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On some topological invariants for one-dimensional discrete-time quantum walks with chiral symmetry

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Declaration

I hereby declare that this thesis does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any university; and that to the best of my knowledge and belief it does not contain any material previously published or written by another person except where due reference is made in the text.

Yohei Tanaka

Abstract

Quantum walk theory is a quantum-mechanical counterpart of the classical random walk theory. Despite its apparent simplicity, this ubiquitous concept has found many useful applications. In general, a concrete quantum walk model is characterised by an associated unitary time-evolution operator. This differs from the usual setting of Schrödinger operators in which we are required to construct the time-evolution operator from a given unbounded hamiltonian via the spectral theorem. The major themes of this dissertation belong to the broad subject of index theory for (discrete-time) chirally symmetric quantum walks. To a chirally symmetric quantum walk model, we wish to assign a certain well-defined index satisfying the following two properties: (i) The index needs to be robust in the sense that it is stable against a wide range of perturbations; (ii) The index gives a lower bound for the number of so-called edge-states. Given (i), if the index turns out to be non-zero, then the associated time-evolution operator has at least one edge-state. This implication, known as the topological protection of edge-states, is an important feature of the bulk-edge correspondence. The present thesis consists of the following two main theorems:

Theorem A states that we can assign two indices satisfying (i), (ii) to a certain variant of Kitagawa's split-step quantum walk on the one-dimensional integer lattice. We impose the so-called asymptotically periodic assumption, the scope of which is beyond that of the existing literature on the bulk-edge correspondence for 2-phase quantum walks. As such, we take a completely new approach by making use of Toeplitz operators.

Theorem B states that we can assign a yet another index to a *non-unitary* version of the split-step model we consider in Theorem A. This index satisfies (i), but it is not known whether or not (ii) also holds true. The main difficulty of this construction lies in the non-unitary feature of the given model. It is expected that Theorem B forms a basis for future mathematical research into the bulk-edge correspondence for non-unitary quantum walks.

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Chapter I

Preface

I.1 Motivation

The major mathematical theme of this dissertation can be broadly described as index theory for *chirally symmetric bounded operators*. More specifically, we focus on an abstract bounded operator U on a Hilbert space $\mathcal{H}$, which satisfies the following algebraic condition;

$$U^* = \varGamma U \varGamma, \tag{I.1}$$

where $\varGamma$ is a unitary self-adjoint operator on $\mathcal{H}$. We repeatedly refer to (I.1) as a ***chiral symmetry condition*** throughout the present thesis. Clearly, the operator U satisfying (I.1) is unitarily equivalent to its adjoint U^*, and so the spectrum of U, denoted by $\sigma(U)$, is symmetric about the real axis. A naive description of what the present thesis tries to achieve is the following;

Aim. Let U be a bounded operator satisfying (I.1), and let λ be a fixed real number. We wish to assign a certain well-defined index to the pair $(\varGamma, U)$, say $\mathrm{ind}_\lambda(\varGamma, U)$, in such a way that the following two conditions are fulfilled:

(i) The index $\mathrm{ind}_\lambda(\varGamma, U)$ is robust in the sense that it is stable against a wide range of perturbations.

(ii) The index $\mathrm{ind}_\lambda(\varGamma, U)$ gives a lower bound for the number of non-trivial eigenstates associated with λ in the sense of $|\mathrm{ind}_\lambda(\varGamma, U)| \leq \dim\ker(U - \lambda)$. Given (i), if the index $\mathrm{ind}_\lambda(\varGamma, U)$ turns out to be non-zero, then the eigenspace $\ker(U - \lambda)$ contains at least one non-trivial eigenstate whose existence is ensured by the robustness of $\mathrm{ind}_{\lambda}(\Gamma, U)$.

We focus on index theory of this kind in the context of (discrete-time) ***quantum walks***. Quantum walk theory is a quantum-mechanical counterpart of the classical random walk theory [Gud88, ADZ93, Mey96, ABNVW01]. Despite its apparent simplicity, this ubiquitous concept has found many useful applications. On one hand, the physical utility of quantum walks is especially confirmed for quantum algorithms [Gro96, ABNVW01], photosynthesis [MRLA08, Per+10], topological phases [KRBD10, OK11, Kit12, AO13], and non-unitary Floquet systems [MKO16, MKKO20]. On the other hand, mathematically rigorous studies have also taken various points of view: localisation and weak-limit theorems [Kon02, IKK04, Kon10, Seg11, CGML12, Suz16, FFS17, FFS18, FFS19], non-linear analysis [MSSSS18b, MSSSS18a, MS19, MSSSS19], scattering-theoretic analysis [ABJ15, Suz16, RST17, RST18, Mor19, Wad19, Wad20, Tie20], quantum walks on graphs [AAKV01, Amb03, Por16], classification by unitary equivalence [Ohn16, Ohn17], and time operators [ST19a, FMSST20].

A concrete quantum walk model is characterised by an associated unitary ***time-evolution operator*** U. This differs from the usual setting of Schrödinger operators in which we are required to construct the time-evolution operator from a given unbounded hamiltonian via the spectral theorem. For concreteness, let us consider the Hilbert space $\ell^2(\mathbb{Z}, \mathbb{C}^n)$ of square-summable $\mathbb{C}^n$-valued sequences indexed by the set $\mathbb{Z}$ of integers. In the physical context, we may regard $\mathcal{H} := \ell^2(\mathbb{Z}, \mathbb{C}^n)$ as the state Hilbert space of an n-state quantum walker on the one-dimensional integer lattice $\mathbb{Z}$. If $U : \mathcal{H} \to \mathcal{H}$ is a unitary time-evolution operator and if $\Psi_0 = (\Psi_0(x))_{x\in\mathbb{Z}}$ is a normalised state vector in $\mathcal{H}$, then the time-evolution of Ψ_0 is given by

$$\Psi_t := U^t \Psi_0, \qquad t \in \mathbb{N}.$$

Given a fixed pair $(t_0, x_0) \in \mathbb{N} \times \mathbb{Z}$, the non-negative number $\|\Psi_{t_0}(x_0)\|^2_{\mathbb{C}^n}$ gives the probability of finding the quantum walker at $(t, x) = (t_0, x_0)$.

I.2 An overview of three main chapters

Apart from the current chapter, this thesis consists of three chapters in total. The main results of the present thesis can be found in three published papers [ST19b, Tan21, AFST21] or two preprints [MST21, MTW21]. Note that some passages have been quoted verbatim from the above sources.

I.2.1 Chapter II. Unitary Models

We consider index theory for chirally symmetric unitary operators in this chapter.

I.2.1.1 Introduction of Chapter II

With the canonical decomposition $\ell^2(\mathbb{Z},\mathbb{C}^2) = \ell^2(\mathbb{Z},\mathbb{C}) \oplus \ell^2(\mathbb{Z},\mathbb{C})$ in mind, we shall consider the following 2×2 block-operator matrix on $\ell^2(\mathbb{Z},\mathbb{C}^2)$ throughout this chapter;

$$U_{\mathrm{suz}} := \begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix} \begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix}, \tag{I.2}$$

where L is the bilateral left-shift operator on $\ell^2(\mathbb{Z}) := \ell^2(\mathbb{Z},\mathbb{C})$ (see §I.3 for definition), and where $p = (p(x))_{x\in\mathbb{Z}}, a = (a(x))_{x\in\mathbb{Z}}$ are two arbitrary real-valued sequences taking values in the closed interval $[-1,1]$. From this point onward, any bounded sequence indexed by $\mathbb{Z}$ shall be identified with the corresponding multiplication operator on $\ell^2(\mathbb{Z})$ throughout the present thesis. The unitary operator U_{suz} defined by (I.2) is called the time-evolution operator of ***Suzuki's (one-dimensional) split-step quantum walk*** [FFS17, FFS18, FFS19, NOW21]. Note first that this unitary operator can be naturally decomposed as the product $U_{\mathrm{suz}} = \varGamma_{\mathrm{suz}}\varGamma'_{\mathrm{suz}}$, where the two unitary self-adjoint operators $\varGamma_{\mathrm{suz}}, \varGamma'_{\mathrm{suz}}$ are defined respectively by

$$\varGamma_{\mathrm{suz}} := \begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix}, \qquad \varGamma'_{\mathrm{suz}} := \begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix}. \tag{I.3}$$

If we let $(\varGamma, U) = (\varGamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ or $(\varGamma, U) = (\varGamma'_{\mathrm{suz}}, U_{\mathrm{suz}})$, then one can easily verify that the chiral symmetry condition (I.1) holds true. This motivates us to consider (I.1) in full generality.

Let U be an arbitrary unitary operator on an abstract Hilbert space $\mathcal{H}$, and let R be the real part of U. If U satisfies the the chiral symmetry condition (I.1), then we obtain the commutation relation $\varGamma R - R\varGamma = 0$. It follows that the self-adjoint operator R admits the following diagonal representation;

$$R = \begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}_{\ker(\varGamma-1)\oplus\ker(\varGamma+1)}, \tag{I.4}$$

where the $\mathbb{Z}_2$-grading of the underlying Hilbert space $\mathcal{H} = \ker(\varGamma - 1) \oplus \ker(\varGamma + 1)$ is given by the unitary self-adjoint operator $\varGamma$. The decomposition (I.4) allows us to introduce the following formal indices:

$$\operatorname{ind}_+(\varGamma, U) := \dim\ker(R_1 - 1) - \dim\ker(R_2 - 1), \tag{I.5}$$

$$\operatorname{ind}_-(\varGamma, U) := \dim\ker(R_1 + 1) - \dim\ker(R_2 + 1). \tag{I.6}$$

It follows from a direct computation that $\ker(U \mp 1) = \ker(R_1 \mp 1) \oplus \ker(R_2 \mp 1)$ (see Lemma II.2 for details), and so the following estimate holds true;

$$|\operatorname{ind}_\pm(\varGamma, U)| \leq \dim\ker(U \mp 1). \tag{I.7}$$

We make the following two observations about (I.7):

(i) The index $\operatorname{ind}_\pm(\varGamma, U)$ is well-defined, if $\ker(U \mp 1)$ is finite-dimensional. In particular, if the essential spectrum of U, denoted by $\sigma_{\mathrm{ess}}(U)$, does not contain ± 1, then $\operatorname{ind}_\pm(\varGamma, U)$ is well-defined.

(ii) If $\operatorname{ind}_\pm(\varGamma, U)$ is non-zero, then the eigenspace $\ker(U \mp 1)$ contains some non-trivial eigenstates. This implication can be regarded as an abstract form of *chiral symmetry protection of eigenstates*.

We are now in a position to introduce the following index formula for U_{suz};

Lemma I.1. *Let* $(\varGamma, U) = (\varGamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ *be defined by* (I.2), (I.3)*, and let us assume the existence of the following limit for each* $\star = -\infty, +\infty$ *and each* $\zeta = p, a$;

$$\zeta(\star) := \lim_{x\to\star} \zeta(\star). \tag{I.8}$$

Then $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ *if and only if* $p(\star) \neq \pm a(\star)$ *for each* $\star = -\infty, +\infty$. *In this case, we have*

$$\operatorname{ind}_{\pm}(\Gamma, U) = \begin{cases} +1, & p(-\infty) \mp a(-\infty) < 0 < p(+\infty) \mp a(+\infty), \\ -1, & p(+\infty) \mp a(+\infty) < 0 < p(-\infty) \mp a(-\infty), \\ 0, & \textit{otherwise}. \end{cases} \tag{I.9}$$

Note that (I.9) is robust in the sense that it depends only on the asymptotic values (I.8). An index formula of this kind is an active theme of mathematical studies on 2-phase quantum walks [CGSVWW16, CGGSVWW18, CGSVWW18, Suz19, ST19b, Mat20, AFST21, Tan21, CGWW21], in which the assumption (I.8) consistently plays an indispensable role (see, for example, [CGGSVWW18, Corollary 4.3]). Following [RST17, RST18] we may refer to (I.8) as an ***anisotropic assumption***. This begs the following natural question. Are there some meaningful ways to generalise Lemma I.1 without imposing the anisotropic assumption (I.8)? One of the main purposes of this chapter is to show that such a non-trivial generalisation actually exists. It is worth mentioning that the scope of this generalisation is beyond that of the existing literature on 2-phase quantum walks mentioned above. As such, we take a completely new approach by making use of Toeplitz operators in this chapter.

We introduce the following terminology to generalise Lemma I.1. A complex-valued sequence $\zeta = (\zeta(x))_{x \in \mathbb{Z}}$ is said to be ***asymptotically periodic***, if there exist $n_{-\infty}, n_{+\infty} \in \mathbb{N}$ with the property that the following limits exist for each $\star = -\infty, +\infty$;

$$\zeta(\star, m) := \lim_{x \to \star} \zeta(n_\star \cdot x + m), \qquad m \in \{0, \dots, n_\star - 1\}. \tag{I.10}$$

In particular, the sequence $\zeta = (\zeta(x))_{x \in \mathbb{Z}}$ is said to be ***anisotropic***, if $n_{-\infty} = n_{+\infty} = 1$. We are now in a position to state the following generalisation of Lemma I.1;

Theorem A. *Let* $(\Gamma, U) = (\Gamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ *be defined by* (I.2), (I.3). *Suppose that limits of the form* (I.10) *exist for each* $\zeta = p, a$ *and each* $\star = -\infty, +\infty$, *and that for each* $\zeta = p, a$ *we have*

$$\sup_{x \in \mathbb{Z}} |\zeta(x)| < 1. \tag{I.11}$$

Let $p(\pm\infty), a(\pm\infty) \in (-1, 1)$ *be uniquely defined through*

$$\frac{\prod_{m=0}^{n_\star - 1} (1 + \zeta(\star, m))}{\prod_{m=0}^{n_\star - 1} (1 - \zeta(\star, m))} = \left(\frac{1 + \zeta(\star)}{1 - \zeta(\star)} \right)^{n_\star}, \qquad \zeta = p, a, \qquad \star = -\infty, +\infty. \tag{I.12}$$

Then $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ *if and only if* $p(\star) \neq \pm a(\star)$ *for each* $\star = -\infty, +\infty$. *In this case, we have:*

(i) **Index formula.** *The index* $\mathrm{ind}_{\pm}(\varGamma, U)$ *is given explicitly by the formula* (I.9). *That is,* $|\mathrm{ind}_{\pm}(\varGamma, U)| = 1$ *if and only if the following inequality holds true for* $j = 1$ *or* $j = 2$:

$$(-1)^j (p(-\infty) \mp a(-\infty)) < 0 < (-1)^j (p(+\infty) \mp a(+\infty)). \tag{I.13}$$

(ii) **Exponential decay.** *We have* $\dim\ker(U \mp 1) = |\mathrm{ind}_{\pm}(\varGamma, U)|$. *In particular, if* (I.13) *holds true for* $j = 1$ *or* $j = 2$, *then any non-zero vector* Ψ *in the one-dimensional eigenspace* $\ker(U \mp 1)$ *admits the following representation;*

$$\Psi = \begin{pmatrix} \mp(-1)^j \sqrt{\frac{1\mp(-1)^j a}{1\pm(-1)^j a}}\psi \\ \psi \end{pmatrix}, \qquad \psi \in \ker\left(L \mp \sqrt{\frac{1+(-1)^j p}{1-(-1)^j p} \frac{1\mp(-1)^j a}{1\pm(-1)^j a}} \right). \tag{I.14}$$

Moreover, the eigenstate Ψ *characterised by* (I.14) *exhibits exponential decay in the sense that there exist positive constants* $c^{\downarrow}_{j,\pm}, c^{\uparrow}_{j,\pm}, \kappa^{\downarrow}_{j,\pm}, \kappa^{\uparrow}_{j,\pm}, x_{\pm}$, *such that*

$$\kappa^{\downarrow}_{j,\pm} e^{-c^{\downarrow}_{j,\pm}|x|} \leq \|\Psi(x)\|^2_{\mathbb{C}^2} \leq \kappa^{\uparrow}_{j,\pm} e^{-c^{\uparrow}_{j,\pm}|x|}, \qquad |x| \geq x_{\pm}. \tag{I.15}$$

Firstly, the denominator $1 - \zeta(\star, m)$ on the left hand side of (I.12) is non-zero. Indeed, the assumption (I.11) ensures $1 > \sup_{x\in\mathbb{Z}} |\zeta(x)| \geq \limsup_{x\to\infty} |\zeta(\pm x)|$, and so $|\zeta(\star, m)| \neq 1$ for each $m \in \{0, \dots, n_\star - 1\}$. Secondly, $\zeta(\star) \in (-1, 1)$ can be uniquely defined through (I.12), since $(-1, 1) \ni s \longmapsto (1+s)/(1-s) \in (0, \infty)$ is a bijection as in Figure I.1.

In the physical context, Theorem A can also be viewed as the *bulk-edge correspondence* of the one-dimensional split-step quantum walk with asymptotically periodic parameters (see §IV.2 for details).

I.2.1.2 Organisation of Chapter II

The ultimate purpose of §II is to prove Theorem A with the aid of the following two preliminary sections:

- In §II.1, we develop index theory for abstract unitary operators U satisfying the chiral symmetry condition (I.1) in full generality. More precisely, we make the formal indices defined by (I.5) to (I.6) precise with the decomposition (I.4) in mind. It is worth mentioning that the two subspaces $\ker(R_2 - 1), \ker(R_1 + 1)$ turn out to be the so-called *birth eigenspaces* in the language of the *spectral mapping theorem for chirally* *symmetric unitary operators* [HKSS14, SS16, SS19](see §II.5.3 for details). In fact, the main results of §II.1 can be obtained via this well-known theorem. Note, however, that the purpose of §II.1 is to show that there is an alternative elementary approach without relying on the spectral mapping theorem.

- In §II.2, we focus on analysis of operators of the form (I.2). For full generality, we consider the following *finite* sum of $n \times n$ block-matrix operators on $\ell^2(\mathbb{Z}, \mathbb{C}^n) = \bigoplus_{j=1}^n \ell^2(\mathbb{Z})$;

$$A = \sum_{y=-k}^{k} \begin{pmatrix} a_{11}(y,\cdot)L^y & \dots & a_{1n}(y,\cdot)L^y \\ \vdots & \ddots & \vdots \\ a_{n1}(y,\cdot)L^y & \dots & a_{nn}(y,\cdot)L^y \end{pmatrix} = \begin{pmatrix} \sum_{y=-k}^{k} a_{11}(y,\cdot)L^y & \dots & \sum_{y=-k}^{k} a_{1n}(y,\cdot)L^y \\ \vdots & \ddots & \vdots \\ \sum_{y=-k}^{k} a_{n1}(y,\cdot)L^y & \dots & \sum_{y=-k}^{k} a_{nn}(y,\cdot)L^y \end{pmatrix}, \tag{I.16}$$

  where each $a_{ij}(y,\cdot) = (a_{ij}(y,x))_{x \in \mathbb{Z}}$ is an arbitrary bounded $\mathbb{C}$-valued sequence viewed as a multiplication operator on $\ell^2(\mathbb{Z})$ as before. We call any operator of the form (I.16) ***strictly local*** following [CGSVWW18, §1.2]. Under the assumption that each sequence $\zeta = a_{ij}(y,\cdot)$ fulfils the asymptotically periodic assumption (I.10), we show in Theorem II.8 that computations of the Fredholm index and Fredholm essential spectrum of A (see §I.3 for definition) can be reduced to finite-dimensional spectral analysis via the language of Toeplitz operators. This approach is entirely motivated by [Mat20]. The novelty of Theorem II.8 lies in the fact that it is applicable to non-normal strictly local operators, and this fact plays an important role when we consider non-unitary quantum walks in §III.

We can then proceed to §II.3 to prove Theorem A (i) via Theorem II.8 mentioned above and a decomposition method outlined in [CGWW21, §3]. Note that we consider Theorem A (ii) as a totally separate problem in §II.4, since Theorem II.8 alone is not sufficient to prove the exponential decay property (I.15). Instead, we shall make use of an elementary difference equation method as outlined in [FFS18] to prove Theorem A (ii). Finally, the present chapter concludes with some discussions and remarks in §II.5.

I.2.2 Chapter III. Non-unitary Models

We consider index theory for chirally symmetric *non-unitary* operators in this chapter.

I.2.2.1 Introduction of Chapter III

Non-unitary quantum walks naturally arise in the physical context. In fact, such models can account for the gain-loss effects of photons in optical network experiments (see §IV.3 for details). From a purely mathematical point of view, whether or not an estimate analogous to (I.7) holds true for non-unitary chirally symmetric (bounded) operators U is a highly non-trivial question. It is worth mentioning that this general problem is in fact far beyond the scope of the present thesis. The main hindrance of the non-unitary setting lies in the fact that the two indices $\mathrm{ind}_+(\varGamma, U), \mathrm{ind}_-(\varGamma, U)$ we have discussed in §I.2.1.1 become ill-defined.

This motivates us to introduce a yet another index, say $\mathrm{ind}\,(\varGamma, U)$, for non-unitary chirally symmetric operators U with the hope that it gives a basis for further investigation of topologically protected eigenstates. More precisely, if U is a (not necessarily unitary) operator satisfying (I.1), then we may focus on the imaginary part Q of U, instead of the real part R. Indeed, the chiral symmetry condition (I.1) immediately implies the anti-commutation relation $\varGamma Q + Q\varGamma = 0$, and so the self-adjoint operator Q admits the following off-diagonal representation (cf (I.4));

$$Q = \begin{pmatrix} 0 & Q_1^* \\ Q_1 & 0 \end{pmatrix}_{\ker(\varGamma-1)\oplus\ker(\varGamma+1)}. \tag{I.17}$$

Under the assumption that Q_1 is Fredholm, we define the new index $\mathrm{ind}\,(\varGamma, U)$ by

$$\mathrm{ind}\,(\varGamma, U) := \mathrm{ind}\, Q_1, \tag{I.18}$$

where the right hand side denotes the Fredholm index of Q_1. It is worth mentioning that if U is unitary and if Q_1 is Fredholm, then we obtain the following results (see Lemma II.2 (ii) for details):

$$\mathrm{ind}\,(\varGamma, U) = \mathrm{ind}_+(\varGamma, U) + \mathrm{ind}_-(\varGamma, U), \tag{I.19}$$

$$|\mathrm{ind}\,(\varGamma, U)| \leq \dim\ker(U-1) + \dim\ker(U+1), \tag{I.20}$$

where (I.20) is a weaker version of (I.7).

As is well-known, the assignment of the Fredholm index on the right hand side of (I.18) to a (possibly unbounded) self-adjoint operator of the form (I.17) is commonly used in *supersymmetric quantum mechanics* (see, for example, [Tha92, §5] or [Ara18, §7.13]). The hamiltonian $Q^2 = Q_1^* Q_1 \oplus Q_1 Q_1^*$ is often referred to as a *superhamiltonian*, and the following obvious equality holds true;

$$\operatorname{ind} Q_1 = \dim\ker Q_1^* Q_1 - \dim\ker Q_1 Q_1^*,$$

where Q_1 is assumed to be Fredholm. On the other hand, the index $\operatorname{ind}(\varGamma, U) = \operatorname{ind} Q_1$, often referred to as the *Witten index*, is the main subject of the existing literature for chirally symmetric *unitary* quantum walks [Suz19, ST19b, Mat20, Tan21]. More precisely, some existing index formulas for Suzuki's one-dimensional split-step quantum walk can be found in [ST19b, Mat20, Tan21](see §II.5.4 for details), and the purpose of the current chapter is to consider their non-unitary variants.

I.2.2.2 Organisation of Chapter III

This chapter is primarily concerned with the following modified version of U_{suz} (cf (I.2));

$$U_1 := \begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix} \begin{pmatrix} e^{-2\gamma(\cdot+1)} a & e^{\gamma-\gamma(\cdot+1)}\sqrt{1-a^2} \\ e^{\gamma-\gamma(\cdot+1)}\sqrt{1-a^2} & -e^{2\gamma} a \end{pmatrix}, \tag{I.21}$$

where $\gamma = (\gamma(x))_{x\in\mathbb{Z}}$ is a bounded $\mathbb{R}$-valued sequence, and where $\gamma(\cdot + 1)$ denotes the sequence $(\gamma(x+1))_{x\in\mathbb{Z}}$. Note that the operator U_1 is non-unitary in general, but it coincides with the unitary operator U_{suz} if we let $\gamma(x) = 0$ for each $x \in \mathbb{Z}$. For simplicity, we assume the existence of a limit of the form (I.8) for each $\star = -\infty, +\infty$ and each $\zeta = \gamma, p, a$ throughout the current chapter, instead of the asymptotically periodic assumption (I.10).

The main theorem of the current chapter, Theorem B, is a two-fold proposition about the pair $(\varGamma, U) := (\varGamma_{\mathrm{suz}}, U_1)$ which clearly satisfies the chiral symmetry condition (I.1) as before. In fact, we consider a slightly more general version of (I.21) by replacing L with L^m for any non-zero integer m in Theorem B, but this generalisation turns out to be mathematically immaterial (note, however, that the case $m = 2$ plays a somewhat important physical role as in the proceeding chapter). The purpose of §III.1 is to give the precise statement of

Theorem B. Firstly, the following complete classification of the index (I.18) can be found in Theorem B (i);

$$\operatorname{ind}(\varGamma, U) = \begin{cases} 0, & |p_\gamma(-\infty)| < |a(-\infty)|,\ |p_\gamma(+\infty)| < |a(+\infty)|, \\ \operatorname{sign} p(+\infty), & |p_\gamma(-\infty)| < |a(-\infty)|,\ |p_\gamma(+\infty)| > |a(+\infty)|, \\ -\operatorname{sign} p(-\infty), & |p_\gamma(-\infty)| > |a(-\infty)|,\ |p_\gamma(+\infty)| < |a(+\infty)|, \\ \operatorname{sign} p(+\infty) - \operatorname{sign} p(-\infty), & |p_\gamma(-\infty)| > |a(-\infty)|,\ |p_\gamma(+\infty)| > |a(+\infty)|, \end{cases} \tag{I.22}$$

where $\operatorname{sign} : \mathbb{R} \to \{-1, 1\}$ is the sign function (see (I.28) for definition), and where $p_\gamma(-\infty), p_\gamma(+\infty) \in \mathbb{R}$ are defined by

$$p_\gamma(\star) := p(\star)\left(p(\star)^2 + (1 - p(\star)^2)\cosh^2(2\gamma(\star))\right)^{-1/2}, \qquad \star = -\infty, +\infty.$$

Secondly, it is shown in Theorem B (ii) that the essential spectrum $\sigma_{\mathrm{ess}}(U_1)$ is a subset of the union of the unit-circle $\mathbb{T}$ and real axis $\mathbb{R}$, and that it is given explicitly by $\sigma_{\mathrm{ess}}(U_1) = \sigma(-\infty) \cup \sigma(+\infty)$, where for each $\star = -\infty, +\infty$ the subset $\sigma(\star)$ of $\mathbb{T} \cup \mathbb{R}$ depends only on the asymptotic values $\gamma(\star), p(\star), a(\star)$. We defer the proof of Theorem B, and directly proceed to discussions in §III.2. In particular, we explain how Theorem B forms a basis for future mathematical research in the context of the bulk-edge correspondence for *non-unitary* chirally symmetric quantum walks (see §III.2.1 for details). Finally, the proof of Theorem B is given in §III.3.

I.2.3 Chapter IV. Unitary Transforms of Some One-dimensional Quantum Walks

The purpose of this short supplementary chapter is to show that the models we consider in §II and §III are unitarily equivalent to some well-known one-dimensional quantum walk models in the physics literature. We make emphasis on the physical utility of such physical models.

I.3 Notation and terminology

By operators we shall always mean everywhere-defined bounded linear operators between Banach spaces throughout this thesis. The identity operator on any Banach space is denoted by 1.

- Let $\ell^2(\mathbb{Z}, \mathbb{C}^n)$ be the Hilbert space of square-summable $\mathbb{C}^n$-valued sequences indexed by the set $\mathbb{Z}$ of integers, and let $\ell^2(\mathbb{Z}) := \ell^2(\mathbb{Z}, \mathbb{C}^1)$. The ***left-shift operator*** L on $\ell^2(\mathbb{Z})$ is the unitary operator defined by

$$L\Psi := \Psi(\cdot + 1), \qquad \Psi \in \ell^2(\mathbb{Z}). \tag{I.23}$$

- An operator A on a Hilbert space $\mathcal{H}$ is said to be ***Fredholm***, if $\ker A, \ker A^*$ are finite-dimensional and if A has a closed range. Given such A, we define the ***Fredholm index*** of A by $\operatorname{ind}(A) := \dim\ker A - \dim\ker A^*$. It is well-known that the Fredholm index is invariant under compact perturbations. That is, given an operator A on $\mathcal{H}$ and a compact operator K on $\mathcal{H}$, we have that A is Fredholm if and only if so is $A + K$, and in this case $\operatorname{ind}(A) = \operatorname{ind}(A + K)$. The (Fredholm) ***essential spectrum*** of an operator A on $\mathcal{H}$ is defined as the set $\sigma_{\mathrm{ess}}(A)$ of all $\lambda \in \mathbb{C}$, such that $A - \lambda$ fails to be Fredholm. Note that $\sigma_{\mathrm{ess}}(A)$ is also stable under compact perturbations.

- We shall make use of the following arithmetic convention for each $r \in (0, \infty]$;

$$r + \infty = \infty + r = \infty, \qquad r \cdot \infty = \infty \cdot r = \infty, \qquad 0^{-1} = \infty, \qquad \infty^{-1} = 0. \tag{I.24}$$

  Note that $0 \cdot \infty = \infty \cdot 0$ is left undefined. This convention allows us to consider a homeomorphism of the form $[0, \infty] \ni s \longmapsto s^{-1} \in [0, \infty]$, where the extended half-line $[0, \infty]$ is viewed as a metric space in the obvious way.

- With the convention (I.24) in mind, we define another homeomorphism $\Lambda : [-1, 1] \to [0, \infty]$ by

$$\Lambda(s) := \frac{1 + s}{1 - s}, \qquad s \in [-1, 1]. \tag{I.25}$$

  The function $s \longmapsto \Lambda(s)$ increases from $\Lambda(-1) = 0$ to $\Lambda(+1) = \infty$ as in the following figure;

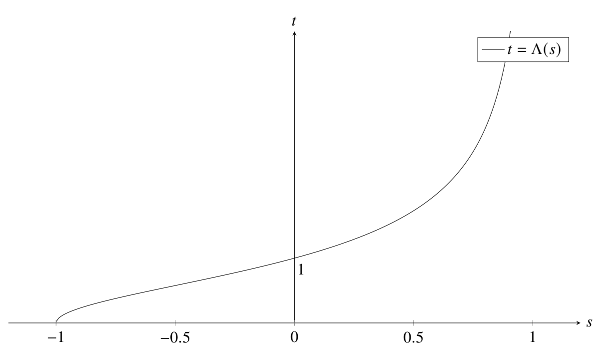


Figure I.1: This figure shows the graph of $t = \Lambda(s)$.

Let $s, s' \in [-1,1]$. We have $\Lambda(-s) = \Lambda(s)^{-1}$. Furthermore, if $ss' \neq -1$, then the product $\Lambda(s)\Lambda(s')$ is a well-defined extended non-negative real number, and the following two assertions hold true:

$$\Lambda(s)\Lambda(s') = \Lambda\left(\frac{s+s'}{1+ss'}\right), \tag{I.26}$$

$$\Lambda(s)\Lambda(s') \lesseqgtr 1 \text{ if and only if } s+s' \lesseqgtr 0, \tag{I.27}$$

where the notation $\lesseqgtr$ in (I.27) simultaneously denotes the three binary relations $>, =, <$.

- The ***sign function*** $\operatorname{sign} : \mathbb{R} \to \{-1,1\}$ is defined by

$$\operatorname{sign} x := \begin{cases} \dfrac{x}{|x|}, & x \neq 0, \\ 1, & x = 0. \end{cases} \tag{I.28}$$

- Let $n_{-\infty}, n_{+\infty} \in \mathbb{N}$ be fixed. A complex-valued sequence $\zeta = (\zeta(x))_{x\in\mathbb{Z}}$ is said to be ***asymptotically periodic***, if limits of the form (I.10) exist for each $\star = -\infty, +\infty$. In particular, the sequence $\zeta = (\zeta(x))_{x\in\mathbb{Z}}$ is said to be ***anisotropic***, if $n_{-\infty} = n_{+\infty} = 1$ (we often let $\zeta(\star) := \zeta(\star, 0)$ in this case). Let us consider the following explicit example;

Example I.2. If $\zeta = (\zeta(x))_{x\in\mathbb{Z}}$ is an asymptotically $(3,2)$-periodic sequence, then we have the following $3+2=5$ limits:

$$\zeta(-\infty,0) = \lim_{x\to-\infty} \zeta(3x+0), \qquad \zeta(+\infty,0) = \lim_{x\to+\infty} \zeta(2x+0),$$
$$\zeta(-\infty,1) = \lim_{x\to-\infty} \zeta(3x+1), \qquad \zeta(+\infty,1) = \lim_{x\to+\infty} \zeta(2x+1).$$
$$\zeta(-\infty,2) = \lim_{x\to-\infty} \zeta(3x+2),$$

On the other hand, one can rearrange $\zeta(x)$ according to the following table;

$\zeta(-\infty,0)$	$\leftarrow$	$\zeta(-9)$	$\zeta(-6)$	$\zeta(-3)$				$\dots$	
$\zeta(-\infty,1)$	$\leftarrow$	$\zeta(-8)$	$\zeta(-5)$	$\zeta(-2)$				$\dots$	
$\zeta(-\infty,2)$	$\leftarrow$	$\zeta(-7)$	$\zeta(-4)$	$\zeta(-1)$				$\dots$	
	$\dots$				$\zeta(0)$	$\zeta(2)$	$\zeta(4)$	$\rightarrow$	$\zeta(+\infty,0)$
	$\dots$				$\zeta(1)$	$\zeta(3)$	$\zeta(5)$	$\rightarrow$	$\zeta(+\infty,1)$

The first three rows show that $\zeta(3x+0), \zeta(3x+1), \zeta(3x+2)$ have well-defined limits as $x \to -\infty$, whereas the last two rows show that $\zeta(2x+0), \zeta(2x+1)$ have well-defined limits as $x \to +\infty$.

We may also speak of the asymptotical periodicity of a matrix-valued sequence in the obvious way.

