A Note on the Spectral Mapping Theorem of Quantum Walk Models

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We discuss the description of eigenspace of a quantum walk model U with an associating linear operator T in abstract settings of quantum walk including the Szegedy walk on graphs. In particular, we provide the spectral mapping theorem of U without the spectral decomposition of T. Arguments in this direction reveal the eigenspaces of U characterized by the generalized kernels of linear operators given by T.

KEYWORDS: quantum walk model, spectral mapping theorem, generalized eigenspace

1. Introduction

Quantum walks are quantum analogues of classical random walks. Their primitive forms of the discrete-time quantum walks on \mathbb{Z} can be seen in Feynman's checker board [1]. It is mathematically shown (e.g. [4]) that this quantum walk has a completely different limiting behavior from classical random walks, which is a typical example showing a difficulty of intuitive description of quantum walks' behavior.

One of main aims of studies of quantum walks from the mathematical point of view is to understand their asymptotic behavior. There are two typical approaches for detecting asymptotic behavior of quantum walks:

- Calculation of density functions for long time limits of quantum walks;
- Description of the spectrum of quantum walks as unitary operators.

In [2], the spectral mapping theorem of the twisted Szegedy walk U is derived with spectral decomposition of the associated self-adjoint operator T. According to [2], the eigenstructure of T induces those of the operator of the form

$$\tilde{T} = \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix},$$

where I is the identity on an appropriate linear space, and eigenstructure of \tilde{T} determines an invariant subspace of U. As mentioned before, their arguments rely on the spectral decomposition and the eigenstructures of T.

In this paper, we propose a spectral analysis method of U without directly using the spectral decomposition of T. The motivation of this study is to overcome the difficulty concerning with spectral structure of T such as a quantum walk model discussed in [5]. As a first step in this direction, we try to apply our new method to the problems whose spectral structures have been well developed, that is, Szegedy walks [7, 10] and abstract quantum walks [6, 8, 9]. We obtain the following new observation of U by this method which has not discussed well before. Let

$$\operatorname{Spec}(A) = \left\{ \lambda \in \mathbb{C} \mid 0 \neq \exists \psi \in \bigcup_{n \in \mathbb{N}} \operatorname{ker}(\lambda I - A)^n \right\}$$
(1.1)

for a linear operator A on a Hilbert space. Here we treat Spec(A) as a multi-set. Then

• As for $\lambda \in \text{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\}$, we have $\ker(\lambda I - U|_{\mathcal{L}}) = L(\ker(\lambda I - \tilde{T}))$.

• As for $\lambda \in \text{Spec}(U|_{\mathcal{L}}) \cap \{\pm 1\}$, we have $\ker(\lambda I - U|_{\mathcal{L}}) = L(\ker(\lambda I - \tilde{T})^2 \setminus \ker(\lambda I - \tilde{T}))$.

Detailed descriptions of U, L and \mathcal{L} are shown in Sections 2 and 3. The new insight of our study is the presence of the generalized eigenspace of the linear operator \tilde{T} . We expect that such generalized eigenstructures reflect not only the geometric feature of underlying graphs such as their bipartiteness and underlying random walks such as their reversibility ([2]), but also performance of quantum search algorithms on graphs [7, 10]. We also expect that our result explicitly reveals such hidden structure and will lead to deeper study of spectra and asymptotic behavior of quantum walks from the viewpoint of functional analysis and geometry.

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Throughout our discussions, we consider an abstract *quantum walk model* given below, which extracts the essence of well-known Szegedy walks on graphs (e.g. [2]). Our study will cover spectral analysis for a general class of quantum walks (e.g. [5,7]).

Remark that there are preceding works of quantum walks in such an abstract setting: [8,9]. There quantum walks on *infinite dimensional* Hilbert spaces are considered. On the other hand, we restrict our considerations to finite dimensional spaces in this paper.

2. Abstract Quantum Walk Models

Throughout this paper, we study the spectrum of quantum walks in the following setting. Note that the following settings are finite dimensional analogue of [8,9].

- K_1 and K_2 : finite dimensional Hilbert spaces over \mathbb{C} with inner products $\langle \cdot, \cdot \rangle_{K_i}$.
- $S: K_2 \rightarrow K_2$: a self-adjoint, unitary operator.
- $d_A: K_2 \to K_1$: a bounded linear operator with the adjoint operator $d_A^*: K_1 \to K_2$.
- $d_B: K_2 \to K_1$: a bounded linear operator given by $d_B = d_A S$. The adjoint operator d_B^* is given by the similar way to d_A^* .
- $T: K_1 \to K_1$: a bounded linear operator given by $T = d_A d_B^*$, which is called *the discriminant operator*.

Note that the linear operator T is actually self-adjoint since $S: K_2 \to K_2$ is self-adjoint and unitary.

Now we assume the following property, which is crucial to our setting.

Assumption 2.1. $d_A d_A^* = I : K_1 \to K_1$.

Lemma 2.2. Under Assumption 2.1, the linear operator $C := 2d_A^*d_A - I : K_2 \to K_2$ is a self-adjoint and unitary operator.

Proof. It easily follows that $d_A^* d_A$ is self-adjoint in K_2 , and so is C. It is thus sufficient to prove that $C^{\dagger}C = C^2 = I : K_2 \to K_2$. We immediately have

$$C^{2} = (2d_{A}^{*}d_{A} - I)^{2} = 4d_{A}^{*}d_{A}d_{A}^{*}d_{A} - 4d_{A}^{*}d_{A} + I = 4d_{A}^{*}d_{A} - 4d_{A}^{*}d_{A} + I = I,$$

which shows the statement. Note that we have used Assumption 2.1 in the above calculation.

Our quantum walk model is given by the following definition.

Definition 2.3 (Quantum walk model). Let *C* be the unitary operator given in Lemma 2.2. Then the operator $U = SC : K_2 \rightarrow K_2$ is also a unitary operator. We shall say the operator *U* a quantum walk model on K_2 associated with the pair (K_1, d_A) of an auxiliary Hilbert space K_1 and the linear operator d_A acting on it.

