Quantum walks defined by digraphs and generalized Hermitian adjacency matrices

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Abstract
We propose a quantum walk defined by digraphs (mixed graphs). This is like Grover walk that is perturbed by a certain complex-valued function defined by digraphs. The discriminant of this quantum walk is a matrix that is a certain normalization of generalized Hermitian adjacency matrices. Furthermore, we give definitions of the positive and negative supports of the transfer matrix and exhibit explicit formulas of supports of their square. Also, we provide tables on the identification of digraphs by their eigenvalues.

Keywords Quantum walk · Twisted Szegedy walk · Positive support · Digraph · Hermitian adjacency matrix · Spectral graph theory

Mathematics Subject Classification 05C50 · 05C20 · 05C81 · 81Q99

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1 Introduction

Since the beginning of the millennium, quantum walks have been actively studied not only in mathematics but also in physics. Several papers and books on the implementation of the experimental setups of them have also been published [7,13,25,26], and quantum walks on networks are reviewed in [2]. Quantum walks on digraphs are also studied as applications of topological phase’s simulators, see, for example, [6]. It can be said that quantum walks are studied in a very wide range of contexts. Due to the wide range of them, fundamental research such as proposing a model defined by digraphs is important for future development of application to quantum walks. In this paper, we introduce a quantum walk model which can define not only undirected graphs but also digraphs. Moreover, it allows us realistic eigenvalue analysis.

The Grover walks are the simplest quantum walks to be defined by providing graphs, and they are recently well studied, including topics on quantum search [27], graph isomorphism problem [5], periodicity [16,21,31,32], relation to the Ihara zeta function [19,20,28], and so on. They are originally defined by undirected graphs, but we will extend them to digraphs. See Sect. 2.2 for readers who want to know details.

In order to define our quantum walk, we introduce a certain complex-valued function \( \theta \) and generalize the shift operator, which can be regarded as perturbations by \( \theta \). We define such function \( \theta \) from digraphs and consider something like Grover walk equipped with \( \theta \). This quantum walk can be seen as the one to have information on digraphs. Moreover, the discriminant of our quantum walk (whose definition is given in (2.3)) coincides with a matrix that is a certain normalization of the Hermitian adjacency matrix, which has been introduced in the context of spectral graph theory [12,23].

As Emms, Hancock, Severini and Wilson [5] attempted to distinguish strongly regular graphs by their spectrum of matrices coming from quantum walks, we also want to use matrices coming from quantum walks to identify digraphs. For this purpose, we exhibit explicit formulas for the positive and negative supports of the square of the transfer matrix of our quantum walk. See Sect. 6 for readers who want to know details. In the case of undirected regular graphs, the eigenvalues of the positive support of the square of the Grover transfer matrices are determined by the eigenvalues of the adjacency matrices [9]. However, we will see that this is not always true for digraphs. Also, we provide tables on the identification of digraphs by their eigenvalues.

This paper is organized as follows: In Sect. 2, we review basic terminologies related to graphs and quantum walks, and define our quantum walk. In Sect. 3, we give a definition of generalized Hermitian adjacency matrices and state that our quantum walk and these matrices are related to each other. In Sect. 4, we show so-called spectral mapping theorem, that is, we show that the eigenvalues of the transfer matrix can be written roughly by those of generalized Hermitian adjacency matrices. In Sect. 5, we calculate the eigenvalues of the transfer matrix of the digraphs cospectral with \( K_n \) in the sense of Hermitian adjacency matrices found by Guo and Mohar [12]. In fact, it can be seen that these digraphs are also cospectral in the sense of our transfer matrix.

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1 This dynamics of the quantum walk treated on a half plain of the two-dimensional lattice [6] can be regarded as a quantum walk on a digraph, which is not symmetric, because a quantum walker moves to \( x \) and \( y \) directions, alternatively.

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In Sect. 6, we give a definition of the positive and negative supports of our transfer matrix to the $n$-th power. For the case of $n = 2$, we show that these matrices can be roughly expressed by the ones of the Grover transfer matrix on the underlying graph. In Sect. 7, we confirm that Guo–Mohar’s digraphs, which could not be identified even by the eigenvalues of our transfer matrix, can be partially identified by the supports of the square. In Sect. 8, consideration on the identification of digraphs by the eigenvalues of matrices newly obtained in this study is given. In this consideration, tables similar to the ones for adjacency matrices and Hermitian adjacency matrices made by Guo and Mohar [12] are given.