Chapter II

Unitary Models

II.1 Indices for chirally symmetric bounded operators (Preliminary 1)

II.1.1 Chiral pairs

A ***chiral pair*** on an abstract Hilbert space $\mathcal{H}$ is any pair $(\varGamma, U)$ of a unitary self-adjoint operator $\varGamma : \mathcal{H} \to \mathcal{H}$ and a (not necessarily normal) operator $U : \mathcal{H} \to \mathcal{H}$, satisfying the chiral symmetry condition (I.1). Note that the underlying Hilbert space $\mathcal{H}$ admits a $\mathbb{Z}_2$-grading of the form $\mathcal{H} = \ker(\varGamma - 1) \oplus \ker(\varGamma + 1)$, and that $\varGamma = 1 \oplus (-1)$ with respect to this orthogonal decomposition. If R, Q denote the real and imaginary parts of U respectively, then the operator U can then be written as $U = R + iQ$, where U is normal if and only if R, Q commute. Furthermore, R, Q admit the following block-operator matrix representation:

$$R = \begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}_{\ker(\varGamma-1)\oplus\ker(\varGamma+1)}, \qquad Q = \begin{pmatrix} 0 & Q_2 \\ Q_1 & 0 \end{pmatrix}_{\ker(\varGamma-1)\oplus\ker(\varGamma+1)}, \tag{II.1}$$

where the first equality follows from the commutation relation $[\varGamma, R] := \varGamma R - R\varGamma = 0$, and where the second equality follows from the anti-commutation relation $\{\varGamma, Q\} := \varGamma Q + Q\varGamma = 0$ (see [Suz19, Lemma 2.2] for details). Since R, Q are self-adjoint, we have $R_j^* = R_j$ for each $j = 1, 2$, and $Q_2 = Q_1^*$. The following formula shall be referred to as the ***standard representation*** of U with respect to $\varGamma$ throughout this chapter;

$$U = \begin{pmatrix} R_1 & iQ_2 \\ iQ_1 & R_2 \end{pmatrix}_{\ker(\varGamma-1)\oplus\ker(\varGamma+1)}. \tag{II.2}$$

Lemma II.1. *Let $\mathcal{H}$ be an abstract Hilbert space, and let $(\varGamma, U)$ be a chiral pair on $\mathcal{H}$. Let U be unitary, and let R, Q be the real and imaginary parts of U respectively. Then*

$$\sigma_{\mathrm{ess}}(R) = \left\{ \frac{z+z^*}{2} \mid z \in \sigma_{\mathrm{ess}}(U) \right\}, \tag{II.3}$$

$$\sigma_{\mathrm{ess}}(Q) = \left\{ \frac{z-z^*}{2i} \mid z \in \sigma_{\mathrm{ess}}(U) \right\}, \tag{II.4}$$

$$\sigma_{\mathrm{ess}}(U) = \left\{ z \in \mathbb{T} \mid \frac{z+z^*}{2} \in \sigma_{\mathrm{ess}}(R) \right\}. \tag{II.5}$$

Furthermore, the operator Q is Fredholm if and only if $-1, +1 \notin \sigma_{\mathrm{ess}}(U)$.

It follows from (II.5) that the essential spectrum of U is also symmetry about the real axis.

Proof. Let $[\cdot]$ be the natural surjection from the C^*-algebra $\mathcal{B}(\mathcal{H})$ of bounded operators on $\mathcal{H}$ onto the Calkin algebra $\mathcal{B}(\mathcal{H})/\mathcal{K}(\mathcal{H})$. As is well-known, we have $\sigma_{\mathrm{ess}}(X) = \sigma([X])$ for each $X \in \mathcal{B}(\mathcal{H})$. If $\rho : \mathbb{T} \to \mathbb{C}$ is a trigonometric polynomial of the form $\rho(z) = \sum_{y=-k}^{k} a(y) z^y$ for each $z \in \mathbb{T}$, then

$$\sigma_{\mathrm{ess}}(\rho(U)) = \sigma\left(\left[\sum_{y=-k}^{k} a(y)U^y\right]\right) = \sigma\left(\sum_{y=-k}^{k} a(y)\,[U]^y\right) = \sigma\left(\rho([U])\right) = \rho(\sigma\left([U]\right)) = \rho(\sigma_{\mathrm{ess}}(U)), \tag{II.6}$$

where the second last equality follows from the spectral mapping theorem. In particular, if we let $\rho(z) := (z+z^*)/2$ (resp. $\rho(z) := (z-z^*)/2i$) for each $z \in \mathbb{T}$, then $\rho(U) = R$ (resp. $\rho(U) = Q$). We obtain (II.3) to (II.4).

We use (II.3) to prove (II.5). It suffices to prove $\{z \in \mathbb{T} \mid \operatorname{Re} z \in \sigma_{\mathrm{ess}}(R)\} \subseteq \sigma_{\mathrm{ess}}(U)$, since the reverse inclusion is obvious. If $z \in \mathbb{T}$ satisfies $\operatorname{Re} z \in \sigma_{\mathrm{ess}}(R)$, then there exists $z_0 \in \sigma_{\mathrm{ess}}(U)$, such that $\operatorname{Re} z = \operatorname{Re} z_0$. That is, either $z = z_0$ or $z = z_0^*$, where $z_0^* \in \sigma_{\mathrm{ess}}(U)$ by the chiral symmetry condition (I.1). We get $z \in \sigma_{\mathrm{ess}}(U)$ in either case. Therefore, (II.5) holds true.

Finally, it immediately follows from (II.4) that Q is Fredholm if and only if $-1, +1 \notin \sigma_{\mathrm{ess}}(U)$. □

II.1.2 Indices for chiral pairs

From this point onward we shall adhere to the convention that whenever we speak of a chiral pair $(\mathit{\Gamma}, U)$, we assume that U is unitary throughout the remaining part of the current chapter. With the standard representation (II.2) in mind, this convention allows us to introduce the following formal indices:

$$\operatorname{ind}_{\pm}(\mathit{\Gamma}, U) := \dim\ker(R_1 \mp 1) - \dim\ker(R_2 \mp 1), \tag{II.7}$$

$$\operatorname{ind}(\mathit{\Gamma}, U) := \dim\ker Q_1 - \dim\ker Q_2. \tag{II.8}$$

Note that if Q_1 is a Fredholm operator, then the formula (II.8) coincides with the definition of the Fredholm index of Q_1, since $Q_2 = Q_1^*$.

Lemma II.2. *Given a chiral pair* $(\mathit{\Gamma}, U)$ *with* (II.2) *being the standard representation of* U*, we have*

$$\ker(U \mp 1) = \ker(R_1 \mp 1) \oplus \ker(R_2 \mp 1), \tag{II.9}$$

$$\ker Q_j = \ker(R_j - 1) \oplus \ker(R_j + 1), \qquad j = 1, 2. \tag{II.10}$$

Moreover, the following assertions hold true:

(i) *The index* $\operatorname{ind}_{\pm}(\mathit{\Gamma}, U)$ *is a well-defined integer, if* $\dim\ker(U \mp 1) < \infty$*. In this case,* (I.7) *holds true.*

(ii) *The index* $\operatorname{ind}(\mathit{\Gamma}, U)$ *is a well-defined integer, if* $\dim\ker(U - 1) + \dim\ker(U + 1) < \infty$*. In this case,* (I.19) *to* (I.20) *hold true.*

Clearly, $\dim\ker(U \mp 1) < \infty$ is a weaker assumption than $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$.

Proof. Since $U = R + iQ$ is unitary and since $[R, Q] = 0$, we have $R^2 + Q^2 = 1$. Firstly, this matrix equality implies $R_j^2 + Q_j^* Q_j = 1$ for each $j = 1, 2$, and so (II.10) follows. Secondly, the same equality implies $(U \mp 1)^*(U \mp 1) = 2(1 \mp R)$. We obtain (II.9) from

$$\ker(U \mp 1) = \ker(U \mp 1)^*(U \mp 1) = \ker(1 \mp R) = \ker(R \mp 1), \tag{II.11}$$

where $\ker(R \mp 1) = \ker(R_1 \mp 1) \oplus \ker(R_2 \mp 1)$, since $R = R_1 \oplus R_2$.

(i) It follows from (II.9) that if $\dim\ker(U \mp 1) < \infty$, then $\dim\ker(R_j \mp 1) < \infty$ for each $j = 1, 2$, and so $\mathrm{ind}_{\pm}(\varGamma, U)$ is well-defined. We have

$$|\mathrm{ind}_{\pm}(\varGamma, U)| \leq \dim\ker(R_1 \mp 1) + \dim\ker(R_2 \mp 1) = \dim\ker(U \mp 1).$$

(ii) It follows from (II.10) that

$$\dim\ker Q_j = \dim\ker(R_j - 1) + \dim\ker(R_j + 1), \qquad j = 1, 2. \tag{II.12}$$

If $\dim\ker(U - 1) \oplus \ker(U + 1) < \infty$, then $\dim\ker(R_j - 1) \oplus \ker(R_j + 1) < \infty$ for each $j = 1, 2$ by (II.11). It follows from (II.12) that

$$\begin{aligned}
\mathrm{ind}\,(\varGamma, U) &= \dim\ker Q_1 - \dim\ker Q_2 \\
&= \dim\ker(R_1 - 1) + \dim\ker(R_1 + 1) - (\dim\ker(R_2 - 1) + \dim\ker(R_2 + 1)) \\
&= \dim\ker(R_1 - 1) - \dim\ker(R_2 - 1) + \dim\ker(R_1 + 1) - \dim\ker(R_2 + 1) \\
&= \mathrm{ind}_{+}(\varGamma, U) + \mathrm{ind}_{-}(\varGamma, U).
\end{aligned}$$

□

Lemma II.3. *Let $(\varGamma_0, U_0), (\varGamma, U)$ be two chiral pairs on Hilbert spaces $\mathcal{H}_0, \mathcal{H}$ respectively. If $(\varGamma_0, U_0), (\varGamma, U)$ are* ***unitarily equivalent*** *in the sense that $(\varGamma_0, U_0) = (\epsilon^* \varGamma \epsilon, \epsilon^* U \epsilon)$ for some unitary operator $\epsilon : \mathcal{H}_0 \to \mathcal{H}$, then the following assertions hold true:*

(i) *If* $\dim\ker(U_0 \mp 1) = \dim\ker(U \mp 1)$ *is finite, then* $\mathrm{ind}_{\pm}(\varGamma_0, U_0) = \mathrm{ind}_{\pm}(\varGamma, U)$.

(ii) *If* $\dim\ker(U_0 - 1) \oplus \ker(U_0 + 1) = \dim\ker(U - 1) \oplus \ker(U + 1)$ *is finite, then* $\mathrm{ind}\,(\varGamma_0, U_0) = \mathrm{ind}\,(\varGamma, U)$.

Proof. Note that the operator $\epsilon : \mathcal{H}_0 \to \mathcal{H}$ admits a block-operator matrix representation of the following form;

$$\epsilon = \begin{pmatrix} \epsilon_+ & \epsilon_{-+} \\ \epsilon_{+-} & \epsilon_- \end{pmatrix}, \qquad \begin{aligned} &\epsilon_+ : \ker(\varGamma_0 - 1) \to \ker(\varGamma - 1), && \epsilon_{-+} : \ker(\varGamma_0 + 1) \to \ker(\varGamma - 1), \\ &\epsilon_{+-} : \ker(\varGamma_0 - 1) \to \ker(\varGamma + 1), && \epsilon_- : \ker(\varGamma_0 + 1) \to \ker(\varGamma + 1). \end{aligned}$$

We show first that the two off-diagonal entries $\epsilon_{+-}, \epsilon_{-+}$ vanish. Indeed, since $\varGamma_0 = 1 \oplus (-1)$ and $\varGamma = 1 \oplus (-1)$, the given equality $0 = \epsilon\varGamma_0 - \varGamma\epsilon$ becomes the following matrix equality;

$$0 = \begin{pmatrix} \epsilon_+ & \epsilon_{-+} \\ \epsilon_{+-} & \epsilon_- \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \epsilon_+ & \epsilon_{-+} \\ \epsilon_{+-} & \epsilon_- \end{pmatrix} = \begin{pmatrix} 0 & -2\epsilon_{-+} \\ 2\epsilon_{+-} & 0 \end{pmatrix}.$$

This implies $\epsilon = \epsilon_+ \oplus \epsilon_- : \ker(\Gamma_0 - 1) \oplus \ker(\Gamma_0 + 1) \to \ker(\Gamma - 1) \oplus \ker(\Gamma + 1)$. Therefore, if U admits the standard representation of the form (II.2), then the standard representation of U_0 is given by the following formula;

$$U_0 = \begin{pmatrix} \epsilon_+^* R_1 \epsilon_+ & i\epsilon_+^* Q_2 \epsilon_- \\ i\epsilon_-^* Q_1 \epsilon_+ & \epsilon_-^* R_2 \epsilon_- \end{pmatrix}_{\ker(\Gamma_0 - 1)\oplus\ker(\Gamma_0+1)}.$$

The claim follows from

$$\dim\ker(R_1 \mp 1) = \dim\ker(\epsilon_+^*(R_1 \mp 1)\epsilon_+) = \dim\ker(\epsilon_+^* R_1 \epsilon_+ \mp 1),$$

$$\dim\ker(R_2 \mp 1) = \dim\ker(\epsilon_-^*(R_2 \mp 1)\epsilon_-) = \dim\ker(\epsilon_-^* R_2 \epsilon_- \mp 1),$$

$$\dim\ker Q_1 = \dim\ker Q_1^* Q_1 = \dim\ker(\epsilon_+^* Q_1^* Q_1 \epsilon_+) = \dim\ker(\epsilon_-^* Q_1 \epsilon_+)^*(\epsilon_-^* Q_1 \epsilon_+) = \dim\ker(\epsilon_-^* Q_1 \epsilon_+),$$

$$\dim\ker Q_2 = \dim\ker Q_2^* Q_2 = \dim\ker(\epsilon_-^* Q_2^* Q_2 \epsilon_-) = \dim\ker(\epsilon_+^* Q_2 \epsilon_-)^*(\epsilon_+^* Q_2 \epsilon_-) = \dim\ker(\epsilon_+^* Q_2 \epsilon_-).$$

□

The fact that the evolution operator of Suzuki's split-step quantum walk (I.2) can be decomposed as the product of two unitary self-adjoint operators defined by (I.3) motivates us to introduce the following general proposition;

Proposition II.4. *Let $\mathcal{H}$ be a Hilbert space, and let Γ, Γ' be two unitary self-adjoint operators on $\mathcal{H}$. If $U := \Gamma\Gamma'$, then $(\Gamma, U), (\Gamma', U)$ are two chiral pairs on $\mathcal{H}$. Moreover, the following assertions hold true:*

(i) *If U admits the standard representation* (II.2)*, then the following equalities hold true for each $j = 1, 2$:*

$$\ker(R_j \mp 1) = \ker(U \mp 1) \cap \ker(\Gamma + (-1)^j) = \ker(\Gamma + (-1)^j) \cap \ker(\Gamma' \mp (-1)^{j+1}). \qquad \text{(II.13)}$$

(ii) *If $\ker(U \mp 1)$ is finite-dimensional, then*

$$\operatorname{ind}_{\pm}(\Gamma, U) = \pm \operatorname{ind}_{\pm}(\Gamma', U). \qquad \text{(II.14)}$$

(iii) *If $\ker(U - 1) \oplus \ker(U + 1)$ is finite-dimensional, then*

$$\operatorname{ind}(\Gamma', U) = \operatorname{ind}_+(\Gamma, U) - \operatorname{ind}_-(\Gamma, U). \qquad \text{(II.15)}$$

Alternatively, if U is a unitary operator on $\mathcal{H}$ satisfying the satisfying the chiral symmetry condition (I.1) for some unitary self-adjoint operator $\varGamma$ on $\mathcal{H}$, then it can be obviously decomposed as $U = \varGamma\varGamma'$, where $\varGamma' := \varGamma U$ is unitary self-adjoint.

Proof. Given two unitary self-adjoint operators $\varGamma, \varGamma'$ on $\mathcal{H}$, we let $U := \varGamma\varGamma'$. It is obvious that $(\varGamma, U)$, $(\varGamma', U)$ are two chiral pairs on $\mathcal{H}$.

(i) We have

$$U \mp 1 = \begin{pmatrix} R_1 \mp 1 & iQ_2 \\ iQ_1 & R_2 \mp 1 \end{pmatrix}.$$

It follows from this equality that

$$\ker(U \mp 1) \cap \ker(\varGamma + (-1)^j) = \ker(R_j \mp 1) \cap \ker Q_j = \ker(R_j \mp 1),$$

where the last equality follows from (II.10). Similarly, we have

$$\varGamma' \mp 1 = \varGamma U \mp 1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} R_1 & iQ_2 \\ iQ_1 & R_2 \end{pmatrix} \mp 1 = \begin{pmatrix} R_1 \mp 1 & iQ_2 \\ -iQ_1 & -(R_2 \pm 1) \end{pmatrix}.$$

We obtain

$$\ker(\varGamma - 1) \cap \ker(\varGamma' \mp 1) = \ker(R_1 \mp 1) \cap \ker Q_1 = \ker(R_1 \mp 1),$$
$$\ker(\varGamma + 1) \cap \ker(\varGamma' \mp 1) = \ker(R_2 \pm 1) \cap \ker Q_2 = \ker(R_2 \pm 1).$$

The above identities can be written as the single formula (II.13).

(ii) Note that $(\varGamma', U)$ is a chiral pair, since $\varGamma' U \varGamma' = \varGamma'(\varGamma\varGamma')\varGamma' = \varGamma'\varGamma = U^*$. Let $\ker(U \mp 1)$ be finite-dimensional, and let

$$m_{j,\pm} := \dim\left(\ker(\varGamma + (-1)^j) \cap \ker(\varGamma' \mp (-1)^{j+1})\right), \tag{II.16}$$
$$m'_{j,\pm} := \dim\left(\ker(\varGamma' + (-1)^j) \cap \ker(\varGamma \mp (-1)^{j+1})\right). \tag{II.17}$$

It follows from (i) that $\operatorname{ind}_\pm(\varGamma, U) = m_{1,\pm} - m_{2,\pm}$ and $\operatorname{ind}_\pm(\varGamma', U) = m'_{1,\pm} - m'_{2,\pm}$. The formula (II.14) is an immediate consequence of the following equalities:

$$m'_{1,+} = m_{1,+}, \qquad m'_{2,+} = m_{2,+},$$

$$m'_{1,-} = m_{2,-}, \qquad m'_{2,-} = m_{1,-}.$$

(iii) This follows from (i) and (ii). □

The proof of Proposition II.4 (ii) above turns out to be an essential tool in verifying the exponential decay property Theorem A (ii). As such, we record it in the following remark for future reference;

Remark II.5. With the notation introduced in Proposition II.4, let $m_{j,\pm}$ be the dimension of the subspace given by (II.13) for each $j = 1, 2$. If $m_{j,\pm} < \infty$ for each $j = 1, 2$, then $\mathrm{ind}_{\pm}(\Gamma, U)$ is well-defined, and we have

$$\mathrm{ind}_{\pm}(\Gamma, U) = m_{1,\pm} - m_{2,\pm}, \tag{II.18}$$

$$\dim\ker(U \mp 1) = m_{1,\pm} + m_{2,\pm}. \tag{II.19}$$

On a side note, we can give an alternative derivation of the formula (II.19) via the so-called *spectral mapping theorem for chirally symmetric unitary operators* [SS16, SS19]. A brief discussion on this supplementary topic can be found in §II.5.3.

Corollary II.6. *Let* (Γ, U) *be a chiral pair, and let* $\ker(U - 1) \oplus \ker(U + 1)$ *be finite-dimensional. Then we have the following formulas:*

$$\mathrm{ind}_{\pm}(\Gamma, -U) = \mathrm{ind}_{\mp}(\Gamma, U), \qquad \mathrm{ind}\,(\Gamma, -U) = \mathrm{ind}\,(\Gamma, U), \tag{II.20}$$

$$\mathrm{ind}_{\pm}(-\Gamma, U) = -\mathrm{ind}_{\pm}(\Gamma, U), \qquad \mathrm{ind}\,(-\Gamma, U) = -\mathrm{ind}\,(\Gamma, U). \tag{II.21}$$

Proof. If U admits the standard representation of the form (II.2) with respect to Γ, then the standard representation of $-U$ is

$$-U = \begin{pmatrix} -R_1 & -iQ_2 \\ -iQ_1 & -R_2 \end{pmatrix}_{\ker(\Gamma-1)\oplus\ker(\Gamma+1)}.$$

It follows that $\operatorname{ind}_{\pm}(\Gamma, -U) = \operatorname{ind}_{\mp}(\Gamma, U)$, and so $\operatorname{ind}(\Gamma, -U) = \operatorname{ind}(\Gamma, U)$ by (I.19). Similarly, the standard representation of U with respect to $-\Gamma$ is

$$U = \begin{pmatrix} R_2 & iQ_1 \\ iQ_2 & R_1 \end{pmatrix}_{\ker(\Gamma+1)\oplus\ker(\Gamma-1)}.$$

We have $\operatorname{ind}_{\pm}(-\Gamma, U) = \dim\ker(R_2 \mp 1) - \dim\ker(R_1 \mp 1) = -\operatorname{ind}_{\mp}(\Gamma, U)$, and so $\operatorname{ind}(-\Gamma, U) = -\operatorname{ind}(\Gamma, U)$.

□

II.2 Strictly local operators (Preliminary 2)

We start with the following main result of [Tan21];

Theorem II.7 ([Tan21, Theorem A])**.** *Let $k_0 \in \mathbb{N}$, and let $A_{-k_0}, \dots, A_{k_0}$ be $n \times n$ matrices-valued sequences on $\mathbb{Z}$ admitting the following limits for $-k_0 \le k \le k_0$;*

$$A_k(\mathrm{L}) := \lim_{x \to -\infty} A_k(x), \qquad A_k(\mathrm{R}) := \lim_{x \to +\infty} A_k(x). \tag{II.22}$$

Let

$$A := \sum_{k=-k_0}^{k_0} A_k \begin{pmatrix} L^k & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & L^k \end{pmatrix}, \tag{II.23}$$

$$\hat{A}(\sharp, z) := \sum_{k=-k_0}^{k_0} A_k(\sharp) \begin{pmatrix} z^k & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & z^k \end{pmatrix}, \qquad z \in \mathbb{T} \qquad \sharp = \mathrm{L}, \mathrm{R}. \tag{II.24}$$

where L is the bilateral left-shift operator on $\ell^2(\mathbb{Z})$, and where each A_k in (II.23) *is viewed as the bounded multiplication operator on $\ell^2(\mathbb{Z}, \mathbb{C}^n)$. Then the following assertions hold true:*

(i) *We have that A is Fredholm if and only if $\mathbb{T} \ni z \longmapsto \det \hat{A}(\sharp, z) \in \mathbb{C}$ is nowhere vanishing on $\mathbb{T}$ for each $\sharp = \mathrm{L}, \mathrm{R}$. In this case, the Fredholm index of A is given by*

$$\operatorname{ind}(A) = \operatorname{wn}\left(\det \hat{A}(\mathrm{R}, \cdot)\right) - \operatorname{wn}\left(\det \hat{A}(\mathrm{L}, \cdot)\right), \tag{II.25}$$

where $\mathrm{wn}\left(\det \hat{A}(\sharp, \cdot)\right)$ *denotes the winding number of the continuous function* $\mathbb{T} \ni z \longmapsto \det \hat{A}(\sharp, z) \in \mathbb{C}$ *with respect to the origin for each* $\sharp = \mathrm{L}, \mathrm{R}$.

(ii) *The essential spectrum of* A *is given by*

$$\sigma_{\mathrm{ess}}(A) = \bigcup_{z \in \mathbb{T}} \sigma\left(\hat{A}(\mathrm{R}, z)\right) \cup \bigcup_{z \in \mathbb{T}} \sigma\left(\hat{A}(\mathrm{L}, z)\right). \tag{II.26}$$

Any operator A of the form (II.23) is referred to as an n-dimensional ***strictly local operator*** on the integer lattice $\mathbb{Z}$ throughout this thesis. The purpose of the current section is to generalise the existing formulas (II.25) to (II.26), by replacing the assumption (II.22) with the so-called ***asymptotically periodic assumption.*** More precisely, we assume that there exist natural numbers $n_{\mathrm{L}}, n_{\mathrm{R}}$ with the property that the following limits exist for $-k_0 \leq k \leq k_0$;

$$A_k(\mathrm{L}, m) := \lim_{x \to -\infty} A_k(n_{\mathrm{L}} \cdot x + m), \qquad m \in \{0, \dots, n_{\mathrm{L}} - 1\}, \tag{II.27}$$

$$A_k(\mathrm{R}, m) := \lim_{x \to +\infty} A_k(n_{\mathrm{R}} \cdot x + m), \qquad m \in \{0, \dots, n_{\mathrm{R}} - 1\}. \tag{II.28}$$

In other words, the doubly-infinite sequences $A_{-k}, \dots, A_k$ are ***asymptotically*** $(n_{\mathrm{L}}, n_{\mathrm{R}})$***-periodic*** in the sense of §I.3. We are now in a position to state the following generalisation of Theorem II.7;

Theorem II.8. *Let* $k_0 \in \mathbb{N}$, *and let* $A_{-k_0}, \dots, A_{k_0}$ *be finitely many* $n \times n$ *matrices-valued sequences on* $\mathbb{Z}$ *admitting the following representations:*

$$A_k(x) = \begin{pmatrix} a^k_{11}(x) & \dots & a^k_{1n}(x) \\ \vdots & \ddots & \vdots \\ a^k_{n1}(x) & \dots & a^k_{nn}(x) \end{pmatrix}, \qquad x \in \mathbb{Z}, \qquad -k_0 \leq k \leq k_0. \tag{II.29}$$

We assume that there exist $n_{\mathrm{L}}, n_{\mathrm{R}} \in \mathbb{N}$ *with the property that the following limits exist for* $1 \leq i, j \leq n$ *and for* $-k_0 \leq k \leq k_0$;

$$a^k_{ij}(\mathrm{L}, m) := \lim_{x \to -\infty} a^k_{ij}(n_{\mathrm{L}} \cdot x + m), \qquad m \in \{0, \dots, n_{\mathrm{L}} - 1\}, \tag{II.30}$$

$$a^k_{ij}(\mathrm{R}, m) := \lim_{x \to +\infty} a^k_{ij}(n_{\mathrm{R}} \cdot x + m), \qquad m \in \{0, \dots, n_{\mathrm{R}} - 1\}. \tag{II.31}$$

For each $\sharp = \mathrm{L}, \mathrm{R}$ *and each* $z \in \mathbb{T}$, *let* $\hat{A}(\sharp, z) = (\hat{A}_{ij}(\sharp, z))_{ij}$ *be the square matrix of dimension* $n \times n_\sharp$ *defined by the following block-matrix representation;*

$$\hat{A}(\sharp, z) := \begin{pmatrix} \hat{A}_{11}(\sharp, z) & \dots & \hat{A}_{1n}(\sharp, z) \\ \vdots & \ddots & \vdots \\ \hat{A}_{1n}(\sharp, z) & \dots & \hat{A}_{nn}(\sharp, z) \end{pmatrix}, \tag{II.32}$$

$$\hat{A}_{ij}(\sharp, z) := \sum_{k=-k_0}^{k_0} \begin{pmatrix} a_{ij}^k(\sharp, 0) & 0 & \dots & 0 \\ 0 & a_{ij}^k(\sharp, 1) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & a_{ij}^k(\sharp, n_\sharp - 1) \end{pmatrix} \begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ z & 0 & \dots & 0 \end{pmatrix}^k, \tag{II.33}$$

where $\mathbf{1}$ *denotes the identity matrix of dimension* $n_\sharp - 1$. *If* A *is a strictly local operator of the form* (II.23), *then the following the following assertions hold true:*

(i) *We have that* A *is Fredholm if and only if* $\mathbb{T} \ni z \longmapsto \det \hat{A}(\sharp, z) \in \mathbb{C}$ *is nowhere vanishing on* $\mathbb{T}$ *for each* $\sharp = \mathrm{L}, \mathrm{R}$. *In this case, the Fredholm index of* A *is given by* (II.25).

(ii) *The essential spectrum of* A *is given by* (II.26).

In general, the Fredholm index and essential spectrum are meaningful only in infinite dimensions. Note, however, that Theorem II.8 allows us to fully classify these two topological invariants for a strictly local operator in the language of linear algebra. In terms of practical applications, Theorem II.8 can be applied to the time-evolution operator of a discrete-time quantum walk defined on the integer lattice $\mathbb{Z}$, provided that it is an operator of the form (II.23) satisfying the asymptotically periodic assumptions (II.30) to (II.31).

Remark II.9. Theorem II.7 is a special case of Theorem II.8. Indeed, with the notation introduced in Theorem II.8, if $n_\sharp = 1$ for each $\sharp = \mathrm{L}, \mathrm{R}$, then (II.30) to (II.31) become:

$$a_{ij}^k(\mathrm{L}, 0) := \lim_{x \to -\infty} a_{ij}^k(x), \qquad a_{ij}^k(\mathrm{R}, 0) := \lim_{x \to +\infty} a_{ij}^k(x).$$

In this case, we show that (II.32) is given by (II.24). We define the two matrices $A_k(\mathrm{L}), A_k(\mathrm{R})$ by (II.22) for each k;

$$A_k(\sharp) := \begin{pmatrix} a^k_{11}(\sharp,0) & \dots & a^k_{1n}(\sharp,0) \\ \vdots & \ddots & \vdots \\ a^k_{n1}(\sharp,0) & \dots & a^k_{nn}(\sharp,0) \end{pmatrix}, \qquad \sharp = \mathrm{L}, \mathrm{R}.$$

We have $\hat{A}_{ij}(\sharp, z) = \sum_{k=-k_0}^{k_0} a^k_{ij}(\sharp, 0) z^k$, and so

$$\hat{A}(\sharp, z) = \begin{pmatrix} \sum_{k=-k_0}^{k_0} a^k_{11}(\sharp,0)z^k & \dots & \sum_{k=-k_0}^{k_0} a^k_{1n}(\sharp,0)z^k \\ \vdots & \ddots & \vdots \\ \sum_{k=-k_0}^{k_0} a^k_{n1}(\sharp,0)z^k & \dots & \sum_{k=-k_0}^{k_0} a^k_{nn}(\sharp,0)z^k \end{pmatrix},$$

which is consistent with (II.24).

II.2.1 Notation

The Hilbert space of all square-summable $\mathbb{C}$-valued sequences $\Psi = (\Psi(x))_{x \in \mathbb{Z}}$ is denoted by the shorthand $\ell^2(\mathbb{Z}) := \ell^2(\mathbb{Z}, \mathbb{C})$. We have a natural orthogonal decomposition $\ell^2(\mathbb{Z}) = \ell^2_{\mathrm{L}}(\mathbb{Z}) \oplus \ell^2_{\mathrm{R}}(\mathbb{Z})$, where

$$\ell^2_{\mathrm{L}}(\mathbb{Z}) := \{\Psi \in \ell^2(\mathbb{Z}) \mid \Psi(x) = 0 \ \forall x \geq 0\}, \qquad \ell^2_{\mathrm{R}}(\mathbb{Z}) := \{\Psi \in \ell^2(\mathbb{Z}) \mid \Psi(x) = 0 \ \forall x < 0\}.$$

The orthogonal projections of $\ell^2(\mathbb{Z})$ onto the above subspaces shall be denoted by P_{L} and $P_{\mathrm{R}} = 1 - P_{\mathrm{L}}$ respectively. For each $\sharp = \mathrm{L}, \mathrm{R}$, the orthogonal projection $P_\sharp$ can be written as $P_\sharp = \iota_\sharp \iota_\sharp^*$, where $\iota_\sharp : \ell^2_\sharp(\mathbb{Z}) \hookrightarrow \ell^2(\mathbb{Z})$ is the inclusion mapping.

For each $m \in \mathbb{N}$ any operator A on $\ell^2(\mathbb{Z}, \mathbb{C}^m) = \bigoplus_{j=1}^m \ell^2(\mathbb{Z})$ admits the following unique block-operator matrix representation;

$$A = \begin{pmatrix} A_{11} & \dots & A_{1m} \\ \vdots & \ddots & \vdots \\ A_{m1} & \dots & A_{mm} \end{pmatrix}_{\bigoplus_{j=1}^m \ell^2(\mathbb{Z})}, \tag{II.34}$$

where each A_{ij} is an operator on $\ell^2(\mathbb{Z})$. We shall agree to use the shorthand $A = (A_{ij})$ to mean that (II.34) holds true. With this representation of A in mind, for each $\sharp = \mathrm{L}, \mathrm{R}$, we define the following compression on

$\ell^2_\sharp(\mathbb{Z},\mathbb{C}^m) := \bigoplus_{j=1}^m \ell^2_\sharp(\mathbb{Z})$;

$$A_\sharp := \begin{pmatrix} \iota_\sharp^* A_{11}\iota_\sharp & \dots & \iota_\sharp^* A_{1m}\iota_\sharp \\ \vdots & \ddots & \vdots \\ \iota_\sharp^* A_{m1}\iota_\sharp & \dots & \iota_\sharp^* A_{mm}\iota_\sharp \end{pmatrix}_{\bigoplus_{j=1}^m \ell^2_\sharp(\mathbb{Z})} . \tag{II.35}$$

II.2.2 A characterisation of strictly local operators

Lemma II.10. *Let $(\delta_x)_{x\in\mathbb{Z}}$ be the standard complete orthonormal basis for $\ell^2(\mathbb{Z})$, and let A be an operator on $\ell^2(\mathbb{Z},\mathbb{C}^n)$ with the block-operator matrix representation* (II.34). *Then the following are equivalent:*

(i) *For each $i,j \in \{1,\dots,n\}$, the operator A_{ij} is a finite sum of the form $A_{ij} = \sum_{y=-k}^k a_{ij}(y,\cdot)L^y$ for some $\mathbb{C}$-valued sequences $a_{ij}(y,\cdot) = (a_{ij}(y,x))_{x\in\mathbb{Z}}$, where $-k \le y \le k$, viewed as multiplication operators on $\ell^2(\mathbb{Z}) = \bigoplus_{x\in\mathbb{Z}}\mathbb{C}$.*

(ii) *There exists a large enough positive integer k, such that for each $x \in \mathbb{Z}$ and for each $i,j \in \{1,\dots,n\}$, the vector $A_{ij}\delta_x \in \ell^2(\mathbb{Z})$ belongs to the linear span of the finite set $\{\delta_{x-y} \mid -k \le y \le k\}$.*

It follows from Lemma II.10 (i) that a strictly local operator A admits a block-operator matrix representation of the following form (I.16).