Note that the discriminant operator T, which is the center of our considerations, and the operator d_B are naturally defined by d_A and S.

Now we have defined the unitary operator U as a quantum walk, while U may not be seen as a "quantum walk" at a glance. The following example shows that this abstract model U includes the well-known quantum walks such as *Grover walk* and *Szegedy walk*.

Example 2.4 (Szegedy walk on a graph). Let G = (V(G), E(G)) be a simple and finite graph, where V(G) is the set of vertices in *G* and E(G) is the set of (undirected) edges in *G*. It can be regarded as the digraph G = (V(G), D(G)), where $D(G) = \{e, \overline{e} \mid e \in E(G)\}$ and $\overline{e} = (v, u)$ for each $e = (u, v), u, v \in V(G)$. For each edge $e = (u, v) \in D(G), o(e) = u$ denotes the origin of *e* and t(e) = v denotes the terminus of *e*.

Now define a \mathbb{C} -linear space $\ell^2(D(G))$ by

$$\ell^{2}(D(G)) := \{ f : D(G) \to \mathbb{C} \mid ||f||_{D(G)} < \infty \}.$$

Here the inner product is given by the standard inner product, that is,

$$\langle f,g\rangle_{D(G)} := \sum_{e \in D(G)} \overline{f(e)}g(e),$$

where $\overline{f(e)}$ denotes the complex conjugate of f(e). Let $\|\cdot\|_{D(G)}$ be the associated norm, namely, $\|f\|_{D(G)} := \langle f, f \rangle_{D(G)}^{1/2}$. We take

$$\delta_e^{(1)}(e') := \begin{cases} 1 & \text{if } e' = e \\ 0 & \text{if } e' \neq e \end{cases}$$

as the standard basis of $\ell^2(D(G))$. One knows that the \mathbb{C} -linear space $\ell^2(D(G))$ associated with the inner product $\langle \cdot, \cdot \rangle_{D(G)}$ is a Hilbert space. We can also define the Hilbert space $\ell^2(V(G))$ in the similar manner.

Next, call a function $w: D(G) \to \mathbb{C}$ a weight if $w(e) \neq 0$ for all $e \in D(G)$ and

$$\sum_{v:o(e)=u} |w(e)|^2 = 1 \quad \text{for all } u \in V(G).$$

Let $S: \ell^2(D(G)) \to \ell^2(D(G))$ be defined by $Sf(e) = f(\overline{e})$, called the shift operator. Under such settings, define $d_A, d_B: \ell^2(D(G)) \to \ell^2(V(G))$ as

$$(d_A\phi)(v) = \sum_{e:o(e)=v} \overline{w(e)}\phi(e), \quad (d_B\phi)(v) = \sum_{e:o(e)=v} \overline{w(e)}\phi(\bar{e}),$$

respectively. It immediately follows that $d_B = d_A S$. Their adjoints $d_A^*, d_B^* : \ell^2(V(G)) \to \ell^2(D(G))$ are defined by

 $(d_A^*\psi)(e) = w(e)\psi(o(e)), \quad (d_B^*\psi)(e) = w(\bar{e})\psi(t(e)),$

from the relationship $\langle \phi, d_J^* \psi \rangle_{D(G)} = \langle d_J \phi, \psi \rangle_{V(G)}$ $(J \in \{A, B\})$ for all $\psi \in \ell^2(V(G))$ and $\phi \in \ell^2(D(G))$. Then, from the property of the weight *w*, we can prove that $d_A d_A^* = d_B d_B^* = I : \ell^2(V(G)) \rightarrow \ell^2(V(G))$ (cf. [2]). In particular, the Szegedy walk $U = SC = S(2d_A^*d_A - I)$ in this setting is contained in our current setting. We often call unitary operators *S* the shift operator and *C* the quantum coin operator. The discriminant operator $T = d_A d_B^*$ is also defined in the natural way.

If we further assume that $w(e) = 1/\sqrt{\deg(o(e))}$ for all $e \in E(G)$, the resulting quantum walk model U is nothing but the Grover walk on G.

3. Spectral Analysis of Abstract Quantum Walk Models

3.1 Invariant Subspaces of U

Now we consider Spec(*U*), the spectrum of *U* in the sense of (1.1). As can be seen in preceding works such as [2], Spec(*U*) consists of eigenvalues inherited from those of a self-adjoint operator $T : K_1 \to K_1$ via the spectral mapping property and specific ones to *U*.

Remark 3.1. Since U is a normal operator, we do not usually need to consider the spectrum in the sense of (1.1). However, in the consideration of the *eigensystem* of U, we need the notion of generalized eigenspaces. This is the reason why we introduce (1.1).

To characterize the spectral mapping property of Spec(U), we consider the following operators. Let $L : K_1^2 \to K_2$ by $L(f,g)^T = d_A^* f + d_B^* g$, where $d_B^* = Sd_A^*$. Note that L is a linear map. Indeed, for any $\alpha_i \in \mathbb{C}$ and $\psi_i = (f_i, g_i)^T \in K_1^2$, i = 1, 2, we have

$$L(\alpha_1\psi_1 + \alpha_2\psi_2) = L(\alpha_1f_1 + \alpha_2f_2, \alpha_1g_1 + \alpha_2g_2)^T$$

= $d_A^*(\alpha_1f_1 + \alpha_2f_2) + d_B^*(\alpha_1g_1 + \alpha_2g_2)$
= $\sum_{i=1}^2 \alpha_i(d_A^*f_i + d_B^*g_i) = \sum_{i=1}^2 \alpha_i L\psi_i.$

Also, let $\tilde{T}: K_1^2 \to K_1^2$ by

$$\tilde{T} = \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix}.$$
(3.1)

Lemma 3.2.

$$UL = L\tilde{T} : K_1^2 \to K_2. \tag{3.2}$$

Proof. Let $\psi = (f, g)^T \in K_1^2$. Direct calculations yield

$$UL\psi = U(d_A^*f + d_B^*g) = S(2d_A^*d_A - I)(d_A^*f + d_B^*g)$$

= $S\{d_A^*f + (2d_A^*T - d_B^*)g\} = d_B^*f + (2d_B^*T - d_A^*)g$

On the other hand,

$$L\tilde{T}\psi = L \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}$$
$$= L \begin{pmatrix} -g \\ f + 2Tg \end{pmatrix} = -d_A^*g + d_B^*(f + 2Tg)$$

and the proof is completed.

