Supersymmetric quantum walks with chiral symmetry

Akito Suzuki *

October 2, 2018

Abstract
Quantum walks have attracted attention as a promising platform realizing topological phenomena and many physicists have introduced various types of indices to characterize topologically protected bound states that are robust against perturbations. In this paper, we introduce an index from a supersymmetric point of view. This allows us to define indices for all chiral symmetric quantum walks such as multidimensional split-step quantum walks and quantum walks on graphs, for which there has been no index theory. Moreover, the index gives a lower bound on the number of bound states robust against compact perturbations. We also calculate the index for several concrete examples including the unitary transformation that appears in Grover’s search algorithm.

1 Introduction
Quantum walks have attracted attention as sources of ideas for quantum algorithms \cite{1, 2, 3, 25, 31, 36}. Motivated by Grover’s quantum search algorithm \cite{14}, Szegedy \cite{38} quantized a Markov chain on a finite bipartite graph and defined a quantum walk, which has been updated \cite{24, 25, 26, 17, 18, 34} to define quantum walks on general (possibly infinite) graphs. What is common to such quantum walks is to have an evolution operator defined as a product of two unitary involutions.

1.1 Spectral mapping and supersymmetry
For two given unitary involutions $\Gamma$ and $C$ on a Hilbert space $\mathcal{H}$, we can introduce a coisometry $d$ from $\mathcal{H}$ to another Hilbert space $\mathcal{K}$ and a self-adjoint operator $T = d\Gamma d^*$ so that $C = 2d^*d - 1$ and $\|T\| \leq 1$. A fascinating property of the product $U = \Gamma C$ of the two unitary involutions is as follows.

*Division of Mathematics and Physics, Faculty of Engineering, Shinshu University, Wakasato, Nagano 380-8553, Japan, e-mail: akito@shinshu-u.ac.jp
Let \( \varphi : S^1 \to [-1, 1] \) be defined as \( \varphi(z) = (z + z^{-1})/2 \). Then the spectrum of \( U \) and the preimage of the spectrum of \( T \) under \( \varphi \) coincide except for the points +1 and -1, i.e.,

\[
\sigma(U_0) = \varphi^{-1} \left( \sigma(T_0) \right),
\]

where \( U_0 = U|_{\ker(U^2 - 1)^\perp} \) and \( T_0 = T|_{\ker(T^2 - 1)^\perp} \) are the restrictions onto \( \ker(U^2 - 1)^\perp \) and \( \ker(T^2 - 1)^\perp \). This property is called the spectral mapping theorem for the product of two unitary involutions. As depicted in Fig. 1, \( \sigma(U_0) \) is divided into two parts, i.e.,

\[
\sigma(U_0) = g_+ \left( \sigma(T_0) \right) \cup g_- \left( \sigma(T_0) \right),
\]

where \( g_{\pm}(\xi) = e^{\pm i \text{arccos} \xi} \) for \( \xi \in [-1, 1] \). Moreover, \( U_0 \) is unitarily equivalent to

\[
e^{i \text{arccos} T_0} \oplus e^{-i \text{arccos} T_0}
\]

(see [10, 35, 18] for more details). This is a sign of supersymmetry. In this paper, we explore the supersymmetry of the two unitary involutions.

On the other hand, the quantum walks have also been viewed as promising platforms to realize topological phenomena [20]. Kita- gawa et al [22, 23] showed that one- and two-dimensional quantum walks exhibit topological phases and experimentally realized topologically protected bound states. To this end, they employed a split-step quantum walk, which possesses chiral symmetry, i.e., the evolution operator \( U \) satisfies

\[
\Gamma U \Gamma = U^{-1}
\]

with some unitary involution \( \Gamma \). Asbóth and Obuse [4] also studied the topological nature of a one-dimensional quantum walk in a chiral symmetric time frame (see also [29, 30]). In the above studies, several types of topological indices were introduced in terms of winding numbers and Chern numbers and they were used for characterizing the topological phenomena. Gross et al [13] also established another index theory in terms of the flow of a walk [19] and Cedzich et al [8, 9] studied topological classifications with various types of symmetry. Topological phenomena for nonunitary PT-symmetric
quantum walks were considered in [28, 41] and topological phenomena for periodically driven systems were studied in [5, 21, 33]. Their definitions and proofs however deeply rely on the spatial dimension and geometry of the quantum walk. There has been no index theory that covers quantum walks on graphs and quantum walks for quantum algorithms. In the present paper, we establish index theory that can cover not only one and two-dimensional quantum walks but also such quantum walks. To this end, we first prove that the evolution operator of every chiral symmetric quantum walk can be written as a product of two unitary involutions and it possesses supersymmetry. Then we define an index for such an evolution operator so that it coincides with the Witten index [40].

1.2 Index formula

To make it more precise, let $U$ obey chiral symmetry (1.2). Then $C := \Gamma U$ is a unitary involution and hence $U = \Gamma C$ can be written as a product of two unitary involutions. Actually, we can prove that every quantum walk with an evolution operator represented as a product of two unitary involutions possesses chiral symmetry. Thus, we find that the above mentioned spectral mapping theorem is applicable for any chiral symmetric quantum walk. Moreover, the spectral mapping theorem [18] implies that

$$\dim \ker(U \mp 1) = m_\mp + M_\mp,$$

where $m_\mp = \dim \ker(T \mp 1)$ and $M_\mp = \dim B_\mp$, and $B_\mp := \ker(\Gamma \mp 1) \cap \ker d$ is called the birth eigenspaces [17, 27, 34]. The supersymmetric structure is introduced as follows. From (1.2), we observe that

$$Q := \frac{1}{2i}[\Gamma, C]$$

plays a role of supercharge: $Q$ anticommutes with $\Gamma$, i.e., $\{\Gamma, Q\} = 0$. Here $[A, B] := AB - BA$ and $\{A, B\} := AB + BA$ are the commutator and anticommutator of $A$ and $B$. From a standard argument of supersymmetric quantum mechanics, the supersymmetric Hamiltonian $H := Q^2$ is decomposed into $H = H_+ \oplus H_-$ on $\ker(\Gamma - 1) \oplus \ker(\Gamma + 1)$. Then we define an index $\ind_{\Gamma}(U)$ for $U$ so that $\ind_{\Gamma}(U)$ agrees with the Witten index of $H$: $\dim \ker H_+ - \dim \ker H_-$. The main result of this paper is the following index formula.

$$\ind_{\Gamma}(U) = (M_- - m_-) - (M_+ - m_+).$$

(1.4)

It is clear from (1.4) that the absolute value on $\ind_{\Gamma}(U)$ gives a lower bound of the number of eigenvalues for $U$:

$$\dim \ker(U - 1) + \dim \ker(U + 1) \geq |\ind_{\Gamma}(U)|.$$

(1.5)
In particular, the equality in (1.5) holds if \( m_- = M_+ = 0 \). We emphasize that \( m_\pm - M_\pm \) depend on the choice of \( \Gamma \) and so is \( \text{ind}_R(U) \), while \( m_\pm + M_\pm = \ker(U \mp 1) \) are independent of the choice of \( \Gamma \). Example 5.2 makes this evident. Therefore (1.5) motivates us to develop a way to know the index without calculating the dimension of the kernels, because it gives a sufficient condition for \( U \) to have eigenvalues \( \pm 1 \). This possibility is explored in a forthcoming paper [37]. As expected, we can prove that in \( \Gamma(U) \) is invariant under compact perturbations if \( H = Q^2 \) is Fredholm. Thus we see that the eigenstates corresponding to \( \pm 1 \) for chiral symmetric quantum walks are robust against perturbations. This phenomena can be interpreted as a topological protection of bound states (see Gesztesy and Simon [12], where the invariance of the Witten index against compact perturbation was called topological invariance). Therefore a nonzero index \( \text{ind}_R(U) \neq 0 \) can mathematically guarantee the existence of topologically protected bound states as found in [4, 22, 23]. Such bound states are also expected to be localized at boundaries. Actually, in [11] we proved exponential decay of bound states in the birth eigenspaces.