Proof. It is obvious that (i) implies (ii), since $L^y\delta_x = \delta_{x-y}$ for each $x,y \in \mathbb{Z}$. This equality shall be repeatedly used throughout the current section. To prove the converse, let (ii) hold true, and let i,j be both fixed. For each $x \in \mathbb{Z}$, there exist finitely many scalars $a'_{ij}(y,x) \in \mathbb{C}$, where $-k \le y \le k$, such that

$$A_{ij}\delta_x = \sum_{y=-k}^{k} a'_{ij}(y,x)\delta_{x-y}. \tag{II.36}$$

Note that $a'_{ij}(y,\cdot) = (a'_{ij}(y,x))_{x\in\mathbb{Z}}$ is a bounded sequence for $-k \le y \le k$;

$$|a'_{ij}(y,x)| = |\left\langle \delta_{x-y}, A_{ij}\delta_x \right\rangle_{\ell^2(\mathbb{Z})}| \le \|A_{ij}\|\|\delta_{x-y}\|_{\ell^2(\mathbb{Z})}\|\delta_x\|_{\ell^2(\mathbb{Z})} \le \|A_{ij}\|, \qquad x \in \mathbb{Z}.$$

Let $a_{ij}(y,x) := a'_{ij}(y,x+y)$ for each x,y. Then we obtain the following equalities for each $x \in \mathbb{Z}$;

$$\sum_{y=-k}^{k} a_{ij}(y,\cdot)L^y\delta_x = \sum_{y=-k}^{k} a_{ij}(y,\cdot)\delta_{x-y} = \sum_{y=-k}^{k} a_{ij}(y,x-y)\delta_{x-y} = \sum_{y=-k}^{k} a'_{ij}(y,x)\delta_{x-y} = A_{ij}\delta_x,$$

where the last equality follows from (II.36). That is, (i) holds true. □

Corollary II.11. *If A is a strictly local operator on $\ell^2(\mathbb{Z}, \mathbb{C}^n)$, then the difference $A - A_\mathrm{L} \oplus A_\mathrm{R}$ is finite-rank. Moreover, the following assertions hold true:*

(i) *The operator A is Fredholm if and only if $A_\mathrm{L}, A_\mathrm{R}$ are both Fredholm. In this case, we have*

$$\mathrm{ind}\,(A) = \mathrm{ind}\,(A_\mathrm{L}) + \mathrm{ind}\,(A_\mathrm{R}). \tag{II.37}$$

(ii) *The essential spectrum of A is given by*

$$\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(A_\mathrm{L}) \cup \sigma_{\mathrm{ess}}(A_\mathrm{R}). \tag{II.38}$$

Proof. Note that $P := \bigoplus_{j=1}^n P_\mathrm{R}$ is the orthogonal projection onto $\ell^2_\mathrm{R}(\mathbb{Z}, \mathbb{C}^n) = \bigoplus_{j=1}^n \ell^2_\mathrm{R}(\mathbb{Z})$. We have

$$A - A_\mathrm{L} \oplus A_\mathrm{R} = PA(1-P) + (1-P)AP = PA - PAP + AP - PAP = P[P, A] + [A, P]P,$$

where $[X, Y] := XY - YX$ denotes the commutator of two operators X, Y. It remains to show that $[A, P]$ is finite-rank, where we may assume without loss of generality that A is of the form (I.16). Since $P = \bigoplus_{j=1}^n P_\mathrm{R}$ is a diagonal block-operator matrix, we obtain

$$[A, P] = \begin{pmatrix} \left[\sum_{y=-k}^k a_{11}(y, \cdot) L^y, P_\mathrm{R}\right] & \dots & \left[\sum_{y=-k}^k a_{1n}(y, \cdot) L^y, P_\mathrm{R}\right] \\ \vdots & \ddots & \vdots \\ \left[\sum_{y=-k}^k a_{n1}(y, \cdot) L^y, P_\mathrm{R}\right] & \dots & \left[\sum_{y=-k}^k a_{nn}(y, \cdot) L^y, P_\mathrm{R}\right] \end{pmatrix}.$$

Since $[-, P_\mathrm{R}]$ is linear with respect to the first variable, each (i, j)-entry of the above block-operator matrix is given by $\sum_{y=-k}^k a_{ij}(y, \cdot)\, [L^y, P_\mathrm{R}]$, where the commutator $[L^y, P_\mathrm{R}]$ is finite-rank for $-k \leq y \leq k$. It follows that $A - A_\mathrm{L} \oplus A_\mathrm{R}$ is finite-rank, and so the remaining assertions immediately follow. □

Note that a strictly local operator of the form (I.16) has the simplest representation, if each sequence $a_{ij}(y, \cdot)$ is constant. Such an operator admits the following characterisation;

Lemma II.12. *Let A be an operator on $\ell^2(\mathbb{Z})$ with the block-operator matrix representation* (II.34)*. Then the following are equivalent:*

(i) *For each $i, j \in \{1, \dots, n\}$, the operator A_{ij} is a finite sum of the form $A_{ij} = \sum_{y=-k}^k a_{ij}(y) L^y$ for some complex numbers $a_{ij}(y)$, where $-k \leq y \leq k$.*

(ii) *The operator A is strictly local and $[A_{ij}, L^x] = 0$ for each $x \in \mathbb{Z}$ and each $i, j \in \{1, \dots, n\}$.*

The operator A is said to be ***uniform***, if it satisfies the above equivalent conditions. It follows from Lemma II.12 (i) that such A admits a block-operator matrix representation of the following form;

$$A = \sum_{y=-k}^{k} \begin{pmatrix} a_{11}(y)L^y & \dots & a_{1n}(y)L^y \\ \vdots & \ddots & \vdots \\ a_{n1}(y)L^y & \dots & a_{nn}(y)L^y \end{pmatrix} = \begin{pmatrix} \sum_{y=-k}^{k} a_{11}(y)L^y & \dots & \sum_{y=-k}^{k} a_{1n}(y)L^y \\ \vdots & \ddots & \vdots \\ \sum_{y=-k}^{k} a_{n1}(y)L^y & \dots & \sum_{y=-k}^{k} a_{nn}(y)L^y \end{pmatrix}. \tag{II.39}$$

Proof. It is obvious that (i) implies (ii). To prove the converse, let $A = (A_{ij})$ be strictly local, and let $[A_{ij}, L^x] = 0$ for each $x \in \mathbb{Z}$ and each $i, j \in \{1, \dots, n\}$. It follows from Lemma II.10 (i) that for each $i, j \in \{1, \dots, n\}$ we have $A_{ij} = \sum_{y=-k}^{k} a_{ij}(y, \cdot)L^y$. It remains to show that the sequence $a_{ij}(y, \cdot) = (a_{ij}(y, x))_{x\in\mathbb{Z}}$ is constant for a fixed pair $i, j \in \{1, \dots, n\}$. Since $A_{ij}\delta_x = \sum_{y=-k}^{k} a_{ij}(y, x-y)\delta_{x-y}$ for each $x \in \mathbb{Z}$, we get

$$A_{ij}\delta_x = A_{ij}L^{-x}\delta_0 = L^{-x}A_{ij}\delta_0 = L^{-x}\left(\sum_{y=-k}^{k} a_{ij}(y, -y)\delta_{-y}\right) = \sum_{y=-k}^{k} a_{ij}(y, -y)\delta_{x-y}.$$

It follows that $a_{ij}(y, x-y) = a_{ij}(y, -y)$ for each $x \in \mathbb{Z}$ and for each $y \in \{-k, \dots, k\}$. The claim follows. $\square$

II.2.3 A characterisation of uniform strictly local operators

The following result is one of the main theorems of the current section;

Theorem II.13. *Let A be a uniform operator on $\ell^2(\mathbb{Z}, \mathbb{C}^n)$ of the form* (II.39)*, and let*

$$\hat{A}(z) := \begin{pmatrix} \sum_{y=-k}^{k} a_{11}(y)z^y & \dots & \sum_{y=-k}^{k} a_{1n}(y)z^y \\ \vdots & \ddots & \vdots \\ \sum_{y=-k}^{k} a_{n1}(y)z^y & \dots & \sum_{y=-k}^{k} a_{nn}(y)z^y \end{pmatrix}, \qquad z \in \mathbb{T}. \tag{II.40}$$

Then the following assertions hold true:

(i) *The operator A is Fredholm if and only if $A_{\mathrm{L}}, A_{\mathrm{R}}$ are both Fredholm if and only if $\mathbb{T} \ni z \longmapsto \det \hat{A}(z) \in \mathbb{C}$ is nowhere vanishing on $\mathbb{T}$. In this case, we have* $\operatorname{ind} A = \operatorname{ind} A_{\mathrm{R}} + \operatorname{ind} A_{\mathrm{L}} = 0$, *and*

$$\operatorname{ind} A_{\mathrm{R}} = \operatorname{wn}\left(\det \hat{A}\right).$$

(ii) *The essential spectrum of A is given by*

$$\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(A_{\mathrm{R}}) = \sigma_{\mathrm{ess}}(A_{\mathrm{L}}) = \bigcup_{z \in \mathbb{T}} \sigma(\hat{A}(z)). \tag{II.41}$$

The proof of Theorem II.13 shall be given at the end of the current subsection. Let us first recall the notion of Toeplitz operators. Let $L^2(\mathbb{T})$ be the Hilbert space of square-summable functions on the unit-circle $\mathbb{T}$, where $\mathbb{T}$ is endowed with the normalised arc-length measure. It is well-known that $L^2(\mathbb{T})$ admits the standard complete orthonormal basis $(e_x)_{x \in \mathbb{Z}}$, where each e_x is defined by $\mathbb{T} \ni z \longmapsto z^x \in \mathbb{C}$. The ***Hardy-Hilbert space*** H^2 is the closure of the linear span of the set $\{e_x \mid x \geq 0\}$. Let $\iota : \mathrm{H}^2 \hookrightarrow L^2(\mathbb{T})$ be the inclusion mapping, and let $f \in \mathbb{C}(\mathbb{T})$. Then the ***Toeplitz operator*** T_f with symbol f is defined by

$$T_f := \iota^* M_f \iota, \tag{II.42}$$

where $M_f : L^2(\mathbb{T}) \to L^2(\mathbb{T})$ is the multiplication operator by f. More generally, let us consider the Banach space $C(\mathbb{T}, \mathbb{C}^{n \times n})$ of continuous matrix-valued functions on $\mathbb{T}$. Given a function $F \in C(\mathbb{T}, \mathbb{C}^{n \times n})$ of the form $F(z) = (f_{ij}(z))$ for each $z \in \mathbb{T}$, the Toeplitz operator with symbol F is defined by

$$T_F := \begin{pmatrix} T_{f_{11}} & \dots & T_{f_{1n}} \\ \vdots & \ddots & \vdots \\ T_{f_{n1}} & \dots & T_{f_{nn}} \end{pmatrix}_{\bigoplus_{j=1}^n \mathrm{H}^2}. \tag{II.43}$$

The following result is standard;

Theorem II.14. *Let $F \in C(\mathbb{T}, \mathbb{C}^{n \times n})$ be a matrix-valued function of the form $F(\cdot) = (f_{ij}(\cdot))$, and let T_F be the corresponding Toeplitz operator given by* (II.43). *Then the following assertions hold true:*

(i) *The Toeplitz operator T_F is Fredholm if and only if $\mathbb{T} \ni z \longmapsto \det F(z) \in \mathbb{C}$ is nowhere vanishing on $\mathbb{T}$. In this case,*

$$\operatorname{ind} T_F = -\operatorname{wn}(\det F). \tag{II.44}$$

(ii) *The essential spectrum of T_F is given by*

$$\sigma_{\mathrm{ess}}(T_F) = \bigcup_{z \in \mathbb{T}} \sigma(F(z)). \tag{II.45}$$

Proof. Note that (i) is the celebrated theorem of Gohberg-Krein (see, for example, [Mur06, Theorem 3.3]). It remains to prove (ii). Let $\mathcal{B}_n(\mathrm{H}^2) := \mathcal{B}\left(\bigoplus_{j=1}^n \mathrm{H}^2\right)$ be the C^*-algebra of operators on $\bigoplus_{j=1}^n \mathrm{H}^2$, and let $\mathcal{K}_n(\mathrm{H}^2) := \mathcal{K}\left(\bigoplus_{j=1}^n \mathrm{H}^2\right)$ be the ideal of compact operators on $\bigoplus_{j=1}^n \mathrm{H}^2$. Let $\mathcal{A}_n(\mathrm{H}^2)$ be the closed $*$-subalgebra of $\mathcal{B}_n(\mathrm{H}^2)$ generated by $\{T_F \mid F \in C(\mathbb{T}, \mathbb{C}^{n\times n})\}$. It is a well-known result that the following mapping is $*$-isomorphic (see, for example, [Dou73, §1]);

$$C(\mathbb{T}, \mathbb{C}^{n\times n}) \ni F \longmapsto [T_F] \in \mathcal{A}_n(\mathrm{H}^2)/\mathcal{K}_n(\mathrm{H}^2).$$

That is, for each $F \in C(\mathbb{T}, \mathbb{C}^{n\times n})$ we have that F is invertible in $C(\mathbb{T}, \mathbb{C}^{n\times n})$ if and only if $[T_F]$ is invertible in the Calkin algebra $\mathcal{B}_n(\mathrm{H}^2)/\mathcal{K}_n(\mathrm{H}^2)$. The equality (II.45) follows. □

Let us consider two unitary operators $\mathcal{F}_{\mathrm{L}} : \mathrm{H}^2 \to \ell^2_{\mathrm{L}}(\mathbb{Z})$ and $\mathcal{F}_{\mathrm{R}} : \mathrm{H}^2 \to \ell^2_{\mathrm{R}}(\mathbb{Z})$ defined respectively by

$$\mathcal{F}_{\mathrm{L}} e_x := \delta_{-x-1}, \qquad \mathcal{F}_{\mathrm{R}} e_x := \delta_x, \qquad x \geq 0,$$

where $(\delta_x)_{x\in\mathbb{Z}}$, $(e_x)_{x\geq 0}$ are the standard bases of $\ell^2(\mathbb{Z}), \mathrm{H}^2$ respectively.

Lemma II.15. *Let A be a uniform operator on $\ell^2(\mathbb{Z}, \mathbb{C}^n)$ of the form* (II.39)*, and let $\hat{A}$ be given by* (II.40)*. Then*

$$\left(\bigoplus_{j=1}^n \mathcal{F}_\sharp^*\right) A_\sharp \left(\bigoplus_{j=1}^n \mathcal{F}_\sharp\right) = \begin{cases} T_{\hat{A}}, & \sharp = \mathrm{L}, \\ T_{\hat{A}(-^*)}, & \sharp = \mathrm{R}, \end{cases} \tag{II.46}$$

where $\hat{A}(-^*)$ denote the matrix-valued function $\mathbb{T} \ni z \longmapsto \hat{A}(z^*) \in \mathbb{C}^{n\times n}$.

Proof. Note first that the inverses of $\mathcal{F}_{\mathrm{L}}, \mathcal{F}_{\mathrm{R}}$ are given respectively by $\mathcal{F}_{\mathrm{L}}^{-1}\delta_x = \mathcal{F}_{\mathrm{L}}^*\delta_x = e_{-x-1}$ for each $x < 0$ and $\mathcal{F}_{\mathrm{R}}^{-1}\delta_x = \mathcal{F}_{\mathrm{R}}^*\delta_x = e_x$ for each $x \geq 0$. Let us first prove the following non-trivial equalities:

$$T_{e_y} = \mathcal{F}_{\mathrm{L}}^* \iota_{\mathrm{L}}^* L^y \iota_{\mathrm{L}} \mathcal{F}_{\mathrm{L}} = \mathcal{F}_{\mathrm{R}}^* \iota_{\mathrm{R}}^* L^{-y} \iota_{\mathrm{R}} \mathcal{F}_{\mathrm{R}}, \qquad y \in \mathbb{Z}. \tag{II.47}$$

Note that for each $y \geq 0$ and each $x \geq 0$ we have

$$T_{e_y} e_x = \iota^* M_{e_y} \iota e_x = \iota^* M_{e_y} e_x = \iota^* e_{x+y} = e_{x+y},$$

$$\mathcal{F}_{\mathrm{L}}^* \iota_{\mathrm{L}}^* L^y \iota_{\mathrm{L}} \mathcal{F}_{\mathrm{L}} e_x = \mathcal{F}_{\mathrm{L}}^* \iota_{\mathrm{L}}^* L^y \iota_{\mathrm{L}} \delta_{-x-1} = \mathcal{F}_{\mathrm{L}}^* \iota_{\mathrm{L}}^* \delta_{-x-y-1} = e_{x+y},$$

$$\mathcal{F}_{\mathrm{R}}^* \iota_{\mathrm{R}}^* L^{-y} \iota_{\mathrm{R}} \mathcal{F}_{\mathrm{R}} e_x = \mathcal{F}_{\mathrm{R}}^* \iota_{\mathrm{R}}^* L^{-y} \iota_{\mathrm{R}} \delta_x = \mathcal{F}_{\mathrm{R}}^* \iota_{\mathrm{R}}^* \delta_{x+y} = e_{x+y}.$$

That is, we have shown that (II.47) holds true for any $y \geq 0$. On the other hand, if $y < 0$, then $-y > 0$, and so

$$T_{e_y} = (T_{e_{-y}})^* = (\mathcal{F}_{\mathrm{L}}^* \iota_{\mathrm{L}}^* L^{-y} \iota_{\mathrm{L}} \mathcal{F}_{\mathrm{L}})^* = (\mathcal{F}_{\mathrm{R}}^* \iota_{\mathrm{R}}^* L^{y} \iota_{\mathrm{R}} \mathcal{F}_{\mathrm{R}})^*, \qquad y < 0.$$

That is, (II.47) holds true for any $y \in \mathbb{Z}$. Let

$$f_{ij}(z) := \sum_{y=-k}^{k} a_{ij}(y) z^y = \sum_{y=-k}^{k} a_{ij}(y) e_y(z), \qquad z \in \mathbb{T}.$$

Then the block-operator matrix representation of A is given by

$$A = \begin{pmatrix} \sum_{y=-k}^{k} a_{11}(y) L^y & \dots & \sum_{y=-k}^{k} a_{1n}(y) L^y \\ \vdots & \ddots & \vdots \\ \sum_{y=-k}^{k} a_{n1}(y) L^y & \dots & \sum_{y=-k}^{k} a_{nn}(y) L^y \end{pmatrix} = \begin{pmatrix} f_{11}(L) & \dots & f_{1n}(L) \\ \vdots & \ddots & \vdots \\ f_{n1}(L) & \dots & f_{nn}(L) \end{pmatrix}.$$

With the representation (II.35) in mind, we obtain

$$\left(\bigoplus_{j=1}^{n} \mathcal{F}_{\sharp}^* \right) A_{\sharp} \left(\bigoplus_{j=1}^{n} \mathcal{F}_{\sharp} \right) = \begin{pmatrix} \mathcal{F}_{\sharp}^* \iota_{\sharp}^* f_{11}(L) \iota_{\sharp} \mathcal{F}_{\sharp} & \dots & \mathcal{F}_{\sharp}^* \iota_{\sharp}^* f_{1n}(L) \iota_{\sharp} \mathcal{F}_{\sharp} \\ \vdots & \ddots & \vdots \\ \mathcal{F}_{\sharp}^* \iota_{\sharp}^* f_{n1}(L) \iota_{\sharp} \mathcal{F}_{\sharp} & \dots & \mathcal{F}_{\sharp}^* \iota_{\sharp}^* f_{nn}(L) \iota_{\sharp} \mathcal{F}_{\sharp} \end{pmatrix}_{\bigoplus_{j=1}^{n} \mathrm{H}^2}, \qquad \sharp = \mathrm{L}, \mathrm{R},$$

where (II.47) gives the following equalities for each $i, j \in \{1, \dots, n\}$:

$$\mathcal{F}_{\sharp}^* \iota_{\sharp}^* f_{ij}(L) \iota_{\sharp} \mathcal{F}_{\sharp} = \sum_{y=-k}^{k} a_{ij}(y) (\mathcal{F}_{\sharp}^* \iota_{\sharp}^* L^y \iota_{\sharp} \mathcal{F}_{\sharp}) = \begin{cases} \sum_{y=-k}^{k} a_{ij}(y) T_{e_y} = T_{f_{ij}}, & \sharp = \mathrm{L}, \\ \sum_{y=-k}^{k} a_{ij}(y) T_{e_y}^* = T_{f_{ij}(-^*)}, & \sharp = \mathrm{R}. \end{cases}$$

It follows that (II.46) holds true, since the Toeplitz operator $T_{\hat{A}}$ is given by (II.43) with $F := \hat{A}$. □

Proof of Theorem II.13. Let A be a uniform operator on $\ell^2(\mathbb{Z}, \mathbb{C}^n)$ of the form (II.39), and let $\hat{A}$ be given by (II.40). It follows from (II.46) that $A_{\mathrm{L}} \cong T_{\hat{A}}$ and $A_{\mathrm{R}} \cong T_{\hat{A}(-^*)}$, where $\cong$ denotes unitary equivalence. The Fredholmness and essential spectra are invariant under unitary transforms.

(i) It follows from Corollary II.11 (i) that the operator A is Fredholm if and only if $A_{\mathrm{L}} \cong T_{\hat{A}}, A_{\mathrm{R}} \cong T_{\hat{A}(-^*)}$ are both Fredholm, and in this case we have $\operatorname{ind} A = \operatorname{ind} T_{\hat{A}} + \operatorname{ind} T_{\hat{A}(-^*)}$. On the other hand, it follows from Theorem II.14 (i) that $A_{\mathrm{L}} \cong T_{\hat{A}}$ is Fredholm if and only if $A_{\mathrm{R}} \cong T_{\hat{A}(-^*)}$ is Fredholm if and only if $\det \hat{A}$ is nowhere vanishing. In this case, we have $\operatorname{ind} A_{\mathrm{L}} = -\operatorname{wn}\left(\det \hat{A}\right)$ and $\operatorname{ind} A_{\mathrm{R}} = -\operatorname{wn}\left(\det \hat{A}(-^*)\right)$. Therefore,

$$\operatorname{ind} A = \operatorname{ind} A_{\mathrm{L}} + \operatorname{ind} A_{\mathrm{R}} = -\operatorname{wn}\left(\det \hat{A}\right) - \operatorname{wn}\left(\det \hat{A}(-^*)\right) = -\operatorname{wn}\left(\det \hat{A}\right) + \operatorname{wn}\left(\det \hat{A}\right) = 0.$$

(ii) It follows from Corollary II.11 (ii) that $\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(A_{\mathrm{L}}) \cup \sigma_{\mathrm{ess}}(A_{\mathrm{R}})$, where $A_{\mathrm{L}} \cong T_{\hat{A}}, A_{\mathrm{R}} \cong T_{\hat{A}(-^*)}$. It follows from Theorem II.14 (ii) that

$$\sigma_{\mathrm{ess}}(A_{\mathrm{L}}) = \sigma_{\mathrm{ess}}(T_{\hat{A}}) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{A}(z)\right) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{A}(z^*)\right) = \sigma_{\mathrm{ess}}\left(T_{\hat{A}(-^*)}\right) = \sigma_{\mathrm{ess}}(A_{\mathrm{R}}),$$

where the third equality follows from the fact that the ranges of $\hat{A}, \hat{A}(-^*)$ are identical. $\square$

II.2.4 Proof of the main theorem (Theorem II.8)

For each $m \in \mathbb{N}$ the operator $\tau_m : \bigoplus_{j=1}^m \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ is defined as the *inverse* of the following unitary operator

$$\ell^2(\mathbb{Z}) \ni \psi \longmapsto \begin{pmatrix} \psi(m\cdot) \\ \vdots \\ \psi(m\cdot + m - 1) \end{pmatrix} \in \bigoplus_{j=1}^m \ell^2(\mathbb{Z}). \tag{II.48}$$

In particular, τ_1 is the identity operator on $\ell^2(\mathbb{Z})$. Similarly, for each $\sharp = \mathrm{L}, \mathrm{R}$ and each $m \in \mathbb{N}$ we define the operator $\tau_{\sharp,m} : \bigoplus_{j=1}^m \ell^2_\sharp(\mathbb{Z}) \to \ell^2_\sharp(\mathbb{Z})$ by

$$\tau_{\sharp,m} := \iota_\sharp^* \tau_m \left(\bigoplus_{j=1}^m \iota_\sharp\right).$$

It is easy to see that $\tau_{\sharp,m}$ is a unitary operator, since its inverse $\tau_\sharp^* = \left(\bigoplus_{j=1}^m \iota_\sharp^*\right) \tau_m^* \iota_\sharp$ is given explicitly by the following formula;

$$\ell^2_\sharp(\mathbb{Z}) \ni \psi \longmapsto \begin{pmatrix} \psi(m\cdot) \\ \vdots \\ \psi(m\cdot + m - 1) \end{pmatrix} \in \bigoplus_{j=1}^m \ell^2_\sharp(\mathbb{Z}), \tag{II.49}$$

where $\psi(m\cdot), \dots, \psi(m\cdot + m - 1) \in \ell^2_\sharp(\mathbb{Z})$.

Lemma II.16. *If $a = (a(x))_{x\in\mathbb{Z}}$ is a bounded $\mathbb{C}$-valued sequence, identified with the associated multiplication* *operator on $\ell^2(\mathbb{Z})$, then for each $n \in \mathbb{N}$ we have*

$$\tau_n^* a \tau_n = \begin{pmatrix} a(n\cdot) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a(n\cdot+n-1) \end{pmatrix}, \tag{II.50}$$

$$\tau_n^* L \tau_n = \begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ L & 0 & \dots & 0 \end{pmatrix}, \tag{II.51}$$

where $\mathbf{1}$ is the identity operator on $\bigoplus_{j=1}^{n-1} \ell^2(\mathbb{Z})$.

Proof. For each $\psi \in \ell^2(\mathbb{Z})$ we have

$$\tau_n^* a\psi = \begin{pmatrix} a(n\cdot)\psi(n\cdot) \\ \vdots \\ a(n\cdot+n-1)\psi(n\cdot+n-1) \end{pmatrix} = \begin{pmatrix} a(n\cdot) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a(n\cdot+n-1) \end{pmatrix} \tau_n^*\psi,$$

$$\tau_n^* L\psi = \begin{pmatrix} \psi(n\cdot+1) \\ \vdots \\ \psi(n\cdot+n) \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ L & 0 & 0 & \dots & 0 \end{pmatrix} \tau_n^*\psi.$$

The claim follows. □

Corollary II.17. *For each $\sharp = \mathrm{L}, \mathrm{R}$ and each $n \in \mathbb{N}$, we have $\tau_n^* P_\sharp \tau_n = \bigoplus_{j=1}^n P_\sharp$.*

Proof. For each $\sharp = \mathrm{L}, \mathrm{R}$, we can identify $P_\sharp$ with the multiplication operator $\delta_\sharp$. It follows from (II.50) that

$$\tau_n^* \delta_\sharp \tau_n = \begin{pmatrix} \delta_\sharp(n\cdot) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \delta_\sharp(n\cdot+n-1) \end{pmatrix},$$

where $\delta_\sharp(n\cdot) = \cdots = \delta_\sharp(n\cdot+n-1) = \delta_\sharp$. Therefore, $\tau_n^* P_\sharp \tau_n = \bigoplus_{j=1}^n P_\sharp$. □

In fact, the special case of Theorem II.8 where $n_{\mathrm{L}} = n_{\mathrm{R}}$ can be easily proved by making use of Lemma II.16. As for the general case $n_{\mathrm{L}} \neq n_{\mathrm{R}}$, we require the following non-trivial fact;

Lemma II.18. *For each* $\sharp = \mathrm{L}, \mathrm{R}$ *and each* $m \in \mathbb{N}$, *we have*

$$\left(\bigoplus_{j=1}^{n} \tau_{\sharp,m}^{*}\right) A_{\sharp} \left(\bigoplus_{j=1}^{n} \tau_{\sharp,m}\right) = \left(\left(\bigoplus_{j=1}^{n} \tau_{m}^{*}\right) A \left(\bigoplus_{j=1}^{n} \tau_{m}\right)\right)_{\sharp}. \tag{II.52}$$

More explicitly, the $m \times n$*-dimensional strictly local operator* $\left(\bigoplus_{j=1}^{n} \tau_{m}^{*}\right) A \left(\bigoplus_{j=1}^{n} \tau_{m}\right)$ *coincides with the block-operator matrix* $B(m)$ *defined by the following formulas:*

$$B(m) := \begin{pmatrix} B_{11}(m) & \cdots & B_{1n}(m) \\ \vdots & \ddots & \vdots \\ B_{n1}(m) & \cdots & B_{nn}(m) \end{pmatrix}, \tag{II.53}$$

$$B_{ij}(m) := \sum_{k=-k_0}^{k_0} \begin{pmatrix} a_{ij}^{k}(m\cdot) & 0 & \dots & 0 \\ 0 & a_{ij}^{k}(m\cdot+1) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & a_{ij}^{k}(m\cdot+m-1) \end{pmatrix} \begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ L & 0 & \cdots & 0 \end{pmatrix}^{k}, \tag{II.54}$$

where $\mathbf{1}$ *denotes the identity operator of dimension* $m-1$.

The formula (II.52) shows that $\sharp$-compression and τ_m-unitary transforms can be interchanged.

Proof. Note that A can be expresses as a block-operator matrix form $A = (A_{ij})$ according to (II.35), where

$$A_{ij} := \sum_{k=-k_0}^{k_0} a_{ij}^{k} L^{k}.$$

Note that the left-hand side of (II.52) becomes;

$$\left(\bigoplus_{j=1}^{n} \tau_{\sharp,m}^{*}\right) A_{\sharp} \left(\bigoplus_{j=1}^{n} \tau_{\sharp,m}\right) = \begin{pmatrix} \tau_{\sharp,m}^{*}(\iota_{\sharp}^{*} A_{11} \iota_{\sharp})\tau_{\sharp,m} & \cdots & \tau_{\sharp,m}^{*}(\iota_{\sharp} A_{1n} \iota_{\sharp})\tau_{\sharp,m} \\ \vdots & \ddots & \vdots \\ \tau_{\sharp,m}^{*}(\iota_{\sharp}^{*} A_{n1} \iota_{\sharp})\tau_{\sharp,m} & \cdots & \tau_{\sharp,m}^{*}(\iota_{\sharp}^{*} A_{nn} \iota_{\sharp})\tau_{\sharp,m} \end{pmatrix}_{\bigoplus_{j=1}^{n} \ell_{\sharp}^{2}(\mathbb{Z},\mathbb{C}^{m})}.$$

Note that for each i, j we obtain

$$\begin{aligned}\tau_{\sharp,m}^*(\iota_\sharp^* A_{ij}\iota_\sharp)\tau_{\sharp,m} &= \left(\bigoplus_{j=1}^m \iota_\sharp^*\right)\tau_m^*\iota_\sharp(\iota_\sharp^* A_{ij}\iota_\sharp)\iota_\sharp^*\tau_m\left(\bigoplus_{j=1}^m \iota_\sharp\right)\\ &= \left(\bigoplus_{j=1}^m \iota_\sharp^*\right)\tau_m^* P_\sharp A_{ij} P_\sharp \tau_m\left(\bigoplus_{j=1}^m \iota_\sharp\right)\\ &= \left(\bigoplus_{j=1}^m \iota_\sharp^*\right)\left(\bigoplus_{j=1}^m P_\sharp\right)\tau_m^* A_{ij}\tau_m\left(\bigoplus_{j=1}^m P_\sharp\right)\left(\bigoplus_{j=1}^m \iota_\sharp\right)\\ &= \left(\bigoplus_{j=1}^m \iota_\sharp^*\right)\tau_m^* A_{ij}\tau_m\left(\bigoplus_{j=1}^m \iota_\sharp\right),\end{aligned}$$

where the second last equality follows from Corollary II.17 and the last equality follows from $\iota_\sharp^*\iota_\sharp = 1$. Therefore, (II.52) holds true. Now,

$$\tau_m^* A_{ij}\tau_m = \sum_{k=-k_0}^{k_0} \tau_m^* a_{ij}^k L^k \tau_m = \sum_{k=-k_0}^{k_0} \tau_m^* a_{ij}^k \tau_m (\tau_m^* L \tau_m)^k.$$

The claim follows from Lemma II.16. □

Lemma II.19. *For each* $\sharp = \mathrm{L}, \mathrm{R}$ *let*

$$A(\sharp) := \begin{pmatrix} A_{11}(\sharp) & \dots & A_{1n}(\sharp)\\ \vdots & \ddots & \vdots \\ A_{1n}(\sharp) & \dots & A_{nn}(\sharp)\end{pmatrix},$$

$$A_{ij}(\sharp) := \sum_{k=-k_0}^{k_0} \begin{pmatrix} a_{ij}^k(\sharp,0) & 0 & \dots & 0\\ 0 & a_{ij}^k(\sharp,1) & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & \dots & \dots & a_{ij}^k(\sharp, n_\sharp - 1)\end{pmatrix}\begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ L & 0 & \dots & 0\end{pmatrix}^k,$$

where $\mathbf{1}$ *denotes the identity operator of dimension* $n_\sharp - 1$. *Then the following operators are compact;*

$$\left(\bigoplus_{j=1}^n \tau_{\sharp,n_\sharp}^*\right) A_\sharp \left(\bigoplus_{j=1}^n \tau_{\sharp,n_\sharp}\right) - A(\sharp)_\sharp, \qquad \sharp = \mathrm{L}, \mathrm{R}.$$

Note that $\hat{A}(\sharp, z)$ defined by (II.33) is nothing but the Fourier transform of $A(\sharp)$.

Proof. It follows from Lemma II.18 that

$$\left(\bigoplus_{j=1}^{n} \tau^*_{\sharp,n_\sharp}\right) A_\sharp \left(\bigoplus_{j=1}^{n} \tau_{\sharp,n_\sharp}\right) - A(\sharp)_\sharp = \big(B(n_\sharp) - A(\sharp)\big)_\sharp ,$$

where $B(n_\sharp) - A(\sharp) = (B_{ij}(n_\sharp) - A_{ij}(\sharp))_{i,j}$. Since $\bigoplus_{j=1}^{n_\sharp} \iota_\sharp^* = \bigoplus_{j=1}^{n_\sharp} \iota_\sharp^* \bigoplus_{j=1}^{n_\sharp} P_\sharp$, it remains to show that $C_{ij}(\sharp) := \left(\bigoplus_{j'=1}^{n_\sharp} P_\sharp\right) \left(B_{ij}(n_\sharp) - A_{ij}(\sharp)\right)$ is compact. We obtain

$$C_{ij}(\sharp) = \sum_{k=-k_0}^{k_0} \begin{pmatrix} \delta_\sharp(a^k_{ij}(\sharp,0) - a^k_{ij}(n_\sharp \bullet)) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \delta_\sharp(a^k_{ij}(n_\sharp \bullet + n_\sharp - 1) - a^k_{ij}(\sharp, n_\sharp - 1)) \end{pmatrix} \begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ L & 0 & \cdots & 0 \end{pmatrix}^k ,$$

where the last equality follows from Lemma II.16. Note that each $\delta_\sharp a^k_{ij}(n_\sharp \bullet + j)$ has the following 2-sided limits:

$$\lim_{x\to-\infty} \delta_\sharp(x) a^k_{ij}(n_\sharp x + j) = \begin{cases} a^k_{ij}(-\infty, j), & \sharp = \mathrm{L}, \\ 0, & \sharp = \mathrm{R}, \end{cases}$$

$$\lim_{x\to+\infty} \delta_\sharp(x) a^k_{ij}(n_\sharp x + j) = \begin{cases} 0, & \sharp = \mathrm{L}, \\ a^k_{ij}(+\infty, j), & \sharp = \mathrm{R}. \end{cases}$$

It follows that $\delta_\sharp(x)(a^k_{ij}(\sharp, j) - a^k_{ij}(n_\sharp x + j)) \to 0$ as $x \to \pm\infty$. The claim follows. □

Proof of Theorem II.8. Note that $A - A_\mathrm{L} \oplus A_\mathrm{R}$ is finite rank by [Tan21, Corollary 2.2]. Since the Fredholm index and essential spectrum are invariant under compact perturbations, it suffices to consider $A' := A_\mathrm{L} \oplus A_\mathrm{R}$ from here on. It follows from Lemma II.19 that the following difference is compact;

$$\left(\bigoplus_{j=1}^{n} \tau^*_{\sharp,n_\sharp}\right) A_\sharp \left(\bigoplus_{j=1}^{n} \tau_{\sharp,n_\sharp}\right) - A(\sharp)_\sharp .$$

(i) Since the Fredholmness is invariant under unitary transforms and compact perturbations, we have that A' is Fredholm if and only if $A(\mathrm{L})_\mathrm{L}, A(\mathrm{R})_\mathrm{R}$ are Fredholm. In this case,

$$\operatorname{ind} A' = \operatorname{ind} A(\mathrm{L})_\mathrm{L} + \operatorname{ind} A(\mathrm{R})_\mathrm{R}.$$

On the other hand, it follows from [Tan21, Theorem 2.4] (i) that for each $\sharp = \mathrm{L}, \mathrm{R}$ the operator $A(\sharp)_\sharp$ is Fredholm if and only if $\mathbb{T} \ni z \longmapsto \det \hat{A}(\sharp, z) \in \mathbb{C}$ is nowhere vanishing on $\mathbb{T}$. In this case, the Fredholm index of $A(\sharp)_\sharp$ is given by

$$\mathrm{ind}\, A(\sharp)_\sharp = \begin{cases} \mathrm{wn}\left(\det \hat{A}(+\infty, \cdot)\right), & \sharp = \mathrm{R}, \\ -\mathrm{wn}\left(\det \hat{A}(-\infty, \cdot)\right), & \sharp = \mathrm{L}. \end{cases}$$

The claim follows.