Let $\mathcal{L} := \text{Im } L = d_A^* K_1 + d_B^* K_1 \subset K_2$, which is the center of our considerations in this paper. First we have the following statement.

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Lemma 3.3. The mapping \tilde{T} is a bijective map on K_1^2 .

Proof. It immediately follows that

$$\begin{pmatrix} 2T & I \\ -I & 0 \end{pmatrix} \tilde{T} = \tilde{T} \begin{pmatrix} 2T & I \\ -I & 0 \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix},$$

which implies that \tilde{T} is bijective.

Using this fact, we obtain the following.

Lemma 3.4.
$$U(\mathcal{L}) = \mathcal{L}$$
.

Proof. For any $\phi \in \mathcal{L}$, there is an element $\psi \in K_1^2$ such that $\phi = L\psi$. Combining the statement of Lemma 3.2, we have $U\phi = UL\psi = L(\tilde{T}\psi) \in \mathcal{L}$,

which yields $U(\mathcal{L}) \subset \mathcal{L}$.

Conversely, for any $\psi \in K_1^2$, there is a unique element $\tilde{\psi} \in K_1^2$ such that $\tilde{T}\tilde{\psi} = \psi$, which follows from Lemma 3.3; namely, \tilde{T} is a bijection from K_1^2 onto itself. Therefore, for any $\psi \in K_1^2$, we have

$$\psi = L \tilde{T} \tilde{\psi} = U L \tilde{\psi} \in U(\mathcal{L}),$$

which yields $\mathcal{L} \subset U(\mathcal{L})$ and the proof is completed.

Definition 3.5. We say the invariant subspace \mathcal{L} the inherited eigenspace of U. The orthogonal complement \mathcal{L}^{\perp} of \mathcal{L} in K is said the birth eigenspace of U.

Easy calculations yield that the subspace \mathcal{L}^{\perp} is characterized by

$$\mathcal{L}^{\perp} = \ker(d_A) \cap \ker(d_B). \tag{3.3}$$

In [2], Spec(U) is studied after decomposing it into two components: $\text{Spec}(U|_{\mathcal{L}})$ and $\text{Spec}(U|_{\mathcal{L}^{\perp}})$. Note that this decomposition makes sense due to Lemma 3.4.

Here we consider the eigenvalue problem on the inherited eigenspace \mathcal{L} :

$$U|_{\mathcal{L}}\phi = \lambda\phi, \quad \phi \in \mathcal{L}. \tag{3.4}$$

By Lemmas 3.2 and 3.4, Eq. (3.4) is equivalent to the following problem: Find $\psi \notin \text{ker}(L)$ and $\lambda \in \mathbb{C}$ such that

$$L(\lambda I - \tilde{T})\psi = 0. \tag{3.5}$$

By Eq. (3.5), there are two possibilities:

(C1)' $\psi \in \ker(\lambda I - \tilde{T})$ and $\psi \notin \ker(L)$.

(C2)' $\psi \notin \ker(\lambda I - \tilde{T}), \psi \in \ker(L(\lambda I - \tilde{T})) \text{ and } \psi \notin \ker(L).$

Now a natural question arises: What role does ker L play in Spec(U)? The following three lemmas answer this question and clarify our focus.

First we have the following.

Lemma 3.6. Let L and \tilde{T} be as above. Then

$$\ker(L) = \ker(I - \tilde{T}^2). \tag{3.6}$$

Proof. First assume that $\psi = (f,g)^T \in \ker L \subset K_1^2$. This implies $d_A^*f + d_B^*g = 0$. Acting the operator d_A on both sides, we have f + Tg = 0. Similarly, acting the operator d_B on both sides, we also have Tf + g = 0. These observations imply

$$f \in \ker(I - T^2), g \in \ker(I - T^2)$$
 with $f = -Tg$.

On the other hand,

$$\tilde{T}^2 = \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix} \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix} = \begin{pmatrix} -I & -2T \\ 2T & 4T^2 - I \end{pmatrix}.$$

Thus

$$(I - \tilde{T}^{2}) \binom{f}{g} = \binom{2I \quad 2T}{-2T \quad -4T^{2} + 2I} \binom{f}{g} = \binom{2f + 2Tg}{-2Tf - 4T^{2}g + 2g} = \binom{0}{0},$$
(3.7)

which implies $\ker(L) \subset \ker(1 - \tilde{T}^2)$.

Conversely, assume $\psi = (f,g)^T \in \ker(I - \tilde{T}^2)$. Then (3.7) (in this case, it is a consequence of the assumption $\psi \in \ker(I - \tilde{T}^2)$) yields f + Tg = 0 and g + Tf = 0, which means $g \in \ker(I - T^2)$. Since $d_A d_A^* = I$ and $d_B d_B^* = I$, these two equations also imply

$$d_A(d_A^*f + d_B^*g) = 0$$
 and $d_B(d_A^*f + d_B^*g) = 0.$

Thus $d_A^* f + d_B^* g \in \ker d_A \cap \ker d_B = \mathcal{L}^{\perp}$ and hence $d_A^* f + d_B^* g \in \mathcal{L} \cap \mathcal{L}^{\perp} = \{0\}$. Finally we have $d_A^* f + d_B^* g = 0$ and hence $\ker(I - \tilde{T}^2) \subset \ker L$.