1.3 Comparison with related work

Avron et al. [6] defined an index for a Fredholm pair \( (P_1, P_2) \) of two projections \( P_1 \) and \( P_2 \) so that \( \text{index}(P_1, P_2) = \dim \ker(P_1 - P_2 - 1) - \dim \ker(P_1 - P_2 + 1) \). This inspires us to introduce the following terminology in order to give a criterion for the Fredholmness of superhamiltonians. For two unitary involutions \( \Gamma \) and \( C \), we say that \( (\Gamma, C) \) is a Fredholm pair if \( H = Q^2 \) is Fredholm with \( Q \) defined in (1.3). Let \( \Gamma_+ \) and \( C_\pm \) be the projections onto \( \ker(\Gamma - 1) \) and \( \ker(C \mp 1) \). The index for two projections and the index we consider in this paper are related as follows.

\[
\text{ind}_R(U) = \text{index}(\Gamma_+, C_+) + \text{index}(\Gamma_+, C_-).
\] (1.6)

Avron et al applied their index to study the charge deficiency [7], in which they took two projections as \( P_1 \) and \( P_2 := WP^* \) with \( W \) a unitary operator and obtained

\[
\text{Index}(P_1, P_2) = \text{Tr}([P_1, W][W^*])^{2n+1}
\]

whenever \( [[P_1, W][W^*]]^{2n+1} \) is trace class. To define an index \( \text{ind}(U) \) for a one-dimensional quantum walk with an evolution \( U \), Gross et al [13] employed the above formula with \( n = 0 \), \( W = U \), and \( P_1 = P \) the projection onto the half line, i.e., \( \text{ind}(U) = \text{Tr}([P, U]U^*) \). Usually, standard one-dimensional quantum walks have evolution operators of the form \( U = SC \), where \( S \) is a shift operator and \( C \) is a coin operator defined by a multiplication operator by \( C(x) \in U(2) \). In such a case, the above index defined by Gross et al. cannot give different indices for different coins, because \( \text{Tr}([P, U]U^*) = \)
\[ \text{Tr}( [P, S] S^* ) \]. In particular, if \( S = S_{ss} := \begin{pmatrix} p & qL \\ qL^* & -p \end{pmatrix} \) with \( p^2 + |q|^2 = 1 \) (\( p \in \mathbb{R} \), \( q \in \mathbb{C} \)) and \( L \) the left-shift operator, a direct calculation yields \( \text{ind}(U) = \text{Tr}( [P, S] S^* ) = 0 \). In [8, 9], Cedzich et al. dealt with indices defined by means of \( \text{Im}U := (U - U^*)/2i \), which is equal to our supercharge \( Q \), because \( [\Gamma, C] = \Gamma C - C \Gamma = U - U^* \). However, their construction and proofs seem to depend on the one-dimensionality. They did not obtain the formula (1.4) and did not mention supersymmetry.

Because \( S_{ss} \) is a unitary involution, all one-dimensional quantum walks given by evolution operators \( U = S_{ss} C \) with \( C(x) \) unitary involution matrices are typical examples of index theory developed in this paper. This model includes all translation invariant standard one-dimensional quantum walks (even if \( C(x) \) is not an involution) and Kitagawa’s one-dimensional quantum walks [23] (see [11, 10] for more details). We calculate the indices for such walks and give a trace formula in a companion paper [37]. Our framework also covers multi-dimensional split-step quantum walks [10], Grover’s search algorithm (see Section 5.2), the Grover walks on graphs (see Section 5.3), the (twisted) Szegedy walks [17], and the Staggered quantum walks [32].

This paper is organized as follows. Section 2 is devoted to defining the index for unitary operators. To this end, we study the relation between chiral symmetry for a unitary operator and supersymmetry for a pair of unitary involutions. In Section 3, we formulate the index formula (1.4) in terms of the spectral mapping theorem for pairs of unitary involutions. Here we also prove several properties for the index formula. In Section 4, we prove the index formula. We close this paper with three examples. In Subsection 5.1, we give finite dimensional toy models. In Subsection 5.2, we calculate the index for a unitary operator that appears in Grover’s search algorithm. Finally, we consider the Grover walks on graphs in Subsection 5.3.

## 2 Chiral symmetry and supersymmetry

Throughout this paper, we assume that all Hilbert spaces are separable. We say that an operator \( X \) is an involution if \( X^2 = 1 \). The following is standard.

**Remark 2.1.** If an operator \( X \) has any two of the following three properties, then it has all three properties: (1) \( X \) is self-adjoint, i.e., \( X^* = X \); (2) \( X \) is unitary, i.e., \( X^* = X^{-1} \); (3) \( X \) is involutory, i.e., \( X^2 = 1 \).

### 2.1 Chiral symmetry

**Definition 2.1.** Let \( U \) be a unitary operator on a Hilbert space \( \mathcal{H} \). Then we say that \( U \) has chiral symmetry if there exists a unitary involution \( \Gamma \) on \( \mathcal{H} \) such that

\[ \Gamma U \Gamma = U^{-1} \].

(2.1)
Lemma 2.1. Let $U$ be a unitary operator on a Hilbert space $\mathcal{H}$. The following are equivalent.

(1) $U$ has chiral symmetry.

(2) $U$ is a product of two unitary involutions.

In particular, if $U$ satisfies (2.1) with a unitary involution $\Gamma$, then $C := \Gamma U$ is a unitary involution and

$$U = \Gamma C. \quad \text{(2.2)}$$

Remark 2.2. The product decomposition of (2) is not necessary unique. In fact, if $U_1$ and $U_2$ are unitary involutions, then $-U_1$ and $-U_2$ are also unitary involutions and $U_1 U_2 = (-U_1)(-U_2)$. See also Example 5.2.

Proof of Lemma 2.1. Let $U$ satisfy (2.1). Then $C = \Gamma U$ is unitary. From (2.1), $C^2 = (\Gamma U)^2 = 1$. Because $\Gamma$ is a unitary involution, $U = \Gamma^2 U = \Gamma \cdot (\Gamma U) = \Gamma C$. Hence (1) implies (2).

Conversely, suppose that $U$ satisfies (2.2) and $\Gamma$ and $C$ are unitary involutions. Then $\Gamma U \Gamma = C \Gamma = U^{-1}$. Hence (2) implies (1).

Thus we have the desired conclusion. \qed

2.2 Supersymmetry

Let $U$ have chiral symmetry with a unitary involution $\Gamma$ satisfying (2.1) and set $C = \Gamma U$. Then

$$R := \frac{1}{2} \{ \Gamma, C \}, \quad Q := \frac{1}{2i} [\Gamma, C]$$

are self-adjoint.

Lemma 2.2. Let $U$ and $\Gamma$ be as stated above. Then

(1) $[\Gamma, R] = 0,$

(2) $\{ \Gamma, Q \} = 0,$

where $[X,Y] := XY - YX$ and $\{X,Y\} := XY + YX$.

