vec{\mathrm{si}}' = 0$. Hence, taken individually, each timeframe has only three phases instead of four.

For the sake of completeness, let us demonstrate that there exist "bridges" between these 0-plaquettes if only one timeframe is considered. We again consider the respective flat-band representatives with parameters corresponding to the centres of the respective plaquette. Since changing from one timeframe to the other amounts to exchanging the parameters θ_1 and θ_2 for the split-step walk, both scenarios correspond to similar flat-band operators, namely

$$U_I = \begin{pmatrix} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \qquad \text{and} \qquad U_{II} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}. \tag{5.95}$$

These are continuously connected on a chiral symmetric path via

$$t \mapsto U_t = \begin{pmatrix} 0 & -e^{it\pi\mathbb{1}} \\ e^{-it\pi\mathbb{1}} & 0 \end{pmatrix}, \quad t \in [0,1], \tag{5.96}$$

with $U_0 = U_I$ and $U_1 = U_{II}$.

In summary, the example above demonstrates that the two timeframes distinguish different regions of topological phases of the driving process. We need to consider both to distinguish all phases in the present example. However, while translation-invariant chiral drivings are described by the three indices $(\vec{\mathrm{ind}}\,(A), \vec{\mathrm{ind}}\,(B), \vec{\mathrm{ind}}\,(C)) \in \mathbb{Z}^3$, there are only the two $(\vec{\mathrm{si}}\,(U), \vec{\mathrm{si}}\,(U')) \in \mathbb{Z}^2$ on the level of timeframes. Therefore, something must be missing on that level.

5.5 Connection to the symmetry indices

Let us further investigate how the symmetry indices of two timeframes U and U' with a common half-step operator F are related to each other. As discussed in Section 3.6 the homotopy type of each timeframe is uniquely labelled by the index triple $(\mathrm{si}, \vec{\mathrm{si}}\,, \mathrm{si}_+)$. In order to streamline notation we often abbreviate $\mathrm{si}(U)$ as si and $\mathrm{si}(U')$ as si' and similarly for $\vec{\mathrm{si}}\,, \vec{\mathrm{si}}\,', \mathrm{si}_\pm$ and $\mathrm{si}'_\pm$. At least one of these six indices must be redundant since the complete classification of half-step walks determines the classification of U and U' in terms of only five indices. Nevertheless, it might well be that the walk indices do not cover the full classification. So what are the restrictions on these six indices for a timeframed setting?

5.5.1 Index relations

We already discovered the necessary condition $\mathrm{si}_\pm = \pm\,\mathrm{si}'_\pm$ in Theorem 5.2.9. Evaluating this condition together with $\mathrm{si} = \mathrm{si}_+ + \mathrm{si}_-$ we find

$$\mathrm{si}_\pm = \pm\,\mathrm{si}'_\pm = \frac{\mathrm{si} \pm \mathrm{si}'}{2}. \tag{5.97}$$

Hence, in a timeframed setting, $\mathrm{si}_\pm$ and $\mathrm{si}'_\pm$ are completely determined by si and si'. This reduces the six indices to four, showing that the walk indices cannot fully describe the driven setting. Moreover, this means that si and si' have to fulfil

$$\mathrm{si} \equiv \mathrm{si}' \bmod 2 \tag{5.98}$$

in order to be realisable by timeframes U and U'. Apart from this condition, the remaining four indices are independent. Combining (5.20), (5.68) and (5.73) we get

$$\begin{aligned} \mathrm{si} &= a_L - b_L - (a_R - b_R) & \vec{\mathrm{si}} &= -(a_R - b_R) \\ \mathrm{si}' &= -(a_L + b_L) + a_R + b_R & \vec{\mathrm{si}}\,' &= a_R + b_R + c \end{aligned} \tag{5.99}$$

for the generating example from Section 5.3.1. Provided that (5.98) is fulfilled, (5.99) can be inverted, which yields

$$(a_L, b_L, a_R, b_R, c) = \left(a_R + \frac{\mathrm{si} - \mathrm{si}'}{2}, a_R - \frac{\mathrm{si} + \mathrm{si}'}{2} + \vec{\mathrm{si}}\,, a_R, a_R + \vec{\mathrm{si}}\,, \vec{\mathrm{si}}\,' - \vec{\mathrm{si}}\, - 2a_R \right). \tag{5.100}$$

Note that a_R is a free parameter, i.e. for each choice of a_R the indices of U and U' of the generating example with (5.100) evaluate to the given values $(\mathrm{si}, \vec{\mathrm{si}}, \mathrm{si}', \vec{\mathrm{si}}')$. Hence, all index combinations $(\mathrm{si}, \vec{\mathrm{si}}, \mathrm{si}' \vec{\mathrm{si}}') \in \mathbb{Z}^4$ fulfilling (5.98) can be realised. Since a_R appears as a summand with coefficient 1 in the other parameters a_L, b_L, b_R, each of these could equally well be chosen freely by adjusting a_R accordingly. It seems that this is not possible for c, because we cannot solve $c = \vec{\mathrm{si}}' - \vec{\mathrm{si}} - 2a_R$ for a_R in general ($\vec{\mathrm{si}}' - \vec{\mathrm{si}}$ is not necessarily even, as the split-step walk shows). However, we will readily see that there is an additional condition on $\vec{\mathrm{si}}$ and $\vec{\mathrm{si}}'$, involving $\vec{\mathrm{ind}}\,(F)$, which is determined by c in the generating example.

Adding $\vec{\mathrm{ind}}\,(F)$ to the four of walk indices supplements them to a complete index set. To see this, let us first verify that $\vec{\mathrm{ind}}\,(F)$ is not already determined by the four walk indices. This can be done, by expressing the walk indices and $\vec{\mathrm{ind}}\,(F)$ as vectors in the space $\mathbb{Z}^5$ of the five complete indices $\big(\mathrm{ind}\,(A), \mathrm{ind}\,(B), \vec{\mathrm{ind}}\,(A), \vec{\mathrm{ind}}\,(B), \vec{\mathrm{ind}}\,(C)\big)$:

$$\begin{aligned} \mathrm{si} &\equiv (1,-1,0,0,0) \qquad & \vec{\mathrm{si}} &\equiv (0,0,1,-1,0) \\ \mathrm{si}' &\equiv (-1,-1,0,0,0) \qquad & \vec{\mathrm{si}}' &\equiv (0,0,-1,0,1) \\ & & \vec{\mathrm{ind}}\,(F) &\equiv (0,0,0,1,1), \end{aligned} \tag{5.101}$$

Clearly these vectors are linearly independent. Using (5.68) and (5.69), we get

$$\vec{\mathrm{ind}}\,(F) + \vec{\mathrm{si}} + \vec{\mathrm{si}}' = 2\,\vec{\mathrm{ind}}\,(C) \equiv 0 \bmod 2. \tag{5.102}$$

With this, $\vec{\mathrm{ind}}\,(F) \pm \vec{\mathrm{si}} \pm \vec{\mathrm{si}}'$ is always even, wherefore (keeping in mind that $c = -\vec{\mathrm{ind}}\,(F)$) we can chose $a_R = 1/2(\vec{\mathrm{si}}' - \vec{\mathrm{si}} + \vec{\mathrm{ind}}\,(F))$ in (5.100). Hence, choosing the parameters (a_L, b_L, a_R, b_R, c) as

$$\left(\frac{\vec{\mathrm{ind}}\,(F) + \overleftarrow{\mathrm{si}} - \overleftarrow{\mathrm{si}}'}{2}, \frac{\vec{\mathrm{ind}}\,(F) - \overleftarrow{\mathrm{si}} - \overleftarrow{\mathrm{si}}'}{2}, \frac{\vec{\mathrm{ind}}\,(F) - \vec{\mathrm{si}} + \vec{\mathrm{si}}'}{2}, \frac{\vec{\mathrm{ind}}\,(F) + \vec{\mathrm{si}} + \vec{\mathrm{si}}'}{2}, -\vec{\mathrm{ind}}\,(F) \right), \tag{5.103}$$

realises any combination of $\big(\mathrm{si}, \vec{\mathrm{si}}, \mathrm{si}', \vec{\mathrm{si}}'\, \vec{\mathrm{ind}}\,(F)\big)$ via the generating example, provided that (5.98) and (5.102) are fulfilled. Note that we used $\overleftarrow{\mathrm{si}} = \mathrm{si} - \vec{\mathrm{si}}$ and $\overleftarrow{\mathrm{si}}' = \mathrm{si}' - \vec{\mathrm{si}}'$, which also fulfil (5.102), in order to shorten the expression.

Corollary 5.5.1. *A quintuple of indices*

$$\big(\mathrm{si}(U), \vec{\mathrm{si}}\,(U), \mathrm{si}(U'), \vec{\mathrm{si}}\,(U'), \vec{\mathrm{ind}}\,(F)\big) \tag{5.104}$$

can be realised by a half-step operator F, if and only if

$$\mathrm{si}(U) \equiv \mathrm{si}(U') \bmod 2 \qquad \textit{and} \qquad \vec{\mathrm{ind}}\,(F) \equiv \vec{\mathrm{si}}\,(U) + \vec{\mathrm{si}}\,(U') \bmod 2. \tag{5.105}$$

Moreover, there is a one-to-one correspondence between this set of indices and the index quintuple from Theorem 5.3.1. Hence, also (5.104) *is a complete set of indices with respect to homotopies and compact perturbations of half-step walks.*

Proof. The first part of the statement was proven above. For the second part, we already know that all five indices are homotopy invariants. As indicated in the corollary, we will

prove the completeness by mapping the indices to the index set in Theorem 5.3.1, which we proved to be complete and realisable for any quintuple in $\mathbb{Z}^5$.