1.1 Histories of quantum walks on digraphs

In this subsection, we review previous works on quantum walks on digraphs. In general, it is difficult to define quantum walks on digraphs themselves. Historically, Severini [29] focused on 1-factors of digraphs and first defined coined quantum walks on digraphs. In 2003, the following year, Severini [30] considered a condition called strong quadrangularity and showed that a line digraph is the digraph of a unitary matrix, if and only if the digraph is Eulerian. From the result, we saw that quantum walks on digraphs can be defined when the digraph is Eulerian. After that, Acevedo and Gobron [1] defined quantum walks on Cayley graphs. The Cayley graphs can be digraphs depending on connection sets, so in this sense, they also defined quantum walks on digraphs. In 2007, Montanaro [24] successfully explained a necessary and sufficient condition for defining a discrete-time quantum walk on a digraph by a property called reversibility. For digraphs that are not reversible, a method called a partially quantum walk has been presented. On the other hand, Hoyer and Meyer [17] gave the first example of faster transport with a quantum walk on digraphs. Other recent studies of quantum walks on digraphs are in [4,10,22,33].

In contrast to previous studies, we propose quantum walks defined by digraphs in another form. Our idea is to generalize the Grover walks. Roughly speaking, we consider the generalized Grover walks on the underlying graphs of digraphs and change the phase using information of the digraphs. By this idea, we can not only easily define quantum walks for any digraphs, but also provide models to allow realistic eigenvalue analysis. Indeed, we explicitly reveal eigenvalues of the transfer matrices of quantum walks defined by digraphs cospectral with the complete graphs.

1.2 A remark for readers

The transfer matrix of our quantum walks is defined by digraphs. However, our quantum walk is not the one on digraphs, so readers should note it.

2 Grover walks and their generalization

First, we review several notations on graphs. Let $G = (V(G), E(G))$ be a finite simple and connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For an edge
uv \in E(G)$, the arc from $u$ to $v$ is denoted by $(u, v)$. The origin and terminus vertices of $e = (u, v)$ are denoted by $o(e), t(e)$, respectively. We express $e^{-1}$ as the inverse arc of $e$. We define $A(G) = \{(u, v), (v, u) | uv \in E(G)\}$, which is the set of the symmetric arcs of $G$.

### 2.1 Grover walks on undirected graphs

Let $G$ be a finite simple and connected graph. Then, $G$ defines the following three complex matrices $K, S, C$. First, $K = K(G)$ is the complex matrix whose rows are indexed by $V(G)$ and columns are indexed by $A(G)$, defined by

$$K_{v,a} = \frac{1}{\sqrt{\deg t(a)}} \delta_{v,t(a)},$$  

where $\delta_{a,b}$ is the Kronecker delta symbol. Note that $KK^* = I$. Second, $S = S(G)$ is the complex matrix indexed by $A(G)$, where

$$S_{ab} = \delta_{a,b^{-1}}.$$  

Third, $C = C(G)$ is the complex matrix indexed by $A(G)$, where

$$C = 2K^*K - I.$$  

The matrices $S$ and $C$ are called the *shift operator* and the *coin operator*, respectively. Usually, it is customary for these matrices $K, S, C$ to be defined as mappings on $l^2$-spaces on $V(G)$ or $A(G)$, but we would like to study quantum walks from the viewpoint of spectral graph theory, so these operators are displayed in matrix and we will discuss by using matrices.

The *Grover transfer matrix* $U = U(G)$ is the product of the shift operator and the coin operator, that is,

$$U = SC.$$  

Since $S$ and $C$ are unitary, $U$ is also a unitary matrix, so $U$ can define a quantum walk on a given graph $G$. We call this quantum walk the *Grover walk*. Note that $U$ is the complex matrix indexed by $A(G)$ and the $(a, b)$-component can be calculated as:

$$U_{ab} = \frac{2}{\deg_G(t(b))} \delta_{t(b),o(a)} - \delta_{a^{-1},b^{-1}},$$  

so some papers directly give a definition of the Grover transfer matrix by this computation. In addition, the *discriminant operator* $T$ of Grover walk is defined by

$$T = KSK^*,$$  

which plays an important role in analyzing spectrum of $U$. 

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2.2 Quantum walks defined by digraphs

Based on the Grover walks, our quantum walks will be defined. Let $G$ be a finite simple and connected graph, and let $\theta : A(G) \to \mathbb{R}$ be a function. The complex matrix $S_\theta = S_\theta(G)$ is the one indexed by $A(G)$, where

$$(S_\theta)_{ab} = e^{\theta(b) i} \delta_{a,b^{-1}}.$$  

We consider a condition where $S_\theta$ is unitary and self-adjoint. The following lemma is easy, but it is essentially important.

**Lemma 2.1** With the above notations, we have the following:
1. $S_\theta$ is unitary;
2. $S_\theta$ is self-adjoint if and only if $\theta(a) + \theta(a^{-1}) \in 2\pi\mathbb{Z}$ for any $a \in A(G)$.