Lemma 3.6 indicates that Eq. (3.5) is equivalent to

$$(I - \tilde{T}^2)(\lambda I - \tilde{T})\psi = 0 \quad \text{and} \quad \psi \notin \ker(I - \tilde{T}^2).$$
 (3.8)

Consequently, the case (C2)' is equivalent to the following:

(C2)" $\psi \notin \ker(\lambda I - \tilde{T}), \psi \notin \ker(I - \tilde{T}^2) \text{ and } (I - \tilde{T}^2)(\lambda I - \tilde{T})\psi = 0.$

We thus have translated the structure of ker L into the corresponding nullspace of \tilde{T} . Thanks to this fact, we can provide the following lemmas.

Lemma 3.7. Let \tilde{T} , U and \mathcal{L} be as above. Then we have

$$\operatorname{Spec}(\tilde{T}) \supset \operatorname{Spec}(U|_{\mathscr{L}}).$$
 (3.9)

Proof. Let $\lambda \in \text{Spec}(U|_{\mathcal{L}})$ and $\phi \in \mathcal{L}$ be a nonzero vector satisfying $U\phi = \lambda\phi$. Since $\mathcal{L} = \text{Im } L$, we have $\phi = L\psi$ with some $\psi \in K_1^2$. Since

$$L\tilde{T}\psi = UL\psi = U\phi = \lambda\phi = \lambda L\psi$$

by Lemma 3.2, $L(\lambda I - \tilde{T})\psi = 0$. Using Lemma 3.6 and the fact that $I - \tilde{T}^2$ and $\lambda I - \tilde{T}$ commute each other, we obtain

$$(\lambda I - \tilde{T})(I - \tilde{T}^2)\psi = (I - \tilde{T}^2)(\lambda I - \tilde{T})\psi = 0.$$

Let us assume that $\lambda \notin \text{Spec}(\tilde{T})$. Since $\lambda I - \tilde{T}$ is injective, it holds that $(I - \tilde{T}^2)\psi = 0$, and thus $L\psi = 0$ by Lemma 3.6, which contradicts to $L\psi = \phi \neq 0$. Consequently, we obtain $\lambda \in \text{Spec}(\tilde{T})$.

The spectra of \tilde{T} and $U|_{\mathcal{L}}$ coincide except ± 1 , as shown in the following lemma.

Lemma 3.8. Let \tilde{T} , U and \mathcal{L} be as above. Then we have

$$\operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\} = \operatorname{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\}.$$

Proof. By Lemma 3.7, $\operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\} \supset \operatorname{Spec}(U|_{\ell}) \setminus \{\pm 1\}$. Now we show the converse: $\operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\} \subset \operatorname{Spec}(U|_{\ell}) \setminus \{\pm 1\}$. If $(\lambda I - \tilde{T})\psi = 0$ for $\lambda \neq \pm 1$, then we have $(I - \tilde{T}^2)\psi \neq 0$, which implies the case (C1)' holds, thus $\lambda \in \operatorname{Spec}(U|_{\ell})$.

We have seen that, from Lemma 3.6, (3.5) is equivalent to (3.8). Using this fact and Lemma 3.8, we have the following equivalences.

Proposition 3.9. (C1)' is equivalent to (C1) $\lambda \in \operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\}$ and (3.8). Similarly, (C2)', namely (C2)'', is equivalent to (C2) $\lambda \in \operatorname{Spec}(\tilde{T}) \cap \{\pm 1\}$ and (3.8).

Proof. It is sufficient to show the equivalence between (C1) and (C1)'.

Since the proof of Lemma 3.8 indicates that (C1) implies (C1)', we will show that (C1)' implies (C1). If not, $\lambda \in \{\pm 1\}$ may also satisfy (C1)'. For example, assume that $\lambda = 1$ satisfies (C1)'. We then have

$$\psi \in \ker(I - \tilde{T}) \subset \ker(I + \tilde{T})(I - \tilde{T}) = \ker(I - \tilde{T}^{2}),$$

which contradicts (3.8). Similar arguments holds for $\lambda = -1$. We thus obtain (C1)' is equivalent to (C1) and complete the proof.

Proposition 3.9 guarantees that the study of $\text{Spec}(U|_{\mathcal{L}})$ is reduced to individual cases (C1) and (C2).

3.2 The Case (C1)

The problem in the setting of case (C1) is reduced to the one that we find $\lambda \in \mathbb{C}$ with $\lambda \neq \pm 1$ and $\psi \neq 0$ such that $(\lambda I - \tilde{T})\psi = 0$. We then have

$$(\lambda I - \tilde{T})\psi = 0 \Leftrightarrow \begin{pmatrix} \lambda I & I \\ -I & \lambda I - 2T \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Leftrightarrow \lambda f + g = 0 \text{ and } - f + (\lambda I - 2T)g = 0$$

$$\Leftrightarrow g \in \ker(\lambda^2 I - 2\lambda T + I) \text{ and } \lambda f + g = 0.$$

Since \tilde{T} is invertible from Lemma 3.3, $0 \notin \operatorname{Spec}(\tilde{T})$ holds, which means $\lambda \neq 0$. The above statement is thus equivalent to

$$g \in \ker\left(\left(\frac{\lambda+\lambda^{-1}}{2}\right)I - T\right)$$
 and $f = -\lambda^{-1}g$.

Therefore we have

$$\ker(\lambda I - \tilde{T}) = \begin{pmatrix} 1 \\ -\lambda \end{pmatrix} \otimes \ker\left(\left(\frac{\lambda + \lambda^{-1}}{2}\right)I - T\right).$$

Putting $\mu = (\lambda + \lambda^{-1})/2$, we have

$$\ker(e^{\pm i \arccos \mu} I - \tilde{T}) = \begin{pmatrix} 1 \\ -e^{\pm i \arccos \mu} \end{pmatrix} \otimes \ker(\mu I - T)$$

Remarking $e^{\pm i \operatorname{arccos} \mu} = \pm 1$ if and only if $\mu = \pm 1$, we have the following lemma, which describes eigenpairs of U associated with $\lambda \neq \pm 1$.