By (5.101), the mapping from the index quintuple of Theorem 5.3.1 to the index set discussed here can be done by applying the invertible matrix M' to the former:

$$M' = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}, \quad \text{with} \quad M'^{-1} = \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 1 \\ 0 & -1 & 0 & -1 & 1 \\ 0 & 1 & 0 & 1 & 1 \end{pmatrix}. \tag{5.106}$$

Note, however, that differently from the conversion matrix M in (5.74), the inverse of M' is not an integer matrix. Nevertheless, applying M'^{-1} only to the allowed index quintuples $\overrightarrow{v} = (\mathrm{si}, \overrightarrow{\mathrm{si}}, \mathrm{si}', \overrightarrow{\mathrm{si}}', \overrightarrow{\mathrm{ind}}(F))$, the result will always be integer-valued and we can reach any vector in $\mathbb{Z}^5$. Indeed, for indices fulfilling (5.105) we can write $\overrightarrow{v} = (\mathrm{si}, \overrightarrow{\mathrm{si}}, \mathrm{si} - 2k, \overrightarrow{\mathrm{si}}', \overrightarrow{\mathrm{si}} + \overrightarrow{\mathrm{si}}' + 2l)$, for some integers $k, l \in \mathbb{Z}$. From this we get

$$\begin{aligned} M'^{-1}\overrightarrow{v} &= \big(\mathrm{ind}(A), \mathrm{ind}(B), \overrightarrow{\mathrm{ind}}(A), \overrightarrow{\mathrm{ind}}(B), \overrightarrow{\mathrm{ind}}(C)\big) \\ &= (k, k - \mathrm{si}, l + \overrightarrow{\mathrm{si}}, l, l + \overrightarrow{\mathrm{si}} + \overrightarrow{\mathrm{si}}'), \end{aligned} \tag{5.107}$$

which span $\mathbb{Z}^5$. □

At this point, one could ask why we did not use the complete index set (5.104) for our classification in the first place. However, the additional constraints in (5.105) were not apparent at all from the beginning, and we only discovered them using the "detour" via the unconstrained index set (5.70) from Theorem 5.3.1. Moreover, taking (5.70) as the classifying set has the advantage of being the more fundamental choice, at least in some sense, since these are given by the well known Fredholm index itself or the right Fredholm index, which we derived from the information flow index in Section 3.3.2.

5.5.2 Bulk-boundary correspondence

For a single walk operator U with chiral symmetry, the bulk-boundary correspondence result in Corollary 3.5.8 predicts a lower bound on the number of eigenstates corresponding to eigenvalues ± 1, given by $|\,\mathrm{si}(U)| = |\overleftarrow{\mathrm{si}}(U) + \overrightarrow{\mathrm{si}}(U)|$. However, it was not possible to distinguish between the eigenvalue $+1$ and -1. Taking into account a second timeframe, allows us to predict the lower number of $+1$ and -1 eigenvalues separately.

Let U and U' be timeframes of some chiral driving, such that they are crossovers of (exactly gapped) bulk walks U_L, U_R, U'_L and U'_R. I.e. U and U' become equal to U_L and U'_L far to the left and to U_R and U'_R far to the right, respectively, in the sense of (3.165) in Corollary 3.5.8. Then we get

$$\mathrm{si}(U) = \overleftarrow{\mathrm{si}}(U_L) + \overrightarrow{\mathrm{si}}(U_R) = \overrightarrow{\mathrm{si}}(U_R) - \overrightarrow{\mathrm{si}}(U_L) \qquad \text{and} \qquad \mathrm{si}(U') = \overrightarrow{\mathrm{si}}(U'_R) - \overrightarrow{\mathrm{si}}(U'_L). \tag{5.108}$$

Inserting this into (5.97), the indices $\mathrm{si}_\pm(U) = \pm\,\mathrm{si}_\pm(U')$ evaluate to

$$\mathrm{si}_\pm(U) = \pm\,\mathrm{si}_\pm(U') = \frac{\big(\overrightarrow{\mathrm{si}}(U_R) \pm \overrightarrow{\mathrm{si}}(U'_R)\big) - \big(\overrightarrow{\mathrm{si}}(U_L) \pm \overrightarrow{\mathrm{si}}(U'_L)\big)}{2}. \tag{5.109}$$

Hence, the second timeframe stabilizes the ± 1 eigenspaces and allows to distinguish them in the bulk-boundary correspondence. This observation can also be understood in the context of non-gentle compact perturbations. In the following section, we will see that there are no non-gentle perturbations of timeframed systems, the possible crossovers are restricted, and those, which would result in shifting an eigenvalue from $+1$ to -1 are excluded. However, before we detail this, let us focus on the present crossover scenario.

If we assume the crossover to be valid also on the level of half-step walks, i.e. F is a crossover of F_L far to the left and F_R far to the right, such that $F_{L/R}$ is the half-step walk for $U_{L/R}$ and $U'_{L/R}$, we can further simplify (5.109). In this case we can express $\overrightarrow{\mathrm{si}}(U_{L/R})$ and $\overrightarrow{\mathrm{si}}(U'_{L/R})$ in terms of the respective chiral blocks of F_L and F_R according to (5.68). We get

$$\mathrm{si}_+(U) = \overrightarrow{\mathrm{ind}}(C_R) - \overrightarrow{\mathrm{ind}}(C_L) = -\left(\overrightarrow{\mathrm{ind}}(B_R) - \overrightarrow{\mathrm{ind}}(B_L)\right) \tag{5.110}$$

and

$$\mathrm{si}_-(U) = \overrightarrow{\mathrm{ind}}(A_R) - \overrightarrow{\mathrm{ind}}(A_L) = -\left(\overrightarrow{\mathrm{ind}}(D_R) - \overrightarrow{\mathrm{ind}}(D_L)\right), \tag{5.111}$$

where we used $\overrightarrow{\mathrm{ind}}(F_L) = \overrightarrow{\mathrm{ind}}(F_R)$, which is a necessary condition for a crossover between F_L and F_R to exist (see Theorem 3.3.19), in combination with (5.69).

These formulas confirm those from [ATD14], and [AO13] if the corresponding winding formulas in case of translation-invariant systems are considered [CGS$^+$18]. Moreover, they generalize the work of [ATD14] to non-translation invariant systems, and, in particular, also to half-step operators that do not stem from continuously driven Floquet process (see also [MBSO20]). This makes the theory applicable to, e.g., the split-step walk[7].

5.6 Compact perturbations and finite systems

A property that quantum walks exhibit in contrast to Hamiltonian or continuously driven systems is the existence of non-gentle perturbations. We discussed this in great detail in Section 3.2. In particular, in Proposition 3.2.8, we saw that $\mathrm{si}_\pm$ decide about the gentleness of a perturbation in case of the tenfold way, i.e., in particular, for chiral walks. The (discretely) driven systems via any F we consider in this section lie somewhat between the Floquet setting and quantum walks considered as a single discrete timestep. This raises the question of whether compact perturbations of a non-continuously driven F can produce non-gently perturbations on the level of U and U' or not, i.e. on which level non-gentle perturbations fail to exist.

5.6.1 Compact perturbations

The complete index quintuple for half-step walks F consists entirely of (right-) Fredholm indices. These are inherently invariant under compact perturbations. Therefore,

[7] The theory was already applied to the Hadamard quantum walk (which is a special case of the split-step walk) in [OANK15, Sect. IV], however, without rigorously proving that the formulas are valid also for $\overrightarrow{\mathrm{ind}}(F) \neq 0$.

no compact perturbation can change the topological class of a given F, and by completeness, every compact perturbation is continuously connected to the identity.

Corollary 5.6.1. *Let F be a half-step walk for a chiral symmetric protocol. Then any compact perturbation of F is gentle.*

Proof. We already argued above why this is true, using the completeness result for half-step walks. However, this can also be seen on the level of U and U': Clearly, any compact perturbation of F results in a compact perturbation of U and U'. Now, by Theorem 3.5.7, the symmetry indices $\mathrm{si}(U)$ and $\mathrm{si}(U')$ are invariant under compact perturbations. Since these also determine $\mathrm{si}_+(U) = \mathrm{si}_+(U')$ (see (5.97)) in the timeframed setting, also those are invariant under compact perturbations of F. Finally, Proposition 3.2.8 tells us that the perturbations of U and U' are gentle.

□

The corollary above seems to raise a contradiction: We know from Corollary 5.2.11 that every chiral symmetric walk with essential gaps exhibits a half-step walk F. In particular, we also find an F after non-gently perturbing a given walk U. This apparent contradiction is resolved by the following observation:

Corollary 5.6.2. *Let F_1 and F_2 be two half-step walks, such that U_1 and U_2 (both in the same timeframe, e.g. $U_i = \gamma F_i^* \gamma F_i$) are non-gentle compact perturbations of each other. Then $F_1 - F_2$ is not compact, i.e. F_1 and F_2 are non-compact perturbations of each other.*

Let us exemplify this via an example:

Example 5.6.3. *Consider the split-step walk from Section 5.4 with the parameters $(\theta_1, \theta_2) = (0, -\pi/2)$. I.e. we get $F = R(-\pi/2)S_\uparrow R(\pi/4)$, which results in $U = \bigoplus_x (i\sigma_y)^x$, where the superscript denotes the cell, in which the respective block acts.*

The arch-typical example of a non-gentle perturbation is to replace the θ_2-rotating coin in the split-step protocol by σ_x in a single cell, e.g. at $x = 1$ [CGG+18, Sta15]. In the present example this changes the action of $\widetilde{U} = VU$ only at $x = 0$, where $i\sigma_y$ is replaced by σ_z.

$$\widetilde{U} = \left[\bigoplus_{x<0} (i\sigma_y)^x\right] \oplus (\sigma_z)^0 \oplus \left[\bigoplus_{0<x} (i\sigma_y)^x\right] \quad \equiv \quad \cdots\!-\!(i\sigma_y)\!-\!(i\sigma_y)\!-\!(\sigma_z)\!-\!(i\sigma_y)\!-\!(i\sigma_y)\!-\!\cdots \qquad (5.112)$$

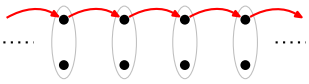
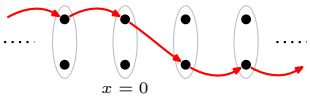
$x = 0$

Since the cells are in chiral eigenbasis, we can directly read off the change in the symmetry indices. Being block-diagonal and purely off-diagonal inside each block, we trivially had $\mathrm{si}_\pm(U) = 0$ before inserting the σ_x-coin. After the perturbation on the other hand, we get $\mathrm{si}_\pm(\widetilde{U}) = \pm 1$. Hence, the perturbation is non-gentle by Proposition 3.2.8. By Corollary 5.2.11, however, there still exists a half-step walk $\widetilde{F}$ for $\widetilde{U}$, which must be a non-compact perturbation of F by Corollary 5.6.2. In fact, the non-gentle perturbation on the level of U will turn out to originate from the joining of two topologically different bulks on the level of F.