(ii) Since the essential spectrum is invariant under unitary transforms and compact perturbations, we have

$$\sigma_{\mathrm{ess}}(A') = \sigma_{\mathrm{ess}}(A(\mathrm{L})_{\mathrm{L}}) \cup \sigma_{\mathrm{ess}}(A(\mathrm{R})_{\mathrm{R}}) = \bigcup_{z \in \mathbb{T}} \sigma\left(\hat{A}(\mathrm{R}, z)\right) \cup \bigcup_{z \in \mathbb{T}} \sigma\left(\hat{A}(\mathrm{L}, z)\right),$$

where the last equality follows from (II.25). □

II.3 Proof of the index formula (Theorem A (i))

The following theorem is a slightly more general version of Theorem A (i);

Theorem II.20. *Let* $(\Gamma, U) = (\Gamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ *be defined by* (I.2), (I.3). *Suppose that there exist* $n_{-\infty}, n_{+\infty} \in \mathbb{N}$ *with the property that limits of the form* (I.10) *exist for each* $\zeta = p, a$, *and each* $\star = -\infty, +\infty$. *Then the following assertions hold true:*

(i) *Then* $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ *if and only if for each* $\star = -\infty, +\infty$

$$\prod_{m=0}^{n_\star - 1} (1 + p(\star, m))(1 \mp a(\star, m)) \neq \prod_{m=0}^{n_\star - 1} (1 - p(\star, m))(1 \pm a(\star, m)). \tag{II.55}$$

(ii) *Let us impose the following condition;*

$$\prod_{m=0}^{n_\star - 1} (1 + p(\star, m))(1 \mp a(\star, m)) + \prod_{m=0}^{n_\star - 1} (1 - p(\star, m))(1 \pm a(\star, m)) > 0. \tag{II.56}$$

For each $\star = -\infty, +\infty$ *let* $p(\star), a(\star) \in [-1, 1]$ *be uniquely defined through* (I.12). *Then* $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ *if and only if* $p(\pm\infty) \neq \pm a(\pm\infty)$. *In this case,* $\mathrm{ind}_\pm(\Gamma, U)$ *is given by* (I.9).

Theorem II.20 (i) states that the assumption (II.56) is a necessary condition for $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$. With the convention (I.24) in mind, the assumption (II.56) ensures that the left-hand side of (I.12) is a well-defined number in $[0,\infty]$, since the problematic case $0/0$ never occurs. It follows that for each $\zeta(\star) \in \{p(\star), a(\star)\}$, the number $\zeta(\star) \in [-1,1]$ can be uniquely defined through (I.12). We shall make use of the following remark to prove Theorem II.20;

Remark II.21. Suppose that $A = \alpha_{-1}L^{-1} + \alpha_0 + \alpha_1 L$ is a one-dimensional strictly local operator, and that there exist $n_{-\infty}, n_{+\infty} \in \mathbb{N}$ with the property that the following limits exist for each $\star = -\infty, +\infty$;

$$\alpha_j(\star, m) := \lim_{x\to\star} \alpha_j(n_\star \cdot x + m), \qquad j = -1,0,1, \qquad m \in \{0,\dots,n_\star - 1\}.$$

We introduce the following matrices according to (II.32) to (II.33) for each $\star = -\infty, +\infty$;

$$\hat{A}(\star, z) := \sum_{j=-1,0,1} \begin{pmatrix} \alpha_j(\star,0) & 0 & 0 & 0 \\ 0 & \alpha_j(\star,1) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \alpha_j(\star, n_\star - 1) \end{pmatrix} \begin{pmatrix} 0 & & & \\ \vdots & & \mathbf{1} & \\ 0 & & & \\ z & 0 & \dots & 0 \end{pmatrix}^j, \qquad z \in \mathbb{T}, \tag{II.57}$$

where $\mathbf{1}$ denotes the identity matrix of dimension $n_\star - 1$. Note that each $\hat{A}(\star, z)$ admits the following explicit representation;

$$\hat{A}(\star,z) = \begin{cases} \alpha_{-1}(\star,0)z^* + \alpha_0(\star,0) + \alpha_1(\star,0)z, & n_\star = 1, \\ \begin{pmatrix} \alpha_0(\star,0) & \alpha_{-1}(\star,0)z^* + \alpha_1(\star,0) \\ \alpha_{-1}(\star,1) + \alpha_1(\star,1)z & \alpha_0(\star,1) \end{pmatrix}, & n_\star = 2, \\ \begin{pmatrix} \alpha_0(\star,0) & \alpha_1(\star,0) & 0 & \cdots & 0 & \alpha_{-1}(\star,0)z^* \\ \alpha_{-1}(\star,1) & \alpha_0(\star,1) & \alpha_1(\star,1) & \cdots & 0 & 0 \\ 0 & \alpha_{-1}(\star,2) & \alpha_0(\star,2) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha_0(\star,n_\star-2) & \alpha_1(\star,n_\star-2) \\ \alpha_1(\star,n_\star-1)z & 0 & 0 & \cdots & \alpha_{-1}(\star,n_\star-1) & \alpha_0(\star,n_\star-1) \end{pmatrix}, & n_\star \geq 3. \end{cases} \tag{II.58}$$

Lemma II.22. *If $(\varGamma, U) = (\varGamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ is defined by* (I.3) *and* (I.2)*, then there exist two unitary operators ϵ, η on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, such that the following four decompositions hold true:*

$$\epsilon^* \varGamma \epsilon = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \epsilon^* U_{\mathrm{suz}} \epsilon = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (\eta^*\epsilon)^* \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (\eta^*\epsilon), \tag{II.59}$$

$$\eta^* \varGamma' \eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \eta^* U_{\mathrm{suz}} \eta = (\eta^*\epsilon) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (\eta^*\epsilon)^* \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{II.60}$$

More explicitly, if we let $\zeta_\pm := \sqrt{1 \pm \zeta}$ for each $\zeta = p, a$, then the unitary operators ϵ, η are given respectively by

$$\epsilon := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix}\begin{pmatrix} p_+ & -p_- \\ p_- & p_+ \end{pmatrix}, \qquad \eta := \frac{1}{\sqrt{2}}\begin{pmatrix} a_+ & -a_- \\ a_- & a_+ \end{pmatrix}. \tag{II.61}$$

Proof. Note first that we have the following unitary diagonalisation for each $\zeta = p, a$ and each $x \in \mathbb{Z}$ (see, for example, [Tan21, Example 3.1]);

$$\begin{pmatrix} \frac{\zeta_+(x)}{\sqrt{2}} & \frac{-\zeta_-(x)}{\sqrt{2}} \\ \frac{\zeta_-(x)}{\sqrt{2}} & \frac{\zeta_+(x)}{\sqrt{2}} \end{pmatrix}^* \begin{pmatrix} \zeta(x) & \sqrt{1-\zeta(x)^2} \\ \sqrt{1-\zeta(x)^2} & -\zeta(x) \end{pmatrix}\begin{pmatrix} \frac{\zeta_+(x)}{\sqrt{2}} & \frac{-\zeta_-(x)}{\sqrt{2}} \\ \frac{\zeta_-(x)}{\sqrt{2}} & \frac{\zeta_+(x)}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

This result motivates us to introduce the unitary operators ϵ, η defined by (II.61). Indeed,

$$\epsilon^*\varGamma\epsilon = \begin{pmatrix} \frac{p_+}{\sqrt{2}} & \frac{-p_-}{\sqrt{2}} \\ \frac{p_-}{\sqrt{2}} & \frac{p_+}{\sqrt{2}} \end{pmatrix}^* \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix}\begin{pmatrix} \frac{p_+}{\sqrt{2}} & \frac{-p_-}{\sqrt{2}} \\ \frac{p_-}{\sqrt{2}} & \frac{p_+}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\eta^*\varGamma'\eta = \begin{pmatrix} \frac{a_+}{\sqrt{2}} & \frac{-a_-}{\sqrt{2}} \\ \frac{a_-}{\sqrt{2}} & \frac{a_+}{\sqrt{2}} \end{pmatrix}^* \begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix}\begin{pmatrix} \frac{a_+}{\sqrt{2}} & \frac{-a_-}{\sqrt{2}} \\ \frac{a_-}{\sqrt{2}} & \frac{a_+}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

On the other hand,

$$\epsilon^* U_{\mathrm{suz}}\epsilon = \epsilon^*\varGamma\varGamma'\epsilon = (\epsilon^*\varGamma\epsilon)(\epsilon^*\eta)(\epsilon^*\varGamma\epsilon)(\eta^*\epsilon) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}(\eta^*\epsilon)^*\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}(\eta^*\epsilon),$$

$$\eta^* U_{\mathrm{suz}}\eta = \eta^*\varGamma\varGamma'\eta = (\eta^*\epsilon)(\eta^*\varGamma'\eta)(\epsilon^*\eta)(\eta^*\varGamma'\eta) = (\eta^*\epsilon)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}(\eta^*\epsilon)^*\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

□

With the notation introduced in Lemma II.22, it is easy to see that the operator $F := \eta^*\epsilon$ is given explicitly by

$$F = \frac{1}{2}\begin{pmatrix} p_+a_+ + a_-L^*p_- & -p_-a_+ + a_-L^*p_+ \\ -p_+a_- + a_+L^*p_- & p_-a_- + a_+L^*p_+ \end{pmatrix} =: \begin{pmatrix} F_{1,-} & F_{2,+} \\ F_{1,+} & F_{2,-} \end{pmatrix}. \tag{II.62}$$

It follows from [CGWW21, Lemma 3.2] that $U \mp 1$ is Fredholm if and only if $F_{1,\pm}, F_{2,\pm}$ are Fredholm. In this case, we have

$$\operatorname{ind}_\pm(\varGamma, U) = \operatorname{ind}_\pm(\epsilon^*\varGamma\epsilon, \epsilon^*U\epsilon) = \operatorname{ind} F_{1,\pm} = -\operatorname{ind} F_{2,\pm},$$

where the first equality follows from the unitary invariance of the indices $\mathrm{ind}_{\pm}$, and where the last two equalities follow from [CGWW21, Lemma 3.2]. Therefore, it remains to compute the Fredholm index of the strictly local operators $F_{1,\pm} = \mp p_+ a_\mp + p_-(\cdot - 1)a_\pm L^*$ with the aid of the following lemma;

Lemma II.23. *Let $\alpha, \beta \in \mathbb{R}$, and let $f(z) := \alpha + \beta z^*$ for each $z \in \mathbb{T}$. Then f is nowhere vanishing if and only if $|\alpha| \neq |\beta|$. In this case, we have*

$$\mathrm{wn}(f) = \begin{cases} -1, & |\alpha| < |\beta|, \\ 0, & |\alpha| > |\beta|. \end{cases}$$

Proof. On one hand, if $\beta = 0$, then the constant function $f = \alpha$ is nowhere vanishing with $\mathrm{wn}(f) = 0$ if and only if $|\alpha| \neq 0$. On the other hand, if $\beta \neq 0$, then the image of f is the circle centred at α with the non-zero radius $|\beta|$. Note that the intersection of the circle and the real line $\mathbb{R}$ is the two-point set $\{\alpha - |\beta|, \alpha + |\beta|\}$. It follows that f is nowhere vanishing if and only if $|\alpha| \neq |\beta|$, where the winding number of f is either -1 or 0. We have $\mathrm{wn}(f) = -1$ if and only if $\alpha - |\beta| < 0 < \alpha + |\beta|$ if and only if $|\alpha| < |\beta|$. Similarly, $\mathrm{wn}(f) = 0$ if and only if $|\alpha| > |\beta|$. □

Proof of Theorem II.20. Note first that the formula (I.9) can be rewritten as

$$\mathrm{ind}_{\pm}(\varGamma, U) = \frac{\mathrm{sign}\,(p(+\infty) \mp a(+\infty)) - \mathrm{sign}\,(p(-\infty) \mp a(-\infty))}{2}, \tag{II.63}$$

where the sign function sign is defined by (I.28).

For each $\zeta = p, a$, and each $\star = -\infty, +\infty$, let

$$\zeta_\pm(\star, m) := \sqrt{1 \pm \zeta(\star, m)}, \qquad m \in \{0, \dots, n_\star - 1\}.$$

If we let $f_{0,\pm} := \mp p_+ a_\mp$ and $f_{-1,\pm} := p_-(\cdot - 1)a_\pm$, then $F_{1,\pm} = f_{-1,\pm}L^* + f_{0,\pm} + 0L$. For each $z \in \mathbb{T}$ we introduce the following matrix according to (II.58);

$$2\hat{F}_{1,\pm}(\star, z) := \begin{cases} f_{0,\pm}(\star, 0) + f_{-1,\pm}(\star, 0)z^*, & n_\star = 1, \\ \begin{pmatrix} f_{0,\pm}(\star,0) & f_{-1,\pm}(\star,0)z^* \\ f_{-1,\pm}(\star,1) & f_{0,\pm}(\star,1) \end{pmatrix}, & n_\star = 2, \\ \begin{pmatrix} f_{0,\pm}(\star,0) & 0 & 0 & \cdots & 0 & f_{-1,\pm}(\star,0)z^* \\ f_{-1,\pm}(\star,1) & f_{0,\pm}(\star,1) & 0 & \cdots & 0 & 0 \\ 0 & f_{-1,\pm}(\star,2) & f_{0,\pm}(\star,2) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & f_{0,\pm}(\star,n_\star-2) & 0 \\ 0 & 0 & 0 & \cdots & f_{-1,\pm}(\star,n_\star-1) & f_{0,\pm}(\star,n_\star-1) \end{pmatrix}, & n_\star \geq 3. \end{cases}$$

(i) Note first that the following equality holds true, if $n_\star = 1, 2$;

$$\det(2\hat{F}_{1,\pm}(\star, z)) = \prod_{m=0}^{n_\star-1} f_{0,\pm}(\star, m) + (-1)^{n_\star+1} \left(\prod_{m=0}^{n_\star-1} f_{-1,\pm}(\star, m) \right) z^*. \tag{II.64}$$

In fact, the co-factor expansion easily allows us to prove that (II.64) also holds true for any $n_\star \geq 3$, since the determinant of any triangular matrix is the product of its diagonal entries. It follows from (II.64) that

$$\det(2\hat{F}_{1,\pm}(\star, z)) = \prod_{m=0}^{n_\star-1} \mp p_+(\star, m)a_\mp(\star, m) + \left((-1)^{n_\star+1} \prod_{m=0}^{n_\star-1} p_-(\star, m)a_\pm(\star, m) \right) z^*,$$

since $p'_- := p_-(\cdot - 1)$ satisfies

$$\prod_{m=0}^{n_\star-1} p'_-(\star, m) = p_-(\star, n_\star - 1)p_-(\star, 0) \dots p_-(\star, n_\star - 2) = \prod_{m=0}^{n_\star-1} p_-(\star, m).$$

It follows from Lemma II.23 that $z \longmapsto \det \hat{F}_{1,\pm}(\star, z)$ is nowhere vanishing if and only if (II.55) holds true for each $\star = -\infty, +\infty$, since

$$\prod_{m=0}^{n_\star-1} \mp p_+(\star, m)a_\mp(\star, m) = (\mp 1)^{n_\star} \left(\prod_{m=0}^{n_\star-1} (1 + p(\star, m))(1 \mp a(\star, m)) \right)^{1/2},$$

$$(-1)^{n_\star+1} \prod_{m=0}^{n_\star-1} p_-(\star, m)a_\pm(\star, m) = (-1)^{n_\star+1} \left(\prod_{m=0}^{n_\star-1} (1 - p(\star, m))(1 \pm a(\star, m)) \right)^{1/2}.$$

Moreover, if (II.55) holds true, then $w_\pm(\star) := \mathrm{wn}(\det \hat{F}_{1,\pm}(\star, \cdot))$ is given by

$$w_\pm(\star) = \begin{cases} -1, & \prod_{m=0}^{n_\star-1} (1 + p(\star, m))(1 \mp a(\star, m)) < \prod_{m=0}^{n_\star-1} (1 - p(\star, m))(1 \pm a(\star, m)), \\ 0, & \prod_{m=0}^{n_\star-1} (1 + p(\star, m))(1 \mp a(\star, m)) > \prod_{m=0}^{n_\star-1} (1 - p(\star, m))(1 \pm a(\star, m)). \end{cases} \tag{II.65}$$

(ii) We shall make use of (I.25) throughout this proof. Suppose that (II.56) holds true. Note that

$$\Lambda(-\zeta(\star))^{n_\star} = (\Lambda(\zeta(\star))^{n_\star})^{-1} = \left(\frac{\prod_{m=0}^{n_\star-1}(1+\zeta(\star,m))}{\prod_{m=0}^{n_\star-1}(1-\zeta(\star,m))}\right)^{-1} = \frac{\prod_{m=0}^{n_\star-1}(1-\zeta(\star,m))}{\prod_{m=0}^{n_\star-1}(1+\zeta(\star,m))}.$$

We consider

$$\prod_{m=0}^{n_\star-1}(1+p(\star,m))\prod_{m=0}^{n_\star-1}(1\mp a(\star,m)) \lesseqgtr \prod_{m=0}^{n_\star-1}(1-p(\star,m))\prod_{m=0}^{n_\star-1}(1\pm a(\star,m)), \tag{II.66}$$

where the notation $\lesseqgtr$ simultaneously denotes the three binary relations $>, =, <$. On one hand, if $\prod_{m=0}^{n_\star-1}(1-p(\star,m))(1\pm a(\star,m)) > 0$, then (II.66) is equivalent to

$$\Lambda(p(\star))^{n_\star}\Lambda(\mp a(\star))^{n_\star} \lesseqgtr 1 \text{ if and only if } \Lambda(p(\star))\Lambda(\mp a(\star)) \lesseqgtr 1 \text{ if and only if } p(\star)\mp a(\star) \lesseqgtr 0,$$

where the first equivalence follows from the fact that $[0,\infty] \ni s \longmapsto s^{n_\star} \in [0,\infty]$ is an increasing function. On the other hand, if $\prod_{m=0}^{n_\star-1}(1+p(\star,m))(1\mp a(\star,m)) \neq 0$, then (II.66) is equivalent to

$$1 \lesseqgtr \Lambda(-p(\star))^{n_\star}\Lambda(\pm a(\star))^{n_\star} \text{ if and only if } 0 \lesseqgtr -p(\star)\pm a(\star) \text{ if and only if } p(\star)\mp a(\star) \lesseqgtr 0.$$

It follows that (II.66) is equivalent to $p(\star)\mp a(\star) \lesseqgtr 0$. It follows from (i) that $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ if and only if $p(\star)\mp a(\star) \neq 0$. In this case, (II.65) becomes

$$\begin{aligned} w_\pm(\star) &= \begin{cases} -1, & p(\star)\mp a(\star) < 0, \\ 0, & p(\star)\mp a(\star) > 0, \end{cases} \\ &= \frac{\operatorname{sign}(p(\star)\mp a(\star)) - 1}{2}. \end{aligned}$$

We obtain (II.63) as follows;

$$\operatorname{ind}_\pm(\Gamma, U) = w_\pm(+\infty) - w_\pm(-\infty) = \frac{\operatorname{sign}(p(+\infty)\mp a(+\infty)) - \operatorname{sign}(p(-\infty)\mp a(-\infty))}{2}.$$

The claim follows. □

Proof of Theorem A (i). The claim immediately follows from Theorem II.20. □

II.4 Proof of the exponential decay property (Theorem A (ii))

We shall obtain Theorem A (ii) as a special case of the following result;

Theorem II.24. *Let $U = U_{\mathrm{suz}}$ be the evolution operator of Suzuki's split-step quantum walk given by* (I.3)*, and let the following inequality hold true for each $\zeta = p, a$;*

$$\sup_{x \in \mathbb{Z}} |\zeta(x)| < 1. \tag{II.67}$$

With (I.25) *in mind, let us introduce the following notation for each $j = 1, 2$:*

$$\delta_{j,\pm}(y) := \pm\sqrt{\Lambda((-1)^j p(y))\Lambda(\mp(-1)^j a(y))}, \qquad y \in \mathbb{Z}, \tag{II.68}$$

$$\Delta_{j,\pm} := \sum_{x=1}^{\infty}\left(\prod_{y=0}^{x-1} |\delta_{j,\pm}(-y-1)|^{-2}\right) + \sum_{x=1}^{\infty}\left(\prod_{y=0}^{x-1} |\delta_{j,\pm}(y)|^{2}\right), \tag{II.69}$$

Then $\Delta_{1,\pm}$ and $\Delta_{2,\pm}$ cannot be simultaneously finite, and the following assertions hold true:

(i) *The dimension of* $\ker(U \mp 1)$ *is at most* 1*. More explicitly, we have*

$$|\mathrm{ind}_{\pm}(\varGamma, U)| = \dim\ker(U \mp 1), \tag{II.70}$$

$$\mathrm{ind}_{\pm}(\varGamma, U) = \begin{cases} +1, & \Delta_{1,\pm} < \infty, \\ -1, & \Delta_{2,\pm} < \infty, \\ 0, & \Delta_{1,\pm} = \Delta_{2,\pm} = \infty. \end{cases} \tag{II.71}$$

In particular, if $\Delta_{j,\pm} < \infty$ holds true for $j = 1$ or $j = 2$, then $\Psi \in \ker(U \mp 1)$ if and only if there exists $\psi \in \ker(L - \delta_{j,\pm})$ such that the following equality holds true;

$$\Psi = \begin{pmatrix} \mp(-1)^j\sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix}. \tag{II.72}$$

(ii) *For each $j = 1, 2$, let*

$$\delta^{\downarrow}_{j,\pm} := \min\left\{\liminf_{x\to\infty}\left(\prod_{y=1}^{x}|\delta_{j,\pm}(-y)|^{-2}\right)^{1/x}, \qquad \liminf_{x\to\infty}\left(\prod_{y=0}^{x-1}|\delta_{j,\pm}(y)|^{2}\right)^{1/x}\right\}, \tag{II.73}$$

$$\delta^{\uparrow}_{j,\pm} := \max\left\{\limsup_{x\to\infty}\left(\prod_{y=1}^{x}|\delta_{j,\pm}(-y)|^{-2}\right)^{1/x}, \qquad \limsup_{x\to\infty}\left(\prod_{y=0}^{x-1}|\delta_{j,\pm}(y)|^{2}\right)^{1/x}\right\}, \tag{II.74}$$

$$\Lambda^{\downarrow}_{j,\pm} := \inf_{x\in\mathbb{Z}}\Lambda(\mp(-1)^j a(x)) + 1, \tag{II.75}$$

$$\Lambda^{\uparrow}_{j,\pm} := \sup_{x\in\mathbb{Z}}\Lambda(\mp(-1)^j a(x)) + 1. \tag{II.76}$$

If $0 < \delta^{\downarrow}_{j,\pm} \leq \delta^{\uparrow}_{j,\pm} < 1$ holds true for $j = 1$ or $j = 2$, then $\Delta_{j,\pm} < \infty$. Moreover, in this case, for any $\epsilon > 0$ satisfying $0 < \delta^{\downarrow}_{j,\pm} - \epsilon < \delta^{\uparrow}_{j,\pm} + \epsilon < 1$, there exists $x_\pm \in \mathbb{N}$ with the property that if $\psi \in \ker(L - \delta_{j,\pm})$ is a non-zero vector and if Ψ is given by (II.72)*, then one has the following exponential decay property;*

$$\Lambda^{\downarrow}_{j,\pm}\left(\delta^{\downarrow}_{j,\pm} - \epsilon\right)^{|x|} \leq \frac{\|\Psi(x)\|^2}{|\psi(0)|^2} \leq \Lambda^{\uparrow}_{j,\pm}\left(\delta^{\uparrow}_{j,\pm} + \epsilon\right)^{|x|}, \qquad |x| \geq x_\pm. \tag{II.77}$$

As we shall see shortly, Theorem II.24 is a generalisation of [FFS18] (see §II.5.3 for details).

Remark II.25.

(i) Note that (II.77) can be rewritten as

$$\Lambda^{\downarrow}_{j,\pm}e^{\log\left(\delta^{\downarrow}_{j,\pm}-\epsilon\right)|x|} \leq \frac{\|\Psi(x)\|^2}{|\psi(0)|^2} \leq \Lambda^{\uparrow}_{j,\pm}e^{\log\left(\delta^{\uparrow}_{j,\pm}+\epsilon\right)|x|}, \qquad |x| \geq x_\pm,$$

where $\epsilon > 0$ is any fixed number satisfying $0 < \delta^{\downarrow}_{j,\pm} - \epsilon < \delta^{\uparrow}_{j,\pm} + \epsilon < 1$,

(ii) It is in general difficult to compute $\delta^{\downarrow}_{j,\pm}, \delta^{\uparrow}_{j,\pm}$, but the following estimates may be useful:

$$\delta^{\downarrow}_{j,\pm} \geq \min\left\{\liminf_{x\to\infty}|\delta_{j,\pm}(-x)|^{-2}, \qquad \liminf_{x\to\infty}|\delta_{j,\pm}(x)|^{2}\right\}, \tag{II.78}$$

$$\delta^{\uparrow}_{j,\pm} \leq \max\left\{\limsup_{x\to\infty}|\delta_{j,\pm}(-x)|^{-2}, \qquad \limsup_{x\to\infty}|\delta_{j,\pm}(x)|^{2}\right\}. \tag{II.79}$$

Note that the estimates (II.78) to (II.79) can be easily proved by the following well-known fact (see, for example, [Rud76, Theorem 3.37]). Given a sequence $(\alpha(x))_{x\in\mathbb{N}}$ of positive numbers, we have

$$\liminf_{x\to\infty}\frac{\alpha(x+1)}{\alpha(x)} \leq \liminf_{x\to\infty}\alpha(x)^{1/x} \leq \limsup_{x\to\infty}\alpha(x)^{1/x} \leq \limsup_{x\to\infty}\frac{\alpha(x+1)}{\alpha(x)}.$$

II.4.1 Proof of the general case (Theorem II.24)

The purpose of the current section is to prove Theorem II.24 with the aid of two lemmas. It follows from Theorem II.24 (i) that (II.72) allows us to construct an explicit linear isomorphism from the vector space $\ker(L - \delta_{j,\pm})$ onto the one-dimensional eigenspace $\ker(U \mp 1)$, under the assumption $\Delta_{j,\pm} < \infty$ for some $j = 1, 2$. This isomorphism turns out to be a key ingredient in the following result;

Lemma II.26. *If* (II.67) *holds true for each* $\zeta = p, a$, *then we have the following well-defined linear isomorphism for each* $j = 1, 2$;

$$\ker(L - \delta_{j,\pm}) \ni \psi \longmapsto \begin{pmatrix} \mp(-1)^j \sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix} \in \ker(\varGamma + (-1)^j) \cap \ker(\varGamma' \mp (-1)^{j+1}), \tag{II.80}$$

where the bounded sequence $\delta_{j,\pm}$ *is defined by* (II.68).

That is,

$$\ker(\varGamma + (-1)^j) \cap \ker(\varGamma' \mp (-1)^{j+1}) = \left\{ \begin{pmatrix} \mp(-1)^j \sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix} \mid \psi \in \ker(L - \delta_{j,\pm}) \right\}, \qquad j = 1, 2.$$

Proof. To compute $\ker(\varGamma' \mp 1)$ we consider the following $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$-valued sequence;

$$(\varGamma' \mp 1)\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} a \mp 1 & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -(a \pm 1) \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \mp(1 \mp a) & \sqrt{1-a^2} \\ \sqrt{1-a^2} & \mp(1 \pm a) \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \mp(1 \mp a)\psi_1 + \sqrt{1-a^2}\psi_2 \\ \sqrt{1-a^2}\psi_1 \mp (1 \pm a)\psi_2 \end{pmatrix},$$

where $\psi_1, \psi_2 \in \ell^2(\mathbb{Z})$. Then $\mp(1 \mp a)\psi_1 + \sqrt{1-a^2}\psi_2 = 0$ if and only if $\sqrt{1-a^2}\psi_1 \mp (1 \pm a)\psi_2 = 0$, since

$$\frac{\sqrt{1-a^2}}{1 \mp a} = \frac{1 \pm a}{\sqrt{1-a^2}} = \frac{1 \pm a}{\sqrt{(1 \pm a)(1 \mp a)}} = \sqrt{\frac{1 \pm a}{1 \mp a}} = \sqrt{\Lambda(\pm a)}.$$

It follows that the following equalities hold true;

$$\ker(\varGamma' \mp 1) = \ker\left(\begin{pmatrix} a & \sqrt{1-a^2} \\ \sqrt{1-a^2} & -a \end{pmatrix} \mp 1\right) = \left\{ \begin{pmatrix} \pm\sqrt{\Lambda(\pm a)}\psi \\ \psi \end{pmatrix} \mid \psi \in \ell^2(\mathbb{Z}) \right\}.$$

On the other hand,

$$\ker(\varGamma \mp 1) = \ker\begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix}\left(\begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \mp 1\right)\begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & L^* \end{pmatrix}\begin{pmatrix} \pm\sqrt{\Lambda(\pm p)}\psi \\ \psi \end{pmatrix} \mid \psi \in \ell^2(\mathbb{Z}) \right\},$$

We obtain the following equalities for each $j = 1, 2$:

$$\ker(\Gamma' \mp (-1)^{j+1}) = \left\{ \begin{pmatrix} \mp(-1)^j \sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix} \mid \psi \in \ell^2(\mathbb{Z}) \right\}, \tag{II.81}$$

$$\ker(\Gamma + (-1)^j) = \left\{ \begin{pmatrix} (-1)^{j+1} \sqrt{\Lambda((-1)^{j+1} p)} L\psi \\ \psi \end{pmatrix} \mid \psi \in \ell^2(\mathbb{Z}) \right\}. \tag{II.82}$$

Next, we show that (II.80) is a well-defined linear transform, where $\delta_{j,\pm} = \pm\sqrt{\Lambda((-1)^j p)\Lambda(\mp(-1)^j a)}$. Given $\psi \in \ell^2(\mathbb{Z})$, we have that $\psi \in \ker(L - \delta_{j,\pm})$ if and only if $L\psi = \pm\sqrt{\Lambda((-1)^j p)\Lambda(\mp(-1)^j a)}\psi$. Therefore, if $\psi \in \ker(L - \delta_{j,\pm})$, then

$$\begin{aligned} (-1)^{j+1}\sqrt{\Lambda((-1)^{j+1}p)} L\psi &= \pm(-1)^{j+1}\sqrt{\Lambda((-1)^{j+1}p)}\sqrt{\Lambda((-1)^j p)\Lambda(\mp(-1)^j a)}\psi \\ &= \mp(-1)^j\sqrt{\Lambda(-(-1)^j p)\Lambda((-1)^j p)\Lambda(\mp(-1)^j a)}\psi \\ &= \mp(-1)^j\sqrt{\Lambda(\mp(-1)^j a)}\psi, \end{aligned}$$

where the last equality follows from $\Lambda(-(-1)^j p) = \Lambda((-1)^j p)^{-1}$. It follows that (II.80) is a well-defined injective linear transform. With (II.81) to (II.82) that (II.80) in mind, the surjectivity of (II.80) can be verified in an analogous fashion. The claim follows. □

Lemma II.27. *Let $\delta = (\delta(x))_{x\in\mathbb{Z}}$ be a bounded sequence of non-zero complex numbers, and let*

$$\Delta := \sum_{x=1}^{\infty} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right) + \sum_{x=1}^{\infty} \left(\prod_{y=0}^{x-1} |\delta(y)|^{2} \right).$$

Then the following assertions hold true:

(i) *We have*

$$\dim\ker(L - \delta) = \begin{cases} 1, & \Delta < \infty, \\ 0, & \Delta = \infty. \end{cases} \tag{II.83}$$

(ii) *Let*

$$\delta^{\downarrow} := \min\left\{ \liminf_{x\to\infty} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right)^{1/x}, \quad \liminf_{x\to\infty} \left(\prod_{y=0}^{x-1} |\delta(y)|^{2} \right)^{1/x} \right\}, \tag{II.84}$$

$$\delta^{\uparrow} := \max\left\{ \limsup_{x\to\infty} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right)^{1/x}, \quad \limsup_{x\to\infty} \left(\prod_{y=0}^{x-1} |\delta(y)|^{2} \right)^{1/x} \right\}. \tag{II.85}$$

If $0 < \delta^{\downarrow} \leq \delta^{\uparrow} < 1$, *then* $\dim \ker (L - \delta) = 1$. *Moreover, in this case, for any* $\epsilon > 0$ *satisfying* $0 < \delta^{\downarrow} - \epsilon \leq \delta^{\uparrow} + \epsilon < 1$, *there exists* $x_\epsilon \in \mathbb{N}$, *such that for any* $\psi \in \ker (L - \delta)$ *we have*

$$|\psi(0)|^2 (\delta^{\downarrow} - \epsilon)^{|x|} \leq |\psi(x)|^2 \leq |\psi(0)|^2 (\delta^{\uparrow} + \epsilon)^{|x|}, \qquad |x| \geq x_\epsilon. \tag{II.86}$$

Note that (i) shows that $\dim \ker (L - \delta)$ depends only on $|\delta|$.

Proof. (i) We need to solve a difference equation of the form;

$$\psi(x+1) = \delta(x)\psi(x), \qquad \forall x \in \mathbb{Z}. \tag{II.87}$$

Since each $\delta(x)$ is non-zero, such a solution is uniquely determined by the initial value $\psi(0)$. In particular, if $\psi, \psi' \in \ker (L - \delta)$ are non-zero vectors, then $\psi(0), \psi'(0)$ are non-zero, and so the linear combination $\psi'(0)\psi - \psi(0)\psi'$ is the zero vector. It follows that ψ, ψ' are linearly independent, and so $\dim \ker (L - \delta) \leq 1$. Suppose that we have a bounded sequence $\psi = (\psi(x))_{x \in \mathbb{Z}}$ satisfying (II.87). We have

$$\psi(x) = \prod_{y=0}^{x-1} \delta(y)\psi(0), \qquad \psi(-x) = \prod_{y=1}^{x} \delta(-y)^{-1}\psi(0), \qquad x \geq 1. \tag{II.88}$$

Since $\sum_{x \in \mathbb{Z}} |\psi(x)|^2 = |\psi(0)|^2 + \sum_{x \in \mathbb{N}} |\psi(-x)|^2 + \sum_{x \in \mathbb{N}} |\psi(x)|^2$, we get

$$\sum_{x \in \mathbb{Z}} |\psi(x)|^2 = |\psi(0)|^2 + |\psi(0)|^2 \sum_{x \in \mathbb{N}} \prod_{y=1}^{x} |\delta(-y)|^{-2} + |\psi(0)|^2 \sum_{x \in \mathbb{N}} \prod_{y=0}^{x-1} |\delta(y)|^2.$$

That is, $\dim \ker(L - \delta) = 1$ if and only if $\Delta := \sum_{x=1}^{\infty} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right) + \sum_{x=1}^{\infty} \left(\prod_{y=0}^{x-1} |\delta(y)|^2 \right) < \infty$.