Lemma 3.10. The eigenpair of U associated with $\lambda \in \text{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\}$ is characterized by the following.

$$\operatorname{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\} = \{e^{\pm i \operatorname{arccos} \mu} | \mu \in \operatorname{Spec}(T) \setminus \{\pm 1\}\},\$$
$$\operatorname{ker}(e^{\pm i \operatorname{arccos} \mu} I - U|_{\mathcal{L}}) = (d_A^* - e^{\pm i \operatorname{arccos} \mu} d_B^*) \operatorname{ker}(\mu I - T).$$

3.3 The Case (C2)

Our main aim here is the complete description of $\text{Spec}(U|_{\mathcal{L}})$ in the case (C2). The key point is the structure of the eigenspaces ker $(I \pm \tilde{T})$ as well as the *generalized eigenspaces* ker $(I \pm \tilde{T})^n$, $n \ge 2$. To this end, we provide the following lemma.

Lemma 3.11. For each $n \ge 1$, we have

$$(I - \tilde{T})^{2n} = 2^n (-\tilde{T})^n \begin{pmatrix} (I - T)^n & 0\\ 0 & (I - T)^n \end{pmatrix},$$
(3.10)

$$(I+\tilde{T})^{2n} = 2^n \tilde{T}^n \begin{pmatrix} (I+T)^n & 0\\ 0 & (I+T)^n \end{pmatrix}.$$
(3.11)

Proof. First consider $(I - \tilde{T})^{2n}$. The case n = 0 is trivial. We have

$$(I - \tilde{T})^2 = \begin{pmatrix} I & I \\ -I & I - 2T \end{pmatrix} \begin{pmatrix} I & I \\ -I & I - 2T \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 2(I - T) \\ -2(I - T) & -4T(I - T) \end{pmatrix} = 2 \begin{pmatrix} 0 & I \\ -I & -2T \end{pmatrix} \begin{pmatrix} I - T & 0 \\ 0 & I - T \end{pmatrix},$$

which means (3.10) for n = 1. Notice that

$$\begin{pmatrix} I-T & 0\\ 0 & I-T \end{pmatrix} \begin{pmatrix} 0 & I\\ -I & -2T \end{pmatrix} = \begin{pmatrix} 0 & I\\ -I & -2T \end{pmatrix} \begin{pmatrix} I-T & 0\\ 0 & I-T \end{pmatrix}.$$
(3.12)

Assume that (3.10) holds for some $n = n_0 \ge 1$. Then

$$(I - \tilde{T})^{2(n_0+1)} = 2^{n_0} (-\tilde{T})^{n_0} \begin{pmatrix} (I - T)^{n_0} & 0 \\ 0 & (I - T)^{n_0} \end{pmatrix} \begin{pmatrix} 0 & 2(I - T) \\ -2(I - T) & -4T(I - T) \end{pmatrix}$$
$$= 2^{n_0+1} (-\tilde{T})^{n_0} \begin{pmatrix} (I - T)^{n_0} & 0 \\ 0 & (I - T)^{n_0} \end{pmatrix} (-\tilde{T}) \begin{pmatrix} I - T & 0 \\ 0 & I - T \end{pmatrix}$$
$$= 2^{n_0+1} (-\tilde{T})^{n_0+1} \begin{pmatrix} (I - T)^{n_0+1} & 0 \\ 0 & (I - T)^{n_0+1} \end{pmatrix}$$

by (3.12), which proves (3.10) for $n = n_0 + 1$. By induction, (3.10) holds for all $n \ge 0$.

Next consider $(I + \tilde{T})^{2n}$. The case n = 0 is trivial. We have

$$(I + \tilde{T})^{2} = \begin{pmatrix} I & -I \\ I & I + 2T \end{pmatrix} \begin{pmatrix} I & -I \\ I & I + 2T \end{pmatrix}$$
$$= \begin{pmatrix} 0 & -2(I+T) \\ 2(I+T) & 4T(I+T) \end{pmatrix} = 2 \begin{pmatrix} 0 & -I \\ I & 2T \end{pmatrix} \begin{pmatrix} I+T & 0 \\ 0 & I+T \end{pmatrix},$$

which means (3.11) for n = 1. By the same arguments as the proof of (3.10) we obtain (3.11).

With the help of Lemma 3.11, we can prove the following, which gives us the description of eigenspaces of \tilde{T} associated with eigenvalues $\lambda = \pm 1$.

Proposition 3.12.

$$\ker(I - \tilde{T}) = \begin{pmatrix} 1\\ -1 \end{pmatrix} \otimes \ker(I - T), \tag{3.13}$$

$$\ker(I - \tilde{T})^n = \mathbb{C}^2 \otimes \ker(I - T) \ (n \ge 2), \tag{3.14}$$

$$\ker(I + \tilde{T}) = \begin{pmatrix} 1\\1 \end{pmatrix} \otimes \ker(I + T), \tag{3.15}$$

$$\ker(I+\tilde{T})^n = \mathbb{C}^2 \otimes \ker(I+T) \ (n \ge 2). \tag{3.16}$$

Proof. We only prove (3.13) and (3.14). Remaining statements (3.15) and (3.16) can be proved by the same arguments. First we have

$$I - \tilde{T} = \begin{pmatrix} I & I \\ -I & I - 2T \end{pmatrix}, \quad (I - \tilde{T})^2 = \begin{pmatrix} 0 & 2(I - T) \\ -2(I - T) & -4T(I - T) \end{pmatrix}.$$
(3.17)

For $\psi = (f, g)^T \in \ker(I - \tilde{T})$, we have

$$\begin{pmatrix} I & I \\ -I & I - 2T \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} f + g \\ -f + (I - 2T)g \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

which yields f = -g and Tf = f, and hence $\ker(I - \tilde{T}) \subset \{(f, -f)^T : f \in \ker(I - T)\}$. The converse is trivial and (3.13) holds true.