Proof. Because $C = \Gamma U$, we observe that

$$R = \text{Re} U := \frac{U + U^*}{2}, \quad Q = \text{Im} U := \frac{U - U^*}{2i}.$$

By (2.1), $\Gamma U = U^* \Gamma$ and $U \Gamma = \Gamma U^*$. Hence, $\Gamma R = R \Gamma$ and $\Gamma Q = -Q \Gamma$. This proves (1) and (2). \qed
From Remark 2.1, the spectrum of $\Gamma$ is $\sigma(\Gamma) = \{1, -1\}$ and the spectral decomposition of $\Gamma$ is
$$\Gamma = \Gamma_+ - \Gamma_-,$$
where $\Gamma_{\pm} = (1 \pm \Gamma)/2$ is the projection onto $\ker(\Gamma \mp 1)$. With the identification $\mathcal{H} = \operatorname{Ran}\Gamma_+ \oplus \operatorname{Ran}\Gamma_-$, $\Gamma$ is written as
$$\Gamma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
With this notation, (2) of Lemma 2.2 yields
$$Q = \begin{pmatrix} 0 & \alpha^* \\ \alpha & 0 \end{pmatrix},$$
(2.3)
where $\alpha = \Gamma_+ Q \Gamma_+$ is an operator from $\operatorname{Ran}\Gamma_+ \to \operatorname{Ran}\Gamma_-$. We set $H = Q^2$ and write
$$H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix},$$
where $H_+ = \alpha^* \alpha$ and $H_- = \alpha \alpha^*$. In the context of supersymmetry, $Q$ is called a supercharge and $H$ is a superhamiltonian 40 (see also 39). The Witten index of $H$ is defined as
$$\Delta(H) = \dim \ker H_+ - \dim \ker H_-.$$

2.3 Index of a Fredholm pair

In this paper, we introduce an index for a pair $(U, \Gamma)$ of a unitary operator $U$ and a unitary involution $\Gamma$ satisfying (2.1). Before that, inspired by 6, we introduce the following terminology. We say that a pair $(C_1, C_2)$ of two unitary involutions is a Fredholm pair if $([C_1, C_2]/2)i$ is Fredholm. By definition, the pair $(\Gamma, C)$ of unitary involutions with $C := \Gamma U$ is a Fredholm pair if and only if $H = Q^2$ is Fredholm.

**Definition 2.2.** Let $U$ and $\Gamma$ satisfy (2.1) and let $\alpha$ be as stated above. We say that $(U, \Gamma)$ is a Fredholm pair if $\alpha$ is Fredholm, i.e., $\dim \ker \alpha < \infty$, $\dim \ker \alpha^* < \infty$, and $\operatorname{Ran}(\alpha)$ is closed. In this case, the index of the pair $(U, \Gamma)$ is defined by
$$\text{ind}_\Gamma(U) = \text{index}(\alpha),$$
(2.4)
where $\text{index}(\alpha) := \dim \ker \alpha - \dim \ker \alpha^*$ is the Fredholm index of $\alpha$.

**Proposition 2.3.** Let $U$ be unitary and $\Gamma$, $\Gamma'$ be unitary involutions satisfying $\Gamma U \Gamma' = U^{-1}$ and $\Gamma' U \Gamma = U^{-1}$. If $(U, \Gamma)$ is a Fredholm pair, then so is $(U, \Gamma')$. 

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Proof. Observe that the operator $\alpha$ is Fredholm if and only if
\[
\dim \ker H_+ < \infty \quad \text{and} \quad \inf \sigma(H_+) \setminus \{0\} > 0. \tag{2.5}
\]
Moreover, (2.5) is equivalent to saying that $H$ is Fredholm (see [6, 39] for more details). Because $H = (\Im U)^2$ is independent of the choice of $\Gamma$, we obtained the desired assertion.

Remark 2.3. Because from the above proof, $\alpha$ is Fredholm if and only if $H$ is Fredholm, $(U, \Gamma)$ is a Fredholm pair if and only if so is $(\Gamma, C)$. Therefore we henceforth only consider the Fredholmness of pairs $(U, \Gamma)$ of a unitary operator $U$ and a unitary involution $\Gamma$. Moreover, we observe from (2.5) that if $(U, \Gamma)$ is a Fredholm pair, then $\text{index}(\alpha) = \Delta(H)$. Because the Hamiltonian $H$ is independent of the choice of $\Gamma$, one may feel that the index is also independent of the choice of $\Gamma$. However, the definition of the Witten index depends on the choice of $\Gamma$, because $H_\pm$ are determined by $\Gamma$.

As mentioned in Remark 2.2, the decomposition $U = \Gamma C$ by two unitary involutions $\Gamma$ and $C$ is not necessary unique. Hence, it is possible that there are two unitary involutions $\Gamma_i$ such that $\Gamma_i U \Gamma_i = U^{-1}$ $(i = 1, 2)$. Indeed, Example 5.2 reveals that there are Fredholm pairs $(U, \Gamma)$ and $(U, \Gamma')$ such that $\text{ind}_{\Gamma'}(U) \neq \text{ind}_{\Gamma}(U)$. That is why we define an index for a pair $(U, \Gamma)$ and not for $U$ itself.

3 Index formula

Throughout this section, we assume that $U$ is a unitary operator on a Hilbert space $H$ and it has chiral symmetry. Then Lemma 2.1 says that $U$ is written as a product of two unitary involutions $\Gamma$ and $C$, i.e., $U = \Gamma C$. Without loss of generality, we can suppose that $\ker(C - 1) \neq \{0\}$, because if $\ker(C - 1) = \{0\}$, then $-C = 1$ and $-\Gamma$ are unitary involutions and $U = (-\Gamma)(-C)$ is a product of two unitary involutions.

In this section, we give an explicit expression for $\text{ind}_{\Gamma}(U)$ defined in (2.4). To this end, we review a previous result [18, 35] on a spectral mapping theorem for a product of two unitary involutions.

Theorem 3.1 ([18, 35]). Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces. Let $\gamma$ be a unitary involution on $\mathcal{H}$ and $\partial: \mathcal{H} \to \mathcal{K}$ be a coisometry, i.e., $\partial \partial^* = 1$ on $\mathcal{K}$.

(i) $\tau := \partial \gamma \partial^*$ is bounded and self-adjoint on $\mathcal{K}$ with $\|\tau\| \leq 1$.

(ii) $u := \gamma(2\partial^* \partial - 1)$ is unitary and
\[
\sigma_\mathcal{K}(u) = \varphi^{-1}(\sigma_\mathcal{K}(\tau)), \quad \varphi(c, ac, sc, \ldots),
\]
where $\varphi(z) = (z + z^{-1})/2$. 

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(iii) For $\lambda \in \sigma_p(u)$,

$$\dim \ker(u - \lambda) = \begin{cases} 
\dim \ker(\tau - \varphi(\lambda)), & \lambda \neq \pm 1 \\
m_\pm + M_\pm, & \lambda = \pm 1,
\end{cases}$$

where $m_\pm := \dim \ker(\tau \mp 1)$ and $M_\pm := \dim \ker(\gamma \pm 1) \cap \ker \partial$.

We now give different expressions for $m_\pm$ and $M_\pm$.

**Corollary 3.2.** Let $\gamma$, $\partial$, and $m_\pm$ be as stated in Theorem 3.1.

$$m_\pm = \dim \ker(\gamma \mp 1) \cap \ker(c - 1), \quad (3.1)$$

$$M_\pm = \dim \ker(\gamma \pm 1) \cap \ker(c + 1), \quad (3.2)$$

where $c := 2\partial^*\partial - 1$.