(ii) If $0 < \delta^{\downarrow} \leq \delta^{\uparrow} < 1$, then $\dim \ker (L - \delta) = 1$ by the root test. Let $\epsilon > 0$ be any number satisfying $0 < \delta^{\downarrow} - \epsilon \leq \delta^{\uparrow} + \epsilon < 1$. It follows that there exists $x_\epsilon \in \mathbb{N}$, such that

$$\delta^{\downarrow} - \epsilon < \min \left\{ \inf_{x \geq x_\epsilon} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right)^{1/x}, \inf_{x \geq x_\epsilon} \left(\prod_{y=0}^{x-1} |\delta(y)|^2 \right)^{1/x} \right\}, \tag{II.89}$$

$$\delta^{\uparrow} + \epsilon > \max \left\{ \sup_{x \geq x_\epsilon} \left(\prod_{y=1}^{x} |\delta(-y)|^{-2} \right)^{1/x}, \sup_{x \geq x_\epsilon} \left(\prod_{y=0}^{x-1} |\delta(y)|^2 \right)^{1/x} \right\}. \tag{II.90}$$

Let $\psi \in \ker(L - \delta)$, and let $|x| \geq x_\epsilon$. On one hand, if $x \geq x_\epsilon$, then $|\psi(x)|^2 = \prod_{y=0}^{x-1} |\delta(y)|^2 |\psi(0)|^2$, and so

$$(\delta^{\downarrow} - \epsilon)^x |\psi(0)|^2 < |\psi(x)|^2 < (\delta^{\uparrow} + \epsilon)^x |\psi(0)|^2.$$

On the other hand, if $-x \geq x_\epsilon$, then $|\psi(x)|^2 = \prod_{y=1}^{-x} |\delta(-y)|^{-2}|\psi(0)|^2$, and so

$$(\delta^{\downarrow} - \epsilon)^{-x}|\psi(0)|^2 < |\psi(x)|^2 < (\delta^{\uparrow} + \epsilon)^{-x}|\psi(0)|^2.$$

The claim follows. $\square$

Proof of Theorem II.24. With the notation introduced in Remark II.5, for each $j = 1, 2$, we obtain

$$m_{j,\pm} = \dim\left(\ker(\varGamma + (-1)^j) \cap \ker(\varGamma' \mp (-1)^{j+1})\right) = \dim\ker(L - \delta_{j,\pm}),$$

where the last equality follows from Lemma II.26. Clearly, Lemma II.27 is applicable to the pair $(\delta, \Delta) := (\delta_{j,\pm}, \Delta_{j,\pm})$, and so we obtain

$$m_{j,\pm} = \begin{cases} 1, & \Delta_{j,\pm} < \infty, \\ 0, & \text{otherwise}. \end{cases} \tag{II.91}$$

Assume the contrary that $\Delta_{j,\pm} < \infty$ for each $j = 1, 2$. In this case, for each $j = 1, 2$, we have $\prod_{y=0}^{x-1} |\delta_{j,\pm}(y)|^2 \to 0$ as $x \to \infty$. Therefore, $\prod_{y=0}^{x-1} |\delta_{1,\pm}(y)|^2|\delta_{2,\pm}(y)|^2 \to 0$ as $x \to \infty$. Note, however, that this is impossible, since for each $y = 0, \dots, x-1$ we have

$$|\delta_{1,\pm}(y)|^2|\delta_{2,\pm}(y)|^2 = \Lambda(p(y))^{-1}\Lambda(\mp a(y))^{-1}\Lambda(p(y))\Lambda(\mp a(y)) = 1.$$

This contradiction shows $\Delta_{1,\pm} + \Delta_{2,\pm} = \infty$.

(i) If $\Delta_{1,\pm} = \Delta_{2,\pm} = \infty$, then we get the trivial equalities $\operatorname{ind}_\pm(\varGamma, U) = 0 = \dim\ker(U \mp 1)$. On one hand, if $\Delta_{1,\pm} < \infty$, then $\operatorname{ind}_\pm(\varGamma, U) = 1 - 0$ and $\dim\ker(U \mp 1) = 1 + 0$. On the other hand, if $\Delta_{2,\pm} < \infty$, then $\operatorname{ind}_\pm(\varGamma, U) = 0 - 1$ and $\dim\ker(U \mp 1) = 0 + 1$. Thus, the formulas (II.70) to (II.71) have been verified. If $\Delta_{j,\pm} < \infty$ holds true for $j = 1$ or $j = 2$, then the linear isomorphism (II.80) becomes

$$\ker(L - \delta_{j,\pm}) \ni \psi \longmapsto \begin{pmatrix} \mp(-1)^j\sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix} \in \ker(U \mp 1),$$

since $\ker(U \mp 1) = \ker(\varGamma + (-1)^j) \cap \ker(\varGamma' \mp (-1)^{j+1})$.

(ii) If $0 < \delta^{\downarrow}_{j,\pm} \leq \delta^{\uparrow}_{j,\pm} < 1$ for some $j = 1, 2$, then $\Delta_{j,\pm} < \infty$ by the root test. Let $\epsilon > 0$ be any number satisfying $0 < \delta^{\downarrow}_{j,\pm} - \epsilon < \delta^{\uparrow}_{j,\pm} + \epsilon < 1$. It follows from Lemma II.27 (ii) that there exists $x_\pm \in \mathbb{N}$, such that for any non-zero $\psi \in \ker(L - \delta_{j,\pm})$, we have

$$(\delta_{j,\pm}^{\downarrow} - \epsilon)^{|x|} \leq \frac{|\psi(x)|^2}{|\psi(0)|^2} \leq (\delta_{j,\pm}^{\uparrow} + \epsilon)^{|x|}, \qquad |x| \geq x_\epsilon.$$

Let Ψ be defined by (II.72). With (II.72) in mind, we have $\|\Psi(x)\|^2 = (\Lambda(\mp(-1)^j a(x)) + 1)|\psi(x)|^2$. for each $x \in \mathbb{Z}$. The claim follows. □

II.4.2 Proof of the special case (Theorem A (ii))

We shall prove Theorem A (ii) via Theorem II.24 and the following lemma;

Lemma II.28. *Let $(\alpha(x))_{x=0}^{\infty}$ be a sequence of positive numbers, and let us assume that there exists a natural number $n_0 \in \mathbb{N}$ such that the following limits exist in $(0, \infty)$:*

$$\alpha(+\infty, m) := \lim_{x\to\infty} \alpha(n_0 x + m), \qquad m \in \{0, \ldots, n_0 - 1\}. \tag{II.92}$$

Then $\left(\prod_{m=0}^{x-1} \alpha(m)\right)^{1/x} \to \left(\prod_{m=0}^{n_0-1} \alpha(+\infty, m)\right)^{1/n_0}$ as $x \to \infty$.

Note that the special case $n_0 = 1$ is nothing but the well-known result that the geometric mean of a convergent positive sequence converges to its limit, and that we shall make use of this result in the proof below.

Proof. Let $m_0 \in \{1, \ldots, n_0\}$ be fixed. If let $\beta(x) = \left(\prod_{m=0}^{x-1} \alpha(m)\right)^{1/x}$ for each $x \in \mathbb{N}$, then

$$\begin{aligned}
\beta(n_0 x + m_0) &= \left(\prod_{m=0}^{n_0 x - 1} \alpha(m) \prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right) \\
&= \left(\prod_{m=0}^{n_0 x - 1} \alpha(m)\right)\left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right) \\
&= \prod_{m=0}^{n_0-1}\left(\prod_{x_m=0}^{x-1} \alpha(x_m n_0 + m)\right)\left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right),
\end{aligned}$$

where $\left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right)_{x\in\mathbb{N}}$ converges to the positive number $\prod_{m=0}^{m_0-1} \alpha(+\infty, m)$. Moreover, we get as $x \to \infty$

$$\log\left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right)^{\frac{1}{n_0 x + m_0}} = \frac{\log \prod_{m=0}^{m_0-1} \alpha(n_0 x + m)}{n_0 x + m_0} \to 0,$$

where the last step follows from the fact that $\left(\log \prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right)_{x\in\mathbb{N}}$ is a bounded sequence. It follows from the continuity of the exponential function that

$$\left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right)^{\frac{1}{n_0 x + m_0}} \to e^0 = 1. \tag{II.93}$$

On the other hand, it follows that as $x \to \infty$

$$\prod_{m=0}^{n_0-1} \prod_{x_m=0}^{x-1} \alpha(x_m n_0 + m)^{\frac{1}{x}} \to \prod_{m=0}^{n_0-1} \alpha(+\infty, m)^{\frac{1}{x_0}}. \tag{II.94}$$

It follows from (II.93) to (II.94) as $x \to \infty$ we have

$$\begin{aligned}\beta(n_0 x + m_0)^{\frac{1}{n_0 x + m_0}} &= \left(\prod_{m=0}^{n_0-1} \prod_{x_m=0}^{x-1} \alpha(x_m n_0 + m)^{1/x}\right)^{\frac{x}{n_0 x + m_0}} \left(\prod_{m=0}^{m_0-1} \alpha(n_0 x + m)\right)^{\frac{1}{n_0 x + m_0}} \\ &\to \left(\prod_{m=0}^{n_0-1} \alpha(+\infty, m)\right)^{\frac{1}{x_0}}.\end{aligned}$$

It follows that any subsequence of $(\beta(x)^{1/x})_{x\in\mathbb{N}}$ also converges to $\left(\prod_{m=0}^{n_0-1} \alpha(+\infty, m)\right)^{\frac{1}{x_0}}$, since the constant m_0 was chosen arbitrarily. The claim follows. □

Proof of Theorem A (ii). Let $\delta_{j,\pm}(y)$ be defined by (II.68), and let $\Delta_{j,\pm}$ be defined by (II.69).

(i) Note first that the two non-negative numbers $\Delta_{1,\pm}$ and $\Delta_{2,\pm}$ cannot be simultaneously finite, since $|\delta_{1,\pm}(y)\delta_{2,\pm}(y)|^2 = 1$ for each $y \in \mathbb{Z}$. With this result in mind, it follows from Theorem II.24 (i) that $|\mathrm{ind}_\pm(\Gamma, U)| = \dim\ker(U \mp 1)$, where $\mathrm{ind}_\pm(\Gamma, U)$ is given explicitly by (II.71). We are required to show that (II.71) agrees with (I.9) by making use of the root test. Since the function Λ is continuous, for each $\zeta = -p, +p, -a, +a$ and each $\star = -\infty, +\infty$, the following numbers belong to $(0, \infty)$;

$$\Lambda(\zeta(\star, y)) = \lim_{x\to\star} \Lambda(\zeta(n_\star \cdot x + y)), \qquad y \in \{0, \dots, n_\star - 1\},$$

where $|\zeta(\star, n_0)| < 1$. It follows from Lemma II.28 that as $x \to \infty$

$$\lim_{x\to\infty} \left(\prod_{y=0}^{x-1} \Lambda(\zeta(-y-1))\right)^{\frac{1}{x}} = \left(\prod_{y=0}^{n_{-\infty}-1} \Lambda(\zeta(-\infty, y))\right)^{\frac{1}{n_{-\infty}}},$$

$$\lim_{x\to\infty} \left(\prod_{y=0}^{x-1} \Lambda(\zeta(y))\right)^{\frac{1}{x}} = \left(\prod_{y=0}^{n_{+\infty}-1} \Lambda(\zeta(\infty, y))\right)^{\frac{1}{n_{+\infty}}}.$$

Since $|\delta_{j,\pm}(y)|^2 = (\Lambda(p(y))\Lambda(\mp a(y)))^{(-1)^j}$ for each $y \in \mathbb{Z}$, we have

$$\lim_{x\to\infty}\left(\prod_{y=0}^{x-1}|\delta_{j,\pm}(-y-1)|^{-2}\right)^{1/x} = (\Lambda(p(-\infty))\Lambda(\mp a(-\infty)))^{(-1)^{j+1}},$$

$$\lim_{x\to\infty}\left(\prod_{y=0}^{x-1}|\delta_{j,\pm}(y)|^{2}\right)^{1/x} = (\Lambda(p(+\infty))\Lambda(\mp a(+\infty)))^{(-1)^{j}},$$

where $\Lambda(p(\star))\Lambda(\mp a(\star)) \neq 1$ for each $\star = -\infty, +\infty$, since we assume $p(\star) \mp a(\star) \neq 0$. That is, the root test is applicable to each of the two infinite series on the right hand side of (II.69), and we obtain the following equivalence for each $j = 1, 2$;

$$\Delta_{j,\pm} < \infty \text{ if and only if } (-1)^j(p(+\infty) \mp a(+\infty)) < 0 < (-1)^j(p(-\infty) \mp a(-\infty)). \tag{II.95}$$

It is now easy to see that (II.71) becomes (I.9).

(ii) Let $\Delta_{j,\pm} < \infty$ for some $j = 1, 2$ throughout. It follows from Theorem II.24 (ii) that we have the following linear isomorphism;

$$\ker(L - \delta_{j,\pm}) \ni \psi \longmapsto \begin{pmatrix} \mp(-1)^j\sqrt{\Lambda(\mp(-1)^j a)}\psi \\ \psi \end{pmatrix} \in \ker(U \mp 1), \tag{II.96}$$

where $\dim\ker(U \mp 1) = 1$. In other words, for any non-zero vector $\Psi_\pm \in \ker(U \mp 1)$ there exists a unique non-zero vector $\psi_\pm \in \ker\left(L + \sqrt{\Lambda((-1)^j p)\Lambda(\mp(-1)^j a)}\right)$, such that $\Psi_\pm$ is given explicitly by

$$\Psi_\pm = \begin{pmatrix} \mp(-1)^j\sqrt{\Lambda(\mp(-1)^j a)}\psi_\pm \\ \psi_\pm \end{pmatrix}. \tag{II.97}$$

Finally, we introduce the following positive constants to show that $\Psi_\pm$ exhibits exponential decay.

$$\delta^{\downarrow}_{j,\pm} := \min\left\{(\Lambda(p(-\infty))\Lambda(\mp a(-\infty)))^{(-1)^{j+1}}, (\Lambda(p(+\infty))\Lambda(\mp a(+\infty)))^{(-1)^{j}}\right\}, \tag{II.98}$$

$$\delta^{\uparrow}_{j,\pm} := \max\left\{(\Lambda(p(-\infty))\Lambda(\mp a(-\infty)))^{(-1)^{j+1}}, (\Lambda(p(+\infty))\Lambda(\mp a(+\infty)))^{(-1)^{j}}\right\}, \tag{II.99}$$

$$\Lambda^{\downarrow}_{j,\pm} := \inf_{x\in\mathbb{Z}}\Lambda(\mp(-1)^j a(x)) + 1, \tag{II.100}$$

$$\Lambda^{\uparrow}_{j,\pm} := \sup_{x\in\mathbb{Z}}\Lambda(\mp(-1)^j a(x)) + 1. \tag{II.101}$$

Note that $0 < \delta^{\downarrow}_{j,\pm} \leq \delta^{\uparrow}_{j,\pm} < 1$, where the last inequality follows from (II.95) with $\Delta_{j,\pm} < \infty$. Let $\epsilon > 0$ be small enough, so that $0 < \delta^{\downarrow}_{j,\pm} - \epsilon < \delta^{\uparrow}_{j,\pm} + \epsilon < 1$ holds true. It then follows from Theorem II.24 (iii) that there exists $x_{\pm} \in \mathbb{N}$, such that (II.77) holds true. We obtain (I.15), if we let

$$\kappa^{\downarrow}_{j,\pm} := |\psi(0)|^2 \Lambda^{\downarrow}_{j,\pm}, \qquad c^{\downarrow}_{j,\pm} := -\log\left(\delta^{\downarrow}_{j,\pm} - \epsilon\right), \tag{II.102}$$

$$\kappa^{\uparrow}_{j,\pm} := |\psi(0)|^2 \Lambda^{\uparrow}_{j,\pm}, \qquad c^{\uparrow}_{j,\pm} := -\log\left(\delta^{\uparrow}_{j,\pm} + \epsilon\right). \tag{II.103}$$

□

Remark II.29. The proof of Theorem A (ii) above gives yet another derivation of the index formula (I.9) via (II.71). This latter derivation relies only on elementary analysis of first-order difference equations inspired by [FFS18], while the former derivation outlined in §II.3 makes extensive use of Toeplitz operators. Note, however, that despite its simplicity the latter method alone is insufficient to justify where the technical assumption $p(\pm\infty) \neq \pm a(\pm\infty)$ comes from. It is precisely the language of Toeplitz operators that allows us to establish the non-trivial equivalence of this assumption and the essential gap condition $\pm 1 \notin \sigma_{\mathrm{ess}}(U)$ (see Theorem II.20 (ii) for details).

II.5 Discussion

II.5.1 The essential spectrum

Further classifications for the essential spectrum of the evolution operator associated with Suzuki's one-dimensional split-step quantum walk can be found in this subsection. We start with the following broad description of the essential spectrum;

Theorem II.30. *Let* $(\Gamma, U) = (\Gamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ *be defined by* (I.2), (I.3). *Suppose that there exist* $n_{-\infty}, n_{+\infty} \in \mathbb{N}$ *with the property that limits of the form* (I.10) *exist for each* $\zeta = p, a$. *Let* $\hat{R}_{+}(\star, z), \hat{R}_{-}(\star, z)$ *be the* $n_{\star} \times n_{\star}$ *matrices* *defined by the following formula;*

$$2\hat{R}_\pm(\star, z) := \begin{cases} r_{1,\pm}(\star,0)z^* + r_{0,\pm}(\star,0) + r_{1,\pm}(\star,0)z, & n_\star = 1, \\ \begin{pmatrix} r_{0,\pm}(\star,0) & r_{1,\pm}(\star,0)+r_{1,\pm}(\star,1)z^* \\ r_{1,\pm}(\star,0)+r_{1,\pm}(\star,1)z & r_{0,\pm}(\star,1) \end{pmatrix}, & n_\star = 2, \\ \begin{pmatrix} r_{0,\pm}(\star,0) & r_{1,\pm}(\star,0) & 0 & \cdots & 0 & r_{1,\pm}(\star,n_\star-1)z^* \\ r_{1,\pm}(\star,0) & r_{0,\pm}(\star,1) & r_{1,\pm}(\star,1) & \cdots & 0 & 0 \\ 0 & r_{1,\pm}(\star,1) & r_{0,\pm}(\star,2) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & r_{0,\pm}(\star,n_\star-2) & r_{1,\pm}(\star,n_\star-2) \\ r_{1,\pm}(\star,n_\star-1)z & 0 & 0 & \cdots & r_{1,\pm}(\star,n_\star-2) & r_{0,\pm}(\star,n_\star-1) \end{pmatrix}, & n_\star \geq 3, \end{cases} \tag{II.104}$$

$$r_{0,\pm}(\star, m) := (p(\star,m) \pm 1)a(\star,m) + (p(\star,m) \mp 1)a(\star,m+1), \tag{II.105}$$

$$r_{1,\pm}(\star, m) := \sqrt{(1 \mp p(\star,m))(1 \pm p(\star,m+1))(1 - a(\star,m+1)^2)}, \tag{II.106}$$

where we let $p(\star, n_\star) := p(\star, 0)$ *and* $a(\star, n_\star) := a(\star, 0)$*. Then*

$$\sigma_{\mathrm{ess}}(U) = \sigma(-\infty) \cup \sigma(+\infty), \tag{II.107}$$

$$\sigma(\star) := \left\{ z \in \mathbb{T} \mid \operatorname{Re} z \in \sigma\left(\hat{R}_-(\star,z)\right) \cup \sigma\left(\hat{R}_+(\star,z)\right) \right\}, \qquad \star = -\infty, +\infty. \tag{II.108}$$

Note that U_{suz} in Theorem II.30 is a 2-dimensional strictly local operator. In theory, it is possible to compute $\sigma_{\mathrm{ess}}(U_{\mathrm{suz}})$ by making use of Theorem II.8 (ii), but we shall end up with spectral analysis of $2n_\star \times 2n_\star$ matrices according to (II.32). In order to reduce the complexity of computations, we shall make use of the following lemma;

Lemma II.31. *With the notation introduced in Lemma II.22, let* R, Q *be the real and imaginary parts of* U_{suz}*. Then the unitary operator* ϵ *gives the following decomposition;*

$$\epsilon^* R \epsilon = \begin{pmatrix} R_{\epsilon_1} & 0 \\ 0 & R_{\epsilon_2} \end{pmatrix}, \qquad \epsilon^* Q \epsilon = \begin{pmatrix} 0 & Q_{\epsilon_0}^* \\ Q_{\epsilon_0} & 0 \end{pmatrix}, \tag{II.109}$$

where the three operators $R_{\epsilon_1}, R_{\epsilon_2}, Q_{\epsilon_0}$ *are defined respectively by*

$$2R_{\epsilon_1} := p_- L p_+ \sqrt{1-a^2} + p_+ \sqrt{1-a^2} L^* p_- + (1+p)a - (1-p)a(\cdot + 1), \tag{II.110}$$

$$2R_{\epsilon_2} := p_+ L p_- \sqrt{1-a^2} + p_- \sqrt{1-a^2} L^* p_+ - (1-p)a + (1+p)a(\cdot + 1), \tag{II.111}$$

$$-2iQ_{\epsilon_0} := p_+ L p_+ \sqrt{1-a^2} - p_- \sqrt{1-a^2} L^* p_- - \sqrt{1-p^2}(a + a(\cdot + 1)). \tag{II.112}$$

Proof. Recall that $F := \eta^* \epsilon$ is given by (II.62). It follows from the second equality in (II.59) that

$$\epsilon^* U_{\mathrm{suz}} \epsilon = \begin{pmatrix} F_{1,-}^* F_{1,-} - F_{1,+}^* F_{1,+} & -(F_{2,-}^* F_{1,+} - F_{2,+}^* F_{1,-})^* \\ F_{2,-}^* F_{1,+} - F_{2,+}^* F_{1,-} & F_{2,-}^* F_{2,-} - F_{2,+}^* F_{2,+} \end{pmatrix}.$$

Since $\epsilon^* R \epsilon, \epsilon^* Q \epsilon$ are the real and imaginary parts of $\epsilon^* U_{\mathrm{suz}} \epsilon$ respectively, we get

$$\epsilon^* R \epsilon = \begin{pmatrix} F_{1,-}^* F_{1,-} - F_{1,+}^* F_{1,+} & 0 \\ 0 & F_{2,-}^* F_{2,-} - F_{2,+}^* F_{2,+} \end{pmatrix},$$

$$\epsilon^* Q \epsilon = \begin{pmatrix} 0 & i(F_{2,-}^* F_{1,+} - F_{2,+}^* F_{1,-})^* \\ -i(F_{2,-}^* F_{1,+} - F_{2,+}^* F_{1,-}) & 0 \end{pmatrix},$$

where $2F_{1,\pm} = \mp p_+ a_\mp + a_\pm L^* p_-$ and $2F_{2,\pm} = \mp p_- a_\pm + a_\mp L^* p_+$. The claim follows from the following direct computations;

$$4(F_{1,-}^* F_{1,-} - F_{1,+}^* F_{1,+}) = 4R_{\epsilon_1},$$

$$4(F_{2,-}^* F_{2,-} - F_{2,+}^* F_{2,+}) = 4R_{\epsilon_2},$$

$$4(F_{2,-}^* F_{1,+} - F_{2,+}^* F_{1,-}) = 4iQ_{\epsilon_0}.$$

□

Remark II.32. It immediately follows from (II.5) and (II.109) that

$$\sigma_{\mathrm{ess}}(U) = \left\{ z \in \mathbb{T} \mid \operatorname{Re} z \in \sigma_{\mathrm{ess}}(R_{\epsilon_1}) \cup \sigma_{\mathrm{ess}}(R_{\epsilon_2}) \right\}, \tag{II.113}$$

where each R_{ϵ_j} is a one-dimensional strictly local operator, unlike the evolution operator U itself. We are now in a position to apply the argument outlined in Remark II.21 to R_{ϵ_j}.

Proof of Theorem II.30. Note that the two operators $R_+ := R_{\epsilon_1}$ and $R_- := R_{\epsilon_2}$, defined respectively by (II.110) to (II.111), are operators of the form $2R_\pm = r_{1,\pm}(\cdot - 1)L^{-1} + r_{0,\pm} + r_{1,\pm}L$. The formula (II.58) motivates us to define $\hat{R}_\pm(\star, z)$ by (II.104). It follows from Theorem II.8 (ii) that

$$\sigma_{\mathrm{ess}}(R_\pm) = \bigcup_{\star = -\infty, +\infty} \left(\bigcup_{z \in \mathbb{T}} \sigma\left(\hat{R}_\pm(\star, z) \right) \right). \tag{II.114}$$

We get

$$\sigma_{\mathrm{ess}}(U) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in \sigma_{\mathrm{ess}}(R_-) \cup \sigma_{\mathrm{ess}}(R_+)\} = \bigcup_{\star=-\infty,+\infty} \sigma(\star),$$

where the first equality follows from (II.113), and where the last equality follows from (II.114). $\square$

It is shown in Theorem II.30 that $\sigma_{\mathrm{ess}}(U) = \sigma(-\infty) \cup \sigma(+\infty)$, where for each $\star = -\infty, +\infty$ the subset $\sigma(\star)$ of $\mathbb{T}$ is defined by (II.108). The purpose of this subsection is to give a further classification of $\sigma(\star)$ by restricting attention to $n_\star = 1$ and $n_\star = 2$. We introduce the following notation for simplicity;

$$q := \sqrt{1 - p^2}, \qquad b := \sqrt{1 - a^2}. \tag{II.115}$$

Given a fixed real number r_0 and a compact interval $[r_1, r_2]$ in $\mathbb{R}$, we let

$$r_0 + [r_1, r_2] := [r_0 + r_1, r_0 + r_2], \qquad r_0 - [r_1, r_2] := [r_0 - r_2, r_0 - r_1].$$

II.5.1.1 The asymptotically 1-periodic case

We focus on the case $n_\star = 1$ first. The following proposition can be found in [Tan21], but we give an alternative derivation via Theorem II.30.

Proposition II.33 ([Tan21, Theorem B(ii)]). *With the notation introduced in Theorem II.30 in mind, if* $n_\star = 1$, *then we have* $\sigma(\star) = \sigma\left(\hat{R}_+(\star, z)\right) = \sigma\left(\hat{R}_-(\star, z)\right)$ *for each* $z \in \mathbb{T}$. *More precisely,*

$$\sigma(\star) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in I(\star)\}, \tag{II.116}$$

where the closed subinterval $I(\star)$ *of* $[-1, 1]$ *is defined by*

$$I(\star) := p(\star, 0)a(\star, 0) + [-q(\star, 0)b(\star, 0), q(\star, 0)b(\star, 0)]. \tag{II.117}$$

Moreover, $\pm 1 \notin \sigma(\star)$ *if and only if* $p(\star) \neq \pm a(\star)$.

Proof. It follows from (II.104) that if $n_\star = 1$, then

$$2\hat{R}_\pm(\star, e^{it}) = r_{0,\pm}(\star, 0) + 2r_{1,\pm}(\star, 0)\cos(t),$$

where

$$r_{0,\pm}(\star,0) = (p(\star,0) \pm 1)a(\star,0) + (p(\star,0) \mp 1)a(\star,0) = 2p(\star,0)a(\star,0),$$
$$r_{1,\pm}(\star,0) = \sqrt{(1 \mp p(\star,0))(1 \pm p(\star,0))(1 - a(\star,0)^2)} = q(\star,0)b(\star,0).$$

It follows that $\hat{R}_+(\star,e^{it}) = \hat{R}_-(\star,e^{it}) =: \hat{R}_0(\star,e^{it})$ for each $t \in [0,2\pi]$, and we get (II.116). It is easy to see that $I(\star) = [p(\star,0)a(\star,0) - q(\star,0)b(\star,0), p(\star,0)a(\star,0) + q(\star,0)b(\star,0)]$ is a subset of $[-1,1]$;

$$|p(\star,0)a(\star,0)| + q(\star,0)b(\star,0) \le \frac{p(\star,0)^2 + a(\star,0)^2}{2} + \frac{(1-p(\star,0)^2) + (1-a(\star,0)^2)}{2} \le 1.$$

It remains to show that $\pm 1 \notin \sigma(\star)$ is equivalent to $p(\star) \neq \pm a(\star)$, but we defer the proof until Remark II.35. □

II.5.1.2 The asymptotically 2-periodic case

Next, we focus on the case $n_\star = 2$.

Theorem II.34. *With the notation introduced in Theorem II.30 in mind, if $n_\star = 2$, then we have $\sigma(\star) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{R}_+(\star,z)\right) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{R}_-(\star,z)\right)$ for each $z \in \mathbb{T}$. More precisely,*

$$\sigma(\star) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in I_1(\star) \cup I_2(\star)\}, \tag{II.118}$$

where each closed subinterval $I_j(\star)$ of $[-1,1]$ is defined by

$$I_j(\star) := d(\star) + (-1)^j \left[\sqrt{d(\star)^2 + d_1(\star)}, \sqrt{d(\star)^2 + d_2(\star)}\right], \tag{II.119}$$
$$d(\star) := \frac{(p(\star,0) + p(\star,1))(a(\star,0) + a(\star,1))}{4}, \tag{II.120}$$
$$d_j(\star) := \frac{2 - (1 + p(\star,0)p(\star,1))(1 + a(\star,0)a(\star,1)) + (-1)^j \prod_{m=0,1} q(\star,m)b(\star,m)}{2}. \tag{II.121}$$

Furthermore, we have the following assertions:

(i) *The set $I_j(\star)$ given by* (II.119) *is a well-defined closed interval in the sense that $0 \le d(\star)^2 + d_1(\star) \le d(\star)^2 + d_2(\star)$. Moreover, $I_1(\star)$ lies to the left of $I_2(\star)$.*

(ii) *We have $\pm 1 \notin \sigma(\star)$ if and only if*

$$\prod_{m=0,1} (1 + p(\star,m))(1 \mp a(\star,m)) \neq \prod_{m=0,1} (1 - p(\star,m))(1 \pm a(\star,m)) \tag{II.122}$$

(iii) *If* $\prod_{m=0,1}(1+p(\star,m))(1\mp a(\star,m))+\prod_{m=0,1}(1-p(\star,m))(1\pm a(\star,m))>0$, *then we uniquely define* $p(\star), a(\star)\in[-1,1]$ *through*

$$\frac{\prod_{m=0}^{n_\star-1}(1+\zeta(\star,m))}{\prod_{m=0}^{n_\star-1}(1-\zeta(\star,m))}=\left(\frac{1+\zeta(\star)}{1-\zeta(\star)}\right)^2,\qquad \zeta=p,a. \tag{II.123}$$

Then $\pm1\notin\sigma(\star)$ *if and only if* $p(\star)\neq\pm a(\star)$.

(iv) *The sets* $I_1(\star), I_2(\star)$ *are singleton sets if and only if* $\{p(\star,0),p(\star,1),a(\star,0),a(\star,1)\}$ *contains either* -1 *or* $+1$. *In this case, each* $I_j(\star)$ *is given explicitly by*

$$I_j(\star)=\left\{d(\star)+(-1)^j\sqrt{d(\star)^2+\frac{2-(1+p(\star,0)p(\star,1))(1+a(\star,0)a(\star,1))}{2}}\right\}.$$

We show first that Proposition II.33 is a special case of Theorem II.34.

Remark II.35. With the notation introduced in Theorem II.30 in mind, let $n_\star=2$. If $p(\star,0)=p(\star,1)$ and if $a(\star,0)=a(\star,1)$, then

$$d(\star)=\frac{(p(\star,0)+p(\star,1))(a(\star,0)+a(\star,1))}{4}=p(\star,0)a(\star,0),$$
$$d_j(\star)=\frac{2-(1+p(\star,0)^2)(1+a(\star,0)^2)+(-1)^j(1-p(\star,0)^2)(1-a(\star,0)^2)}{2}.$$

It follows that $d(\star)^2+d_1(\star)=0$, and that $d(\star)^2+d_2(\star)=(1-p(\star,0)^2)(1-a(\star,0)^2)$.

$$I_1(\star)=[p(\star,0)a(\star,0)-q(\star,0)b(\star,0),p(\star,0)a(\star,0)],$$
$$I_2(\star)=[p(\star,0)a(\star,0),p(\star,0)a(\star,0)+q(\star,0)b(\star,0)].$$

Therefore, $I_1(\star)\cup I_2(\star)=[p(\star,0)a(\star,0)-q(\star,0)b(\star,0),p(\star,0)a(\star,0)+q(\star,0)b(\star,0)]$ coincides with $I(\star)$ given by (II.117). It follows from Theorem II.34 (ii),(iii) that $\pm1\notin\sigma(\star)$ if and only if $p(\star)\neq\pm a(\star)$.

We prove Theorem II.34 with the aid of the following lemma;

Lemma II.36. *Given* $\alpha_1,\alpha_2\in\mathbb{R}$ *and* $\beta_1,\beta_2\geq0$, *let us consider the one-parameter family* $\{R(z)\}_{z\in\mathbb{T}}$ *of* 2×2 *Hermitian matrices defined by the following formula;*

$$R(z):=\frac{1}{2}\begin{pmatrix}\alpha_1 & \beta_1+\beta_2z^*\\ \beta_1+\beta_2z & \alpha_2\end{pmatrix},\qquad z\in\mathbb{T}. \tag{II.124}$$

For each $j = 1, 2$, *let*

$$I_j := \frac{\alpha_1+\alpha_2}{4} + (-1)^j \left[\frac{\sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1-\beta_2)^2}}{4}, \frac{\sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1+\beta_2)^2}}{4} \right].$$

Then the following assertions hold true:

(i) *We have* $\bigcup_{z\in\mathbb{T}} \sigma(R(z)) = I_1 \cup I_2$, *where* I_1 *lies to the left of* I_2.

(ii) *The set* $I_1 \cup I_2$ *is connected if and only if* $\alpha_1 = \alpha_2$ *and* $\beta_1 = \beta_2$. *In this case, we have* $I_1 \cup I_2 = [\alpha_1/2 - \beta_1, \alpha_1/2 + \beta_1]$.

Note that I_1, I_2 are well-defined, since $(\beta_1-\beta_2)^2 \le (\beta_1+\beta_2)^2$ follows from $(\beta_1 \pm \beta_2)^2 = \beta_1^2 \pm 2\beta_1\beta_2 + \beta_2^2$.

Proof. We shall identify the unit-circle $\mathbb{T}$ with $[0, 1]$ through $[0, 1] \ni t \longmapsto e^{it} \in \mathbb{T}$.