A possible half-step operator for $\widetilde{U}$ is

$$\widetilde{F} = R(-\pi/2)\widetilde{S}_\uparrow R(\pi/4), \qquad \text{with} \qquad \widetilde{S}_\uparrow = (P_{\leq 0} + P_{>0}\sigma_x)\, S_\uparrow\, (P_{\leq 0} + P_{>0}\sigma_x)\,, \quad (5.113)$$

i.e. $\widetilde{F}$ originates from F, by effectively replacing the shift $S_\uparrow$ by $S_\downarrow^*$ on the right half of the chain:

$S_\uparrow \equiv$  $\mapsto$ $\widetilde{S}_\uparrow \equiv$  (5.114)

Clearly, $\widetilde{F}$ is a non-compact perturbation of F. Moreover, $\widetilde{F}$ is the crossover between the two bulks

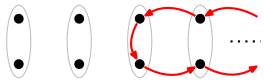
$$F_L = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ -S & S \end{pmatrix} \qquad \text{and} \qquad F_R = \frac{1}{\sqrt{2}} \begin{pmatrix} S & S \\ -\mathbb{1} & \mathbb{1} \end{pmatrix}, \tag{5.115}$$

with indices $(0,0,0,0,-1)_L$ and $(0,0,-1,-1,0)_R$. Inserting these index values into (5.110) *and* (5.111) *we get $\mathrm{si}_\pm(\widetilde{U}) = \pm 1$, confirming the observations above.*

The example demonstrates a non-gentle compact perturbation, which stems from a bulk-boundary scenario on the level of F. This raises the question of whether all non-gentle perturbations of chiral quantum walks U are just bulk-boundary settings of the underlying protocol in disguise. We answer this question in the affirmative, at least to some extend: It turns out that up to a gentle compact perturbation on the walk level, every non-gentle perturbation can be realized via a crossover between topologically different half-step operators F_L and F_R. Alternatively, phrased more casually, a compact perturbation's "non-gentleness" can always be realized via a bulk-boundary scenario of half-step walks.

Corollary 5.6.4. *Any non-gentle compact perturbation of an essentially gapped chiral walk U is a gentle compact perturbation of a crossover between two topologically different half-step walks F_L and F_R for U.*

Proof. Let U be some chiral walk with half-step operator F and $\widehat{U}$ a compact non-gentle perturbation of U with $\mathrm{si}(\widehat{U} : U) = \mathrm{si}_-(\widehat{U}) - \mathrm{si}_-(U) = n$ (see Proposition 3.2.8). Moreover similarly to the example above, we denote by $S_\uparrow$ the partial shift up. Note that in general we have $\dim \mathcal{H}_x \neq 2$, but we can simply chose a basis vector in the Γ_+ subspace in each cell and shift it to the right. We again construct $\widetilde{S}_\uparrow$ similarly to the example above, with a generalized σ_x, swapping the full $\Gamma_\pm$ eigenspaces in each cell whenever $\dim \mathcal{H}_x > 2$. Let $V = S_\uparrow^* \widetilde{S}_\uparrow$, which, expressed in the same pictorial way as in the example above, acts as

$V \equiv$  (5.116)

and set

$$\widetilde{F} = V^n F. \tag{5.117}$$

Then $\widetilde{F}$ is a crossover between $F_L = F$ and $F_R = \left(\begin{smallmatrix} S^* & 0 \\ 0 & S \end{smallmatrix}\right) F$. By Lemma 5.2.12 F_L and F_R result in the same walk U but they are clearly in different topological classes of half-step walks. In particular we get $\vec{\mathrm{ind}}\,(A_R) = \vec{\mathrm{ind}}\,(A_L) + n$, $\vec{\mathrm{ind}}\,(B_R) = \vec{\mathrm{ind}}\,(B_L) + n$, and $\vec{\mathrm{ind}}\,(C_R) = \vec{\mathrm{ind}}\,(C_L) - n$, while $\mathrm{ind}\,(A_R) = \mathrm{ind}\,(A_L)$ and $\mathrm{ind}\,(B_R) = \mathrm{ind}\,(B_L)$.

The corresponding walk $\widetilde{U} = \gamma \widetilde{F}^* \gamma \widetilde{F}$ is a compact perturbation of U, with

$$\mathrm{si}_-(\widetilde{U}) = \mathrm{ind}\,(\widetilde{A}) = \mathrm{ind}\,(A) + n = \mathrm{si}_-(U) + n = \mathrm{si}_-(\widehat{U}). \tag{5.118}$$

Hence, by Theorem 3.2.6 and Proposition 3.2.8, $\widehat{U}$ is a gentle compact perturbation of the crossover $\widetilde{U}$. □

5.6.2 Finite systems

Corollary 5.6.2 has an important consequence on perturbations of half-step walks on finite systems. In finite systems there exist chiral walks, which are not driven by a half-step operator F: given any finite F with timeframes U and U', let $\widetilde{U}$ be a non-gentle perturbation of U. Then for any half-step operator $\widetilde{F}$ of $\widetilde{U}$, $F - \widetilde{F}$ would have to be non-compact, which is not possible on a finite-dimensional Hilbert space. So what are the conditions for a half-step operator to exist for a given chiral unitary U on a finite system?

We begin by considering general chiral unitaries without taking a possible spatial structure or locality assumption into account.

Lemma 5.6.5. *Let U be a chiral unitary on a finite-dimensional Hilbert space with a balanced representation of the chiral symmetry*[8]*. Then there exists a half-step operator F, such that $U = \gamma F^* \gamma F$ if and only if*

$$\mathrm{si}_-(U) = 0. \tag{5.119}$$

Proof. For the only if part, it suffices to find an example unitary U_0 with half-step operator F_0, such that $\mathrm{si}_-(U_0) = 0$. Then, by the arguments above, every other U exhibiting a half-step operator F has to be a gentle perturbation of U_0, i.e. by Proposition 3.2.8 we get $\mathrm{si}_-(U) = \mathrm{si}_-(U_0) = 0$. This U_0 is easily found by choosing

$$F_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ \mathbb{1} & -\mathbb{1} \end{pmatrix} \tag{5.120}$$

as in the proof of Lemma 5.3.5, yielding $U_0 = i\sigma_y \otimes \mathbb{1}$. This is exactly gapped, wherefore we get $\mathrm{si}_-(U_0) = 0$.

For the converse, let U be chiral symmetric with $\mathrm{si}(U) = \mathrm{si}_+(U) = \mathrm{si}_-(U) = 0$. We can then use the same construction as in the proof of Theorem 5.2.9, and set

$$F = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}_+ \oplus \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}_- \oplus \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{\mathbb{1}+\alpha} & V_\beta \sqrt{\mathbb{1}-\delta} \\ -V_\beta^* \sqrt{\mathbb{1}-\alpha} & \sqrt{\mathbb{1}+\delta} \end{pmatrix}_{\mathcal{K}}, \tag{5.121}$$

where the splitting $F = F_+ \oplus F_- \oplus F_{\mathcal{K}}$ is again with respect to $\mathcal{H}_\pm$ and their complement $\mathcal{K}$ and α, β, δ refer to the matrix elements of U restricted to $\mathcal{K}$. □

Taking also a second timeframe U' into account, it is clear that the index condition $\mathrm{si}_\pm(U) = \pm\,\mathrm{si}_\pm(U)$ in Theorem 5.2.9 becomes void for $\mathrm{si}_\pm(U) = \mathrm{si}_\pm(U') = 0$. Moreover, the trivial indices also simplify the extra condition on the unitary equivalence operator there:

Corollary 5.6.6. *Let U and U' be two chiral walks with $\mathrm{si}_-(U) = \mathrm{si}_-(U') = 0$ on a finite-dimensional Hilbert space with a balanced representation of the chiral symmetry. Then there exists a half-step unitary F with U and U' as its timeframes if and only if there exists a unitary V, such that*

$$U' = VUV^* \qquad \text{and} \qquad V\gamma = \gamma V. \tag{5.122}$$

[8] Note that the purpose of assuming a balanced representation, i.e. $\mathrm{tr}\,\gamma = 0$, is to guarantee a trivial reference for the symmetry index (see Assumption 3.1.1 and the discussion thereafter). Any non-trivial value for $\mathrm{tr}\,\gamma$ would just shift this reference, and the condition for an F to exist would change to $\mathrm{si}_-(U) = \mathrm{tr}\,\gamma$.