**Proof.** Because $\ker \partial = \ker(c + 1)$, (3.2) is obtained from

$$\ker(\gamma \pm 1) \cap \ker(c + 1) = \ker(\gamma \pm 1) \cap \ker \partial. \quad (3.3)$$

We prove (3.1). Because $\partial^*$ is a bijection from $\ker(\tau \mp 1)$ to $\partial^* \ker(\tau \mp 1)$, we need only prove

$$\partial^* \ker(\tau \mp 1) = \ker(\gamma \mp 1) \cap \ker(c - 1). \quad (3.4)$$

Because $\text{Ran}(\partial^*) = \ker(c - 1)$,

$$\ker(\gamma \mp 1) \cap \ker(c - 1) = \{ \partial^* f \mid \gamma \partial^* f = \pm \partial^* f \}.$$

If $\gamma \partial^* f = \pm \partial^* f$, then $\tau f = \partial \gamma \partial^* f = \pm f$. Hence $f \in \ker(\tau \mp 1)$. Conversely, if $f \in \ker(\tau \mp 1)$, then

$$\langle \partial^* f, S \partial^* f \rangle = \langle f, T f \rangle = \pm \|f\|^2 = \pm \|\partial^* f\|^2.$$

Subtracting the right-hand side from the left-hand side yields $\|\gamma \mp 1\| \partial^* f\|^2 = 0$, because $(1 \pm \gamma)/2$ is a projection. Hence $\partial^* f \in \ker(\tau \mp 1)$ and (3.1) is proved. This concludes the desired assertion.

To apply Theorem 3.1 and Corollary 3.2 to the operator $U = \Gamma C$, we will represent $C$ using a coisometry. Let $\{\chi_j\}_{j \in V}$ be a CONS of $\ker(C - 1)$, where $V$ is a countable set. We use $\mathcal{K}$ to denote the Hilbert space $\ell^2(V)$ of square summable functions on $V$. We introduce an operator $d : \mathcal{H} \to \mathcal{K}$ as follows. For $\psi \in \mathcal{H}$, $d\psi \in \mathcal{K}$ is defined as a function on $V$ such that

$$(d\psi)(j) = \langle \chi_j, \psi \rangle, \quad j \in V,$$

where $\langle \cdot, \cdot \rangle$ on the right-hand side is the inner product on $\mathcal{H}$. The Bessel inequality guarantees the boundedness of $d$. The following lemma is straightforward. For a proof, the reader can consult [15].
Lemma 3.3. Let $d$ be as stated above.

(i) The operator $d$ is a coisometry, i.e., $dd^* = 1$ on $K$.

(ii) The adjoint $d^* : K \to H$ is an isometry and is given by

$$d^* f = \sum_{j \in V} f(j) \chi_j, \quad f \in K.$$ 

(iii) $d^* d = \sum_{j \in V} |j\rangle \langle j|$ is the projection onto $\ker(C - 1)$.

(iv) $C = 2d^* d - 1$.

Because, from the above lemma, any chiral symmetric unitary operator $U$ can be written as $U = \Gamma(2d^* d - 1)$ with a unitary involution $\Gamma$ and a coisometry $d$, Theorem 3.1 is applicable for $U$. Let $m_{\pm} = \dim \ker(T \mp 1)$ and $M_{\pm} = \dim B_{\pm}$, where $T = d\Gamma d^*$ is called the discriminant of $U$ and $B_{\pm} = \ker(\Gamma \pm 1) \cap \ker d$ is called the birth eigenspaces [31, 27]. From the proof of Corollary 3.2,

$$B_{\pm} = \ker(\Gamma \pm 1) \cap \ker(C + 1). \quad (3.5)$$

In this paper, we introduce inherited eigenspaces $T_{\pm}$ by

$$T_{\pm} = \ker(\Gamma \mp 1) \cap \ker(C - 1). \quad (3.6)$$

Corollary 3.2 says that $m_{\pm} = \dim T_{\pm}$.

Remark 3.1. It is worthy noting that the inherited eigenspaces and the birth eigenspaces can be represented as

$$T_{\pm} = d^* \ker(T \mp 1), \quad B_{\pm} = \ker(\Gamma \mp 1) \cap \ker d \quad (3.7)$$

and

$$\ker(U \mp 1) = T_{\pm} \oplus B_{\pm}. \quad (3.8)$$

Here (3.7) has already been proved in (3.1) and (3.3). For the proof of (3.8), the reader can consult [35], [35], [35], and [35] prove (3.9).

In terms of the spectral mapping theorem, we obtain the following index theorem.

Theorem 3.4. Let $U, \Gamma, T = d\Gamma d^*, m_{\pm}$, and $M_{\pm}$ be as stated above.

(i) $(U, \Gamma)$ is a Fredholm pair if and only if $1 - T^2$ is Fredholm and $M_{\pm} < \infty$. 

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(ii) If \((U, \Gamma)\) is a Fredholm pair,

\[
\text{ind}_F(U) = (M_- - m_-) - (M_+ - m_+). \tag{3.9}
\]

In particular,

\[
\dim \ker(U - 1) + \dim \ker(U + 1) \geq |\text{ind}_F(U)|, \tag{3.10}
\]

where the equality holds if \(m_- = 0\) and \(M_+ = 0\).

(iii) If \((U, \Gamma)\) and \((U', \Gamma')\) are Fredholm pairs and \(U' - U\) is compact, then

\[
\text{ind}_F(U') = \text{ind}_F(U). \tag{3.11}
\]

We postpone the proof until the next section. In what follows, we give several corollaries of Theorem 3.4.

**Corollary 3.5.** Let \(U, \Gamma, T, \) and \(M_{\pm}\) be as stated above. If \(\|T\| < 1\) and \(M_{\pm} < \infty\), then \((U, \Gamma)\) is a Fredholm pair, \(m_{\pm} = 0\), and

\[
\text{ind}_F(U) = M_- - M_+. \tag{3.12}
\]

**Proof.** By assumption, there exists a positive \(\epsilon\) such that \(\|T\| = 1 - \epsilon\). This implies \(1 - T^2 \geq \epsilon\). Hence \(1 - T^2\) is Fredholm and \(m_{\pm} = 0\). Applying Theorem 3.4, we have the desired assertion. \(\square\)

The following corollary indicates unitary invariance of the index.

**Corollary 3.6.** Let \(U\) and \(\Gamma\) be as above. Let \(V\) be a unitary operator from \(H\) to a Hilbert space \(H'\) and set \(U' = VUV^{-1}\) and \(\Gamma' = V\Gamma V^{-1}\). If \((U, \Gamma)\) is a Fredholm pair, then so is \((U', \Gamma')\) and

\[
\text{ind}_F(U') = \text{ind}_F(U). \tag{3.11}
\]

In particular, \((U^{-1}, \Gamma)\) is a Fredholm pair and

\[
\text{ind}_F(U^{-1}) = \text{ind}_F(U). \tag{3.12}
\]

**Proof.** We first prove (3.11). By Lemma 3.3, \(\Gamma U = C = 2d^*d - 1\) and \(d\) is a coisometry. Then \(d' := dV^{-1}\) is a coisometry from \(H'\) to \(K\). Indeed, \(d'(d')^* = dV^{-1} \cdot Vd^* = dd^* = 1\) on \(K\). Observe that \(U' = \Gamma' C'\) is a product of two unitary involutions \(\Gamma'\) and \(C' := VCV'\). Moreover, \(C' = V(2d^*d - 1)V^{-1} = 2(d')^*d' - 1\). The discriminant \(T'\) of \(U'\) is equal to \(T\), because it is given by

\[
T' = d'd'\Gamma(d')^* = dV^{-1} \cdot V\Gamma V^{-1} \cdot Vd^* = d\Gamma d^* = T.
\]
Let $M_\pm$ be the dimension of $B'_\pm = \ker(I' \pm 1) \cap \ker d'$ and $m'_\pm = \ker(I' \mp 1)$. Since $T' = T$, $m'_\pm = m_\pm$. By definition,

$$B'_\pm = \{ \psi \mid d' \psi = 0, \ (I' \pm 1) \psi = 0 \} = \{ \psi \mid d(V^{-1} \psi) = 0, \ (I \mp 1)(V^{-1} \psi) = 0 \} = VB'_\pm,$$

which implies $M'_\pm = M_\pm$. Thus we find from Theorem 3.4 that if $(U, \Gamma)$ is a Fredholm pair, then so is $(U', \Gamma)$ and

$$\text{ind}_\Gamma(U') = (M'_+ - m'_-) - (M'_- - m'_+) = \text{ind}_\Gamma(U).$$

Hence, (3.11) is proved.