Secondly, consider $(I - \tilde{T})^2 \psi = 0$. (3.17) immediately yields

$$(I - \tilde{T})^2 \psi = \begin{pmatrix} 0 & 2(I - T) \\ -2(I - T) & -4T(I - T) \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Leftrightarrow \quad f \in \ker(I - T), \quad g \in \ker(I - T).$$

Next consider $(I - \tilde{T})^4 \psi = 0$. By Lemma 3.11 with n = 2, we have

$$(I - \tilde{T})^4 \psi = 2^2 (-\tilde{T})^2 \begin{pmatrix} (I - T)^2 & 0\\ 0 & (I - T)^2 \end{pmatrix} \begin{pmatrix} f\\ g \end{pmatrix} = \begin{pmatrix} 0\\ 0 \end{pmatrix}$$

Since the operator $-\tilde{T}$ is invertible by Lemma 3.3, the above equation implies $f \in \ker(I-T)^2$ and $g \in \ker(I-T)^2$.

Here note that ker $(I - T)^2 = \text{ker}(I - T)$, since T is Hermitian and hence diagonalizable and it implies ker $(I - T)^2 =$ $\ker(I-T)$. Thus we observe that $f \in \ker(I-T)$ and $g \in \ker(I-T)$. In particular, $\ker(I-\tilde{T})^4 = \ker(I-\tilde{T})^2$ holds. The similar arguments hold for all *n* by Lemma 3.11 and the invertibility of $-\tilde{T}$.

In general, $\ker(I - \tilde{T})^n \subset \ker(I - \tilde{T})^{n+1}$ holds for all *n*, which is a fundamental property from linear algebra. Combining the fact $\ker(I - \tilde{T})^4 = \ker(I - \tilde{T})^2$, we have $\ker(I - \tilde{T})^2 \subset \ker(I - \tilde{T})^3 \subset \ker(I - \tilde{T})^4 = \ker(I - \tilde{T})^2$. Finally we have $\ker(I - \tilde{T})^n = \ker(I - \tilde{T})^2$ for all $n \ge 2$ by recursive arguments and the proof is completed.

Remark 3.13. In the proof of Proposition 3.12, the operator T being self-adjoint is used to guarantee $ker(I - T)^2 = ker(I - T)$. Our arguments here also hold even for diagonalizable matrices which are not necessarily self-adjoint.

The following proposition characterizes the eigenvalues ± 1 of $U|_{\mathcal{L}}$.

Proposition 3.14. For $\psi = (f, g)^T \in K_1^2$, the following four statements are equivalent.

(i) $UL\psi = \pm L\psi \neq 0.$

- (ii) $\psi \in Z_{\pm} \setminus \ker(L)$, where $Z_{\pm} = \ker(I \mp \tilde{T})^2 (I \pm \tilde{T})$.
- (iii) $\psi = \psi_1 + \psi_2$, such that $\psi_1 \in X_{\pm} \equiv \ker(I \mp \tilde{T})^2 \setminus \ker(I \mp \tilde{T})$ and that $\psi_2 \in \ker(L)$.
- (iv) $f = f_1 + f_2$ and $g = g_1 + g_2$, such that $f_1, g_1 \in \ker(I \mp T)$ with $f_1 \pm g_1 \neq 0$ and that $(f_2, g_2)^T \in \ker(L)$.

Proof. We first claim that $X_{\pm} \subset Z_{\pm}$ by Lemma 3.6 and that $\ker(L) \subset Z_{\pm}$. In what follows, we consider $\lambda =$ $+1 \in \text{Spec}(U|_{\mathcal{L}})$ with $Z = Z_+$ and $X = X_+$. The similar arguments to below yield the corresponding equivalence for the eigenvalue $\lambda = -1$.

Notice that since $I - \tilde{T}^2 = (I + \tilde{T})(I - \tilde{T})$, if $\tilde{T}\psi = \pm \psi \neq 0$, then $L\psi = 0$ by Lemma 3.6, and thus $L\psi$ is not an eigenfunction of $U|_{\mathcal{F}}$.

Since $+1 \in \text{Spec}(U|_{\mathcal{L}})$ if and only if there exists $\phi \in \mathcal{L}$ such that $U\phi = \phi \neq 0$, we can see that $1 \in \text{Spec}(U|_{\mathcal{L}})$ is equivalent to that there exists $\psi \in K_1^2$ such that

$$L\psi \neq 0$$
 and $L(I - \tilde{T})\psi = 0$,

which is also equivalent to

$$L\psi \neq 0$$
 and $(I + \tilde{T})(I - \tilde{T})^2\psi = 0$

by Lemma 3.6. This is also equivalent to

 $\psi \notin \ker(L)$ and $\psi \in Z$.

Thus we obtain that (i) and (ii) are equivalent to each other.

Now we assume $\psi \in Z \setminus \ker(L)$. Then there are two vectors $\psi_1 \in \ker(I - \tilde{T})^2$ and $\psi_2 \in \ker(I + \tilde{T})$ such that $\psi = \psi_1 + \psi_2 \notin \ker(L)$. Now it holds that $\psi_2 \in \ker(I + \tilde{T}) \subset \ker(L)$. If ψ_1 belongs to $\ker(I - \tilde{T})$, then $\psi_1 \in \ker(L)$ also holds and hence $\psi = \psi_1 + \psi_2 \in \ker(L)$, which is contradiction. Therefore $\psi_1 \in \ker(I - \tilde{T})^2 \setminus \ker(I - \tilde{T}) = X$. This shows "(ii) \Rightarrow (iii)".