Proof. By $\operatorname{tr}\gamma_\pm = \operatorname{tr}\gamma'_\pm = 0$[9] on the real eigenspaces of U and U', we get $\gamma_\pm \equiv \gamma'_\pm$[10]. We again use the construction from the proof of Theorem 5.2.9, but instead of the V there, we are free to replace the mapping $V_\pm$ from $\mathcal{H}_\pm$ onto $\mathcal{H}'_\pm$ by any unitary blocks without changing the relation between U and U', which are equal to $\pm\mathbb{1}$ on these spaces. In particular we can chose $V_\pm = \mathbb{1}_2 \otimes \widetilde{V}_\pm$. With these we get $V\gamma_\pm = \gamma'_\pm V_\pm$ and together with the relation (5.42) this condition indeed becomes $V\gamma = \gamma V$.

On the other hand, given any γ-commuting unitary equivalence operator V for U and U', we can set $F = VF_U$, with F_U as in (5.121). This gives

$$\gamma F^*\gamma F = \gamma F_U^* V^*\gamma V F_U = \gamma F_U^*\gamma F_U = U \tag{5.123}$$

and

$$F\gamma F^*\gamma = VF_U\gamma F_U^*\gamma V^* = VUV^* = U'. \tag{5.124}$$

In the second relation, we used $\gamma F_U^*\gamma = F_U(\mathbb{1} - 2P_-)$ and $F_U^2 = U(\mathbb{1} - 2P_-)$, which are both straightforward consequences of the definition of F_U (keeping in mind that the right summand of F_U is a chiral symmetric square root of $U_\mathcal{K}$, as we discussed in the proof of Theorem 5.2.9). □

The absence of **globally** non-gentle perturbations of the timeframes does not exclude **locally** non-gentle perturbations. That is, globally gentle perturbations of a finite system consisting of multiple localized perturbations on separate regions cancelling each other out. So let us, once again, assume a local structure, which we can do in two ways: The most obvious is just a finite piece of chain, which might emerge from an infinite system by decoupling at two positions and cutting out the middle piece. On the other hand, we can think of a system on a ring. While this might seem unnatural initially, especially in the limit of many cells, it shares more properties with the infinite system than the chain. In particular, it is possible to have a non-trivial flow index on the ring (although not defined via a Fredholm index) whereas this is not possible on the finite chain. Moreover, we can always assume a chain to be part of a ring system with a finite perturbation, decoupling it at some position.

Things change significantly compared to the infinite system when it comes to the locality assumption on the unitary operators themselves. Essential locality and band dominatedness are not useful for finite systems: On a finite-dimensional Hilbert space any operator is compact, such that also every operator is essentially local. Moreover, any operator is banded. Therefore we assume strict locality in this setting, with an interaction that is small compared to the system size.

We can still define a flow index according to Definition 3.3.12, but the summation has to be stopped at some point larger than the localization length. Otherwise, the contributions from the left side would interfere with those of the right-hand side. However, for strictly local unitaries, the flow index is a locally computable invariant [GNVW12], and therefore, it makes sense to consider only a finite piece for the calculation. Any chain-like system, on the other hand, can be considered as a decoupled ring or middle

[9] Abbreviating $\gamma_\pm = \gamma|_{\mathcal{H}_\pm}$ and $\gamma'_\pm = \gamma|_{\mathcal{H}'_\pm}$.

[10] Note that these still act with respect to different subspaces $\mathcal{H}_\pm$, resp. $\mathcal{H}'_\pm$ of $\mathcal{H}$.

piece of a twice decoupled infinite system. Hence, the flow index can only be trivial (see Theorem 3.3.19).

Denote by N the number of cells in a ring system. Similar to infinite systems, a shift (with respect to the shift register spanned by φ_x) is then defined via

$$S\varphi_x = \varphi_{x+1 \bmod N}, \tag{5.125}$$

where incrementing the subscript is taken modulo N to close the ring between the N'th and the first cell. As discussed above, we can then locally compute its index, which evaluates to $\overrightarrow{\mathrm{ind}}\,(S) = -1$. Coin operations act in each cell separately anyhow, such that no further adjustments are needed.

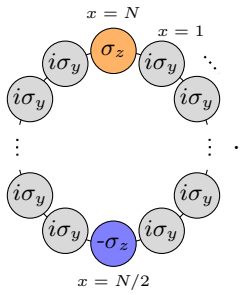
Let us resume Example 5.6.3 and wrap it onto a ring in order to construct an example for two locally non-gentle perturbations on the ring.

Example 5.6.7. *In the scenario of Example 5.6.3 we identify N and 0 in order to wrap the system onto a ring of N cells. This way, the non-gently perturbed walk $\widetilde{U}$ equals σ_z at $x = N$. By Lemma 5.6.5 there exists no F for $\widetilde{U}$. However, let us reverse the line of argument of the infinite example and start with an $\widetilde{F}$ composed of two different bulks, both of which produce the same U when they are considered individually. Let*

$$\widetilde{S}_\uparrow = \left((\mathbb{1} \otimes \sigma_x)P_{\leq N/2} + P_{>N}\right) S_\uparrow \left((\mathbb{1} \otimes \sigma_x)P_{\leq N/2} + P_{>N}\right), \tag{5.126}$$

which, again, effectively changes the shift from $S_\uparrow$ to $S_\downarrow^*$ one half of the system. On a ring, however, this produces two crossovers, one between $x = N$ and $x = 1$ and the other between $x = N/2 - 1$ and $x = N/2$. In addition to the perturbation at $x = N$, this introduces another "opposite" non-gentle perturbation, changing U from $i\sigma_y$ to $-\sigma_z$ (instead of σ_z) at $x = N/2$. We get

$$\widetilde{U} = \left[\bigoplus_{x=1}^{N/2-1} (i\sigma_y)^x\right] \oplus (-\sigma_z)^{N/2} \oplus \left[\bigoplus_{x=N/2+1}^{N} (i\sigma_y)^x\right] \oplus (\sigma_z)^N \equiv$$



(5.127)

We can again read off the indices, which evaluate to $\mathrm{si}_\pm(\widetilde{U}) = 0$. Thereby, the perturbation at $x = n$ provides the same contribution to $\mathrm{si}_\pm$ as in the previous example, namely ± 1, but the perturbation on the other end of the ring cancels this out via contributing ∓ 1. This can also be evaluated via (5.110) and (5.111) with swapped bulks F_L and F_R compared to Example 5.6.3.

The discussion and example above demonstrate that finite systems on a ring provide a well suited model to simulate the effects of infinite one-dimensional quantum walk protocols with chiral symmetry. On the one hand, they exhibit non-trivial information flow indices. On the other, while a single non-gentle perturbation of protocols always stems from a bulk-edge scenario needing two semi-infinite half-chains, the above demonstrated concept of two opposite non-gentle perturbations allows to simulate a single non-gentle perturbation on one side of the ring, by simply "forgetting" about the other side.

Conclusion and outlook

In this thesis, we provided a topological classification of one-dimensional quantum walks with discrete symmetries. Thereby, we approached the topic from different perspectives and emphasised their respective influence on the classification.

We began with a detailed analysis of the possible types of symmetries. Assuming an arbitrary group of involutive symmetries with continuous action on unitary operators, we tackled the question of which non-trivial types of symmetries exist for a topological classification of unitary operators on discrete spatial structures. We developed a reduction procedure to identify the non-trivial differences in arbitrarily large but finite symmetry groups. Thereby, we identified 38 fundamentally different classes. These 38 classes contain and generalise the well-known tenfold way for self-adjoint operators to the setting of unitary operators, i.e. quantum walks. Aiming for a topological classification of operators with symmetry protected topological eigenspaces, we defined an equivalence relation for finite-dimensional representations of these 38 symmetry types. We showed that the resulting equivalence classes equipped with the direct sum between representations naturally form a group: the index group. We concluded the first chapter with the computation of these groups for all non-trivial symmetry types.

Turning our attention to the actual topological classification of quantum walks, we took the first perspective and considered quantum walks as single time-step unitaries. Using the index groups, we defined homotopy invariants for unitaries on discrete spatial structures that are essentially gapped at the symmetry invariant parts of the spectrum, the so-called symmetry indices. Using these, we provided a complete classification of compact symmetric perturbations of admissible unitary operators. This classification is independent of the underlying spatial structure and therefore applies to any lattice dimension or any graph with uniformly bounded local cell dimensions that carry a balanced symmetry representation. We thereby generalised our corresponding result from [CGG$^+$18], which originally only applied to the symmetry types of the tenfold way, to all 38 symmetry types.

Taking the structure of a one-dimensional lattice into account, while putting the symmetries to the side for a moment, we added a locality condition to the set of assumptions and detailed a well-known invariant for one-dimensional quantum walks: the information flow index. This index already provides a complete classification of unitaries on the line with finite maximal jump-length. We generalised the locality condition arriving at essential locality, which became the standing assumption for the rest of the thesis. Observing that the information flow index can be expressed as the Fredholm index of the half-space operator, that is, the operator projected to one half of the lattice,

we generalised it to the setting of essentially local unitaries on the one-dimensional lattice. Moreover, we showed that also in this merely essentially local setting, this so-called "right Fredholm index" is complete and, in particular, distinguishes between processes that are driven continuously in time and the purely discrete setting, in the sense that an essentially local unitary admits a continuous driving by an essentially local Hamiltonian if and only if its right Fredholm index is trivial.