By this lemma, the matrix $U_\theta = S_\theta C$ is also unitary, where $C = C(G)$ is the coin operator given in the previous subsection. We call $U_\theta$ the transfer matrix of a graph $G$. In addition, the discriminant operator $T_\theta$ of our quantum walk is defined by

$$T_\theta = KS_\theta K^*.$$  

As we will see later, the discriminant of our quantum walk equipped with an appropriate function $\theta$ will be a meaningful matrix. In this paper, we discuss the quantum walks defined by $U_\theta$.

Now, we check several terminologies on digraphs. A **digraph** $G$ consists of a finite set $V(G)$ of vertices together with a subset $A(G) \subset V(G) \times V(G) \setminus \{(x,x) \mid x \in V(G)\}$ of ordered pairs called arcs. Define $A(G)^{-1} = \{a^{-1} \mid a \in A(G)\}$ and $A(G)^{\pm 1} = A(G) \cup A(G)^{-1}$. The graph $G^\pm = (V(G), A(G)^{\pm 1})$ is so-called the underlying graph of a digraph $G$, and this is often regarded as an undirected graph. If $(x,y) \in A(G) \cap A(G)^{-1}$, we say that the unordered pair $\{x,y\}$ is a **digon** of $G$. For a vertex $x \in V(G)$, define $\deg_G x = \deg_{G^\pm} x$. A digraph $G$ is $k$-regular if $\deg_G x = k$ for any vertex $x \in V(G)$. Throughout this paper, we assume that digraphs are weakly connected, i.e., for any digraph $G$, we suppose that $G^\pm$ is connected.$^2$

A function $\theta$ which satisfies the condition (ii) of Lemma 2.1 can be defined from digraphs as follows: Let $\eta \in \mathbb{R}$. For a digraph $G = (V(G), A(G))$, we define a function $\theta : A(G^\pm) \to \mathbb{R}$ by

$$\theta(a) = \begin{cases} 
\eta & \text{if } a \in A(G) \setminus A(G)^{-1}, \\
-\eta & \text{if } a \in A(G)^{-1} \setminus A(G), \\
0 & \text{if } a \in A(G) \cap A(G)^{-1}.
\end{cases}$$

Clearly,

$$\theta(a) + \theta(a^{-1}) = 0$$  

$^2$ Quantum walks we will define are a generalization of the Grover walks. As we will see later, walkers in our quantum walk are on $G^\pm$. In the case of Grover walks, the connectedness of graphs is usually assumed, so we need assume that $G^\pm$ is connected.
Table 1 The operators (matrices) used in our quantum walk

| Notation | Name          | Indices of rows and columns | Definition                                                                                                                                 |
|----------|---------------|-----------------------------|------------------------------------------------------------------------------------------------------------------------------------------|
| $K$      | Boundary      | $V(G) \times A(G^\pm)$     | $K_{v,a} = \frac{1}{\sqrt{\deg t(a)}} \delta_{v,t(a)}$                                                                                  |
| $C$      | Coin          | $A(G^\pm) \times A(G^\pm)$ | $C = 2K^*K - I$                                                                                                                         |
| $S_{\theta}$ | Shift      | $A(G^\pm) \times A(G^\pm)$ | $(S_{\theta})_{ab} = e^{\theta(b)}i \delta_{a,b-1}$                                                                                   |
| $U_{\theta}$ | Transfer    | $A(G^\pm) \times A(G^\pm)$ | $U_{\theta} = S_{\theta}C$                                                                                                               |
| $T_{\theta}$ | Discriminant | $V(G) \times V(G)$         | $T_{\theta} = KS_{\theta}K^*$                                                                                                           |

Fig. 1 Digraph $G$

holds for any $a \in A(G^\pm)$. We call this the $\eta$-function of a digraph $G$. Then, we can think that a digraph $G$ equipped with an $\eta$-function $\theta$ defines the transfer matrix $U_{\theta} = S_{\theta}(G^\pm)C(G^\pm)$. The operators (matrices) used in our quantum walks are summarized in Table 1, where $G = (V(G), A(G))$ is a digraph equipped with an $\eta$-function $\theta$.

2.3 Example

We provide an example. As mentioned in the previous subsection, our quantum walk is defined by a digraph and a real number $\eta$. Let $G$ be a digraph in Fig. 1. We consider this digraph $G$ and $\eta = \pi/2$.