(i) We have

$$2 \cdot \operatorname{tr} R(t) = \alpha_1 + \alpha_2,$$

$$4 \cdot \det R(t) = \alpha_1\alpha_2 - |\beta_1 + \beta_2 e^{it}|^2 = \alpha_1\alpha_2 - (\beta_1^2 + \beta_2^2) - 2\beta_1\beta_2 \cos t.$$

The eigenvalues of $R(t)$ are given by

$$\lambda_j(t) = \frac{\alpha_1+\alpha_2+(-1)^j\sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1^2+2\beta_1\beta_2\cos t+\beta_2^2)}}{4},$$

where $j = 1, 2$. We get

$$\bigcup_{t\in[0,2\pi]} \sigma(R(t)) = \bigcup_{t\in[0,2\pi]} \{\lambda_1(t)\} \cup \bigcup_{t\in[0,2\pi]} \{\lambda_2(t)\}.$$

The range of $[0, 2\pi] \ni t \longmapsto \sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1^2+2\beta_1\beta_2\cos t+\beta_2^2)} \in \mathbb{R}$ is

$$\left[\sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1-\beta_2)^2}, \sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1+\beta_2)^2} \right],$$

where $(\beta_1-\beta_2)^2 \le (\beta_1+\beta_2)^2$. Therefore, $\bigcup_{t\in[0,2\pi]}\{\lambda_j(t)\} = I_j$ for each $j = 1, 2$. Note also that I_1 is located to the left of I_2;

$$\Delta(I_1, I_2) := \min I_2 - \max I_1 = \sqrt{(\alpha_1-\alpha_2)^2+4(\beta_1-\beta_2)^2} \ge 0.$$

(ii) The gap $\Delta(I_1, I_2)$ becomes 0 if and only if $\alpha_1 - \alpha_2 = 0 = \beta_1 - \beta_2$. In this case,

$$I_1 \cup I_2 = [\alpha_1/2 - \beta_1, \alpha_1/2 + \beta_1].$$

$\square$

Proof of Theorem II.34. Since $n_\star = 2$, it follows from (II.104) that

$$\hat{R}_\pm(\star, z) = \frac{1}{2}\begin{pmatrix} r_{0,\pm}(\star, 0) & r_{1,\pm}(\star, 0) + r_{1,\pm}(\star, 1)z^* \\ r_{1,\pm}(\star, 0) + r_{1,\pm}(\star, 1)z & r_{0,\pm}(\star, 1) \end{pmatrix}. \tag{II.125}$$

Let us first prove that $\bigcup_{z\in\mathbb{T}} \sigma\left(\hat{R}_\pm(\star, z)\right)$ does not depend on the choice of $\pm$ in order to show (II.118). For each $\zeta = p, q, a, b$, and each $m = 0, 1$, we write $\zeta_m := \zeta(\star, m)$ for simplicity from here on. With this convention in mind, we let

$$\begin{aligned}
r_{0,\pm}(\star, 0) &= (p_0 \pm 1)a_0 + (p_0 \mp 1)a_1 =: \alpha_{1,\pm}, \\
r_{0,\pm}(\star, 1) &= (p_1 \pm 1)a_1 + (p_1 \mp 1)a_0 =: \alpha_{2,\pm}, \\
r_{1,\pm}(\star, 0) &= \sqrt{(1 \mp p_0)(1 \pm p_1)}b_1 =: \beta_{1,\pm}, \\
r_{1,\pm}(\star, 1) &= \sqrt{(1 \pm p_0)(1 \mp p_1)}b_0 =: \beta_{2,\pm},
\end{aligned}$$

where $\alpha_{1,\pm}, \alpha_{2,\pm} \in \mathbb{R}$, and where $\beta_{1,\pm}, \beta_{2,\pm} \geq 0$. It follows that (II.125) is a special case of (II.124). We shall make use of the following equalities in order to apply Lemma II.36 (i) to $\hat{R}_\pm(\star, z)$:

$$\begin{aligned}
\alpha_{1,\pm} + \alpha_{2,\pm} &= (p_0 + p_1)(a_0 + a_1), \\
(\alpha_{1,\pm} - \alpha_{2,\pm})^2 &= (p_0 - p_1)^2(a_0 + a_1)^2 + 4(a_0 - a_1)^2 \pm 4(p_0 - p_1)(a_0^2 - a_1^2), \\
(\beta_{1,\pm} + (-1)^j\beta_{2,\pm})^2 &= (1 - p_0p_1)(2 - a_0^2 - a_1^2) + 2(-1)^j q_0q_1b_0b_1 \mp (p_0 - p_1)(a_0^2 - a_1^2),
\end{aligned}$$

where $j = 1, 2$, and where we use $\beta_{1,\pm}^2 + \beta_{2,\pm}^2 = (1 - p_0p_1)(2 - a_0^2 - a_1^2) \mp (p_0 - p_1)(a_0^2 - a_1^2)$ in the last equality. It follows that $d'_j := (\alpha_{1,\pm} - \alpha_{2,\pm})^2 + 4(\beta_{1,\pm} + (-1)^j\beta_{2,\pm})^2 \geq 0$ does not depend on the choice of $\pm$ for each $j = 1, 2$. Moreover,

$$\begin{aligned}
d'_j &= (p_0 - p_1)^2(a_0 + a_1)^2 + 4(a_0 - a_1)^2 + 4(1 - p_0p_1)(2 - a_0^2 - a_1^2) + 8(-1)^j q_0q_1b_0b_1 \\
&= (p_0 + p_1)^2(a_0 + a_1)^2 + 8(2 - (1 + p_0p_1)(1 + a_0a_1) + (-1)^j q_0q_1b_0b_1) \\
&= 16(d(\star)^2 + d_j(\star)),
\end{aligned}$$

where the second equality follows from $(p_0 - p_1)^2 = (p_0 + p_1)^2 - 4p_0p_1$. If we define $I_j(\star)$ according to (II.119), then it follows from Lemma II.36 (i) that

$$\bigcup_{z\in\mathbb{T}} \sigma\left(\hat{R}_+(\star, z)\right) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{R}_-(\star, z)\right) = I_1(\star) \cup I_2(\star).$$

Note that (II.118) follows from Theorem II.30.

(i) It is obvious that $0 \leq d(\star)^2 + d_1(\star) \leq d(\star)^2 + d_2(\star)$, and that $I_1(\star)$ lies to the left of $I_2(\star)$. It remains to show $I_1(\star) \cup I_2(\star) \subseteq [-1, 1]$. Let

$$d_\pm(\star) := d(\star) \pm \sqrt{d(\star)^2 + d_2(\star)},$$

where $d_-(\star)$ (resp. $d_+(\star)$) is the minimum (resp. maximum) of $I_1(\star)\cup I_2(\star)$. Let the notation $\leqq$ simultaneously denote $\leq$ and $=$. We are required to prove that the following equivalent conditions hold true with $|d(\star)| \leq 1$ in mind;

$$\pm\, d_\pm(\star) \leqq 1 \text{ if and only if } 0 \leqq (1 + p_0p_1)(1 + a_0a_1) \mp (p_0 + p_1)(a_0 + a_1) - q_0q_1b_0b_1, \tag{II.126}$$

where $(1 + p_0p_1)(1 + a_0a_1) \mp (p_0 + p_1)(a_0 + a_1) \geq 0$. Indeed,

$$\begin{aligned}&(1 + p_0p_1)(1 + a_0a_1) \mp (p_0 + p_1)(a_0 + a_1)\\ &\qquad = \begin{cases} 0, & p_0p_1 = -1 \text{ or } a_0a_1 = -1,\\ (1 + p_0p_1)(1 + a_0a_1)\left(1 \mp \frac{p_0+p_1}{1+p_0p_1}\frac{a_0+a_1}{1+a_0a_1}\right), & \text{otherwise.}\end{cases}\end{aligned}$$

It remains to prove

$$0 \leqq ((1 + p_0p_1)(1 + a_0a_1) \mp (p_0 + p_1)(a_0 + a_1))^2 - (1 - p_0^2)(1 - p_1^2)(1 - a_0^2)(1 - a_1^2). \tag{II.127}$$

Let

$$s_\pm := ((1 + p_0p_1)(1 + a_0a_1) \mp (p_0 + p_1)(a_0 + a_1))^2,$$

$$s'_\pm := ((1 + p_0p_1)(a_0 + a_1) \mp (1 + a_0a_1)(p_0 + p_1))^2.$$

We show that the right hand side of (II.127) is $s'_\pm \geq 0$;

$$\begin{aligned} s_\pm - s'_\pm &= (1+p_0p_1)^2((1+a_0a_1)^2 - (a_0+a_1)^2) - (p_0+p_1)^2((1+a_0a_1)^2 - (a_0+a_1)^2) \\ &= ((1+p_0p_1)^2 - (p_0+p_1)^2)((1+a_0a_1)^2 - (a_0+a_1)^2) \\ &= (1-p_0^2)(1-p_1^2)(1-a_0^2)(1-a_1^2). \end{aligned}$$

It follows that (II.127) holds true. We get $-1 \leq d_-(\star) \leq d_+(\star) \leq 1$ by (II.126), and so $I_1 \cup I_2 \subseteq [-1,1]$.

(ii) It follows from (i) that

$$d_\pm(\star) = \pm 1 \text{ if and only if } s'_\pm = 0. \tag{II.128}$$

It follows from a direct computation that

$$\prod_{m=0,1}(1+p_m)(1\mp a_m) - \prod_{m=0,1}(1-p_m)(1\pm a_m) = \mp 2((1+p_0p_1)(a_0+a_1) \mp (1+a_0a_1)(p_0+p_1)).$$

Therefore, $\pm 1 \notin \sigma(\star)$ if and only if $\prod_{m=0,1}(1+p_m)(1\mp a_m) \neq \prod_{m=0,1}(1-p_m)(1\pm a_m)$.

(iii) If $\prod_{m=0,1}(1+p_m)(1\mp a_m) + \prod_{m=0,1}(1-p_m)(1\pm a_m) > 0$, then we define $p(\star), a(\star) \in [-1,1]$ through (II.123). Note that (II.122) is equivalent to $p(\star) \mp a(\star) \neq 0$ as in the proof of Theorem II.20 (ii). The claim follows from (ii).

(iv) Note that $I_j(\star)$ given by (II.119) is a singleton set if and only if $d_1(\star) = d_2(\star)$ if and only if $\prod_{m=0,1} q(\star,m)b(\star,m) = 0$. The claim follows. □

II.5.1.3 The general case

It is desirable to give a complete classification of $\sigma(\star)$ in full generality. The special cases $n_\star = 1,2$ we have considered in this subsection are intended as motivating examples for this general approach. It is worth noting that the proof of Theorem II.34 is already far from obvious. The general case $n_\star \geq 3$ naturally leads to spectral analysis of Hermitian matrices of the following form;

$$\begin{pmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 & \gamma_0 \\ \gamma_1 & \alpha_1 & \beta_1 & \cdots & 0 & 0 \\ 0 & \gamma_2 & \alpha_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \alpha_{n-2} & \beta_{n-2} \\ \beta_{n-1} & 0 & 0 & \cdots & \gamma_{n-1} & \alpha_{n-1} \end{pmatrix}. \tag{II.129}$$

It is not known to the author whether or not there is a general standard method for this.

II.5.2 Decay rates and spectral gaps in the essential spectrum

It is shown in the proof of Theorem A (ii) that (II.77) is a more precise version of the exponential decay property (I.15), where we recall that $\delta^{\downarrow}_{j,\pm}, \delta^{\uparrow}_{j,\pm}$ are given respectively by the following formulas (see (II.98) to (II.99)):

$$\delta^{\downarrow}_{j,\pm} = \min\left\{(\Lambda(p(-\infty))\Lambda(\mp a(-\infty)))^{(-1)^{j+1}}, (\Lambda(p(+\infty))\Lambda(\mp a(+\infty)))^{(-1)^{j}}\right\},$$
$$\delta^{\uparrow}_{j,\pm} = \max\left\{(\Lambda(p(-\infty))\Lambda(\mp a(-\infty)))^{(-1)^{j+1}}, (\Lambda(p(+\infty))\Lambda(\mp a(+\infty)))^{(-1)^{j}}\right\}.$$

The purpose of the current subsection is to show that the two numbers $\delta^{\downarrow}_{j,\pm}, \delta^{\uparrow}_{j,\pm}$, viewed as *decay rates* of the symmetry-protected bound state Ψ, depend on the size of spectral gaps in $\sigma_{\mathrm{ess}}(U)$. For simplicity, we assume that the anisotropic assumption (I.8) holds true for each $\star = -\infty, +\infty$ and each $\zeta = p, a$ throughout (that is to say, we let $n_\star = 1$ for each $\star = -\infty, +\infty$). We consider the following two examples:

Example II.37 (half-gapped case)**.** Let $0 < p_0 < 1$, and let

$$p(-\infty) := -p_0, \qquad a(-\infty) := \pm p_0,$$
$$p(+\infty) := p_0, \qquad a(+\infty) := \mp p_0.$$

Since $\pm a(-\infty) = p_0 \neq p(-\infty)$ and $\pm a(+\infty) = -p_0 \neq p(+\infty)$, the essential spectrum of the operator U has a spectral gap at ± 1. Moreover,

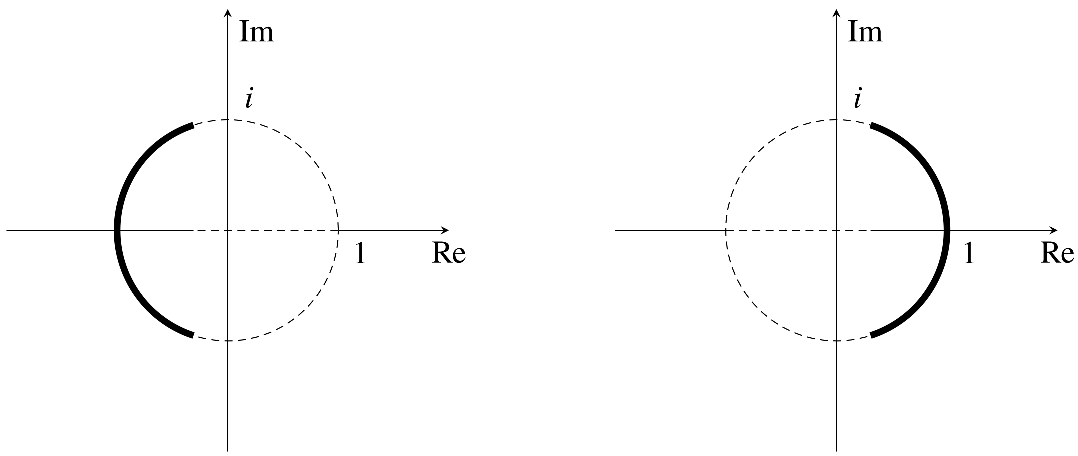
$$p(-\infty) \mp a(-\infty) = -2p_0 < 0 < 2p_0 = p(+\infty) \mp a(+\infty).$$

We get $\operatorname{ind}_{\pm}(\Gamma, U) = \dim\ker(U \mp 1) = 1$. It follows from §II.5.1.1 that the essential spectrum of U is given explicitly by

$$\sigma_{\mathrm{ess}}(U) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in I_{\pm}\}, \qquad I_{\pm} := [\mp p_0^2 - (1 - p_0^2), \mp p_0^2 + (1 - p_0^2)].$$

More precisely, the essential spectrum $\sigma_{\mathrm{ess}}(U)$ can be classified into the following two distinct cases:

(i) $(a(-\infty), a(+\infty)) = (p_0, -p_0)$ (ii) $(a(-\infty), a(+\infty)) = (-p_0, p_0)$



$\sigma_{\mathrm{ess}}(U) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in I_+\}$ $\sigma_{\mathrm{ess}}(U) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in I_-\}$

Figure II.1: The black connected regions depict $\sigma_{\mathrm{ess}}(U)$. We have $-1 \in \sigma_{\mathrm{ess}}(U)$ in Case (i), whereas $+1 \in \sigma_{\mathrm{ess}}(U)$ in Case (ii).

We have $I_+ = [-1, 1 - 2p_0^2]$ in Case (i), and $I_- = [-1 + 2p_0^2, +1]$ in Case (ii). This motivates us to introduce the gap width $\Omega(p_0) := 2p_0^2$. Moreover, we have

$$\delta^{\uparrow}_{1,\pm} = \delta^{\downarrow}_{1,\pm} = \Lambda(-p_0)^2.$$

Note that $\Omega(p_0) = 2p_0^2$ increases as $p_0 \to 1$. In this case, the convergence rates $\delta^{\uparrow}_{1,\pm} = \delta^{\downarrow}_{1,\pm}$ decrease, since $\Lambda(-p_0)^2 \to 0$.

Example II.38 (Double-gapped case)**.** We let $p(x) = 0$ for each $x \in \mathbb{Z}$. We have the following index formula;

$$\operatorname{ind}_{\pm}(\Gamma, U) = \begin{cases} +1, & \mp a(-\infty) < 0 < \mp a(+\infty), \\ -1, & \mp a(+\infty) < 0 < \mp a(-\infty), \\ 0, & \text{otherwise.} \end{cases} \tag{II.130}$$

Note that we have

$$\delta^{\downarrow}_{j,\pm} = \min\left\{\Lambda(\mp(-1)^j a(+\infty)), \frac{1}{\Lambda(\mp(-1)^j a(-\infty))}\right\}, \tag{II.131}$$

$$\delta^{\uparrow}_{j,\pm} = \max\left\{\Lambda(\mp(-1)^j a(+\infty)), \frac{1}{\Lambda(\mp(-1)^j a(-\infty))}\right\}, \tag{II.132}$$

It follows from §II.5.1.1 that

$$\sigma_{\mathrm{ess}}(U) = \bigcup_{\star=\pm\infty} \{z \in \mathbb{T} \mid \operatorname{Re} z \in I(\star)\}, \tag{II.133}$$

$$I(\star) := [-\sqrt{1-a(\star)^2}, \sqrt{1-a(\star)^2}], \qquad \star = \pm\infty. \tag{II.134}$$

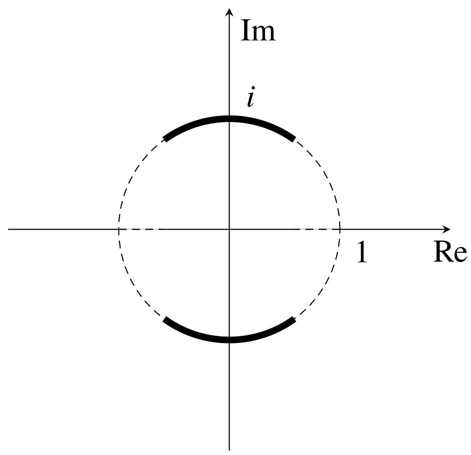


Figure II.2: This figure depicts $\sigma_{\mathrm{ess}}(U)$.

Figure II.2 motivates us to introduce the following gap width;

$$\Omega := \min\{1 - \sqrt{1-a(-\infty)^2}, 1 - \sqrt{1-a(+\infty)^2}\}.$$

Suppose that $\mp a(-\infty) < 0 < \mp a(+\infty)$ holds true. Then $\Lambda(\mp a(-\infty)) < 1$ and $\frac{1}{\Lambda(\mp a(+\infty))} < 1$. Note that Ω increases as $|a(\star)| \to 1$ for each $\star = -\infty, +\infty$. This corresponds to $\mp a(-\infty) \to -1$ and $\mp a(+\infty) \to +1$. Thus, $\Lambda(\mp a(-\infty)) \to 0$ and $\frac{1}{\Lambda(\mp a(+\infty))} \to 0$. It follows that $\delta^{\uparrow}_{2,\pm} \to 0$ and $\delta^{\downarrow}_{2,\pm} \to 0$.

II.5.3 The spectral mapping theorem for chirally symmetric unitary operators

The purpose of the current subsection is to revisit the previously mentioned formula (II.19) in the context of the so-called *spectral mapping theorem for chirally symmetric unitary operators* [HKSS14, SS16, SS19] as mentioned in Remark II.5. Let us start with a brief overview of this well-known theorem under the setting of Proposition II.4. If the underlying Hilbert space $\mathcal{H}$ is separable, then we can canonically decompose the unitary self-adjoint operator Γ' as the difference $\Gamma' = \partial^*\partial - (1 - \partial^*\partial)$ for some operator ∂ from $\mathcal{H} = \ker(\Gamma' - 1) \oplus \ker(\Gamma' + 1)$ into an auxiliary Hilbert space $\mathcal{K}$, satisfying $\partial\partial^* = 1$ (see, for example, [Suz19, Lemma 3.3]). Here, $\partial^*\partial$ (resp. $1-\partial^*\partial$) turns out to be the orthogonal projection onto $\ker(\Gamma'-1)$ (resp. $\ker(\Gamma'+1)$). It is partly shown in the spectral mapping theorem that for each eigenvalue z of U, we have

$$\dim\ker(U-z) = \begin{cases} \dim\ker\left(\partial\Gamma\partial^* - \frac{z+z^*}{2}\right), & |z|<1, \\ \dim\ker(\partial\Gamma\partial^*-1) + \dim\left(\ker(\Gamma+1)\cap\ker\partial\right), & z=1, \\ \dim\ker(\partial\Gamma\partial^*+1) + \dim\left(\ker(\Gamma-1)\cap\ker\partial\right), & z=-1, \end{cases} \tag{II.135}$$

where the spectrum of the self-adjoint operator $T := \partial\Gamma\partial^*$ is a subset of $[-1,1]$, since $\|T\| \leq 1$ immediately follows from $\|\Gamma\| = 1$ and from $\|\partial\|^2 = \|\partial^*\|^2 = \|\partial^*\partial\| = 1$. The complete statement of the spectral mapping theorem can be found, for example, in [SS19, Theorem 1.2]. Mathematical utilities of the spectral mapping theorem are confirmed in the context of chirally symmetric quantum walks [FFS17, FFS18].

If $|z|<1$, then the formula (II.135) has the following graphical interpretation;

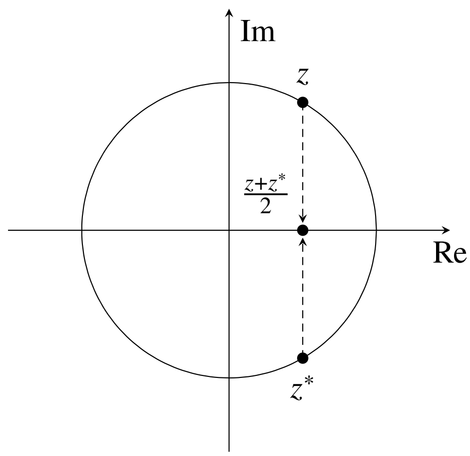


Figure II.3: Given the chirally symmetric unitary operator $U = \Gamma\Gamma'$, where $\Gamma' = \partial^*\partial - (1-\partial^*\partial)$, we have that $z \in \mathbb{T}$ is an eigenvalue of U if and only if so is z^*. In this case, their real part $(z+z^*)/2$ turns out to be an eigenvalue of the self-adjoint operator $T = \partial\Gamma\partial^*$, provided that $|z|<1$.

On the other hand, if $z=-1$ or $z=1$, then special care needs to be taken, since $\dim\ker(U\mp 1)$ is greater than $\dim\ker(T\mp 1)$ in general. More precisely, the formula (II.135) becomes $\dim\ker(U\mp 1) = m_\pm + M_\pm$ in this case, where $m_\pm, M_\pm$ are defined respectively by

$$m_\pm := \dim\ker(T\mp 1), \qquad M_\pm := \dim\left(\ker(\Gamma\pm 1)\cap\ker\partial\right). \tag{II.136}$$

In fact, it is shown in [Suz19, Theorem 3.1] that

$$\partial^* \ker(T \mp 1) = \ker(\varGamma \mp 1) \cap \ker(\varGamma' - 1), \tag{II.137}$$

$$\ker(\varGamma \pm 1) \cap \ker \partial = \ker(\varGamma \pm 1) \cap \ker(\varGamma' + 1), \tag{II.138}$$

where the isometry ∂^* in (II.137) gives a bijective linear transform $\ker(T \mp 1) \ni \psi \longmapsto \partial^*\psi \in \partial^* \ker(T \mp 1)$. It follows that the four numbers defined by (II.136) can be fully characterised by $\varGamma, \varGamma'$ without referring to ∂. More precisely, we obtain the following four equalities by Remark II.5:

$$m_+ = \dim\left(\ker(\varGamma - 1) \cap \ker(\varGamma' - 1)\right) = m_{1,+}, \tag{II.139}$$

$$m_- = \dim\left(\ker(\varGamma + 1) \cap \ker(\varGamma' - 1)\right) = m_{2,-}, \tag{II.140}$$

$$M_+ = \dim\left(\ker(\varGamma + 1) \cap \ker(\varGamma' + 1)\right) = m_{2,+}, \tag{II.141}$$

$$M_- = \dim\left(\ker(\varGamma - 1) \cap \ker(\varGamma' + 1)\right) = m_{1,-}. \tag{II.142}$$

It follows that $\dim\ker(U \mp 1) = m_\pm + M_\pm$ is indeed consistent with the previously mentioned formula (II.19). In particular, if $\dim\ker(U \mp 1) < \infty$, then (II.18) can be analogously interpreted as

$$\operatorname{ind}_\pm(\varGamma, U) = \pm(m_\pm - M_\pm). \tag{II.143}$$

It is worth recalling at this point that the four numbers $m_\pm, M_\pm$ previously mentioned are originally defined by the formula (II.136) in the statement of the spectral mapping theorem (see, for example, [SS16, SS19]). In particular, we may refer to each of $\mathcal{B}_\pm := \ker(\varGamma \pm 1) \cap \ker \partial$ as a ***birth eigenspace*** following [Seg13, MOS17]. For concreteness, let us consider [FFS18], the primary focus of which is a characterisation of the birth eigenspaces for the evolution operator of Suzuki's split-step quantum walk given by (I.2) under the extra assumption of $p = (p(x))_{x \in \mathbb{Z}}$ being a constant sequence. This classification implicitly makes use of (II.138), where $\ker(\varGamma' + 1) = \ker \partial$ immediately follows from $\varGamma' + 1 = 2\partial^*\partial$. On the other hand, at the time of writing [FFS18], the authors were presumably unaware of the less trivial equality (II.137). Otherwise, (II.137) would have immediately led to an analogous classification result for $\ker(T \mp 1)$.

On a final note, we draw the following conclusion. It is certainly possible to start with (II.143) as a defining property of $\operatorname{ind}_\pm(\varGamma, U)$ via the spectral mapping theorem in contrast to the setting of §II.1.2. Note, however, that this method of defining $\mathrm{ind}_{\pm}(\Gamma, U)$ has the following significant drawback. As in the concrete example mentioned above, it is not easy to directly deduce from the formula (II.143) that $m_{\pm}$ and $M_{\pm}$ are analogous in the sense that (II.139) to (II.142) actually hold true. This is partly due to the technical nature of the spectral mapping theorem. In fact, the ultimate purpose of §II.1.2 is to show that the indices $\mathrm{ind}_{\pm}(\Gamma, U)$ admit a yet another caracterisation. Recall that the key step to this elementary construction, which makes no use of the spectral mapping theorem at all, lies in the canonical decomposision of the real part $R := \mathrm{Re}\, U$ into $R = R_1 \oplus R_2$ based on the $\mathbb{Z}_2$-grading of the underlying Hilbert space $\ker(\Gamma - 1) \oplus \ker(\Gamma + 1)$. It follows from a direct algebraic computation that $\ker(U \mp 1) = \ker(R_1 \mp 1) \oplus \ker(R_1 \mp 2)$, and this motivates us to let $\mathrm{ind}_{\pm}(\Gamma, U) := \dim\ker(R_1 \mp 1) - \dim\ker(R_2 \mp 1)$. Note that each $m_{j,\pm} = \dim\ker(R_j \mp 1)$ satisfies (II.139) to (II.142) according to Remark II.5 as mentioned previously.

II.5.4 A new derivation of the existing index formulas

Let $U_{\mathrm{suz}}, \Gamma_{\mathrm{suz}}, \Gamma'_{\mathrm{suz}}$ be given respectively by (I.2), (I.3), and let $(U, \Gamma, \Gamma') := (U_{\mathrm{suz}}, \Gamma_{\mathrm{suz}}, \Gamma'_{\mathrm{suz}})$ for simplicity. Classification of the indices $\mathrm{ind}\,(\Gamma, U), \mathrm{ind}\,(\Gamma', U)$ is one of the main subjects of [ST19b, Mat20, Tan21] under the assumption that a limit of the form (I.8) exists for each $\star = -\infty, +\infty$ and each $\zeta = p, a$. More precisely, it is shown in [Tan21, Theorem B] that we have $|p(\star)| \neq |a(\star)|$ for each $\star = -\infty, +\infty$ if and only if $-1, 1 \notin \sigma_{\mathrm{ess}}(U)$.

In this case, we have

$$\operatorname{ind}(\varGamma, U) = \begin{cases} 0, & |p(-\infty)| < |a(-\infty)| \text{ and } |p(+\infty)| < |a(+\infty)|, \\ +\operatorname{sign} p(+\infty), & |p(-\infty)| < |a(-\infty)| \text{ and } |p(+\infty)| > |a(+\infty)|, \\ -\operatorname{sign} p(-\infty), & |p(-\infty)| > |a(-\infty)| \text{ and } |p(+\infty)| < |a(+\infty)|, \\ +\operatorname{sign} p(+\infty) - \operatorname{sign} p(-\infty), & |p(-\infty)| > |a(-\infty)| \text{ and } |p(+\infty)| > |a(+\infty)|, \end{cases} \tag{II.144}$$

$$\operatorname{ind}(\varGamma', U) = \begin{cases} -\operatorname{sign} a(+\infty) + \operatorname{sign} a(-\infty), & |p(-\infty)| < |a(-\infty)| \text{ and } |p(+\infty)| < |a(+\infty)|, \\ +\operatorname{sign} a(-\infty), & |p(-\infty)| < |a(-\infty)| \text{ and } |p(+\infty)| > |a(+\infty)|, \\ -\operatorname{sign} a(+\infty), & |p(-\infty)| > |a(-\infty)| \text{ and } |p(+\infty)| < |a(+\infty)|, \\ 0, & |p(-\infty)| > |a(-\infty)| \text{ and } |p(+\infty)| > |a(+\infty)|, \end{cases} \tag{II.145}$$

where the sign function sign is given by (I.28). Note that (I.22) coincides with (II.144), if we let $\gamma(x) = 0$ for each $x \in \mathbb{Z}$. The purpose of the current subsection is to show that the same formulas (II.144) to (II.145) still hold true, even if we replace the anisotropic assumption (I.8) by (I.10) for each $\zeta = p, a$.

Theorem II.39. *With the notation introduced in Theorem II.20 in mind, we have $|p(\star)| \neq |a(\star)|$ for each $\star = -\infty, +\infty$ if and only if $-1, 1 \notin \sigma_{\mathrm{ess}}(U)$. In this case, the indices* $\operatorname{ind}(\varGamma, U), \operatorname{ind}(\varGamma', U)$ *are given respectively by* (II.144) *to* (II.145).

This theorem is a generalisation of [Tan21, Theorem B] mentioned above.

Proof. The first part immediately follows from Theorem II.20 (ii). We shall make use of the formula (II.63) throughout. Let i_1 (resp. i_2) be defined by the right hand side of (II.144) (resp. of (II.145)). We are required to show $i_1 = \operatorname{ind}(\varGamma, U)$ and $i_2 = \operatorname{ind}(\varGamma', U)$. For each $\alpha_1, \alpha_2 \in [-1, 1]$ such that $\alpha_1 \neq \alpha_2$, let

$$w_j(\alpha_1, \alpha_2) := \frac{\operatorname{sign}(\alpha_1 - \alpha_2) + (-1)^{j+1} \operatorname{sign}(\alpha_1 + \alpha_2)}{2}, \qquad j = 1, 2.$$

We have $-w_2(\alpha_2, \alpha_1) = w_1(\alpha_1, \alpha_2)$, where

$$w(\alpha_1, \alpha_2) = \begin{cases} \operatorname{sign} \alpha_1, & |\alpha_1| > |\alpha_2|, \\ 0, & |\alpha_1| < |\alpha_2|. \end{cases}$$

With this result in mind, we obtain $i_j = w_j(p(+\infty), a(+\infty)) - w_j(p(-\infty), a(-\infty))$ for each $j = 1, 2$. On the other hand, direct computations show

$$\mathrm{ind}_+(\varGamma, U) + (-1)^{j+1}\mathrm{ind}_-(\varGamma, U) = w_j(p(+\infty), a(+\infty)) - w_j(p(-\infty), a(-\infty)).$$

The claim follows. □

II.5.5 The square of the evolution operator

Theorem II.24 gives a concrete quantum walk example with the property that the estimate (I.7) becomes an equality. The purpose of the current subsection is to show that this is not always the case. Our counter example is based on the following simple proposition.

Proposition II.40. *If $(\varGamma, U)$ is an abstract chiral pair on a Hilbert space $\mathcal{H}$, then $(\varGamma, U^2)$ and $(\varGamma'\varGamma\varGamma', U^2)$ are unitarily equivalent chiral pairs. Moreover, the following assertions hold true:*

(i) *If* $\ker(U^2 - 1) = \ker(U - 1) \oplus \ker(U + 1)$ *is finite-dimensional, then*

$$\mathrm{ind}_+(\varGamma, U^2) = \mathrm{ind}\,(\varGamma, U). \tag{II.146}$$

(ii) *If* $\ker(U^2 + 1) = \ker(U - i) \oplus \ker(U + i)$ *is finite-dimensional, then*

$$\mathrm{ind}_-(\varGamma, U^2) = 0. \tag{II.147}$$

(iii) *If* $\ker(U^2 - 1) \oplus \ker(U^2 + 1)$ *is finite-dimensional, then* $\mathrm{ind}\,(\varGamma, U^2) = \mathrm{ind}\,(\varGamma, U)$.

Proof. Note that $(\varGamma, U^2)$ and $(\varGamma'\varGamma\varGamma', U^2)$ are chiral pairs, since $U^2 = \varGamma(\varGamma'\varGamma\varGamma')$. We have

$$(\varGamma, U^2) = (\varGamma, \varGamma\varGamma'\varGamma\varGamma') \cong (\varGamma'\varGamma\varGamma', \varGamma'(\varGamma\varGamma'\varGamma\varGamma')\varGamma') = (\varGamma'\varGamma\varGamma', \varGamma'\varGamma\varGamma'\varGamma) = (\varGamma'\varGamma\varGamma', (U^2)^*) \cong (\varGamma'\varGamma\varGamma', U^2), \tag{II.148}$$

where $\cong$ represents unitary equivalence. If U admits the standard representation of the form (II.2), then U^2 admits the following standard representation;

$$U^2 = \begin{pmatrix} 2R_1^2 - 1 & 2iQ_2R_2 \\ 2iQ_1R_1 & 2R_2^2 - 1 \end{pmatrix}. \tag{II.149}$$

It follows that

$$\operatorname{ind}_{\pm}(\Gamma, U^2) := \dim\ker((2R_1^2 - 1) \mp 1) - \dim\ker((2R_2^2 - 1) \mp 1). \tag{II.150}$$

(i) If $\ker(U^2 - 1) = \ker(U - 1) \oplus \ker(U + 1)$ is finite-dimensional, then $\ker(U - 1) = \ker(R - 1)$ and $\ker(U + 1) = \ker(R + 1)$ are finite-dimensional. In this case,

$$\begin{aligned}
\operatorname{ind}_{+}(\Gamma, U^2) &= \dim\ker((2R_1^2 - 1) - 1) - \dim\ker((2R_2^2 - 1) - 1) \\
&= \dim\ker(R_1^2 - 1) - \dim\ker(R_2^2 - 1) \\
&= \dim\ker(R_1 - 1) + \dim\ker(R_1 + 1) - (\dim\ker(R_2 - 1) + \dim\ker(R_2 - 1)) \\
&= \dim\ker(R_1 - 1) - \dim\ker(R_2 - 1) + \dim\ker(R_1 + 1) - \dim\ker(R_2 - 1) \\
&= \operatorname{ind}_{+}(\Gamma, U) + \operatorname{ind}_{-}(\Gamma, U) \\
&= \operatorname{ind}(\Gamma, U).
\end{aligned}$$

(ii) If $\ker(U^2 + 1) = \ker(U - i) \oplus \ker(U + i)$ is finite-dimensional, then it follows from (II.148) that

$$\operatorname{ind}_{-}(\Gamma, U^2) = \operatorname{ind}_{-}(\Gamma'\Gamma\Gamma', U^2) = -\operatorname{ind}_{-}(\Gamma, U^2),$$

where the last equality follows from (II.14). We get $\operatorname{ind}_{-}(\Gamma, U^2) = 0$.

(iii) This follows from (i) and (ii). □

Remark II.41. If $\ker(U^2 + 1) = \ker(U - i) \oplus \ker(U + i)$ is finite-dimensional, then $\operatorname{ind}_{-}(\Gamma, U^2) = 0$. It follows from (II.150) that $\ker R_1$ and $\ker R_2$ have the same finite dimension, say, n. We get $\dim(\ker(U^2 + 1)) = 2n$.

Example II.42. Let U be the evolution operator of Suzuki's split-step quantum walk, and let $p(x) = 0$ for each $x \in \mathbb{Z}$. Suppose that there exists $a_0 \in (0, 1)$ with the property that $a(x) \to \pm a_0$ as $x \to \pm\infty$. We make use of the index formula (II.130). Since $a(-\infty) = -a_0 < 0 < a_0 = a(+\infty)$, we have $\operatorname{ind}_{+}(\Gamma, U) = -1$ and $\operatorname{ind}_{-}(\Gamma, U) = 1$. Thus $\operatorname{ind}_{+}(\Gamma, U^2) = 0$. On the other hand, we get

$$\dim\ker(U^2 - 1) = \dim(\ker(U - 1) \oplus \ker(U + 1)) = |\operatorname{ind}_{+}(\Gamma, U)| + |\operatorname{ind}_{-}(\Gamma, U)| = 2.$$

Then $\dim\ker(U^2 - 1) = 2$ and $\operatorname{ind}_{+}(\Gamma, U^2) = 0$. That is, $|\operatorname{ind}_{+}(\Gamma, U^2)| \neq \dim\ker(U^2 - 1)$.