An essential technique in proving the completeness of the information flow index and the right Fredholm index in their respective scenarios was the gentle decoupling construction, which splits an (essentially) local unitary into two separate unitaries on the two halves of a one-dimensional system via a gentle and compact perturbation. Taking the symmetries into account again, we continued investigating the existence of such gentle decouplings under the presence of symmetries. This led to the definition of the left and right symmetry indices associated with the two halves of a one-dimensional symmetric quantum walk. These indices add up to the general symmetry index from before, are robust with respect to local perturbations, and therefore, depend only on the semi-infinite halves of the system and not on how the crossover between the two halves is engineered. This way, they serve as the second ingredient for the so-called bulk-boundary correspondence, connecting the properties of the two bulks of a one-dimensional system with the finite-dimensional eigenspaces associated with the boundary between these bulks. For the symmetry types of the tenfold way, the left and right symmetry indices are proper homotopy invariants even for merely essentially unitary essentially local operators on the line. We sketched the proof for the completeness of a subset of three symmetry indices of quantum walks that are admissible for a symmetry type of the tenfold way. In general, i.e. beyond the tenfold way, we could not lift the left and right symmetry indices to similarly robust invariants. However, we provided a partial classification and demonstrated that for some cases it is possible to infer part of the strong invariance properties via tenfold way subtypes of the respective symmetry types. We discussed this based on three different examples and thereby touched upon the problems to tackle beyond the tenfold way.

Our second perspective for the topological classification of quantum walks was that of driven processes. These are either continuously driven (Floquet) systems or discrete protocols. We first affirmatively answered the long-standing question of whether every quantum walk with finite jump length on a one-dimensional lattice with finite-dimensional local cells can be factorised into shift and coin operations with respect to the given cell structure. We then analysed such protocols in the presence of chiral symmetry. For these, we provided a complete classification in terms of five Fredholm type integer-valued indices depending on the half-step operator.

Moreover, we investigated the conditions for a half-step operator for a chiral symmetric quantum walk or a pair of chiral symmetric timeframes to exist in the first place. Precisely pinning down the differences in the topological classification of different underlying concepts of a quantum walk, we resolved an apparent contradiction between our topological classification of single time-step quantum walks and other ansatzes in the literature. We closed the chapter with a discussion on the implications of the theory for the infinite one-dimensional lattice to finite systems. There, we found that the existence of a half-step operator is more restricted in finite systems. In particular, no quan-

tum walk on a finite-dimensional system with a non-gentle perturbation can be realised via a chiral symmetric protocol. However, opposite pairs of non-gentle perturbations turned out to be possible, which restores the feasibility of studying such phenomena on finite-dimensional systems, e.g. via simulation, by only paying attention to a part of the system.

Outlook

For any thesis, one has to find an end at some point, and this always comes with the slightly unsatisfactory feeling of leaving open ends behind and untrodden paths in front. Hence, let us finally comment on a collection of topics we did not discuss and, in particular, possible further directions of research.

Complete classification of band dominated unitaries
A point we only briefly touched upon in Section 3.3 are band dominated operators. While the right Fredholm index is a valid homotopy invariant also in this case, it is to our knowledge not known whether it is complete in that scenario, but, as already mentioned in Section 3.3 was conjectured in [KKT20a] (see the open question on page 115). Proving this would also guarantee a continuous driving to exist for every band dominated unitary on the one-dimensional lattice with vanishing right Fredholm index.

Complete classification of unitaries for the 38-fold way
The most apparent open end in Chapter 3 is the complete classification of symmetric quantum walks with an essential gap for all symmetry types of the 38 fold way. For the symmetry types of the tenfold way, we saw that the set of symmetry indices $(\mathrm{si}, \overrightarrow{\mathrm{si}}, \mathrm{si}_+)$ provides such complete classification. In that case, we could express the right symmetry index for unitary operators as a symmetry index of a corresponding Hamiltonian, which enabled us to generalise it to essentially unitary and essentially local operators, providing the necessary homotopy stability and deformation freedom for the completeness proof. Beyond the tenfold way, however, no such direct correspondence exists. To fix this gap, one has to tackle the general homotopy classification of symmetric essentially gapped and essentially unitary operators also beyond the tenfold way. Such classification might, however, well exceed the considerations in terms of symmetry indices.

Optimal shift-coin sequences for strictly local walks
We left open the question of optimising the shift-coin sequence in Chapter 4. We approached the topic out of mathematical curiosity and, therefore, only focused on proving the existence of such a sequence for every strictly local walk. However, minimising the number of factors would be an important point for algorithmic applications or experimental realisations that rely on a shift-coin sequence.

Additional symmetries for protocols
In Chapter 5 we focused on chiral symmetry exclusively when we discussed the classification of protocols. An obvious extension of the discussion would be to add additional

symmetries, e.g. like the particle-hole or time-reversal symmetry. For continuously driven two-dimensional systems, this has been addressed, e.g. in [CDFG15, CDF$^+$15]. The generic example of a quantum walk protocol that cannot be realised by a continuously driven process is the split-step walk. This model is already symmetric with respect to the particle-hole and time-reversal symmetry and the classification in terms of symmetry indices does not change when these symmetries are added, since the types AIII and BDI share the same index properties. However, on the protocol level, further subtleties might enter the classification and, in particular, the existence of a half-step operator for a given walk included a condition involving the chiral symmetry. The half-step operator is also singled out by the time-reversal symmetry, such that a classification in terms of F seems to be feasible also in that case. The decomposition with respect to the symmetry eigenbasis is, however, not possible without a unitary symmetry. Hence, a careful investigation of the influence of further symmetries is required.

Higher lattice dimensions
The complete classification of compact perturbations we provided in Section 3.2, does not assume any locality condition at all. Moreover, in every spatially finite dimension, every local perturbation is compact. Hence, our classification of compact perturbation is already valid in any lattice dimension. All our considerations beyond that are concerned with the one-dimensional lattice. Hence, a direction for generalisation that immediately comes to mind is to consider quantum walks on higher dimensional lattices. There exist a variety examples and model systems in that direction in the literature [KRBD10, Kit12, GP13, RLBL13, CDFG15, CDF$^+$15, AE15, GT18, CDQ$^+$18, SAM$^+$19, MBSO20, AM20]. However, similar to the one-dimensional case, these are often concerned with translation invariant systems, continuous-time systems, are model driven, or only consider part of the symmetries from the tenfold way.

One of the phenomena, e.g., in two-dimensional systems, is the appearance of symmetry protected edge currents along the edge between two topologically distinct phases of a two-dimensional material, similar to the quantum Hall effect. The main problem for tackling such a phenomenon with the theory presented in this thesis is that it heavily depends on the finite-dimensional symmetry protected eigenspaces. While this restriction is capable of dealing with edge states at the boundaries of one-dimensional systems, an edge current corresponds to the essential part of the spectrum, wherefore we would have to waive the essential gap assumption.

Another difficulty in directly generalising our results is to properly define the essential locality condition, which we formulate via compactness of the commutator between the walk and a half-space projection, on higher dimensional lattices. It is highly dependent on the one-dimensional structure of the lattice, namely on the fact that the edge between two halves of the system is zero-dimensional. Consider, for example, a two-dimensional lattice. Then, the edge between two halves is a one-dimensional line, and even a simple shift in the lattice direction perpendicular to this line shifts an infinite-dimensional subspace across the edge. Experimenting with different versions of half-space commutator like conditions, we so far could not develop a reasonable generalisation of essential locality in terms of commutators.

This concerns the definition of essential locality. Band-dominated operators on the

other hand do not rely on such a condition bound to one dimension. An operator (on the one-dimensional lattice) is called band dominated if it is the limit of banded operators, i.e. ones with strictly finite jump length. Although the operators are not necessarily "banded" anymore in higher dimensions, limits of finite jump-length operators make perfect sense also there. So one option would be to just stick with band dominated unitaries as the definition for quantum walks.

Another possibility would be to tackle the question of locality from a more abstract point of view, via course structures [Roe03]. It would exceed the scope of this outlook to define the concept of a coarse structure properly. Hence, we limit this discussion to only a coarse introduction and some general comments. A coarse structure on a lattice X can be thought of as a collection of neighbourhoods for allowed interactions, that is, sets $\Lambda_i \subset X \times X$ of pairs (x, y), which decide whether the interaction term $\langle y, Ax\rangle$ of an operator A is non-zero or not. The collection of these sets has to be closed under taking subsets, taking inverses $((x, y) \mapsto (y, x), \forall(x, y) \in \Lambda))$, under composition $((x, y) \in \Lambda_1, (y, z) \in \Lambda_2 \to (x, z) \in \Lambda_3)$, and under unions. An operator is said to be controlled by the coarse structure if its non-trivial interaction terms are contained in a set Λ. Thereby, the rules guarantee that the multiplication and addition of two local operators and their adjoints and inverses are again local. In other words, the controlled operators with respect to a coarse structure form a $*$-algebra. The norm-closure of this algebra is called the uniform Roe algebra of the coarse structure.

The algebra of band dominated operators corresponds to the uniform Roe algebra of the metric coarse structure on $\mathbb{Z}$, that is, the controlled sets consist of pairs $(x, y) \in \mathbb{Z}\times\mathbb{Z}$ for which there exists an $l \in \mathbb{N}$, such that $\|x - y\| < l$. Operators controlled by this coarse structure are precisely given by the strictly local operators on the underlying lattice. This works in any lattice dimension, and hence, as mentioned above, there is no problem of generalisation to higher dimensions. Identifying the appropriate uniform Roe algebra for essentially local operators helps to generalise the concept to higher dimensions. For this, one needs yet another concept of a coarse structure: To every compactification $\overline{X}$ (with edge $\partial X = \overline{X} \setminus X$) of the underlying lattice X, there corresponds a so-called topological coarse structure [Roe03]. Roughly speaking, it consists of sets of pairs $(x_i, y_i) \in X \times X$, such that $\lim x_i = \lim y_i = \omega$, i.e. $\{x_i\}$ and $\{y_i\}$ have the same limit point $\omega \in \partial X$.