We next prove (3.12). Let $V = \Gamma$. We obtain $U' = \Gamma U \Gamma = U^{-1}$, $I' = I$, $\text{ind}_\Gamma(U') = \text{ind}_\Gamma(U^{-1})$. Applying (3.11) yields (3.12). The proof is completed.

**Remark 3.2.** In general, the Fredholm index satisfies

$$\text{Index}(A^*) = -\text{Index}(A).$$

Hence, (3.12) may seem strange. It should be noted that $\text{ind}_\Gamma(U)$ (or equivalently the Witten index $\Delta(H)$) is defined through the Hamiltonian. Because the Hamiltonian $H$ for $U$ is equal to $H'$ for $U^{-1}$, (3.12) is correct. Indeed, $H' = (\text{Im}(U^{-1}))^2 = (\text{Im}U)^2 = H$. As seen below, even if $U$ and $U'$ have the same Hamiltonian, it is possible to have different indices. See also Remark 2.3 and Example 5.2.

Using (3.5) and (3.6), we obtain the following. **Corollary 3.7.** Let $U$ and $\Gamma$ be as stated above. If $(U, \Gamma)$ is a Fredholm pair, then so are $(-U, \Gamma)$ and $(U, -\Gamma)$ and

$$\text{ind}_\Gamma(-U) = \text{ind}_\Gamma(U), \quad \text{ind}_{-\Gamma}(U) = -\text{ind}_\Gamma(U).$$

*Proof.* Let $H$ be the Hamiltonian for $U$. Then the Hamiltonian for $-U$ is equal to $H$, because $(\text{Im}(-U))^2 = (\text{Im}(U))^2 = H$. Hence, from an argument similar to the proof of Proposition 2.3 if $(U, \Gamma)$ is a Fredholm pair, then so are $(-U, \Gamma)$ and $(U, -\Gamma)$.

We now write $B_\pm(U, \Gamma)$ and $T_\pm(U, \Gamma)$ for the birth eigenspaces (3.5) and the inherited eigenspaces (3.10) to make the dependence on $U$ and $\Gamma$ explicit. For the pair $(-U, \Gamma)$, $U$ is decomposed into $-U = \Gamma(-C)$, (3.5) and (3.6) say that

$$B_\pm(-U, \Gamma) = \ker(\Gamma \pm 1) \cap \ker(-C + 1) = T_\pm(U, \Gamma),$$
$$T_\pm(-U, \Gamma) = \ker(\Gamma \mp 1) \cap \ker(-C - 1) = B_\pm(U, \Gamma).$$
which, combined with (3.9), imply that
\[
\text{ind}_F(-U) = (\dim \mathcal{T}_+(U,\Gamma) - \dim \mathcal{B}_+(U,\Gamma)) \\
- (\dim \mathcal{T}_-(U,\Gamma) - \dim \mathcal{B}_-(U,\Gamma)) \\
= \text{ind}_F(U).
\]
Similarly, \( U = (-\Gamma)(-C) \) implies that
\[
\mathcal{B}_\pm(U,-\Gamma) = \ker(-\Gamma \pm 1) \cap \ker(-C + 1) \\
= \ker(\Gamma \mp 1) \cap \ker(C - 1) = \mathcal{T}_\pm(U,\Gamma),
\]
\[
\mathcal{T}_\pm(U,-\Gamma) = \ker(-\Gamma \mp 1) \cap \ker(-C - 1) \\
= \ker(\Gamma \pm 1) \cap \ker(C + 1) = \mathcal{B}_\pm(U,\Gamma),
\]
which yields
\[
\text{ind}_{-F}(U) = (\dim \mathcal{T}_-(U,\Gamma) - \dim \mathcal{B}_-(U,\Gamma)) \\
- (\dim \mathcal{T}_+(U,\Gamma) - \dim \mathcal{B}_+(U,\Gamma)) \\
= -\text{ind}_F(U).
\]
This completes the proof.

We conclude this section with \( \mathcal{H} \) finite dimensional.

**Corollary 3.8.** Let \( U, \Gamma, T, m_\pm, \) and \( M_\pm \) be as stated in Theorem 3.4 and suppose that \( \dim \mathcal{H} < \infty \). Then \((U,\Gamma)\) is a Fredholm pair and (3.9) holds. Moreover, if \( \dim \ker(\Gamma + 1) = \dim \ker(\Gamma - 1) \), then
\[
\text{ind}_F(U) = 0.
\]

**Proof.** Since \( \dim \mathcal{H} < \infty \), \( \alpha \) is automatically Fredholm. Hence, from Theorem 3.4 (3.9) holds. If \( n = \dim \ker(\Gamma + 1) = \dim \ker(\Gamma - 1) \), then \( \alpha \) is viewed as a square matrix of order \( n \) and hence \( \dim \ker \alpha = \dim \ker \alpha^* \). By definition, \( \text{ind}_F(U) = \ker \alpha - \ker \alpha^* = 0 \). This completes the proof.

**4 Proof of the index formula**

In this section, we prove Theorem 3.4. Throughout this section, we assume that a unitary operator \( U \) and a unitary involution \( \Gamma \) satisfy \( \Gamma U \Gamma = U^{-1} \).

We use the notations in Sections 2 and 3. We prove (i)-(ii) of Theorem 3.4 in Subsections 4.1-4.3.
4.1 Fredholmness

In this subsection, we prove (i) of Theorem 3.4, i.e., \((U, \Gamma)\) is a Fredholm pair if and only if \(1 - T^2\) is Fredholm and \(M_\pm < \infty\).

**Proof of Theorem 3.4 (i).** By Remark 2.3, \((U, \Gamma)\) is a Fredholm pair if and only if \(H\) is Fredholm. Thus we find that the following proposition concludes the proof. \(\square\)

**Proposition 4.1.** The following are equivalent.

(i) \(H\) is Fredholm.

(ii) \(1 - T^2\) is Fredholm and \(M_\pm < \infty\).

**Proof.** By [35, Theorem 4.1 and Proposition 5.3], \(H\) is unitarily equivalent to \(\ker(1 - T^2) \perp \ker(1 - T^2) \perp \ker(1 - U) \perp \ker(1 + U)\) and with this identification

\[U \simeq e^{i\arccos T} \oplus e^{-i\arccos T} \oplus 1 \oplus (-1).\]

Because \(e^{\pm \arccos T} = T \pm \sqrt{1 - T^2}\),

\[Q = \text{Im} U \simeq \sqrt{1 - T^2} \oplus \sqrt{1 - T^2} \oplus 0 \oplus 0\]

and hence

\[H = Q^2 \simeq 1 - T^2 \oplus 1 - T^2 \oplus 0 \oplus 0.\]

Therefore,

\[\inf \sigma(H) \setminus \{0\} = \inf \sigma(1 - T^2) \setminus \{0\}. \tag{4.1}\]

Because, by Theorem 3.1, \(\dim \ker(1 \mp U) = m_\pm + M_\pm\) and by definition, \(m_+ + m_- = \ker(1 - T^2)\),

\[
\dim \ker H = \dim \ker(1 - U) \oplus \ker(1 + U)
= m_+ + M_+ + m_- + M_-
= \dim \ker(1 - T^2) + M_+ + M_- \tag{4.2}
\]

(4.1) and (4.2) conclude the desired assertion. \(\square\)

4.2 \(\ker \alpha\) and \(\ker \alpha^*\)

In this section, we prove Theorem 3.4 (ii), i.e., if \((U, \Gamma)\) is a Fredholm pair, then

\[\text{ind}_\Gamma(U) = (M_- - m_-) - (M_+ - m_+). \tag{3.11}\]

(3.10) can be easily proved by the above equation.
Proof of Theorem 3.4 (ii). Because the right-hand side of (3.9) is
\[(m_+ + M_-) - (M_+ + M_-) = (\dim \ker(1 - T) + \dim B_-) - (\dim \ker(1 + T) + \dim B_+),\]
it suffices to prove
\[
dim \ker \alpha = \dim \ker(1 - T) + \dim B_-, \quad \dim \ker \alpha^* = \dim \ker(1 + T) + \dim B_+.
\]
Because \(d^*\) is a bijection from \(\dim \ker(1 - T) = \dim d^* \ker(1 - T)\), the following proposition prove the desired assertion.