Chapter III

Non-unitary Models

III.1 The statement of the main theorem (Theorem B)

We consider index theory for non-unitary operators U satisfying the chiral symmetry condition (I.1) in this chapter. We start with the following definition;

Definition III.1. Let $(\varGamma, U)$ be a chiral pair on a Hilbert space $\mathcal{H}$, and let (II.2) be the standard representation of U with respect to $\varGamma$. We say that $(\varGamma, U)$ is ***Fredholm***, if Q_1 is Fredholm (or, equivalently, $Q_2 = Q_1^*$ is Fredholm). In this case, we define $\operatorname{ind}(\varGamma, U) := \operatorname{ind} Q_1$, where the right hand side is the Fredholm index of Q_1.

We are now in a position to state the main theorem of the current chapter;

Theorem B. *Let m be a fixed non-zero integer, and let $\varGamma_m, U_m$ be two block-operator matrices on $\ell^2(\mathbb{Z}, \mathbb{C}^2) = \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$ defined respectively by*

$$\varGamma_m := \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^{m} \end{pmatrix}, \tag{III.1}$$

$$U_m := \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \begin{pmatrix} p & \sqrt{1-p^2} \\ \sqrt{1-p^2} & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^{m} \end{pmatrix} \begin{pmatrix} e^{-2\gamma(\cdot+1)} a & e^{\gamma-\gamma(\cdot+1)}\sqrt{1-a^2} \\ e^{\gamma-\gamma(\cdot+1)}\sqrt{1-a^2} & -e^{2\gamma} a \end{pmatrix}, \tag{III.2}$$

where $\gamma = (\gamma(x))_{x \in \mathbb{Z}}$ is a bounded $\mathbb{R}$-valued sequence, and where $p = (p(x))_{x \in \mathbb{Z}}, a = (a(x))_{x \in \mathbb{Z}}$ are two $\mathbb{R}$-valued sequences satisfying $p(x), a(x) \in [-1, 1]$ for each $x \in \mathbb{Z}$. If a limit of the form (I.8) *exists for each*

$\star = -\infty, +\infty$ *and each* $\zeta = \gamma, p, a$, *then the following two assertions hold true:*

(i) **Index formula.** *For each* $\star = -\infty, +\infty$, *we let*

$$p_\gamma(\star) := \frac{p(\star)}{\sqrt{p(\star)^2 + (1 - p(\star)^2)\cosh^2(2\gamma(\star))}}. \tag{III.3}$$

Then the chiral pair $(\varGamma_m, U_m)$ *is Fredholm if and only if* $|p_\gamma(\star)| \neq |a(\star)|$ *for each* $\star = -\infty, +\infty$. *In this case, we have* $\operatorname{ind}(\varGamma_m, U_m) \in \{-2m, -m, 0, m, 2m\}$, *and*

$$\frac{\operatorname{ind}(\varGamma_m, U_m)}{m} = \begin{cases} 0, & |p_\gamma(-\infty)| < |a(-\infty)| \text{ and } |p_\gamma(+\infty)| < |a(+\infty)|, \\ +\operatorname{sign} p(+\infty), & |p_\gamma(-\infty)| < |a(-\infty)| \text{ and } |p_\gamma(+\infty)| > |a(+\infty)|, \\ -\operatorname{sign} p(-\infty), & |p_\gamma(-\infty)| > |a(-\infty)| \text{ and } |p_\gamma(+\infty)| < |a(+\infty)|, \\ \operatorname{sign} p(+\infty) - \operatorname{sign} p(-\infty), & |p_\gamma(-\infty)| > |a(-\infty)| \text{ and } |p_\gamma(+\infty)| > |a(+\infty)|, \end{cases} \tag{III.4}$$

where the sign function sign *is defined by* (I.28).

(ii) **Essential spectrum.** *There exist two subsets* $\sigma(-\infty), \sigma(+\infty)$ *of* $\mathbb{T} \cup \mathbb{R}$, *such that*

$$\sigma_{\mathrm{ess}}(U_m) = \sigma(-\infty) \cup \sigma(+\infty).$$

More precisely, for each $\star = -\infty, +\infty$ *the set* $\sigma(\star)$ *is given explicitly by the following formulas:*

$$s(\star) := \operatorname{sign}(p(\star)a(\star)), \tag{III.5}$$

$$\Lambda_\pm(\star) := |p(\star)a(\star)|\cosh(2\gamma(\star)) \pm \sqrt{(1 - p(\star)^2)(1 - a(\star)^2)}, \tag{III.6}$$

$$\sigma(\star) := \bigcup_{n \in \{-1,1\}} \left\{ \left(x + \sqrt{x^2 - 1}\right)^n \,\middle|\, s(\star)x \in [\Lambda_-(\star), \Lambda_+(\star)] \right\}. \tag{III.7}$$

Furthermore, for each $\star = -\infty, +\infty$, *there exists a well-defined closed interval* $[\gamma_-(\star), \gamma_+(\star)] \subseteq [0, \infty]$, *such that the set* $\sigma(\star)$ *admits the following further classification:*

Case I. *If* $|\gamma(\star)| \leq \gamma_-(\star)$, *then* $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [-1, 1]$, *and so* $\sigma(\star)$ *is a subset of* $\mathbb{T}$.

Case II. *If* $\gamma_-(\star) < |\gamma(\star)| < \gamma_+(\star)$, *then* $[\Lambda_-(\star), 1] \subseteq [-1, 1]$ *and* $[1, \Lambda_+(\star)] \subseteq [1, \infty)$, *and so* $\sigma(\star)$ *is a connected subset of* $\mathbb{T} \cup \mathbb{R}$ *containing* $s(\star)$.

Case III. *If* $\gamma_+(\star) \leq |\gamma(\star)|$, *then* $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [1, \infty)$, *and so* $\sigma(\star)$ *is a subset of* $\mathbb{R}$.

More precisely, for each $\star = -\infty, +\infty$, *the two numbers* $\gamma_-(\star), \gamma_+(\star)$ *mentioned above are given by*

$$\gamma_\pm(\star) := \begin{cases} \frac{1}{2}\cosh^{-1}\left(\frac{1 \pm \sqrt{(1-p(\star)^2)(1-a(\star)^2)}}{|p(\star)a(\star)|}\right), & p(\star)a(\star) \neq 0, \\ \infty, & p(\star)a(\star) = 0, \end{cases} \tag{III.8}$$

where $\cosh^{-1}$ *denotes the inverse function of* $[0,\infty) \ni x \longmapsto \cosh x \in [1,\infty)$.

Remark III.2. We have the following remarks:

(i) If γ is identically 0 and if $m = 1$, then $(\varGamma_1, U_1) = (\varGamma_{\mathrm{suz}}, U_{\mathrm{suz}})$ with $p_\gamma(\star) = p(\star)$. It is easy to see that in this case the index formula (III.4) becomes the previously mentioned formula (II.144).

(ii) If γ is identically 0, then U_m fails to be unitary. In particular, if $m = 2$, then U_2 turns out to be unitarily equivalent to a certain well-known non-unitary model in the physics literature (see §IV.3 for details).

Note that Figure III.1 below helps us to visualise the classification of the subset $\sigma(\star)$ of $\mathbb{T} \cup \mathbb{R}$ in Theorem B (ii).

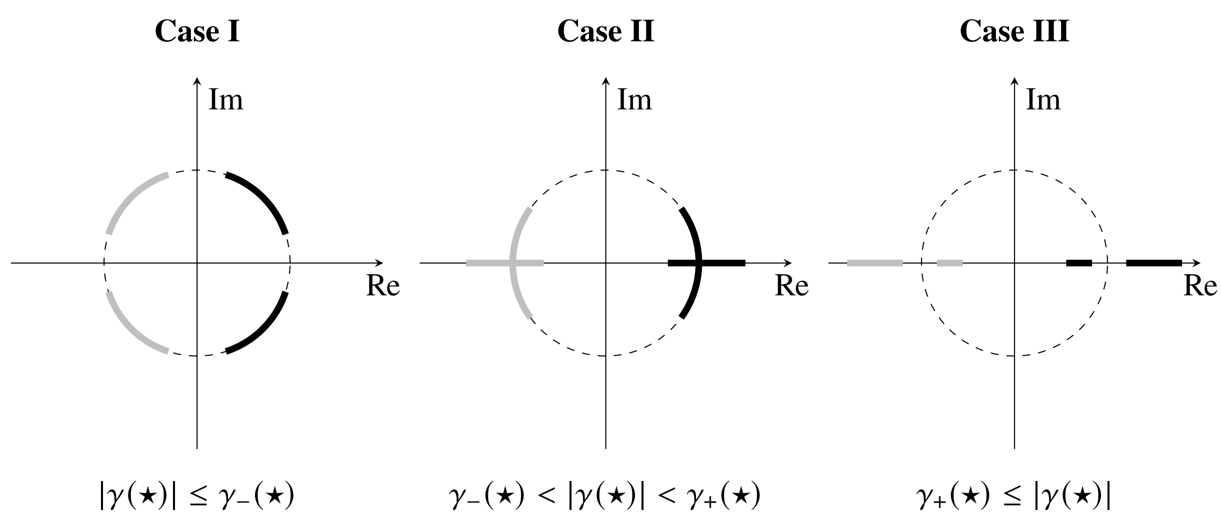


Figure III.1: For each $\star = -\infty, +\infty$, the subset $\sigma(\star)$ of $\mathbb{T} \cup \mathbb{R}$ is classified into Cases I, II, III as above according to the size of $|\gamma(\star)|$. With (III.5) in mind, if $s(\star) = 1$ (resp. if $s(\star) = -1$), then the black regions (resp. gray regions) in each of the above three cases depict the subset $\sigma(\star)$. Therefore, there are six distinct cases in total. In particular, $\sigma(\star)$ is a connected subset of $\mathbb{T} \cup \mathbb{R}$ containing either -1 or $+1$ in Case II.

More explicit formulas for $\sigma(\star)$ will be given shortly in §III.2.2. The proof of Theorem B will be deferred to §III.3, and we directly proceed to the following discussion;

III.2 Discussion

III.2.1 Symmetry protection of bound states for non-unitary quantum walks

Whether or not an estimate analogous to (I.20) holds true for non-unitary U is a highly non-trivial open question. This problem is in fact far beyond the scope of the present thesis. Nevertheless, it is expected that Theorem B forms a basis for further investigation into symmetry protection of eigenstates for non-unitary quantum walks based on the following reasons. Firstly, Theorem B (i) states that the index $\operatorname{ind}(\varGamma, U)$ on the left hand side of (I.20) remains as a robust quantity, even if we consider the non-unitary variant of Suzuki's split-step quantum walk characterised by (III.1) to (III.2). Evidently, we are required to make an appropriate modification to the right hand side of (I.20) somehow. To do so, the following procedure might be useful. With the notation introduced in Theorem B, if we let $\gamma(x) = 0$ for each $x \in \mathbb{Z}$, then the evolution operator U_m becomes a unitary operator. We can then alter the asymptotic values $p(\star), a(\star)$ in such a way that the index (III.4) becomes non-zero, in which case (I.20) ensures the existence of at least one eigenvalue $\lambda_0 \in \{-1, +1\}$. As we monotonically increase $\gamma(\star)$ from 0, the evolution operator U_m becomes non-unitary. In this case, we might be able to keep track of the continuous movement of the eigenvalue λ_0 in a mathematically rigorous fashion; one of the obvious candidates for this investigation is the *transfer matrix method* (see, for example, [KS21]), since it is applicable to non-unitary time-evolutions. This is work in progress.

III.2.2 The gapless case

We start with the following result;

Theorem III.3. *With the notation introduced in Theorem B, suppose that the following two conditions hold true for each* $\star = -\infty, +\infty$:

$$|p_\gamma(\star)| \neq |a(\star)|, \qquad \gamma_-(\star) < |\gamma(\star)| < \gamma_+(\star). \tag{III.9}$$

Then $(\varGamma_m, U_m)$ *is Fredholm, yet the essential spectrum of* U_m *contains* -1 *or* 1. *That is, the characterisation* (II.4) *does not hold true in general for non-unitary* U.

Proof. Let us first start with the following explicit classification of $\sigma_{\mathrm{ess}}(U_m)$. We consider the $\mathbb{R}$-valued function g defined by

$$g(x) := x + \sqrt{x^2 - 1}, \qquad x \in (-\infty, -1] \cup [1, \infty).$$

Figure III.2 shows the graphs of $g, 1/g$;

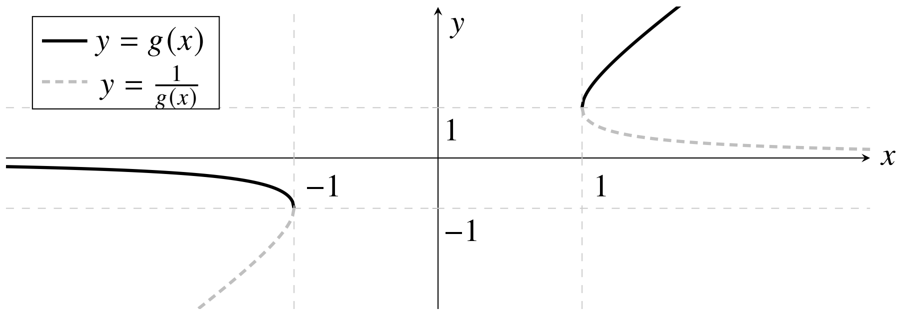


Figure III.2: The black graph corresponds to g, while the gray graph corresponds to $1/g$.

Evidently, $g(x)g(-x)^{-1} = -1$ for $|x| \geq 1$. It follows that for each $\star = -\infty, +\infty$ the set $\sigma(\star)$ is classified into the following six distinct cases:

Case I. If $|\gamma(\star)| \leq \gamma_-(\star)$, then

$$\sigma(\star) = \begin{cases} \left\{x \pm i\sqrt{1 - x^2}\right\}_{x \in [\Lambda_-(\star), \Lambda_+(\star)]}, & s(\star) = 1, \\ \left\{x \pm i\sqrt{1 - x^2}\right\}_{x \in [-\Lambda_+(\star), -\Lambda_-(\star)]}, & s(\star) = -1. \end{cases}$$

Case II. If $\gamma_-(\star) < |\gamma(\star)| < \gamma_+(\star)$, then

$$\sigma(\star) = \begin{cases} \left\{x \pm i\sqrt{1 - x^2}\right\}_{x \in [\Lambda_-(\star), 1]} \cup [g(\Lambda_+(\star))^{-1}, g(\Lambda_+(\star))], & s(\star) = 1, \\ \left\{x \pm i\sqrt{1 - x^2}\right\}_{x \in [-1, -\Lambda_-(\star)]} \cup [-g(\Lambda_+(\star)), -g(\Lambda_+(\star))^{-1}], & s(\star) = -1. \end{cases}$$

Case III. If $\gamma_+(\star) \leq |\gamma(\star)|$, then

$$\sigma(\star) = \begin{cases} [g(\Lambda_+(\star))^{-1}, g(\Lambda_-(\star))^{-1}] \cup [g(\Lambda_-(\star)), g(\Lambda_+(\star))], & s(\star) = 1, \\ [-g(\Lambda_+(\star)), -g(\Lambda_-(\star))] \cup [-g(\Lambda_-(\star))^{-1}, -g(\Lambda_+(\star))^{-1}], & s(\star) = -1. \end{cases}$$

It immediately follows from Theorem B and (III.9) that $(\varGamma_m, U_m)$ is Fredholm, and that $\sigma_{\mathrm{ess}}(U_m) = \sigma(-\infty) \cup \sigma(+\infty)$. In particular, for each $\star = -\infty, +\infty$, the set $\sigma(\star)$ is classified as Case II. That is, each $\sigma(\star)$ is a connected subset of $\mathbb{T} \cup \mathbb{R}$ containing either -1 or $+1$. The claim follows. $\square$

Theorem III.3 motivates us to consider the following explicit example;

Example III.4. Let $(\varGamma_m, U_m)$ be the chiral pair in Theorem B. Let

$$\gamma_0 := 0.7, \qquad p_0 := 0.7, \qquad a_0 := 0.3.$$

If $a(\pm\infty) := \pm a_0$ and $p(\pm\infty) := \pm p_0$, then (III.8) becomes

$$\gamma_-(-\infty) = \gamma_-(+\infty) = \frac{1}{2}\cosh^{-1}\left(\frac{1 - \sqrt{1-p_0^2}\sqrt{1-a_0^2}}{|p_0 a_0|}\right) \approx 0.4891,$$
$$\gamma_+(-\infty) = \gamma_+(+\infty) = \frac{1}{2}\cosh^{-1}\left(\frac{1 + \sqrt{1-p_0^2}\sqrt{1-a_0^2}}{|p_0 a_0|}\right) \approx 1.3847.$$

If we let $\gamma(\pm\infty) := \gamma_0$, then $\gamma_-(\pm\infty) < |\gamma_0| < \gamma_+(\pm\infty)$. It follows from Theorem B (ii) that $\sigma_{\mathrm{ess}}(U_m) = \sigma(-\infty) = \sigma(+\infty)$, since $s(-\infty) = s(+\infty) = 1$ and $\Lambda_\pm(-\infty) = \Lambda_\pm(+\infty) =: \Lambda_\pm$.

$$\sigma_{\mathrm{ess}}(U_m) = \{z \in \mathbb{T} \mid \operatorname{Re} z \in [\Lambda_-, 1]\} \cup [g(\Lambda_+)^{-1}, g(\Lambda_+)],$$
$$\Lambda_\pm = p_0 a_0 \cosh(2\gamma_0) \pm \sqrt{1-p_0^2}\sqrt{1-a_0^2}.$$

The connected black region in Case II of Figure III.1 depicts the subset $\sigma_{\mathrm{ess}}(U_m)$ containing 1. Furthermore, (III.3) becomes

$$|p_\gamma(\pm\infty)| = \frac{|p_0|}{\sqrt{p_0^2 + (1-p_0^2)\cosh^2(2\gamma_0)}} \approx 0.4147 > |a(\pm\infty)| = 0.3.$$

It follows that $(\varGamma_m, U_m)$ is Fredholm, and that $\operatorname{ind}(\varGamma_m, U_m) = m(+1-(-1)) = 2m$ by the index formula (III.4). That is, we have chosen the asymptotic values $\gamma(\pm\infty), p(\pm\infty), a(\pm\infty)$, in such a way that the essential spectrum of U_m is gapless at 1, yet $\operatorname{ind}(\varGamma_m, U_m) = 2m$ is well-defined.

III.2.3 Numerical spectral analysis

It is shown in Theorem B (ii) that $\sigma_{\mathrm{ess}}(U_m)$ is a subset of $\mathbb{R} \cup \mathbb{T}$ under the assumption that a limit of the form (I.8) exists for each $\star = -\infty, +\infty$ and each $\zeta = \gamma, p, a$. The purpose of the current subsection is to numerically show that this is not the case in general, if we replace (I.8) by the asymptotically periodic assumption (I.10);

Lemma III.5. *For each $\star = -\infty, +\infty$ let*

$$\zeta(\star, m) := \lim_{x \to \star} \zeta(2x + m), \qquad \zeta \in \{\gamma, p, a\}, \qquad m = 0, 1.$$

Then the essential spectrum of U_m is given by

$$\sigma_{\mathrm{ess}}(U_m) = \bigcup_{\star=\pm\infty} \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{U}_m(\star, z)\right), \tag{III.10}$$

$$\hat{U}_m(\star,z) := \begin{pmatrix} p(\star,0)a(\star,0)e^{-2\gamma(\star,1)} & q(\star,0)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} & p(\star,0)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & -q(\star,0)a(\star,1)e^{2\gamma(\star,1)} \\ q(\star,1)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)}z & p(\star,1)a(\star,1)e^{-2\gamma(\star,0)} & -q(\star,1)a(\star,0)e^{2\gamma(\star,0)}z & p(\star,1)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} \\ -p(\star,1)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & q(\star,1)a(\star,1)e^{-2\gamma(\star,0)}z^* & p(\star,1)a(\star,0)e^{2\gamma(\star,0)} & q(\star,1)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)}z^* \\ q(\star,0)a(\star,0)e^{-2\gamma(\star,1)} & -p(\star,0)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} & q(\star,0)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & p(\star,0)a(\star,1)e^{2\gamma(\star,1)} \end{pmatrix} \tag{III.11}$$

Proof. For simplicity, let $U = U_1$. Note that we have

$$\begin{aligned} U &= \begin{pmatrix} 0L^{-1} + pe^{-2\gamma(\cdot+1)}a + qb(\cdot+1)e^{\gamma(\cdot+1)-\gamma(\cdot+2)}L & 0L^{-1} + pbe^{\gamma-\gamma(\cdot+1)} - qa(\cdot+1)e^{2\gamma(\cdot+1)}L \\ q(\cdot-1)a(\cdot-1)e^{-2\gamma}L^{-1} - p(\cdot-1)be^{\gamma-\gamma(\cdot+1)} + 0L & q(\cdot-1)b(\cdot-1)e^{\gamma(\cdot-1)-\gamma}L^{-1} + p(\cdot-1)ae^{2\gamma} + 0L \end{pmatrix} \\ &=: \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}. \end{aligned}$$

We introduce the following matrices according to Theorem II.8 (ii) and to (II.58);

$$\hat{U}_m(\star,z) := \begin{pmatrix} \hat{U}_{11}(\star,z) & \hat{U}_{12}(\star,z) \\ \hat{U}_{12}(\star,z) & \hat{U}_{22}(\star,z) \end{pmatrix},$$

where

$$\begin{aligned} \hat{U}_{11}(\star,z) &:= \begin{pmatrix} p(\star,0)a(\star,0)e^{-2\gamma(\star,1)} & q(\star,0)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} \\ q(\star,1)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)}z & p(\star,1)a(\star,1)e^{-2\gamma(\star,0)} \end{pmatrix}, \\ \hat{U}_{12}(\star,z) &:= \begin{pmatrix} p(\star,0)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & -q(\star,0)a(\star,1)e^{2\gamma(\star,1)} \\ -q(\star,1)a(\star,0)e^{2\gamma(\star,0)}z & p(\star,1)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} \end{pmatrix}, \\ \hat{U}_{21}(\star,z) &:= \begin{pmatrix} -p(\star,1)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & q(\star,1)a(\star,1)e^{-2\gamma(\star,0)}z^* \\ q(\star,0)a(\star,0)e^{-2\gamma(\star,1)} & -p(\star,0)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)} \end{pmatrix}, \\ \hat{U}_{22}(\star,z) &:= \begin{pmatrix} p(\star,1)a(\star,0)e^{2\gamma(\star,0)} & q(\star,1)b(\star,1)e^{\gamma(\star,1)-\gamma(\star,0)}z^* \\ q(\star,0)b(\star,0)e^{\gamma(\star,0)-\gamma(\star,1)} & p(\star,0)a(\star,1)e^{2\gamma(\star,1)} \end{pmatrix}. \end{aligned}$$

It follows that $\hat{U}_m(\star,z)$ is consistent with (III.11), and that (III.10) holds true by Theorem II.8 (ii). ◻

It follows from Lemma III.5 that in order to determine $\sigma_{\mathrm{ess}}(U_m)$ it is necessary to compute the eigenvalues of the 4×4 matrix $\hat{U}_m(\star, z)$ defined by (III.11). We consider the following Mathematica code in order to plot $\bigcup_{z\in\mathbb{T}} \sigma(\hat{U}_m(\star, z))$.

```
ClearAll["Global`*"]
ComplexSplit = Function[z, {Re@z, Im@z}, Listable];
Tex[tex_] := ToString[ToExpression[tex, TeXForm, HoldForm], TraditionalForm];
U1[p0_, p1_, q0_, q1_, a0_, a1_, b0_, b1_, z_, gamma0_, gamma1_] :=
  {
    {p0*a0*Exp[-2 gamma1], q0*b1*Exp[gamma1 - gamma0], p0*b0*Exp[gamma0 - gamma1], -q0*a1*Exp[2 gamma1]},
    {q1*b0*Exp[gamma0 - gamma1]*z, p1*a1*Exp[-2 gamma0], -q1*a0*z*Exp[2 gamma0], p1*b1*Exp[gamma1 - gamma0]},
    {-p1*b0*Exp[gamma0 - gamma1], q1*a1*Conjugate[z]*Exp[-2 gamma0], p1*a0*Exp[2 gamma0], q1*b1*Exp[gamma1 - gamma0]*Conjugate[z]},
    {q0*a0*Exp[-2 gamma1], -p0*b1*Exp[gamma1 - gamma0], q0*b0*Exp[gamma0 - gamma1], p0*a1*Exp[2 gamma1]}
  };
U2[p0_, p1_, a0_, a1_, z_, gamma0_, gamma1_] := U1[p0, p1, Sqrt[1 - (p0)^2], Sqrt[1 - (p1)^2], a0, a1, Sqrt[1 - (a0)^2], Sqrt[1 - (a1)^2], z, gamma0, gamma1];
ExactEigenvalues[p0_, p1_, a0_, a1_, t_, gamma0_, gamma1_] := ComplexSplit[Eigenvalues[U2[p0, p1, a0, a1, Exp[I*t], gamma0, gamma1]]];
DiscretisedEigenvalues[p0_, p1_, a0_, a1_, gamma0_, gamma1_, n_, j_] := Table[Part[ExactEigenvalues[p0, p1, a0, a1, 2 Pi*(k - 1)/n, gamma0, gamma1], j],{k, n + 1}];
CollectiveEigenvalues[p0_, p1_, a0_, a1_, gamma0_, gamma1_, n_] := Join[
  DiscretisedEigenvalues[p0, p1, a0, a1, gamma0, gamma1, n, 1], DiscretisedEigenvalues[p0, p1, a0, a1, gamma0, gamma1, n, 2],
  DiscretisedEigenvalues[p0, p1, a0, a1, gamma0, gamma1, n, 3], DiscretisedEigenvalues[p0, p1, a0, a1, gamma0, gamma1, n, 4]
];

Manipulate[
  circle = ParametricPlot[{Cos[k], Sin[k]}, {k, 0, 2 Pi}, PlotStyle -> {Black, Thin}, PlotRange -> {{-width, width}, {-1.2, 1.2}}, Ticks -> Automatic];
  plot = ListPlot[CollectiveEigenvalues[p0, p1, a0, a1, gamma0, gamma1, number],
  PlotStyle -> {Blue}, PlotMarkers -> {Automatic, thickness}];
  Show[circle, plot],
  {{gamma0, 0, Tex["\\gamma(\\star,0)"]}, 0, 2, 0.1, Appearance -> "Labeled"},
  {{gamma1, 0, Tex["\\gamma(\\star,1)"]}, 0, 2, 0.1, Appearance -> "Labeled"},
  {{p0, 0.1, Tex["p(\\star,0)" ]}, -1, 1, 0.1, Appearance -> "Labeled"},
  {{p1, 0.1, Tex["p(\\star,1)" ]}, -1, 1, 0.1, Appearance -> "Labeled"},
  {{a0, 0.1, Tex["a(\\star,0)" ]}, -1, 1, 0.1, Appearance -> "Labeled"},
  {{a1, 0.1, Tex["a(\\star,1)" ]}, -1, 1, 0.1, Appearance -> "Labeled"},
  {{width, 2, "Width"}, 1, 10, 0.1, Appearance -> "Labeled"},
  {{thickness, 5, "Thickness"}, 1, 5, 1, Appearance -> "Labeled"},
  {{number, 50, "Sample␣Number"}, 50, 1000, 50, Appearance -> "Labeled"}
 ]
```

The above Mathematica code produces the following interactive object;

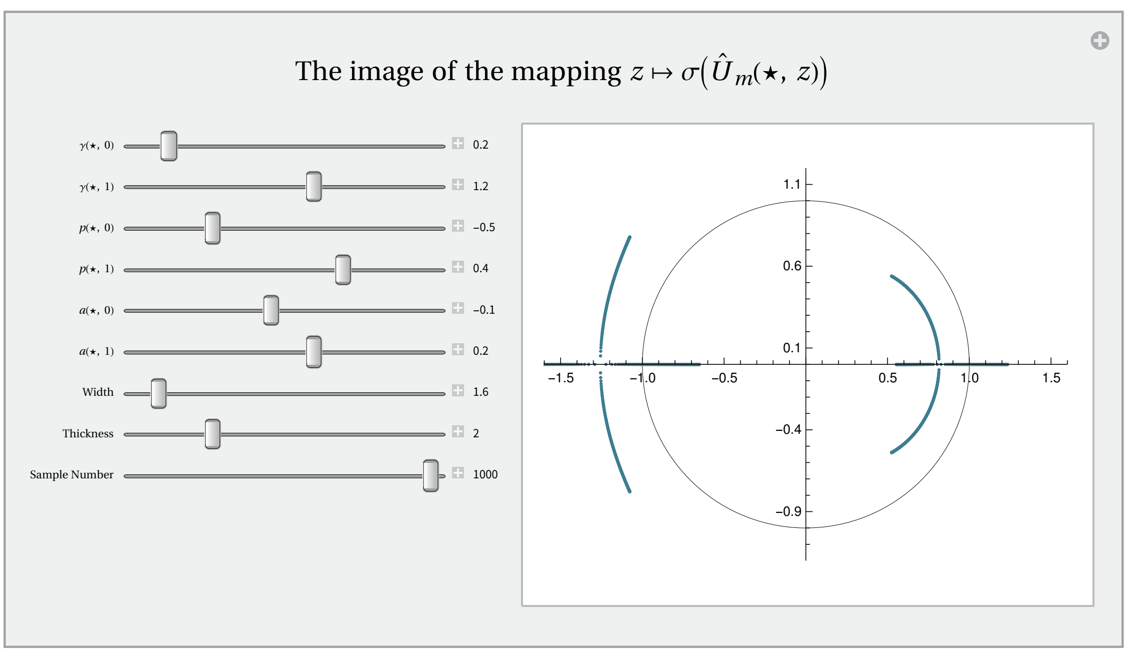


Figure III.3: It is shown in this figure that $\bigcup_{z\in\mathbb{T}} \sigma(\hat{U}_m(\star, z))$ is *not* a subset of $\mathbb{R} \cup \mathbb{T}$, if we set $(\gamma(\star, 0), \gamma(\star, 1), p(\star, 0), p(\star, 1), a(\star, 0), a(\star, 1)) := (0.2, 1.2, -0.5, 0.4, -0.1, 0.2)$.

III.3 Proof of the main theorem (Theorem B)

We are now in a position to prove Theorem B via Theorem II.7 and the following ***unitary invariance property*** of the index;

Lemma III.6. *Let $(\varGamma_0, U_0), (\varGamma, U)$ be two chiral pairs on Hilbert spaces $\mathcal{H}_0, \mathcal{H}$ respectively. If $(\varGamma_0, U_0), (\varGamma, U)$ are **unitarily equivalent** in the sense that $(\varGamma_0, U_0) = (\epsilon^* \varGamma \epsilon, \epsilon^* U \epsilon)$ for some unitary operator $\epsilon : \mathcal{H}_0 \to \mathcal{H}$, then $(\varGamma_0, U_0)$ is Fredholm if and only if so is $(\varGamma, U)$. In this case, we have* $\operatorname{ind}(\varGamma_0, U_0) = \operatorname{ind}(\varGamma, U)$.

Proof. The claim immediately follows from the proof of Lemma II.3 (ii). □

III.3.1 Proof of the index formula (Theorem B (i))

Notation. With the notation introduced in (III.2), we shall also make use of the following notation throughout §III.3.1 for simplicity;

$$(\varGamma, U) := (\varGamma_m, U_m), \qquad C := \begin{pmatrix} \alpha_1 & \beta^* \\ \beta & \alpha_2 \end{pmatrix} := \begin{pmatrix} e^{-2\gamma(\cdot+1)} a & e^{\gamma - \gamma(\cdot+1)} b \\ e^{\gamma - \gamma(\cdot+1)} b & -e^{2\gamma} a \end{pmatrix}.$$

With the above notation, the operator U can be written as $U = \varGamma C$.

In order to compute $\operatorname{ind}(\varGamma, U)$ we shall closely follow [Tan21, §3.2]. Note first that the underlying Hilbert space $\ell^2(\mathbb{Z}, \mathbb{C}^2)$ admits the following two orthogonal decompositions:

$$\ell^2(\mathbb{Z}, \mathbb{C}^2) = \ker(\varGamma - 1) \oplus \ker(\varGamma + 1) = \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z}),$$

where $\ker(\varGamma \mp 1) \neq \ell^2(\mathbb{Z})$. On one hand, the imaginary part Q of U admits an off-diagonal block operator matrix representation with respect to the former decomposition as in the second equality of (II.1), where Q_0 is an operator of the form $Q_0 : \ker(\varGamma - 1) \to \ker(\varGamma + 1)$. On the other hand, the same operator Q can *not* be expressed as an off-diagonal block-operator matrix with respect to the latter decomposition. Lemma III.6 motivates us to construct a unitary operator $\epsilon : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$, in such a way that the imaginary part $\epsilon^* Q \epsilon$ of $\epsilon^* U \epsilon$ become off-diagonal with respect to $\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$.

Lemma III.7. *Let R, Q be the real and imaginary parts of U respectively. For each $x \in \mathbb{Z}$, let $p_\pm(x) := \sqrt{1 \pm p(x)}$. Let*

$$-2iQ_{\epsilon_0} := p_+ L^m \beta p_+ - p_- \beta^* L^{-m} p_- - |q|(\alpha_1 - \alpha_2(\cdot + m)), \tag{III.12}$$

$$2R_{\epsilon_1} := p_- L^m \beta p_+ + p_+ \beta^* L^{-m} p_- + (1+p)\alpha_1 + (1-p)\alpha_2(\cdot + m), \tag{III.13}$$

$$2R_{\epsilon_2} := p_+ L^m \beta p_- + p_- \beta^* L^{-m} p_+ - (1-p)\alpha_1 - (1+p)\alpha_2(\cdot + m). \tag{III.14}$$

Then there exists a unitary operator ϵ on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, such that the following block-operator matrix representations hold true with respect to $\ell^2(\mathbb{Z}, \mathbb{C}^2) = \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$:

$$\epsilon^* \varGamma \epsilon = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \epsilon^* U \epsilon = \begin{pmatrix} R_{\epsilon_1} & iQ_{\epsilon_0}^* \\ iQ_{\epsilon_0} & R_{\epsilon_2} \end{pmatrix}, \qquad \epsilon^* R \epsilon = \begin{pmatrix} R_{\epsilon_1} & 0 \\ 0 & R_{\epsilon_2} \end{pmatrix}, \qquad \epsilon^* Q \epsilon = \begin{pmatrix} 0 & Q_{\epsilon_0}^* \\ Q_{\epsilon_0} & 0 \end{pmatrix},$$

Moreover, the chiral pair $(\varGamma, U)$ is Fredholm if and only if Q_{ϵ_0} is Fredholm. In this case, we have

$$\operatorname{ind}(\varGamma, U) = \operatorname{ind} Q_{\epsilon_0}. \tag{III.15}$$

The derivation of the formula (III.15) as described below only requires the boundedness of the given sequences γ, p, a, q, b, and so (I.8) turns out to be redundant. Note, however, that this assumption is necessary to prove the index formula (III.4).

Proof. Note first that $\varGamma$ can be written as

$$\varGamma = \begin{pmatrix} p & qL^m \\ L^{-m} q & -p(\cdot - m) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \begin{pmatrix} p & q \\ q & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^m \end{pmatrix},$$

where the middle matrix on the right hand side of the second equality admits the following diagonalisation.

$$\epsilon_0^* \begin{pmatrix} p & q \\ q & -p \end{pmatrix} \epsilon_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \epsilon_0 := \frac{1}{\sqrt{2}} \begin{pmatrix} p_+ & -p_- \\ p_- & p_+ \end{pmatrix}. \tag{III.16}$$

Since ϵ_0 is unitary, the following operator is also unitary;

$$\epsilon := \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \epsilon_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \begin{pmatrix} p_+ & -p_- \\ p_- & p_+ \end{pmatrix}.$$

It follows from the first equality that

$$\epsilon^* \varGamma \epsilon = \epsilon_0^* \begin{pmatrix} 1 & 0 \\ 0 & L^m \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \begin{pmatrix} p & q \\ q & -p \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^m \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^{-m} \end{pmatrix} \epsilon_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

where the last equality follows from (III.16).