The algebra of essentially local operators on the one-dimensional lattice equals the uniform Roe algebra of the topological coarse structure corresponding to the two-point compactification of $\mathbb{Z}$ [Sch20]. That is, we distinguish the natural two directions towards infinity on $\mathbb{Z}$. For controlled operators, this means that there are only finitely many jump terms between the two half-chains for every cut point, which yields our definition of essential locality in the norm-closure of controlled operators. We propose the spherical compactifications of the underlying lattice $\mathbb{Z}^n$ (see also [Wil09]) as a reasonable generalisation so higher lattice dimensions.Note, however, that differently from the one-dimensional case, the number of directions towards infinity becomes uncountable, such that a simple $\mathbb{Z}$ valued invariant, measuring the direction of net information flow as in the one-dimensional case becomes unlikely.

Many-particle systems – quantum cellular automata
Another obvious direction for further research whenever quantum walks are under consideration is the generalisation to their many-particle analogues: Quantum cellular automata (QCAs). In the strictly local case, these are defined as automorphisms of the quasilocal algebra corresponding to the lattice system under consideration, with finite interaction length [SW04]. For these, there exists an analogue of the information flow index on the one-dimensional lattice [GNVW12]. It is a multiplicative rational number valued index and can be thought of as the ratio (instead of the difference) of the net information flow from left to right over right to left. This index is complete, i.e. there exists a strongly continuous path of automorphisms between two QCAs on the same cell structure, if and only if they share the same index. Moreover, a QCA can be decoupled similarly to walks, if and only if it has a trivial index of 1. Recently, this index has been generalised to weaker notions of locality [RWW20], which could make the index applicable as an invariant describing the edge current in two-dimensional chiral Floquet systems as described in [PFM$^+$16] (see also the discussion in [RWW20]). The question of local implementability of QCAs with trivial index was also addressed in [WW20]. Beyond that, several works on the topological classification of QCAs were published in recent years, including one-dimensional as well as higher dimensional systems with or without symmetry [Has13, CPGSV17, ŞSBC18, RHR18, HFH18, SNBV$^+$19, GSSC20, FH20, Haa21].

In two of these works, strictly local QCAs are identified with matrix product unitaries (MPUs) [CPGSV17, ŞSBC18]. In [CPGSV17], the authors also consider involutive symmetries of the MPU, which may be identified with some of the symmetries in the tenfold way, and classify the corresponding MPUs with respect to continuous deformations. These considerations are restricted to strictly local QCAs. It is an interesting question whether the considerations in [CPGSV17] can be combined with the generalisation to weaker locality conditions in [RWW20].

Another possible direction of research is investigating the possibility of decomposing QCA into fundamental building blocks like shift and coin operations, similarly to the factorisation of quantum walks. Similar to quantum walks, a QCA is locally implementable if and only if it has a trivial index [GNVW12]. This means that there exist two subdivisions of the lattice into finite collections of cells, respectively, with respect to which the QCA can be implemented by successively applying local operations in these finite blocks (compare (4.22)). A similar construction as in Chapter 4 might be possible in order to decompose these blocks into fundamental operations, respecting the individual cells given from the outset. Such decomposition could then serve as a compiling step in order to implement a desired QCA in a limited experimental setup.

A Decoupling conditions for all symmetry types (proof of Lemma 3.4.9)

Similar to the proof of Lemma 3.4.5, where we established the decoupling on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ for the symmetry types of the tenfold way, we will construct a decoupling unitary V separately for every type. The decoupling unitary V on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ has to swap the spaces $\mathcal{H}_{ij}$, and therefore must be of the form

$$V = \begin{pmatrix} & V_{10} \\ V_{10} & \end{pmatrix}, \tag{A.1}$$

where we labelled the blocks V_{ij} with the pair $\{ij\}$ of the respective target space, i.e. $V_{ij} \colon \mathcal{H}_{ji} \to \mathcal{H}_{ij}$. We guarantee that the decoupling is gentle via the condition $V^2 = -\mathbb{1}$, which implies that the -1-eigenspace is empty. Note that V has to be admissible for the perturbation type $\widetilde{\rho}$, i.e. with respect to $\widetilde{\rho}_g V \widetilde{\rho}_g^* = V^{ur_g}$, according to Lemma 3.2.3. In the following list of symmetry types we therefore already consider the perturbation type $\widetilde{\rho}$, without displaying the twiddle every time.

Similar to the proof of Lemma 3.4.5 we build appropriate bases $\{\chi_n\}$ and $\{\varphi_n\}$, with $n = 1, \ldots, d_{ij}$, for $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$, respectively, incorporating the action of the symmetries via their commutation relations. This way, we get explicit representations of the symmetry types, with respect to which we can construct admissible swapping unitaries V. The relevant dimensions are denoted by

$$d_{ij} = \dim \mathcal{H}_{ij} \qquad \text{and} \qquad d_{ij}^{\pm} = \dim \left(\ker(\sigma \mp \mathbb{1}) \cap \mathcal{H}_{ij} \right). \tag{A.2}$$

When σ is part of the symmetry type, we chose the bases to be σ-eigenbases and indicate this via $\{\chi_n^{\pm}\}$ and $\{\varphi_n^{\pm}\}$, with

$$\sigma \chi_n^{\pm} = \pm \chi_n^{\pm} \qquad \text{and} \qquad \sigma \varphi_n^{\pm} = \pm \varphi_n^{\pm}. \tag{A.3}$$

In this basis σ is of the form (3.103) and a decoupling unitary V further decomposes into blocks as in (3.104). Let us display both again here, for easier reference:

$$\sigma = \begin{pmatrix} \mathbb{1}_{d_{10}^+} & & & \\ & -\mathbb{1}_{d_{10}^-} & & \\ & & \mathbb{1}_{d_{01}^+} & \\ & & & -\mathbb{1}_{d_{01}^-} \end{pmatrix}, \qquad V = \begin{pmatrix} & & V_{10}^+ & \\ & & & V_{10}^- \\ V_{01}^+ & & & \\ & V_{01}^- & & \end{pmatrix}. \tag{A.4}$$

For each group in the following list, we display the generators in angle brackets. Note that we choose the generators such that the constructions for the present task are as simple as possible. Hence, these choices occasionally differ from those in Section 2.3.1, where we computed the index groups for the (non-perturbation) symmetry types. The different symmetry types are then indicated via their distinguishing properties. That is, the value of the commutation character $c_{gh}\colon (g,h) \mapsto \pm 1$ on the generators, and the square of the antiunitary generator.

Group and type 1 (A), $\langle \mathbb{1} \rangle$**:** Decoupling condition: None.
This is the trivial group with only the trivial symmetry type. The existence of a decoupling is guaranteed by the gap condition (see Theorem 3.3.19 and Lemma 3.4.1).

Group and type 2, $\langle \sigma \rangle$**:** Decoupling condition: $d_{10}^{\pm} = d_{01}^{\pm}$.
We already established the condition for symmetry type 2 in Section 3.4.3.

Group and type 3 (AIII), $\langle \gamma \rangle$**:** Decoupling condition: None.
This group is part of the tenfold way. There always exists a decoupling (see Lemma 3.4.5).

Group 4, $\langle \tau \rangle$**:** The two types 4 (AI, $\tau^2 = \mathbb{1}$) and 5 (AII, $\tau^2 = -\mathbb{1}$) of this group belong to the tenfold way. For AI there always exists a decoupling and for AII we need to assume $d_{10} = 0 \bmod 2$ (see Lemma 3.4.5).

Group 5, $\langle \sigma_\tau \rangle$**:** The two types 6 and 7 of this group are equivalent to the types of group 4 (AI and AII), due to the action of the perturbation symmetry type we consider here (see Lemma 3.2.3). Hence, no condition is needed for symmetry type 6, whereas we need to assume $d_{10} = 0 \bmod 2$ for symmetry type 7.

Group 6, $\langle \eta \rangle$**:** The two types 8 (D, $\eta^2 = \mathbb{1}$) and 9 (C, $\eta^2 = -\mathbb{1}$) for this group belong to the tenfold way and there always exists a decoupling (see Lemma 3.4.5).

Group 7, $\langle \sigma, \gamma \rangle$**:**

Type 10, $c_{\sigma\gamma} = 1$**:** Decoupling condition: None.
Because γ is a σ-commuting unitary that swaps the $\mathcal{H}_{ij}$, the extra condition $d_{10}^{\pm} = d_{01}^{\pm}$ is automatically fulfilled. Choosing a basis with σ as in (A.4) and $\gamma = \sigma_x \otimes \mathbb{1}_{d_{10}}$ we find $V = i\sigma_y \otimes \mathbb{1}_{d_{10}}$, which is admissible and fulfils $V^2 = -\mathbb{1}$.

Type 11, $c_{\sigma\gamma} = -1$**:** Decoupling condition: $d_{10}^{\pm} = d_{01}^{\pm}$.
For this type γ anti-commutes with σ, such that the necessary condition $d_{10}^{\pm} = d_{01}^{\pm}$ is not automatically fulfilled. Assuming it, on the other hand, is sufficient: Let $\{\chi_n^{\pm}\}$ be a σ-eigenbasis for $\mathcal{H}_{10}$. Since γ swaps the $\mathcal{H}_{ij}$, we can define a basis $\{\varphi_n^{\pm}\}$ of $\mathcal{H}_{01}$ via $\varphi_n^{\pm} = \gamma\chi_n^{\mp}$. By $c_{\gamma\sigma} = -1$ it follows that $\sigma\varphi_n^{\pm} = \pm\varphi_n^{\pm}$, i.e. in this basis σ is again of the form (A.4). We find the same admissible $V = i\sigma_y \otimes \mathbb{1}_{d_{10}}$ as for type 10.