Proposition 4.2. (i) \(\ker \alpha = d^* \ker(1 - T) \oplus B_-\).

(ii) \(\ker \alpha^* = d^* \ker(1 + T) \oplus B_+\).

The proof of Proposition 4.2 splits into several lemmas.

Lemma 4.3. \(\ker Q = \ker(1 - U^2)\).

Proof. Supposing \(\varphi \in \ker(1 - U^2)\), we have \((U - U^*)\varphi = 0\) and hence \((1 - U^2)\varphi = U(U - U^*)\varphi = 0\). Therefore, \(\varphi \in \ker(1 - U^2)\).

Conversely, suppose that \(\varphi \in \ker(1 - U^2)\). Then \(U^2 \varphi = \varphi\) and hence \(U \varphi = U^* \varphi\). Hence, \(Q \varphi = (U - U^*) \varphi / 2i = 0\). This completes the proof.

Lemma 4.4. (i) \(\ker \alpha = \ker Q \cap \ker(\Gamma - 1)\)

(ii) \(\ker \alpha^* = \ker Q \cap \ker(\Gamma + 1)\)

Proof. Since \(\alpha = \Gamma_- Q \Gamma_+\) is an operator from \(\text{Ran} \Gamma_+\) to \(\text{Ran} \Gamma_-\),
\[
\ker \alpha = \{ \varphi \in \text{Ran} \Gamma_+ \mid \Gamma_- Q \varphi = 0 \}.
\]
Supposing that \(\varphi \in \ker \alpha\), we have \((1 - \Gamma) Q \varphi = 0\). Because, by Lemma 2.2, \(Q\) anticommutes with \(\Gamma\), we obtain \(Q \varphi = \Gamma Q \varphi = -Q \Gamma \varphi\). Hence, \(Q(1 + \Gamma) \varphi = 0\). Because \(\varphi \in \text{Ran} \Gamma_+, Q \varphi = 0\). Thus, we see that \(\varphi \in \ker Q \cap \ker(\Gamma - 1)\).

Conversely, suppose that \(\varphi \in \ker Q \cap \ker(\Gamma - 1)\). Then \(\varphi \in \text{Ran}(\Gamma_+)\) and \(Q \varphi = 0\). Hence, \(\varphi \ker \alpha\). Therefore (i) is proved. The same proof works for (ii).

Lemma 4.5. Let \(C_\pm = (1 \pm C)/2\). For any \(\varphi \in \ker \alpha\),
\[UC_\pm \varphi = \pm C_\pm \varphi.\]
Proof. Observe that $C_\pm$ is the projection onto $\ker(C \mp 1)$. Let $\varphi \in \ker \alpha$. By Lemmas 4.3 and 4.4, $\varphi$ belongs to $\ker(1 - U^2)$ and $\ker(\Gamma - 1)$. Hence, $U^2 \varphi = \varphi$ and

$$U \varphi = U^* \varphi = C \Gamma \varphi = C \varphi. \quad (4.3)$$

By (4.3),

$$UC \varphi = U^2 \varphi = \varphi. \quad (4.4)$$

By (4.3) and (4.4),

$$U \left( \frac{1 \pm C}{2} \right) \varphi = \frac{C \pm 1}{2} \varphi,$$

which proves the lemma.

We now prove Proposition 4.2, using Lemmas 4.3, 4.4, and 4.5.

Proof of Proposition 4.2. Suppose that $\varphi \in \ker \alpha$. With the decomposition $\mathcal{H} = \text{Ran} d^* \oplus \ker d$, we can write

$$\varphi = d^* f + \varphi_0,$$

where $f \in \mathcal{K}$, $\varphi_0 \in \ker d$. Since $C_\pm$ is the projection onto $\ker(C \mp 1)$ Lemma 3.3 says that $C_\mp = d^* d$. Hence, $\text{Ran} d^* = \ker(C - 1)$ and $\ker d = \ker(C + 1)$. Because $d$ is a coisometry,

$$C_+ \varphi = d^* f,$$

$$C_- \varphi = \varphi_0. \quad (4.5)$$

By (4.5),

$$\Gamma d^* f = \Gamma C_+ \varphi = \Gamma C C_+ \varphi = U C_+ \varphi = C_+ \varphi = d^* f,$$

where we have used Lemma 4.5 in the second last equality. Hence,

$$T f = d(\Gamma d^* f) = d(d^* f) = f$$

and therefore $f \in \ker(T - 1)$. Similarly, by (4.6),

$$U \varphi_0 = U C_- \varphi = -C_- \varphi = -\varphi_0, \quad (4.7)$$

where we have used Lemma 4.5 again in the second last equality. Because $\varphi_0 \in \ker(C + 1)$,

$$U \varphi_0 = \Gamma C \varphi_0 = -\Gamma \varphi_0. \quad (4.8)$$

By (4.7) and (4.8), $\Gamma \varphi_0 = \varphi_0$. Hence, $\varphi_0 \in \ker(\Gamma - 1) \cap \ker d = \mathcal{B}_\mp$. Thus we see that $\varphi \in d^* \ker(T - 1) \oplus \mathcal{B}_\mp$. Conversely, supposing that $\varphi \in d^* \ker(T - 1) \oplus \mathcal{B}_\mp$, we can write

$$\varphi = d^* f + \varphi_0. \quad (4.9)$$
where $f \in \ker(T - 1)$ and $\varphi_0 \in B_-$. We now claim that

$$d^* f \in \ker(\Gamma - 1). \quad (4.10)$$

Indeed, an argument similar to the proof of Corollary 3.2 yields (4.10). Since $\varphi_0 \in B_- \subset \ker(\Gamma - 1)$, (4.9) and (4.10) imply $\varphi \in \ker(\Gamma - 1)$. We next prove that $\varphi \in \ker Q$. Combining (4.10) and (iii) of Lemma 3.3, we have

$$2iQd^* f = (U - U^*)d^* f = \Gamma d^* f - C\Gamma d^* f = (1 - C)d^* f = 2C_\varphi d^* f = 0.$$ 

Hence, $d^* f \in \ker Q$. Similarly, using $\varphi_0 \in \ker(C + 1)$, we have

$$2iQ\varphi_0 = (U - U^*)\varphi_0 = -\Gamma\varphi_0 - C\Gamma\varphi_0 = -C_\varphi \varphi_0 = 0.$$ 

Hence, $\varphi_0 \in \ker Q$. Thus we see that $\varphi = d^* f + \varphi_0 \in \ker Q$. Summarizing, we have $\varphi \in \ker Q \cap \ker(\Gamma - 1)$. By Lemma 4.4, we obtain $\varphi \in \ker \alpha$. Thus (i) is proved.

A similar proof works for (ii).

4.3 Topological invariance

In this subsection, we prove Theorem 3.4 (iii), i.e., if $(U, \Gamma)$ and $(U', \Gamma')$ are Fredholm pairs and $U' - U$ is compact, then $\text{ind}_\Gamma(U') = \text{ind}_\Gamma(U)$.