Conversely, we assume (iii); namely, $\psi = \psi_1 + \psi_2$ with $0 \neq \psi_1 \in X \subset Z$ and $\psi_2 \in \ker(L) \subset Z$. Then we have $\psi \in Z$. Note that *Z* is a vector space. Let us prove $\psi \notin \ker(L)$. Since $\psi_2 \in \ker(L)$, it is sufficient to prove that $\psi_1 \notin \ker(L)$. Suppose the converse; namely, $\psi_1 \in \ker(L) = \ker(I - \tilde{T})(I + \tilde{T})$. Since $\psi_1 \in X \subset \ker(I - \tilde{T})^2$, we obtain that $(I - \tilde{T})\psi_1 \in \ker(I + \tilde{T}) \cap \ker(I - \tilde{T}) = \{0\}$. Therefore, we have $(I - \tilde{T})\psi_1 = 0$, which contradicts the assumption $0 \neq \psi_1 \in X$. We thus obtain $\psi_1 \notin \ker(L)$ and $\psi \in Z \setminus \ker(L)$.

Consequently, (ii) and (iii) are equivalent.

Next assume $\psi = \psi_1 + \psi_2$ with $0 \neq \psi_1 \in X$ and $\psi_2 \in \ker(L)$. Write $\psi_i = (f_i, g_i)^T \in K_1^2$ for i = 1, 2. By (3.13) and (3.14) in Proposition 3.12, $\psi_1 = (f_1, g_1)^T$ with $f_1 + g_1 \neq 0$ and $f_1, g_1 \in \ker(I - T)$ hold true. This implies "(iii) \Rightarrow (iv)". The converse also follows from Proposition 3.12.

This proposition indicates that the eigenfunctions of $U|_{\mathcal{L}}$ associated with the eigenvalues $\lambda = \pm 1$ are characterized by purely generalized kernels $X_{\mp} = \ker(I \mp \tilde{T})^2 \setminus \ker(I \mp \tilde{T})$ up to $\ker(L)$.

3.4 The Final Result

Summarizing the above arguments, we have the following spectral mapping theorem of U.

Theorem 3.15 (Spectral Mapping Theorem of U). Let $\varphi_{OW}(x) = (x + x^{-1})/2$ be the Joukowsky transform. Then

$$\ker(\lambda I - U|_{\mathcal{L}}) = \begin{cases} L(\ker(\lambda I - \tilde{T})) & \text{if } \lambda \notin \{\pm 1\}, \\ \{L\psi \mid \psi = (f,g)^{T}, f,g \in \ker(I-T), f+g \neq 0\} \\ = L(\ker(I - \tilde{T})^{2} \setminus \ker(I - \tilde{T})) & \text{if } \lambda = 1, \\ \{L\psi \mid \psi = (f,g)^{T}, f,g \in \ker(I+T), f-g \neq 0\} \\ = L(\ker(I + \tilde{T})^{2} \setminus \ker(I + \tilde{T})) & \text{if } \lambda = -1. \end{cases}$$
(3.18)

In particular, we have

$$\operatorname{Spec}(U|_{\mathcal{L}}) = \operatorname{Spec}(\tilde{T}) = \varphi_{OW}^{-1}(\operatorname{Spec}(T)).$$
(3.19)

For $\lambda \in \text{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\}$, the eigenspace $L(\text{ker}(\lambda I - \tilde{T}))$ is given by

$$d_A^* f_{\varphi_{OW}(\lambda)} - \lambda d_B^* f_{\varphi_{OW}(\lambda)} \mid f_{\varphi_{OW}(\lambda)} \in \ker(\varphi_{QW}(\lambda)I - T)\}.$$

The spectrum of $U|_{\ell^{\perp}}$ has the following relationship : $\operatorname{Spec}(U|_{\ell^{\perp}}) = \operatorname{Spec}(-S)$. Moreover, we have

$$\ker(\lambda I - U|_{\mathcal{L}^{\perp}}) = \begin{cases} 0 & \text{if } \lambda \neq \pm 1, \\ \ker(d_A) \cap \ker(I + S) & \text{if } \lambda = 1, \\ \ker(d_A) \cap \ker(I - S) & \text{if } \lambda = -1. \end{cases}$$
(3.20)

Proof. Eigenstructures of $U|_{\mathcal{L}}$ with $\lambda = \pm 1$ directly follow from Proposition 3.14. Note that $\varphi_{QW}(\pm 1) = \pm 1$, which yield $\ker(\varphi_{QW}(\pm 1)I - T) = \ker(I \mp T)$. For $\lambda \neq \pm 1$, Lemma 3.8 says $\operatorname{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\} = \operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\}$. The spectral mapping property $\operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\} = \varphi_{QW}^{-1}(\operatorname{Spec}(\tilde{T}) \setminus \{\pm 1\}) = \varphi_{QW}^{-1}(\operatorname{Spec}(\tilde{T})) \setminus \{\pm 1\}$ is the consequence of Lemma 3.10.

Let $\phi \in \mathcal{L}^{\perp}$ be an eigenfunction of U. Then $U\phi = S(2d_A^*d_A - I)\psi = -S\phi$ and hence ϕ is an eigenfunction of -S. Note that $\text{Spec}(S) = \{\pm 1\}$, since S is an involution, namely, self-adjoint and unitary. In such a case, we also have $d_B\phi = d_AS\phi = \mp d_A\phi = 0$. Thus the statement $\phi \in \mathcal{L}^{\perp} \cap \ker(I \pm S)$ is consequently equivalent to $\phi \in \ker(d_A) \cap \ker(I \pm S)$. Combination of these results yields our statement.

Before stating the corollary of Theorem 3.15, we provide the following lemma.

Lemma 3.16. For $f \in K_1$, $f \in \text{ker}(I \mp T)$ holds if and only if $d_A^* f = \pm d_B^* f$.