Group 8, $\langle\sigma,\tau\rangle$:

Type 12, $(c_{\sigma\tau},\tau^2)=(1,\mathbb{1})$: Decoupling condition: None.
Let $\{\chi_n^\pm\}$ and $\{\varphi_k^\pm\}$ be σ-eigenbases for $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$, respectively. Since σ and τ commute and τ swaps the spaces $\mathcal{H}_{ij}$ with $\tau^2=\mathbb{1}$, these can be chosen such that $\tau\chi_n^\pm=\varphi_n^\pm$ and $\tau\varphi_n^\pm=\chi_n^\pm$. Hence, $d_{10}^\pm=d_{01}^\pm$ is fulfilled. We can define an admissible V with $V^2=-\mathbb{1}$ via $V\chi_n^\pm=\varphi_n^\pm$ and $V\varphi_n^\pm=-\chi_n^\pm$.

Type 13, $(c_{\sigma\tau},\tau^2)=(1,-\mathbb{1})$: Decoupling condition: $d_{ij}^\pm=0 \bmod 2$.
As before, we have $d_{10}^\pm=d_{01}^\pm$, because τ leaves invariant the σ-eigenspaces but swaps the spaces $\mathcal{H}_{ij}$. In the basis introduced in type 12, τ acts as $\tau\chi_n^\pm=\varphi_n^\pm$ and $\tau\varphi_n^\pm=-\chi_n^\pm$. Now, since any V is of the form (A.4), the admissibility condition for τ forces each of the four blocks V_{ij} of V to fulfil $V_{ij}=-V_{ij}^T$ (compare type 5 (AII) of the tenfold way). This means that the eigenspaces of σ, restricted to the individual $\mathcal{H}_{ij}$ have to be even or, equivalently, a multiple of four on the whole space (since they are equally distributed between $\mathcal{H}_{10}$ and $\mathcal{H}_{01}$). Assuming this condition to be met, we can define $V\chi_{2k-1}^\pm=\varphi_{2k}^\pm$, $V\chi_{2k}^\pm=-\varphi_{2k-1}^\pm$, $V\varphi_{2k-1}^\pm=\chi_{2k}^\pm$ and $V\varphi_{2k}^\pm=-\chi_{2k-1}^\pm$, which fulfils the requirements for a gentle decoupling.

Type 14, $(c_{\sigma\tau},\tau^2)=(-1,\mathbb{1})$: Decoupling condition: $d_{10}^\pm=d_{01}^\pm$.
We need to assume the condition from type 2, since there is no $\mathcal{H}_{ij}$-swapping symmetry that leaves invariant the σ-eigenspaces. Assuming $d_{10}^\pm=d_{01}^\pm=d^\pm$, we also get $d^+=d^-$, because τ swaps the eigenspaces of σ. In the basis chosen above τ acts as $\tau\chi_n^\pm=\varphi_n^\mp$ and $\tau\varphi_n^\pm=\chi_n^\mp$. V can then again be chosen as for type 12.

Type 15, $(c_{\sigma\tau},\tau^2)=(-1,-\mathbb{1})$: Decoupling condition: $d_{10}^\pm=d_{01}^\pm$.
This type can be treated exactly as type 14, replacing τ by σ_τ, which acts on V and $\mathcal{H}_{ij}$ in the same way.

Group 9, $\langle\sigma,\eta\rangle$: Both, σ and η leave $\mathcal{H}_{ij}$ invariant. Hence, $d_{10}^\pm=d_{01}^\pm$ is a necessary condition for all types of this group. Moreover, it is also sufficient in all cases. For all cases we construct a σ-eigenbasis according to the action of η, respectively.

Type 16, $(c_{\sigma\eta},\eta^2)=(1,\mathbb{1})$: Decoupling condition: $d_{10}^\pm=d_{01}^\pm$.
η leaves invariant the eigenspaces of σ. Hence, we can choose η to be just the complex conjugation with respect to the σ-eigenbasis. Assuming $d_{10}^\pm=d_{01}^\pm$, we can define $V=i\sigma_y\otimes\mathbb{1}_{d^++d^-}$ as before.

Type 17, $(c_{\sigma\eta},\eta^2)=(1,-\mathbb{1})$: Decoupling condition: $d_{10}^\pm=d_{01}^\pm$.
This time, $\eta^2=-\mathbb{1}$ further forces $d_{ij}^\pm$ to be even. We can choose the bases such that $\eta\zeta_{2k-1}^\pm=-\zeta_{2k}^\pm$ and $\eta\zeta_{2k}^\pm=\zeta_{2k-1}^\pm$, for $\zeta\in\{\chi,\varphi\}$. We again get the admissible $V=i\sigma_y\otimes\mathbb{1}_{d_++d_-}$.

Type 18, $(c_{\sigma\eta},\eta^2)=(-1,\mathbb{1})$: Decoupling condition: $d_{10}^\pm=d_{01}^\pm$.
By $c_{\sigma\eta}$, we get $d^+=d^-$ and we can choose the basis such that $\eta\zeta_n^\pm=\eta\zeta_n^\mp$ for $\zeta\in\{\chi,\varphi\}$. Once again we can choose $V=i\sigma_y\otimes\mathbb{1}_{d_++d_-}$.

Type 19, $(c_{\sigma\eta}, \eta^2) = (-1, -\mathbb{1})$**:** Decoupling condition: $d_{10}^{\pm} = d_{01}^{\pm}$.
Similar to the equivalence between the types 14 and 15, the considerations for type 19 are equivalent those to type 18, after replacing η by σ_η

Group10, $\langle \gamma, \eta \rangle$**:** This group exhibits the symmetry types $20-23$ (BDI, CII, CI and DIII), which are part of the tenfold way (see Lemma 3.4.5).

Group 11, $\langle \gamma, \sigma_\tau \rangle$**:** This group exhibits the symmetry types $24 - 27$. Due to the action of the perturbation symmetry type (see Lemma 3.2.3), these are equivalent to the four types of the tenfold way (in the same order). However, the symmetry type 27 is special:

Type 27, $(c_{\gamma\sigma_\tau}, \sigma_\tau) = (-1, -\mathbb{1})$**:** Decoupling condition: $d_{10} = 0 \bmod 2$.
This symmetry type is equivalent to DIII, but we need to assume $\dim \mathcal{H}_{10} = 0 \bmod 2$. For type DIII this follows from the fact that the representation on $\mathcal{H}_{10} \oplus \mathcal{H}_{01}$ is balanced, which is equivalent to the overall dimension being a multiple of four and hence, $\dim \mathcal{H}_{10} = 0 \bmod 2$. This is not necessarily true for the symemtry types beyond the tenfold way (see Lemma 3.4.4). Hence, we cannot use this argument here but have to assume the condition instead.

Group 12, $\langle \sigma, \gamma, \eta \rangle$**:** For the following 8 types, the condition $d_{10}^{\pm} = d_{01}^{\pm}$ is always guaranteed by γ, since σ and γ commute in these cases. Hence, we write $d^{\pm} := d_{10}^{\pm} = d_{01}^{\pm}$.

Type 28, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, 1, 1, \mathbb{1})$**:** Decoupling condition: None.
We can consider this type as type 10 with an additional symmetry $\eta = K$ acting as the complex conjugation. Since the construction for type 10 was real-valued, nothing changes by adding η.

Type 29, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, 1, 1, -\mathbb{1})$**:** Decoupling condition: None.
Again, we consider this type as type 10 and add η, which squares to $-\mathbb{1}$. Since the representation is still abelian, η leaves invariant all eigenspaces and also the $\mathcal{H}_{ij}$. Therefore, the dimension of each space is doubled, and η is given by $\eta = \mathbb{1}_{d^+ + d^-} \otimes i\sigma_y$. This does not interfere with V from type 10, making it an appropriate choice also in this case.

Type 30, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, 1, -1, -\mathbb{1})$**:** Decoupling condition: None.
Because η commutes with σ and fulfils $\eta^2 = -\mathbb{1}$, d^+ and d^- are even. Hence, we can choose a σ-eigenbasis, such that $\eta\chi_{2k-1}^{\pm} = -\chi_{2k}^{\pm}$ and $\eta\chi_{2k}^{\pm} = \chi_{2k-1}^{\pm}$. We then extend this basis to $\mathcal{H}_{01}$ via $\varphi_n^{\pm} = \gamma\chi_n^{\pm}$ (and vice versa via $\gamma^2 = \mathbb{1}$), which is again a σ-eigenbasis with $\eta\varphi_{2k-1}^{\pm} = \varphi_{2k}^{\pm}$ and $\eta\varphi_{2k}^{\pm} = -\varphi_{2k-1}^{\pm}$ due to the commutation relations between the symmetries. With respect to these bases we define V via $V\chi_n^{\pm} = (-1)^n\varphi_n^{\pm}$ and $V\varphi_n^{\pm} = (-1)^{n-1}\chi_n^{\pm}$ for a suitable decoupling.

Type 31, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, 1, -1, \mathbb{1})$**:** Decoupling condition: $d_{ij}^{\pm} = 0 \bmod 2$.
We can choose an η-invariant σ-eigenbasis for $\mathcal{H}_{10}$ and extend it to $\mathcal{H}_{01}$ via γ. Because of $c_{\gamma\eta} = -1$, η then acts as $-K$ on $\mathcal{H}_{01}$. That is, we get $\gamma = \sigma_x \otimes \mathbb{1}_{d_{10}}$ and $\eta = (\sigma_z \otimes \mathbb{1}_{d_{10}})K$. The admissibility conditions now force every block V_{ij} of V (see (A.4)) to fulfil $V_{ij} = V_{ij}^*$ due to γ and $V_{ij} = -\overline{V_{ij}}$ due to η. This implies

$V_{ij} = -V_{ij}^T$, which can only be realized by a unitary in even dimensions. On the other hand, assuming $d^\pm$ to be even is sufficient. Indeed, defining the blocks V_{ij} as $V_{13} = \mathbb{1}_{d^+/2} \otimes \sigma_y$, $V_{24} = \mathbb{1}_{d^-/2} \otimes \sigma_y$ and $V_{ji} = -V_{ij}^*$, generates a suitable decoupling unitary V.