**Proof of Theorem 3.4 (iii).** Let $C_1 = \Gamma U$ and $C_2 = \Gamma U'$. By assumption, $C_i$ is written as $C_i = 2P_i - 1$ with the projection onto $\ker(C_i - 1)$ ($i = 1, 2$) and $2(P_1 - P_2) = C_1 - C_2 = \Gamma(U - U')$ is compact. Because supercharges $Q_i$ for $U_i := \Gamma C_i$ ($i = 1, 2$) are $Q_i = (\Gamma, P_1)/i$, 

$$Q_1 - Q_2 = \frac{1}{i} [\Gamma, P_1 - P_2]$$

is compact. Let $\alpha_i = \Gamma Q_i \Gamma_+$. Because $\alpha_1 - \alpha_2 = \Gamma_-(Q_1 - Q_2)\Gamma_+$ is compact, the Fredholm index $\text{index}(\alpha_1)$ is equal to $\text{index}(\alpha_2)$. By definition, this means that $\text{ind}_\Gamma(U) = \text{ind}_\Gamma(U')$. This completes the proof.

**Remark 4.1.** Similarly to the above proof, we can relax the condition of Theorem 3.4 (iii). Indeed, we can prove the following. Suppose that $\Gamma U$ and $\Gamma U'$ are unitary involutions and $U - U'$ is compact. If $(U, \Gamma)$ is a Fredholm pair, then so is $(U', \Gamma)$ and $\text{ind}_\Gamma(U) = \text{ind}_\Gamma(U')$.

5 Examples

Based on the supersymmetric structure discussed above, we will call a quantum walk with a chiral symmetric evolution a supersymmetric quantum walk (SUSYQW). After considering a finite dimensional toy model in Subsection 5.1, we present SUSYQWs. In Subsection 5.2, we give an application to Grover’s algorithm, which is viewed as a SUSYQW. In Subsection 5.3, we treat the Grover walk on a graph.

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5.1 finite dimensional toy models

In this subsection, we demonstrate how to calculate the index \( \text{ind}_\Gamma(U) \) for a finite dimensional toy model, which reveals that the index depends on the choice of \( \Gamma \). For the finite dimensional case, Corollary 3.8 says that the index \( \text{ind}_\Gamma(U) \) is given by the formula (3.9) for every pair \((U, \Gamma)\) of a unitary \( U \) and a unitary involution \( \Gamma \) obeying (2.2).

Example 5.1 (Two dimensional case). Fix \( \beta \in \mathbb{R} \) and set

\[
U = \begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}.
\]

For \( \gamma, c \in \mathbb{R} \) with \( \beta = \gamma - c \), it follows that \( U = \Gamma C \), where

\[
\Gamma = \begin{pmatrix} 0 & e^{i\gamma} \\ e^{-i\gamma} & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & e^{ic} \\ e^{-ic} & 0 \end{pmatrix}.
\]

Because \( \Gamma \) and \( C \) are unitary involutions, \((U, \Gamma)\) becomes a Fredholm pair for every \( \gamma \in \mathbb{R} \) with \( c = \gamma - \beta \). Thus we find that there are infinitely many choices of \( \Gamma \) such that \((U, \Gamma)\) is a Fredholm pair. In this case, Corollary 3.8 says that \( \text{ind}_\Gamma(U) = 0 \), because \( \ker(\Gamma \pm 1) = 1 \).

We next study the birth eigenspaces \( B_\pm \) and the inherited eigenspaces \( T_\pm \). Since \( \text{ind}_\Gamma(U) = 0 \),

\[
M_+ - M_- = m_+ - m_-.
\]

Combining this with \( \dim \ker(U \mp 1) = M_\pm + m_\pm \), we can conclude the following assertion.

- If \( \beta \in \pi \mathbb{Z} \), then either of the following two holds:
  1. \( M_+ = m_+ = 1 \), i.e., \( B_+ = T_- = \{0\} \);
  2. \( M_- = m_- = 1 \), i.e., \( B_- = T_+ = \{0\} \).

- Otherwise, \( \ker(U - 1) = \ker(U + 1) = \{0\} \) and hence \( M_+ = M_- = m_+ = m_- = 0 \), i.e., \( B_+ = B_- = T_+ = T_- = \{0\} \).

The above assertions can be checked directly. Indeed, \( \ker(\Gamma \mp 1) = \text{span}\{v_{\pm 1}(\gamma)\} \) and \( \ker(C \mp 1) = \text{span}\{v_{\pm 1}(c)\} \), where \( v_{\pm 1}(\theta) = \begin{pmatrix} \pm e^{i\theta} \\ 1 \end{pmatrix} \) and \( \langle v_j(\gamma), v_k(c) \rangle = 1 + jk e^{-i\beta} \) with \( j, k = \pm 1 \). For instance, in the case of \( j = -1, k = +1 \), this implies \( B_+ = \ker(\Gamma + 1) \cap \ker(C - 1) = \{0\} \) if \( \beta \in 2\pi \mathbb{Z} \).

Example 5.2 (Four dimensional case). Let \( \mathcal{H} = \mathbb{C}^4 \) and consider

\[
U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.
\]

The following table indicates \( m_\pm, M_\pm \), and \( I := \text{ind}_\Gamma(U) \) for several pairs \((\Gamma, C)\) of two unitary involutions such that \( U = \Gamma C \).
### 5.2 Grover’s search algorithm

Grover’s searching algorithm [14] consists of operators acting on the Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes n} \otimes \mathbb{C}^2$, where $(\mathbb{C}^2)^{\otimes n}$ describes $n$-qubit states and the oracle operator acts on $\mathbb{C}^2$. Let $N = 2^n$ and $V = \{0, 1, \cdots, N - 1\}$. We use $|x\rangle$ to denote $|j_0\rangle \otimes \cdots \otimes |j_{n-1}\rangle \in (\mathbb{C}^2)^{\otimes n}$ where $\{j_i\}_{i=0}^{n-1}$ is the standard basis of $\mathbb{C}^2$ and $j_i \in \{0, 1\}$ ($i = 0, \cdots, n - 1$) are the 2-adic digits, i.e., the 2-adic expansion of $x$ is given by $\sum_{i=0}^{n-1} j_i 2^i$. It is useful to identify $(\mathbb{C}^2)^{\otimes n}$ with the Hilbert space $\ell^2(V)$ of functions on $V$, in which case $|x\rangle$ is identified with a function $\delta_x$, i.e., $\delta_x(y) = 1$ if $y = x$ and $\delta_x(y) = 0$ otherwise. With this identification, we write $\mathcal{H} = \ell^2(V) \otimes \mathbb{C}^2$ and consider the ONB $\{|x\rangle \otimes |\ast\rangle \mid x \in V, \ast = \pm\}$ of $\mathcal{H}$, where we use $|\pm\rangle$ to denote vectors $(|0\rangle \pm |1\rangle)/\sqrt{2} \in \mathbb{C}^2$.

We now introduce two operators on $\mathcal{H}$ known as the oracle operator and the diffusion operator. For a fixed $x_0 \in V$, we set $|\chi_0\rangle = |x_0\rangle \otimes |\ast\rangle$. The oracle operator is defined as

$$C = 1 - 2|\chi_0\rangle\langle\chi_0|.$$ 

Let $|\phi_0\rangle = \sum_{x \in V} |x\rangle/\sqrt{N} \in \ell^2(V)$ and set $D_0 = 2|\phi_0\rangle\langle\phi_0| - 1$. The diffusion operator $\Gamma$ is defined as

$$\Gamma = D_0 \otimes 1.$$ 

Let $U = \Gamma C$. In Grover’s algorithm, after transforming the state $\Psi_0 = |\phi_0\rangle \otimes |\ast\rangle$ by $U^t$, we detect $x_0$ with a probability

$$p_t(x_0) = \|(|x\rangle \otimes 1)U^t \Psi_0\|^2_H.$$ 

| $\Gamma$ | $C$ | $M_+$ | $M_-$ | $m_+$ | $m_-$ | $I$ |
|-------|-----|----|----|----|----|----|
| $-1$  | $-U$ | 3  | 0  | 0  | 1  | -4 |
| $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ | 2  | 0  | 1  | 1  | -2 |
| $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ | 1  | 0  | 2  | 1  | 0  |
| $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$ | 1  | 1  | 2  | 0  | 2  |
| 1     | $U$  | 0  | 1  | 3  | 0  | 4  |
This is viewed as the probability of finding a quantum walker on $V$ at a position $x_0 \in V$. In this case, $U^t\Psi_0$ is the state of the walker at time $t$ when $\Psi_0$ is the initial state. From this viewpoint, $U = \Gamma C$ is the evolution operator of a SUSYQW, because $\Gamma$ and $C$ are unitary involutions, as is easily verified.