Proof. We immediately have

$$f \in \ker(I - T) \Leftrightarrow d_B d_A^* f = f \Leftrightarrow d_B (d_A^* f - d_B^* f) = d_A (d_A^* f - d_B^* f) = 0$$

$$\Leftrightarrow d_A^* f - d_B^* f \in \mathcal{L} \cap (\ker d_A \cap \ker d_B) = \mathcal{L} \cap \mathcal{L}^\perp = \{0\}$$

$$\Leftrightarrow d_A^* f = d_B^* f.$$

The same calculations yield $f \in \ker(I+T) \Leftrightarrow d_A^* f = -d_B^* f$.

Summarizing the above statements with the preceding work [2], we obtain the complete characterization of the spectrum of quantum walks on graphs.

Corollary 3.17 ([2], Complete eigenstructure of U on the graph G). Assume that a connected graph G is finite; namely, |V(G)|, $|E(G)| < \infty$. Consider the Szegedy walk on G given in Example 2.4. Then we have the following statements.

(1) Integers $m_{\pm 1} \in \{0, 1\}$ denote the multiplicity of eigenvalues ± 1 of *T*, respectively, which are given by

$$m_{+1} = \begin{cases} 1 & \text{if } 1 \in \operatorname{Spec}(T) \\ 0 & \text{otherwise} \end{cases}, \quad m_{-1} = \begin{cases} 1 & \text{if } 1 \in \operatorname{Spec}(T) \text{ and } G \text{ is bipartite} \\ 0 & \text{otherwise} \end{cases}$$

See [2] for details of these definitions.

Let $\varphi_{QW} : \mathbb{C} \to \mathbb{C}$ be the Joukowsky transform given by $\varphi_{QW}(x) = (x + x^{-1})/2$. Then we have

$$\operatorname{Spec}(U) = \varphi_{OW}^{-1}(\operatorname{Spec}(T)) \cup \{+1\} \cup \{-1\},$$

where the multiplicity of +1 and -1 are $M_{+1} = \max\{0, |E| - |V| + m_{+1}\}$ and $M_{-1} = \max\{0, |E| - |V| + m_{-1}\}$, respectively.

(2) The eigenfunctions of the eigenvalue $\lambda \in \varphi_{QW}^{-1}(\operatorname{Spec}(T))$ generating \mathcal{L} are given by

$$\begin{cases} \frac{1}{\sqrt{2}|\sin\lambda|} (I - e^{i\lambda}S)d_A^*f, \text{ where } f \in \ker(\varphi_{QW}(\lambda)I - T) & \text{if } \lambda \neq \pm 1, \\ d_A^*f, \text{ where } f \in \ker(I - T) & \text{if } \lambda = 1. \end{cases}$$

If G is further assumed to be bipartite, then $U|_{\mathcal{L}}$ has the eigenvalue -1 and its eigenfunction is given by

$$d_A^*f$$
, where $f \in \ker(I+T)$.

The eigenspaces associated with the eigenvalues +1 with multiplicity M_{+1} and -1 with multiplicity M_{-1} except those corresponding to $\varphi_{OW}^{-1}(\pm 1)$ are described by

$$\ker(d_A) \cap \mathcal{H}_{-1}^{\mathcal{S}} \quad and \quad \ker(d_A) \cap \mathcal{H}_{+1}^{\mathcal{S}}, \tag{3.21}$$

respectively. Here $\mathcal{H}_{\pm 1}^{S} = \ker(I \mp S)$.

Proof. By definition of m_{+1} , we have dim ker(I - T) = 1. Thus $\psi = (f, g)^T$ in (3.18) is written as $(f, \alpha f)^T$ for $\alpha \in \mathbb{R} \setminus \{-1\}$. By Lemma 3.16, we have $d_A^* f = d_B^* f$. It thus follows that the eigenfunction $L\psi$ of $U|_{\mathcal{L}}$ is written as $\beta d_A^* f$ for some $\beta \in \mathbb{R} \setminus \{0\}$.

Properties that G is bipartite, we have dim ker(I + T) = 1 by definition of m_{-1} (cf. [2]). The same arguments as above thus yield (3.21).

All remaining statements follow from Theorem 3.15.

Remark 3.18. It is shown in [2] that the discriminant operator *T* has the eigenvalue 1 *if and only if the underlying* random walk on a finite graph *G* is reversible. Moreover, the operator *T* has the eigenvalue -1 if and only if the graph *G* is bipartite, namely, its set of vertices can be partitioned into two parts V_1 and V_2 such that each edge has one vertex in V_1 and one vertex in V_2 . Spectral properties around 1 of the twisted random walks has been well studied in [3] and also its induced quantum walk has been studied in [2]. Analysis in [2] also indicates that the eigenstructure of $\text{Spec}(U|_{\mathcal{L}^{\perp}})$ induces localization of *U*. Roughly, a cycle structure on *G* induces localization, since the geometric multiplicities of $\{\pm 1\} \cap U|_{\mathcal{L}^{\perp}}$ are described with the first Betti number of *G*, which becomes a motivation of extend quantum walks on graphs to new quantum walks on simplicial complexes [5]. See [2] for more detailed description of $\ker(I \pm U|_{\mathcal{L}^{\perp}})$.

4. Conclusion

In this paper, we have discussed the spectral mapping theorem of quantum walks of the general form containing

well-known Grover and Szegedy walks on finite graphs. We have derived the spectral mapping theorem of $U|_{\mathcal{L}}$ without using the spectral decomposition of the discriminant operator T to obtain the description of eigenstructures.

We have seen that all eigenvalues of \tilde{T} describe whole eigenvalues of $U|_{\mathcal{L}}$ even if \tilde{T} is not diagonalizable. We also have obtained that $\ker(\lambda I - U|_{\mathcal{L}}) = L(\ker(\lambda I - \tilde{T}))$ for $\lambda \in \operatorname{Spec}(U|_{\mathcal{L}}) \setminus \{\pm 1\}$. On the other hand, if the eigenvalue λ has degenerate geometric multiplicity, then $\ker(\lambda I - U|_{\mathcal{L}})$ is described by purely generalized eigenspace of $\lambda I - \tilde{T}$. This observation is a by-product of introducing our new method.

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