Given an operator X on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, we introduce the shorthand $X_\epsilon := \epsilon^* X \epsilon$. With this convention in mind, we have $[\varGamma_\epsilon, R_\epsilon] = 0 = \{\varGamma_\epsilon, Q_\epsilon\}$, where $\varGamma_\epsilon = 1 \oplus (-1)$ with respect to $\ell^2(\mathbb{Z}, \mathbb{C}^2) = \ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})$. It follows that we have the following representations:

$$R_\epsilon = \begin{pmatrix} R'_{\epsilon_1} & 0 \\ 0 & R'_{\epsilon_2} \end{pmatrix}, \qquad Q_\epsilon = \begin{pmatrix} 0 & (Q'_{\epsilon_0})^* \\ Q'_{\epsilon_0} & 0 \end{pmatrix}, \qquad U_\epsilon = R_\epsilon + iQ_\epsilon = \begin{pmatrix} R'_{\epsilon_1} & i(Q'_{\epsilon_0})^* \\ iQ'_{\epsilon_0} & R'_{\epsilon_2} \end{pmatrix}. \tag{III.17}$$

On one hand, we get

$$2C_\epsilon = \varGamma_\epsilon (2U_\epsilon) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 2R'_{\epsilon_1} & 2i(Q'_{\epsilon_0})^* \\ 2iQ'_{\epsilon_0} & 2R'_{\epsilon_2} \end{pmatrix} = \begin{pmatrix} 2R'_{\epsilon_1} & 2i(Q'_{\epsilon_0})^* \\ -2iQ'_{\epsilon_0} & -2R'_{\epsilon_2} \end{pmatrix}. \tag{III.18}$$

On the other hand, a direct computation gives

$$2C_\epsilon = 2\epsilon^* \begin{pmatrix} 0 & \beta^* \\ \beta & 0 \end{pmatrix} \epsilon + 2\epsilon^* \begin{pmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{pmatrix} \epsilon = \begin{pmatrix} 2R_{\epsilon_1} & 2iQ^*_{\epsilon_0} \\ -2iQ_{\epsilon_0} & -2R_{\epsilon_2} \end{pmatrix}. \tag{III.19}$$

By comparing (III.18) with (III.19), the three operators $Q'_{\epsilon_0}, R'_{\epsilon_1}, R'_{\epsilon_2}$ coincide with the ones defined by the formulas (III.12) to (III.14).

On one hand, the operator Q_ϵ admits the following representations;

$$Q_\epsilon = \begin{pmatrix} 0 & Q^*_{\epsilon_0} \\ Q_{\epsilon_0} & 0 \end{pmatrix}_{\ell^2(\mathbb{Z}) \oplus \ell^2(\mathbb{Z})} = \begin{pmatrix} 0 & 0 & 0 & Q_{\epsilon_0} \\ 0 & 0 & \mathbf{0} & 0 \\ 0 & \mathbf{0} & 0 & 0 \\ Q_{\epsilon_0} & 0 & 0 & 0 \end{pmatrix}_{\ell^2(\mathbb{Z}) \oplus \{0\} \oplus \{0\} \oplus \ell^2(\mathbb{Z})}, \tag{III.20}$$

where $\mathbf{0}$ denotes the zero operator of the form $\mathbf{0} : \{0\} \to \{0\}$. On the other hand, the imaginary part Q_ϵ of U_ϵ admits the following off-diagonal block-operator matrix representation as in the second equality in (II.1);

$$Q_\epsilon = \begin{pmatrix} 0 & (Q'_0)^* \\ Q'_0 & 0 \end{pmatrix}_{\ker(\varGamma_\epsilon - 1) \oplus \ker(\varGamma_\epsilon + 1)} = \begin{pmatrix} 0 & (Q'_0)^* \\ Q'_0 & 0 \end{pmatrix}_{(\ell^2(\mathbb{Z}) \oplus \{0\}) \oplus (\{0\} \oplus \ell^2(\mathbb{Z}))}. \tag{III.21}$$

It follows from (III.20) to (III.21) that Q_0' is an off-diagonal block-operator matrix of the form;

$$Q_0' = \begin{pmatrix} 0 & \mathbf{0} \\ Q_{\epsilon_0} & 0 \end{pmatrix}.$$

Since $\mathbf{0}$ is a Fredholm operator of zero index, we have that Q_0' is Fredholm if and only if Q_{ϵ_0} is Fredholm. In this case, we have $\operatorname{ind} Q_0' = \operatorname{ind} Q_{\epsilon_0}$. The claim follows from Lemma III.6. □

We are now in a position to apply Theorem II.7 (i) to Q_{ϵ_0}. We introduce the following notation;

$$c(\star) := |q(\star)|a(\star)\cosh(2\gamma(\star)), \tag{III.22}$$

$$f(\star, z) := \frac{(p(\star)+1)b(\star)z^m + (p(\star)-1)b(\star)z^{-m} - 2c(\star)}{-2i}, \tag{III.23}$$

where $\star = \pm\infty$ and $z \in \mathbb{T}$. It follows from Theorem II.7 (i) that $A = Q_{\epsilon_0}$ is Fredholm if and only if $f(\star, \cdot)$ is nowhere vanishing on $\mathbb{T}$ for each $\star = -\infty, +\infty$. In this case, we have

$$\operatorname{ind}(\varGamma, U) = \operatorname{ind} A = \operatorname{wn}(f(+\infty, \cdot)) - \operatorname{wn}(f(-\infty, \cdot)). \tag{III.24}$$

It remains to compute the winding number of $f(\star, \cdot)$.

Lemma III.8. *For each $\star = -\infty, +\infty$, let $f(\star, \cdot)$ be defined by* (III.22) *to* (III.23)*, and let $p_\gamma(\star)$ be defined by* (III.3)*. Then the function $\mathbb{T} \ni z \longmapsto f(\star, z) \in \mathbb{C}$ is nowhere vanishing if and only if $|p_\gamma(\star)| \neq |a(\star)|$. In this case, we have*

$$\operatorname{wn}(f(\star, \cdot)) = \begin{cases} m \cdot \operatorname{sign} p(\star), & |p_\gamma(\star)| > |a(\star)|, \\ 0, & |p_\gamma(\star)| < |a(\star)|. \end{cases} \tag{III.25}$$

Proof. Let us first prove that the function $\mathbb{T} \ni z \longmapsto f(\star, z) \in \mathbb{C}$ is nowhere vanishing if and only if $|p(\star)b(\star)| \neq |c(\star)|$, and that in this case

$$\operatorname{wn}(f(\star, \cdot)) = \begin{cases} m \cdot \operatorname{sign} p(\star), & |p(\star)b(\star)| > |c(\star)|, \\ 0, & |p(\star)b(\star)| < |c(\star)|. \end{cases} \tag{III.26}$$

Let us consider the following function on $\mathbb{R}$;

$$2F(s) := (|p(\star)b(\star)| + |b(\star)|)e^{is} + (|p(\star)b(\star)| - |b(\star)|)e^{-is}, \qquad s \in \mathbb{R}.$$

We have $2F(s) = 2|p(\star)b(\star)|\cos s + i2|b(\star)|\sin s$ for each $s \in \mathbb{R}$. Since $p(\star) = \operatorname{sign} p(\star)|p(\star)|$, we get the following for each $t \in [0, 2\pi]$;

$$\begin{aligned} -2if(\star, e^{it}) + 2c(\star) &= (p(\star)+1)b(\star)e^{imt} + (p(\star)-1)b(\star)e^{-imt} \\ &= \operatorname{sign} p(\star) \cdot 2F(\operatorname{sign} p(\star)mt)). \end{aligned}$$

It follows that $-if(\star, e^{it}) = \operatorname{sign} p(\star) \cdot F(\operatorname{sign} p(\star)mt) - c(\star)$ for each $t \in [0, 2\pi]$, where the constant $-i$ does not play any significant role in this proof. On one hand, if $p(\star)b(\star) = 0$, then the image of the function $-if(\star, \cdot)$ coincides with that of the vertical line segment $[-1, 1] \ni t \longmapsto -c(\star) + i|b(\star)|t \in \mathbb{C}$ passing through $-c(\star)$. That is, the function $f(\star, \cdot)$ is nowhere vanishing if and only if $|c(\star)| \neq 0 = |p(\star)b(\star)|$, and in this case $\operatorname{wn}(f(\star, \cdot)) = 0$. This is a special case of (III.26). On the other hand, if $p(\star)b(\star) \neq 0$, then the image of $-if(\star, \cdot)$ is an ellipse as in Figure III.4. The winding number of the curve $[0, 2\pi] \ni t \longmapsto -if(\star, e^{it}) \in \mathbb{C}$ with respect to its center $-c(\star)$ on the real axis is $m \cdot \operatorname{sign} p(\star)$.

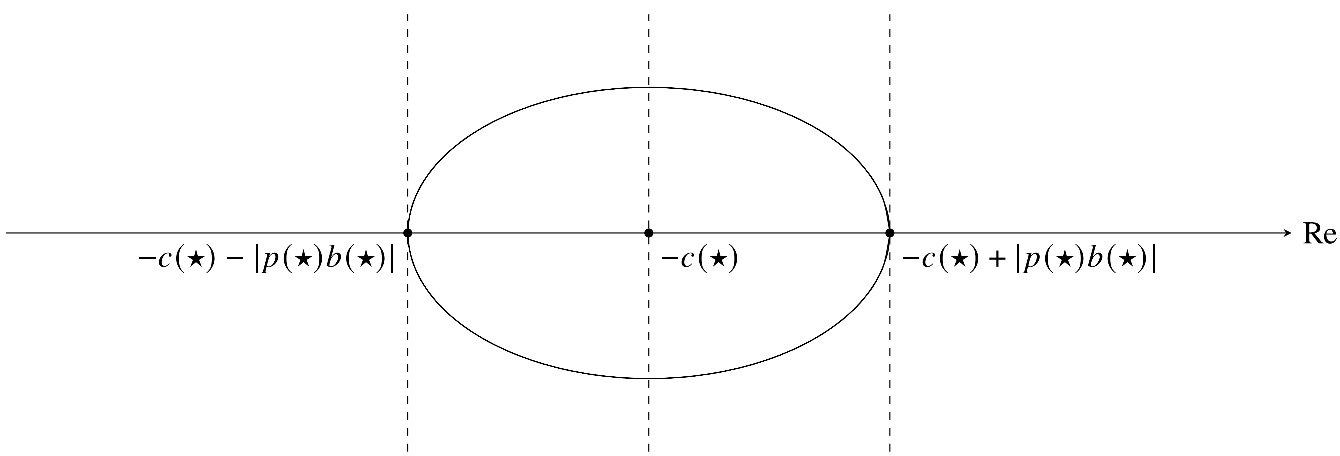


Figure III.4: This figure shows the image of the curve $[0, 2\pi] \ni t \longmapsto -if(\star, e^{it}) \in \mathbb{C}$.

If $|p(\star)b(\star)| > |c(\star)|$, then the origin is inside the interior of the ellipse, and so $\operatorname{wn}(f(\star, \cdot)) = \operatorname{wn}(-if(\star, \cdot)) = m \cdot \operatorname{sign} p(\star)$. If $|p(\star)b(\star)| < |c(\star)|$, then the origin is inside the exterior of the ellipse, and so $\operatorname{wn}(f(\star, \cdot)) = 0$. Clearly, the curve $[0, 2\pi] \ni t \longmapsto -if(\star, e^{it}) \in \mathbb{C}$ passes through the origin if and only if $|p(\star)b(\star)| = |c(\star)|$. It follows that (III.26) holds true.

It remains to check that (III.26) coincides with (III.25). If the notation $\lesseqgtr$ simultaneously denotes $>, =, <$, then $|p(\star)b(\star)| \lesseqgtr |c(\star)|$ if and only if $p(\star)^2(1 - a(\star)^2) \lesseqgtr |q(\star)|^2 a(\star)^2 \cosh^2(2\gamma(\star))$. It follows from the obvious rearrangement that $|p(\star)b(\star)| \lesseqgtr |c(\star)|$ if and only if $|p_\gamma(\star)| \lesseqgtr |a(\star)|$. The claim follows. □

Proof of Theorem B (i). The index formula (III.4) immediately follows from (III.24) and (III.25). □

III.3.2 Proof of the classification formula (Theorem B (ii))

Proof of Theorem B (ii). Note first that U_m is a strictly local operator of the form

$$U_m = \begin{pmatrix} pe^{-2\gamma(\cdot+1)}a + qL^m e^{\gamma-\gamma(\cdot+1)}b & pe^{\gamma-\gamma(\cdot+1)}b - qL^m e^{2\gamma}a \\ L^{-m}qe^{-2\gamma(\cdot+1)}a - p(\cdot-m)e^{\gamma-\gamma(\cdot+1)}b & L^{-m}qe^{\gamma-\gamma(\cdot+1)}b + p(\cdot-m)e^{2\gamma}a \end{pmatrix}.$$

For each $\star = -\infty, +\infty$, we let

$$U_m(\star) := \begin{pmatrix} q(\star)b(\star)L^m + p(\star)a(\star)e^{-2\gamma(\star)} & -q(\star)a(\star)e^{2\gamma(\star)}L^m + p(\star)b(\star) \\ q(\star)a(\star)e^{-2\gamma(\star)}L^{-m} - p(\star)b(\star) & q(\star)b(\star)L^{-m} + p(\star)a(\star)e^{2\gamma(\star)} \end{pmatrix}.$$

The above 2×2 matrix with L replaced by the complex variable $z \in \mathbb{T}$ will be denoted by $\hat{U}_m(\star, z)$. It follows from Theorem II.7 (ii) that

$$\sigma_{\mathrm{ess}}(U_m) = \sigma_{\mathrm{ess}}(U_m(-\infty)) \cup \sigma_{\mathrm{ess}}(U_m(+\infty)),$$

$$\sigma_{\mathrm{ess}}(U_m(\star)) = \bigcup_{z\in\mathbb{T}} \sigma\left(\hat{U}_m(\star, z)\right), \qquad \star = \pm\infty.$$

Let us first prove that $\sigma'(\star) := \bigcup_{t\in[0,2\pi]} \sigma\left(\hat{U}_m(\star, e^{it})\right)$ coincides with $\sigma(\star)$ given by (III.7) for each fixed $\star = \pm\infty$. Let

$$\hat{U}_m(\star, e^{it}) =: \begin{pmatrix} X_1(e^{it}) & -Y_1(e^{it}) \\ Y_2(e^{it}) & X_2(e^{it}) \end{pmatrix}, \qquad t \in [0, 2\pi].$$

We obtain the following two equalities for each $t \in [0, 2\pi]$:

$$\frac{\operatorname{tr} \hat{U}_m(\star, e^{it})}{2} = p(\star)a(\star)\cosh(2\gamma(\star)) + |q(\star)b(\star)|\cos(mt),$$

$$\det \hat{U}_m(\star, e^{it}) = 1.$$

This result motivates us to introduce the following notation;

$$\Lambda(\star, s) := p(\star)a(\star)\cosh(2\gamma(\star)) + |q(\star)b(\star)|s, \qquad -1 \le s \le 1,$$

$$\lambda_\pm(\star, s) := \Lambda(\star, s) \pm \sqrt{\Lambda(\star, s)^2 - 1}, \qquad -1 \le s \le 1.$$

Indeed, for each $t \in [0, 2\pi]$ the eigenvalues of $\hat{U}_m(\star, e^{it})$ are given by

$$\frac{\operatorname{tr} \hat{U}_m(\star, e^{it}) \pm \sqrt{(\operatorname{tr} \hat{U}_m(\star, e^{it}))^2 - 4}}{2} = \lambda_\pm(\star, \cos(mt)).$$

We have

$$\sigma'(\star) = \bigcup_{t \in [0,2\pi]} \sigma\left(\hat{U}_m(\star, e^{it})\right) = \bigcup_{s \in [-1,1]} \{\lambda_\pm(\star, s)\} = \bigcup_{s \in [-1,1]} \{\lambda_+(\star, s)^{\pm 1}\},$$

where the second equality follows from the fact that the range of the cosine function is $[-1, 1]$, and the last equality follows from $\lambda_+(\star, t)\lambda_-(\star, t) = 1$ for each $t \in [0, 2\pi]$. It follows that $\sigma'(\star) = \sigma(\star)$, and so $\sigma_{\mathrm{ess}}(U_m) = \sigma(-\infty) \cup \sigma(+\infty)$. Note first that (III.8) is well-defined, because of the following estimate;

$$|p(\star)a(\star)| + |q(\star)b(\star)| \leq \frac{|p(\star)|^2 + |a(\star)|^2}{2} + \frac{|q(\star)|^2 + |b(\star)|^2}{2} \leq 1.$$

Note also that $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [-1, \infty)$ follows from

$$-1 \leq -|q(\star)b(\star)| \leq |p(\star)a(\star)| \cosh(2\gamma(\star)) - |q(\star)b(\star)| = \Lambda_-(\star).$$

If $p(\star)a(\star) = 0$, then $\Lambda_+(\star) = |q(\star)b(\star)| \leq 1$. This is a special case of Case I, since $\gamma_-(\star) = \gamma_+(\star) = \infty$ according to (III.8). It remains to consider the case $p(\star)a(\star) \neq 0$. We shall make use of the fact that the hyperbolic cosine is an even function throughout. It follows from (III.8) that

$$|p(\star)a(\star)| \cosh(2\gamma_\pm(\star)) = 1 \pm |q(\star)b(\star)|. \tag{III.27}$$

Case I. If $|\gamma(\star)| \leq \gamma_-(\star)$, then

$$\Lambda_+(\star) \leq |p(\star)a(\star)| \cosh(2\gamma_-(\star)) + |q(\star)b(\star)| = 1,$$

where the first inequality follows from $\cosh(2\gamma(\star)) \leq \cosh(2\gamma_-(\star))$, and the last equality follows from (III.27). Thus $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [-1, 1]$.

Case II. If $\gamma_-(\star) < |\gamma(\star)| < \gamma_+(\star)$, then it follows from (III.27) that $\Lambda_-(\star) < 1 < \Lambda_+(\star)$. It follows that the interval $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [-1, \infty)$ can be written as $[\Lambda_-(\star), \Lambda_+(\star)] = [\Lambda_-(\star), 1] \cup [1, \Lambda_+(\star)]$.

Case III. If $\gamma_+(\star) \leq |\gamma(\star)|$. Then $[\Lambda_-(\star), \Lambda_+(\star)] \subseteq [1, \infty)$ follows from

$$1 = |p(\star)a(\star)| \cosh(2\gamma_+(\star)) - |q(\star)b(\star)| \leq \Lambda_-(\star),$$

where the first equality follows from (III.27) and the last inequality follows from $\cosh(2\gamma_+(\star)) \le \cosh(2\gamma(\star))$.

$\square$

On a final note, a typical computation of the essential spectrum makes use of the discrete Fourier transform and Weyl's criterion in the setting of 2-phase quantum walks (see, for example, [FFS17, Lemma 3.3]). Weyl's criterion is applicable to, for example, non-compact perturbations (see, for example, [SS17]), but its usage is restricted to normal operators. This is why the method described above is not suitable for proving Theorem B (ii).

Chapter IV

Unitary Transforms of Some One-dimensional Quantum Walks

The following one-dimensional models in the physics literature can be viewed as variants of the non-unitary model U_m defined by (III.2):

- ***Kitagawa's split-step quantum walk*** [KRBD10, Kit+12, Kit12].
- ***Mochizuki-Kim-Obuse model*** [MKO16].

The purpose of this supplementary chapter is to show that U_m completely unifies the above two models. We start with the following preliminary section.

IV.1 Elimination of the phase terms

Theorem IV.1. *Let* $m \in \mathbb{Z} \setminus \{0\}$, *and let*

$$S := \begin{pmatrix} \alpha_1 & \beta_1 L^m \\ L^{-m}\beta_1^* & \alpha_1'(\cdot - m) \end{pmatrix}, \qquad C := \begin{pmatrix} \alpha_2 & \beta_2 \\ \beta_2^* & \alpha_2' \end{pmatrix}, \tag{IV.1}$$

where $\alpha_1, \alpha_1', \alpha_2, \alpha_2'$ are bounded $\mathbb{R}$-valued sequences, and where β_1, β_2 are bounded $\mathbb{C}$-valued sequences. Then there exist $\mathbb{R}$-valued sequences f, g, such that the following two equalities hold true:

$$\begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig} \end{pmatrix} S \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig} \end{pmatrix} = \begin{pmatrix} \alpha_1 & |\beta_1| L^m \\ L^{-m}|\beta_1| & \alpha_1'(\cdot - m) \end{pmatrix},$$

$$\begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig} \end{pmatrix} C \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig} \end{pmatrix} = \begin{pmatrix} \alpha_2 & |\beta_2| \\ |\beta_2| & \alpha_2' \end{pmatrix}.$$

Note that this unitary transform is strongly based on the method of proof of [NOW21, Corollary 4.4], and we give a direct proof merely for the convenience of the reader.

Proof. We only prove the case for $m > 0$. For each $j = 1, 2$, let $\theta_j = (\theta_j(x))_{x \in \mathbb{Z}}$ be any $\mathbb{R}$-valued sequence, such that $\beta_j(x) = e^{i\theta_j(x)}|\beta_j(x)|$. Note that we have

$$\begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig} \end{pmatrix} S \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & L^{-y} \end{pmatrix} \begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig(\cdot + m)} \end{pmatrix} \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_1^* & \alpha_1' \end{pmatrix} \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig(\cdot + m)} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & L^m \end{pmatrix}.$$

We obtain the following two unitary transforms of the given multiplication operators:

$$\begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig(\cdot + m)} \end{pmatrix} \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_1^* & \alpha_1' \end{pmatrix} \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig(\cdot + m)} \end{pmatrix} = \begin{pmatrix} \alpha_1 & |\beta_1| e^{i(\theta_1 + g(\cdot + m) - f)} \\ |\beta_1| e^{-i(\theta_1 + g(\cdot + m) - f)} & \alpha_1' \end{pmatrix}, \tag{IV.2}$$

$$\begin{pmatrix} e^{-if} & 0 \\ 0 & e^{-ig} \end{pmatrix} \begin{pmatrix} \alpha_2 & \beta_2 \\ \beta_2^* & \alpha_2' \end{pmatrix} \begin{pmatrix} e^{if} & 0 \\ 0 & e^{ig} \end{pmatrix} = \begin{pmatrix} \alpha_2 & |\beta_2| e^{i(\theta_2 + g - f)} \\ |\beta_2| e^{-i(\theta_2 + g - f)} & \alpha_2' \end{pmatrix}. \tag{IV.3}$$

The unitary transform (IV.3) motivates us to define $g := f - \theta_2$. It remains to define f in such a way that $\theta_1 + g(\cdot + m) - f = 0$ holds true. If we let $\phi := \theta_2(\cdot + m) - \theta_1$, then this equality is equivalent to

$$f(x + m) - f(x) = \phi(x) \qquad \forall x \in \mathbb{Z}. \tag{IV.4}$$

For each $x \in \mathbb{Z}$, we consider $Z_x := \{mx + 0, \dots, mx + (m-1)\}$ consisting of m integers. It is obvious that $\mathbb{Z}$ partitions into the disjoint union $\mathbb{Z} = \bigcup_{x \in \mathbb{Z}} Z_x$. We let $f(n) := 0$ for each $n \in Z_0$. Note that any arbitrary number in $\mathbb{Z} \setminus Z_0$ can be uniquely written as $mx + n$, where $x \in \mathbb{Z} \setminus \{0\}$, and where $n \in Z_0$. This allows us to let

$$f(mx + n) := \begin{cases} + \sum_{y=0}^{x-1} \phi(my + n), & x \geq 1, \\ - \sum_{y=1}^{-x} \phi(-my + n), & x \leq -1. \end{cases} \tag{IV.5}$$

Let us first prove that (IV.4) holds true on $Z_{-1} \cup Z_0$. If $n \in Z_0$, then $f(n) = 0$ by construction, and so

$$f(n+m) - f(n) = f(n+m) - 0 = f(m \times 1 + n) = \phi(m \times 0 + n) = \phi(n),$$
$$f((n-m)+m) - f(n-m) = f(n) - f(n-m) = 0 - f(m \times (-1) + n) = \phi(m \times (-1) + n) = \phi(n-m),$$

where $n - m$ belongs to $Z_{-1} = Z_0 - m$. Let $x' \notin Z_{-1} \cup Z_0$. On one hand, if $x \geq 1$ and if $x' = mx + n$, then

$$f(x'+m) - f(x') = f(m(x+1)+n) - f(mx+n) = \sum_{y=0}^{x} \phi(my+n) - \sum_{y=0}^{x-1} \phi(my+n) = \phi(mx+n) = \phi(x').$$

On the other hand, if $x \leq -2$ and if $x' = mx + n$, then

$$f(x'+m) - f(x') = f(m(x+1)+n) - f(mx+n) = -\sum_{y=1}^{-x-1} \phi(-my+n) + \sum_{y=1}^{-x} \phi(-my+n) = \phi(mx+n) = \phi(x').$$

□

As can be seen from [Tan21, Lemma 3.4] or [AFST21, Lemma 11], the presence of off-diagonal phase terms often create a non-trivial hindrance in the existing literature. Note, however, that the unitary transform in Theorem IV.1 immediately makes these lemmas completely redundant.

IV.2 Kitagawa's split-step quantum walk

Kitagawa's (one-dimensional) split-step quantum walk [KRBD10, Kit+12, Kit12] can be characterised by the following unitary time-evolution;

$$U_{\mathrm{kit}} := \begin{pmatrix} 1 & 0 \\ 0 & L \end{pmatrix} \begin{pmatrix} \cos\theta_2 & -\sin\theta_2 \\ \sin\theta_2 & \cos\theta_2 \end{pmatrix} \begin{pmatrix} L^* & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{pmatrix}, \tag{IV.6}$$

where $\theta_1 = (\theta_1(x))_{x\in\mathbb{Z}}, \theta_2 = (\theta_2(x))_{x\in\mathbb{Z}}$ are $\mathbb{R}$-valued sequences.

In the physical context, the theme of symmetry-protection of eigenstates we have discussed in §I.2.1.1 belongs to the broad subject of topological phases of matter. It is the works of T. Kitagawa that clearly demonstrate great effectiveness of discrete-time quantum walks in exploring topological phases. Kitagawa's previous studies mentioned above focus on the symmetry-protection of eigenstates associated with (IV.6) and its higher-dimensional variants. In particular, it is shown in [Kit+12] that such eigenstates, often referred to as ***symmetry-protected edge-states***, can be observed in an optical network experiment. This is a brief description of the *bulk-edge correspondence* for chirally symmetric unitary quantum walks [AO13]. Mathematically rigorous studies of the bulk-edge correspondence for various symmetry types, including chiral symmetry (I.1), can be found in the existing literature [CGSVWW16, CGGSVWW18, CGSVWW18].

The following lemma shows that the evolution operator of kitagawa split-step quantum walk can be made unitarily equivalent to that of Suzuki's split-step quantum walk defined by (I.2);

Lemma IV.2. *Let*

$$p := \sin\theta_2(\cdot+1), \qquad q := \cos\theta_2(\cdot+1), \qquad a := -\sin\theta_1, \qquad b := \cos\theta_1.$$

Then

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} U_{\mathrm{kit}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} p & qL \\ L^* q & -p(\cdot-1) \end{pmatrix} \begin{pmatrix} a & b \\ b & -a \end{pmatrix}.$$

It follows from Theorem IV.1 that U_{kit} is unitarily equivalent to U_{suz}.

Proof. Let σ_1 be the first Pauli matrix. Given any $\mathbb{R}$-valued sequence $\theta = (\theta(x))_{x\in\mathbb{Z}}$, we consider the following rotation matrix;

$$R(\theta) := \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

It is obvious that $R(\theta)R(\phi) = R(\theta+\phi)$ for any $\mathbb{R}$-valued sequences θ, ϕ. If we let $\varGamma := \sigma_1(1\oplus L)R(\theta_2)(L^*\oplus 1)$ and $\varGamma' := R(\theta_1)\sigma_1$, then

$$\sigma_1 U_{\mathrm{kit}} \sigma_1 = \varGamma\varGamma'.$$

We have

$$R(\theta_j)\sigma_1 = \begin{pmatrix} \cos\theta_j & -\sin\theta_j \\ \sin\theta_j & \cos\theta_j \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -\sin\theta_j & \cos\theta_j \\ \cos\theta_j & \sin\theta_j \end{pmatrix}.$$

Now

$$\varGamma = \sigma_1(1\oplus L)R(\theta_2)(L^*\oplus 1) = \begin{pmatrix} p & qL \\ L^* q & -p(\cdot-1) \end{pmatrix}.$$

$\square$

IV.3 Mochizuki-Kim-Obuse model

The evolution operator of the ***Mochizuki-Kim-Obuse model*** is characterised by the following operator on $\mathcal{H} = \ell^2(\mathbb{Z}, \mathbb{C}^2)$;

$$U_{\mathrm{mko}} := SG\Phi C_2 SG^{-1}\Phi C_1, \tag{IV.7}$$

where the operators S, G, Φ, C_1, C_2 are defined respectively as the following block-operator matrices on $\mathcal{H} = \ell^2(\mathbb{Z}, \mathbb{C}) \oplus \ell^2(\mathbb{Z}, \mathbb{C})$:

$$S := \begin{pmatrix} L & 0 \\ 0 & L^{-1} \end{pmatrix}, \qquad G := \begin{pmatrix} e^{\gamma} & 0 \\ 0 & e^{-\gamma(\cdot+1)} \end{pmatrix}, \qquad \Phi := \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi(\cdot+1)} \end{pmatrix}, \qquad C_j := \begin{pmatrix} \cos\theta_j & i\sin\theta_j \\ i\sin\theta_j & \cos\theta_j \end{pmatrix},$$

where $\gamma = (\gamma(x))_{x\in\mathbb{Z}}, \phi = (\phi(x))_{x\in\mathbb{Z}}, \theta_1 = (\theta_1(x))_{x\in\mathbb{Z}}, \theta_2 = (\theta_2(x))_{x\in\mathbb{Z}}$ are four $\mathbb{R}$-valued sequences. This model is slightly more general than the homogenous model considered in [MKO16, §III.A]. In particular, (IV.7) is consistent with the optical network experiment setup in [RBMOCP12], where the parameter γ represents the gain-loss effect of photons (see [MKO16, §I-II] for details). If γ is identically zero, then there is no such effect, and so the corresponding time-evolution U_{mko} becomes unitary.

Lemma IV.3. *Let U_{mko} be given by* (IV.7)*. Then there exists a unitary self-adjoint operator $\varGamma_{\mathrm{mko}}$ on $\ell^2(\mathbb{Z}, \mathbb{C}^2)$, such that $(\varGamma_{\mathrm{mko}}, U_{\mathrm{mko}})$ forms a chiral pair. Moreover, the chiral pair $(\varGamma_{\mathrm{mko}}, U_{\mathrm{mko}})$ is unitarily equivalent to the chiral pair $(\varGamma_2, U_2)$ introduced in Theorem B.*

Proof. Let

$$p := -\sin\theta_1(\cdot+1), \qquad q := -i\cos\theta_1(\cdot+1), \qquad a := \sin\theta_2, \qquad b := i\cos\theta_2 e^{i(\phi+\phi(\cdot+1))}. \tag{IV.8}$$

We have

$$
\begin{aligned}
U_{\mathrm{mko}}C_1^{-1} &= S(G\Phi)C_2S(G^{-1}\Phi) \\
&= S\begin{pmatrix} e^{\gamma+i\phi} & 0 \\ 0 & e^{-\gamma(\cdot+1)-i\phi(\cdot+1)} \end{pmatrix}\begin{pmatrix} \cos\theta_2 & i\sin\theta_2 \\ i\sin\theta_2 & \cos\theta_2 \end{pmatrix} S \begin{pmatrix} e^{-\gamma+i\phi} & 0 \\ 0 & e^{\gamma(\cdot+1)-i\phi(\cdot+1)} \end{pmatrix} \\
&= S\begin{pmatrix} e^{\gamma+i\phi} & 0 \\ 0 & e^{-\gamma(\cdot+1)-i\phi(\cdot+1)} \end{pmatrix}\begin{pmatrix} \cos\theta_2 & i\sin\theta_2 \\ i\sin\theta_2 & \cos\theta_2 \end{pmatrix} \begin{pmatrix} e^{-\gamma(\cdot+1)+i\phi(\cdot+1)} & 0 \\ 0 & e^{\gamma-i\phi} \end{pmatrix} S \\
&= S\begin{pmatrix} \cos\theta_2 e^{\gamma-\gamma(\cdot+1)+i(\phi+\phi(\cdot+1))} & i\sin\theta_2 e^{2\gamma} \\ i\sin\theta_2 e^{-2\gamma(\cdot+1)} & \cos\theta_2 e^{\gamma-\gamma(\cdot+1)-i(\phi+\phi(\cdot+1))} \end{pmatrix} S,
\end{aligned}
$$

where the third equality follows from $L^{\pm1}\psi = \psi(\cdot \pm 1)L^{\pm 1}$ for any bounded sequence $\psi = (\psi(x))_{x\in\mathbb{Z}}$, viewed as a multiplication operator on $\ell^2(\mathbb{Z})$. If $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ denotes the second Pauli matrix, then $\sigma_2^2 = 1$, and so

$$
\begin{aligned}
U_{\mathrm{mko}} &= (S\sigma_2)\sigma_2 \begin{pmatrix} \cos\theta_2 e^{\gamma-\gamma(\cdot+1)+i(\phi+\phi(\cdot+1))} & i\sin\theta_2 e^{2\gamma} \\ i\sin\theta_2 e^{-2\gamma(\cdot+1)} & \cos\theta_2 e^{\gamma-\gamma(\cdot+1)-i(\phi+\phi(\cdot+1))} \end{pmatrix} SC_1 \\
&= (S\sigma_2)\begin{pmatrix} \sin\theta_2 e^{-2\gamma(\cdot+1)} & -i\cos\theta_2 e^{\gamma-\gamma(\cdot+1)-i(\phi+\phi(\cdot+1))} \\ i\cos\theta_2 e^{\gamma-\gamma(\cdot+1)+i(\phi+\phi(\cdot+1))} & -\sin\theta_2 e^{2\gamma} \end{pmatrix} SC_1 \\
&= (S\sigma_2)\begin{pmatrix} e^{-2\gamma(\cdot+1)}a & e^{\gamma-\gamma(\cdot+1)}b \\ e^{\gamma-\gamma(\cdot+1)}b & -e^{2\gamma}a \end{pmatrix}(S\sigma_2)(\sigma_2C_1),
\end{aligned}
$$

where the last equality follows from (IV.8). If we let $\eta := (\sigma_2C_1)(S\sigma_2)$, where σ_2C_1 and $S\sigma_2$ are unitary self-adjoint, then

$$
\eta^*U_{\mathrm{mko}}\eta = (S\sigma_2)(\sigma_2C_1)(S\sigma_2)\begin{pmatrix} e^{-2\gamma(\cdot+1)}a & e^{\gamma-\gamma(\cdot+1)}b \\ e^{\gamma-\gamma(\cdot+1)}b & -e^{2\gamma}a \end{pmatrix}.
$$

It remains to compute $(S\sigma_2)(\sigma_2C_1)(S\sigma_2)$;

$$
(S\sigma_2)(\sigma_2C_1)(S\sigma_2) = \begin{pmatrix} 0 & -iL \\ iL^{-1} & 0 \end{pmatrix}\begin{pmatrix} \sin\theta_1 & -i\cos\theta_1 \\ i\cos\theta_1 & -\sin\theta_1 \end{pmatrix}\begin{pmatrix} 0 & -iL \\ iL^{-1} & 0 \end{pmatrix}.
$$

The claim follows from Theorem IV.1. $\square$

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