In what follows, we calculate the index of $U$.

**Theorem 5.1.** Let $U$ and $\Gamma$ be stated as above. Then

$$\text{ind}_\Gamma(U) = 4 - 2N. \quad (5.1)$$

Moreover

$$\sigma(U) = \{ e^{i \arccos(1-2/N)}, e^{-i \arccos(1-2/N)}, 1, -1 \}. \quad (5.2)$$

**Proof.** Form Corollary 3.7, it suffices to calculate the spectrum of $U' := -U = \Gamma C'$, where $C' = -C = 2|x_0\rangle\langle x_0| - 1$. To this end, we define an operator $d : \mathcal{H} \rightarrow \mathcal{K}$ as

$$d\psi = \langle x_0, \psi \rangle, \quad \psi \in \mathcal{H}.$$ 

Then the adjoint $d^* : \mathcal{K} \rightarrow \mathcal{H}$ is given by

$$d^* f = f|x_0\rangle, \quad f \in \mathcal{K}.$$ 

It is straightforward to see that $d$ is a coisometry, i.e., $dd^* = 1$ on $\mathcal{K}$. The discriminant operator is then calculated as follows.

$$T f = d\Gamma d^* f = \langle x_0, (D_0 \otimes 1) x_0 \rangle f$$

$$= (2|\langle x_0, \phi_0 \rangle|^2 - 1) f$$

$$= (2/N - 1)f.$$ 

Hence, $T = 2/N - 1 \neq 0$ and $\sigma(T) = \{2/N - 1\}$. In particular, because $\|T\| < 1$, Corollary 3.5 says that

$$\text{ind}_\Gamma(-U) = M_- - M_+ \quad (5.3)$$

with $M_{\pm} = \dim \ker(\Gamma \pm 1) \cap \ker d$ and $m_{\pm} = 0$.

To count $M_{\pm}$, we calculate the spectrum of $-U$. By Theorem 3.1

$$\sigma(-U) \setminus \{1, -1\} = \varphi^{-1}(2/N - 1) = \{ e^{i \arccos(2/N - 1)}, e^{-i \arccos(2/N - 1)} \}$$

and $\dim \ker(-U - e^{\pm i \arccos(2/N - 1)}) = 1$. Hence,

$$2N = \dim \mathcal{H} = M_+ + M_- + 2. \quad (5.4)$$

Observe that

$$B_- = \ker(\Gamma - 1) \cap \ker d = \text{Ran}(|\phi_0\rangle\langle \phi_0| \otimes 1) \cap \text{Ran}(1 - |\phi_0\rangle \otimes -),$$

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where
\[
\operatorname{Ran} \Gamma_+ = \text{span}\{|\phi_0\rangle \otimes |+\rangle, \ |\phi_0\rangle \otimes |-\rangle\}
\]
and
\[
\ker d = \text{span}\{|x_0\rangle \otimes |+\rangle\} \oplus \text{span}\{|x\rangle \otimes |\ast\rangle \mid \ast = \pm, \ x \neq x_0\}.
\]
Hence,
\[
\mathcal{B}_- = \text{span}\{|\phi_0\rangle \otimes |+\rangle\}
\]
and \( M_- = 1 \). Combining this with (5.3) and (5.4), we obtain \( M_+ = 2N - 3 \) and \( \operatorname{ind}_\Gamma(-U) = 1 - (2N - 3) = 4 - 2N \).
Therefore, Corollary 3.7 proves (5.1).

From the above argument, we observe that
\[
\sigma(U) = \sigma(-U) = \{-e^{i \arccos(2/N - 1)}, -e^{-i \arccos(2/N - 1)}, 1, -1\}.
\]
Because \( -e^{\pm i \arccos(2/N - 1)} = e^{\mp i \arccos(1 - 2/N)} \), we obtain (5.2). This completes the proof.

5.3 The Grover walk

Let \( G = (V, E) \) be a connected undirected graph (having multiple edges and self-loops) with \( V \) the set of vertices and \( E \) the set of edges. For the undirected graph \( G \), we introduce a set \( D \) of directed edges of \( G \) as follows. We first determine a direction for each edge \( e \in E \) and denote the origin by \( o(e) \) and the terminus by \( t(e) \), and next introduce the inverse edge of \( e \) by \( o(\bar{e}) = t(e) \) and \( t(\bar{e}) = o(e) \). We then define the set \( D \) as all such directed edges. By abuse of notation, denoting the set of directed edges determined first by the same symbol \( E \), we can write \( D = E \cup \bar{E} \), where \( \bar{E} = \{\bar{e} \mid e \in E\} \).
Following the definition in [17], we introduce the Grover walk on \( G \) as follows. Let \( \mathcal{H} = l^2(D) \) be the Hilbert space of square summable functions on \( D \). The shift operator \( S \) is defined as
\[
(S\psi)(e) = \psi(\bar{e}), \quad e \in D, \ \psi \in \mathcal{H}.
\]
Let
\[
\chi_v = \frac{1}{\deg v} \sum_{e \in D, o(e) = v} \delta_e,
\]
where \( \deg v = \# \{e \in D \mid o(e) = v\} \) and \( \delta_e \in \mathcal{H} \) is defined by \( \delta_e(f) = 1 \) \((f = e)\); \( \delta_e(f) = 0 \) otherwise. Then a coisometry \( d \) from \( \mathcal{H} \) to \( K := l^2(V) \) is defined as
\[
(d\psi)(v) = \langle \chi_v, \psi \rangle_{\mathcal{H}}, \quad v \in V, \ \psi \in \mathcal{H}.
\]
The coin operator $C$ is defined by
\[ C = 2d^*d - 1. \]
Because $S$ is a unitary involution, $U$ is written as
\[ U = \Gamma C, \]
where $\Gamma = S$ and $C$ are unitary involutions. Hence the Grover walk is a SUSYQW.

$M_\pm$ and $m_\pm$ have already been calculated in [17] for finite graphs and several crystal lattices. See also [15] [16] [18] for magnifier graphs, infinite trees, and the Sierpiński lattice. It is noteworthy that $M_\pm$ are determined by the number of cycles and geometric properties of the graph. In particular, if the total number of all cycles is infinity, then $M_+ = \infty$. From [17] Theorem 1 and Lemma 2) and Theorem 3.4 we observe that $\text{ind}_F(U) = 0$ for all finite graphs. For crystal lattices such as a triangular lattice, a square lattice, and a hexagonal lattice $(U, \Gamma)$ are not Fredholm pairs, because such graphs have infinitely many cycles.

Acknowledgments

This work was supported by JSPS KAKENHI Grant Number JP18K03327 and by the Research Institute for Mathematical Sciences, a Joint Usage/Research Center located in Kyoto University. The author thanks Y. Matsuzawa and Y. Tanaka for helpful comments on the index formula for finite-dimensional cases and for one dimensional split-step quantum walks.

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