Type 32, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, -1, 1, \mathbb{1})$**:** Decoupling condition: None.
Since η swaps the σ-eigenspaces, but leaves invariant $\mathcal{H}_{ij}$ we get $d^+ = d^-$. Hence, we can choose the basis for $\mathcal{H}_{10}$ with $\eta\chi_n^\pm = \chi_n^\mp$. Extending this basis via $\varphi_n^\pm = \gamma\chi_n^\pm$ gives $\eta\varphi_n^\pm = \varphi_n^\mp$. Setting $V = i\sigma_y \otimes \mathbb{1}$ then provides a suitable decoupling unitary.

Type 33, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, -1, 1, -\mathbb{1})$**:** Decoupling condition: None.
This type is quite similar to type 32 above, with the slight adjustments $\eta\chi_n^\pm = \mp\chi_n^\mp$ and $\eta\varphi_n^\pm = \mp\varphi_n^\mp$. We can still use the same V.

Type 34, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, -1, -1, -\mathbb{1})$**:** Decoupling condition: None.
The basis for $\mathcal{H}_{10}$ can be chosen as for type 33, i.e. $\eta\chi_n^\pm = \mp\chi_n^\mp$. The action on $\varphi_n^\pm$ is then determined by $c_{\gamma\eta} = -1$, i.e. $\eta\varphi_n^\pm = \pm\varphi_n^\pm$. This gives $\sigma = \mathbb{1}_2 \otimes \sigma_z \otimes \mathbb{1}_d$ with $d^\pm = d$, $\gamma = \sigma_x \otimes \mathbb{1}_{2d}$ and $\eta = (\sigma_z \otimes i\sigma_y \otimes \mathbb{1}_d)K$. A decoupling is then given by $V = i\sigma_y \otimes \sigma_z \otimes \mathbb{1}_d$.

Type 35, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (1, -1, -1, \mathbb{1})$**:** Decoupling condition: None.
Type 35 relates to 34 as 32 does to 33. Everything stays the same, except η, for which we get $\eta\chi_n^\pm = \chi_n^\mp$ and the same for $\varphi_n^\pm$. That is, $\eta = (\sigma_z \otimes \sigma_x \otimes \mathbb{1}_d)K$, admitting the same V as for 34.

For the remaining eight types, γ swaps the σ-eigenspaces, which gives $d_{10}^\pm = d_{01}^\mp$ instead of the necessary condition $d_{10}^\pm = d_{01}^\pm$. In the following four cases, however, $d_{10}^\pm = d_{01}^\pm$ is fulfilled due to τ, which is swaps the $\mathcal{H}_{ij}$ and commutes with σ. Hence, we have $d_{ij}^\pm = d$. We can therefore fix σ and γ and adjust only η and d to match the conditions of the type. Hence, in all following cases we chose a σ-eigenbasis, such that $\varphi_{10}^\pm = \gamma\chi_{10}^\mp$ and vice versa. Assuming the necessary condition $d_{10}^\pm = d_{01}^\pm = d$ for the types 40-43, we always get

$$\sigma = \mathbb{1}_2 \otimes \sigma_z \otimes \mathbb{1}_d \qquad \text{and} \qquad \gamma = \sigma_x \otimes \sigma_x \otimes \mathbb{1}_d. \tag{A.5}$$

Type 36, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, -1, 1, \mathbb{1})$**:** Decoupling condition: None.
We can choose the basis, such that $\eta\chi_n^\pm = \chi_n^\mp$ and $\varphi_n^\pm = \gamma\chi_n^\mp$, which, by $c_{\gamma\eta} = 1$, induces $\eta\varphi_n^\pm = \varphi_n^\mp$. This gives $\eta = (\mathbb{1}_2 \otimes \sigma_x \otimes \mathbb{1}_d)K$ and we find the admissible $V = i\sigma_y \otimes \mathbb{1}_{2d}$.

Type 37, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, -1, 1, -\mathbb{1})$**:** Decoupling condition: $d_{ij}^\pm = 0 \bmod 2$.
The only difference to type 36 is $\eta^2 = -\mathbb{1}$. Taking this into account during the basis construction, we set $\eta\chi_n^\pm = \pm\chi_n^\mp$ and $\eta\varphi_n^\pm = \mp\varphi_n^\mp$, i.e. $\eta = (\sigma_z \otimes i\sigma_y \otimes \mathbb{1}_d)K$. Now, the $d \times d$ blocks V_{ij} of any admissible V (which must be of the form (3.104)) have to fulfil $V_{24} = V_{13}^* = -\overline{V_{13}}$ and $V_{42} = V_{31}^* = -\overline{V_{31}}$, where the first equalities are due to γ and the second due to η, respectively. This gives $V_{13} = -V_{31}^T$, which is only possible for even d. Assuming d to be even, we can define $V = \sigma_x \otimes \sigma_z \otimes (i\sigma_y \otimes \mathbb{1}_{d/2})$.

Type 38, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, -1, -1, -\mathbb{1})$**:** Decoupling condition: None.
The difference to type 37 is $c_{\gamma\eta} = -1$, which becomes visible in the action of η on $\varphi_n^\pm$. We get $\eta\chi_n^\pm = \pm\chi_n^\mp$ as before, but $\eta\varphi_n^\pm = \pm\varphi_n^\mp$. Hence, $\eta = (\mathbb{1}_2 \otimes i\sigma_y \otimes \mathbb{1}_d)K$ and, once again, $V = i\sigma_y \otimes \mathbb{1}_{2d}$ is admissible.

Type 39, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, -1, -1, \mathbb{1})$**:** Decoupling condition: $d_{ij}^\pm = 0 \bmod 2$.
By $\eta^2 = \mathbb{1}$, we can set $\eta\chi_n^\pm = \chi_n^\pm$ as for type 36. Combining this with $c_{\gamma\eta} = -1$ leads to $\eta\varphi_n^\pm = -\varphi_n^\mp$, i.e. we get $\eta = (\sigma_z \otimes \sigma_x \otimes \mathbb{1}_d)K$. Similar to type 37, this forces the blocks of $V =$ (3.104) to fulfil $V_{ij} = -V_{ij}^T$ and hence, we need $d = 0 \bmod 2$. Assuming this, on the other hand, we can use the same V as for type 37.

In the remaining types, all $\mathcal{H}_{ij}$-swapping symmetries (γ, σ_γ, τ and σ_τ) anti-commute with σ. Hence, we need to assume $d_{10}^\pm = d_{01}^\pm$ for a decoupling to exist. Doing so, we again get $d_{ij}^\pm = d$ due to γ and we can choose a basis in which σ and γ are as in (A.5). In all four cases this assumption is also sufficient:

Type 40, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, 1, 1, \mathbb{1})$**:** Decoupling condition: $d_{10}^\pm = d_{01}^\pm$.
We can choose the basis, such that $\eta\chi_n^\pm = \chi_n^\pm$ and $\eta\varphi_n^\pm = \varphi_n^\pm$. Hence, $\eta = K$ and we find the admissible unitary $V = i\sigma_y \otimes \mathbb{1}_{2d}$.

Type 41, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, 1, 1, -\mathbb{1})$**:** Decoupling condition: $d_{10}^\pm = d_{01}^\pm$.
The only difference to type 40 is $\eta^2 = -\mathbb{1}$. Hence, d is even and we get $\eta = \mathbb{1}_{2d} \otimes i\sigma_y$, which allows for the same V.

Type 42, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, 1, -1, -\mathbb{1})$**:** Decoupling condition: $d_{10}^\pm = d_{01}^\pm$.
Again, d is even due to $\eta^2 = -\mathbb{1}$. We chose the basis, such that $\eta\chi_{2k-1}^\pm = -\chi_{2k}^\pm$ and $\eta\chi_{2k}^\pm = \chi_{2k-1}^\pm$. Combining $c_{\gamma\eta} = -1$ with $\varphi_n^\pm = \gamma\chi_n^\pm$ then gives $\eta\varphi_{2k-1}^\pm = \varphi_{2k}^\pm$ and $\eta\varphi_{2k}^\pm = -\varphi_{2k-1}^\pm$, i.e. $\eta = (\sigma_z \otimes \mathbb{1}_2 \otimes (\mathbb{1}_{d/2} \otimes i\sigma_y))K$. An admissible V is then given by $V = i\sigma_y \otimes \mathbb{1}_2 \otimes (\mathbb{1}_{d/2} \otimes \sigma_z)$.

Type 43, $(c_{\sigma\gamma}, c_{\sigma\eta}, c_{\gamma\eta}, \eta^2) = (-1, 1, -1, \mathbb{1})$**:** Decoupling condition: $d_{10}^\pm = d_{01}^\pm$.
We can choose the basis $\{\chi_n^\pm\}$ η-invariant. For $\{\varphi_n^\pm\}$ this means $\eta\varphi_n^\pm = -\varphi_n^\pm$, due to $c_{\gamma\eta} = -1$ and therefore we get $\eta = (\sigma_z \otimes \mathbb{1}_{2d})K$. An admissible V is then given by $V = i\sigma_x \otimes \sigma_z \otimes \mathbb{1}_d$.

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List of Publications and Preprints

[1] 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. *Ann. Henri Poincaré*, 19(2):325–383, 2018. doi:10.1007/s00023-017-0630-x. arXiv:1611.04439.

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[8] C. Cedzich, T. Geib, and R. F. Werner. An algorithm to factorize quantum walks into shift and coin operations, 2021. arXiv:2102.12951.

Curriculum Vitae

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Academic career

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