For the sets of indices $V(G) = \{v_1, v_2, v_3, v_4\}$ and $A(G^\pm) = \{a, a^{-1}, b, b^{-1}, c, c^{-1}, d, d^{-1}\}$, we have

\[
K = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\
\end{bmatrix},
\]

\[
C = 2K^*K - I = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & \frac{2}{3} & 0 & 0 \\
0 & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \frac{2}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & \frac{2}{3} & \frac{2}{3} & 0 & 0 & -\frac{1}{3} & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\end{bmatrix},
\]
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\[ S_{\theta} = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -i & 0 & 0 & 0 \\
0 & 0 & i & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -i & 0 & 0 \\
0 & 0 & 0 & i & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -i & 0 \\
0 & 0 & 0 & 0 & 0 & i & 0 \\
\end{bmatrix}, \]

so the transfer matrix is

\[ U_{\theta} = S_{\theta} C = \begin{bmatrix}
0 & \frac{1}{3} & 2 \frac{2}{3} & 0 & 0 & \frac{2}{3} & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -i & 0 & 0 \\
0 & \frac{2}{3} i & \frac{1}{3} i & 0 & 0 & \frac{2}{3} i & 0 & 0 \\
0 & -\frac{2}{3} i & -\frac{1}{3} i & 0 & 0 & \frac{1}{3} i & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & i \\
0 & 0 & 0 & 0 & -i & 0 & 0 & 0 \\
0 & 0 & 0 & i & 0 & 0 & 0 & 0 \\
\end{bmatrix}. \]

Unlike the conventional Grover walks, our transfer matrix takes imaginary numbers. It can be seen that these imaginary numbers give information of digraphs.

### 3 Hermitian adjacency matrices

Guo–Mohar [12] and Li–Liu [23] independently defined the Hermitian adjacency matrix as a new matrix determined by a digraph. Since this matrix is Hermitian, the eigenvalues are real numbers and the interlacing theorem can be used, so this is a convenient matrix for estimating invariants of graphs. Basic properties of the Hermitian adjacency matrix can be seen in both papers. In [12], we can see estimation on the maximum eigenvalue and the spectral radius. In [23], consideration of the Hermitian energy is carried out.

For a digraph \( G \), the Hermitian adjacency matrix \( H = H(G) \) is the complex matrix indexed by the vertex set \( V(G) \), where

\[
H_{xy} = \begin{cases} 
1 & \text{if } (x, y) \in A(G) \cap A(G)^{-1}, \\
i & \text{if } (x, y) \in A(G) \setminus A(G)^{-1}, \\
-i & \text{if } (x, y) \in A(G)^{-1} \setminus A(G), \\
0 & \text{otherwise.} 
\end{cases}
\]

When every edge of \( G \) lies in a digon, \( H(G) \) coincides with the adjacency matrix, so in this sense, the Hermitian adjacency matrices can be seen as a generalization of the ordinary adjacency matrices of undirected graphs. We generalize this matrix by interpreting the complex value \( i \) as \( e^{\frac{\pi}{2} i} \). For \( \eta \in \mathbb{R} \) and a digraph \( G \), the \( \eta \)-Hermitian
adjacency matrix $H_\eta = H_\eta(G)$ is the complex matrix indexed by the vertex set $V(G)$, where

$$(H_\eta)_{xy} = \begin{cases} 
1 & \text{if } (x, y) \in A(G) \cap A(G)^{-1}, \\
e_{\eta i} & \text{if } (x, y) \in A(G) \setminus A(G)^{-1}, \\
e_{-\eta i} & \text{if } (x, y) \in A(G)^{-1} \setminus A(G), \\
0 & \text{otherwise.}
\end{cases}$$

Note that $H_\eta = H_\eta$. Due to the spectral mapping theorem which will be described in Sect. 4, the eigenvalues of $U_\theta$ are roughly expressed by those of a matrix indexed by the vertex set, called discriminant. In the case of Grover walks, the discriminant operator corresponds to the transition matrix of the isotropic random walk. As we will see, the discriminant of our quantum walk is a certain normalized Hermitian adjacency matrix. For a digraph $G$, we define the degree matrix $D = D(G)$ by $D_{xy} = (\deg_G x)\delta_{x, y}$ for vertices $x, y \in V(G)$. For $\eta \in \mathbb{R}$, we define the normalized $\eta$-Hermitian adjacency matrix $\tilde{H}_\eta$ by

$$\tilde{H}_\eta = D^{-\frac{1}{2}} H_\eta D^{-\frac{1}{2}}.$$ 

Note that if a digraph $G$ is $k$-regular, then $D^{-\frac{1}{2}} = \frac{1}{\sqrt{k}} I$, so $\tilde{H}_\eta = \frac{1}{k} H_\eta$. This implies that the eigenvalues of $\tilde{H}_\eta$ can be determined by $H_\eta$.

The following can be easily confirmed by calculating each component directly, but this equality is valuable in the sense of connecting quantum walks to spectral graph theory.

**Theorem 3.1** Let $\eta \in \mathbb{R}$ and $G$ be a digraph equipped with the $\eta$-function $\theta$. Then, we have

$$\tilde{H}_\eta(G) = KS_\theta K^*.$$ 

**Proof** Indeed,

$$(KS_\theta K^*)_{xy} = \sum_{a, b \in A(G^\pm)} K_{x, a}(S_\theta)_{ab} K_{y, b}$$

$$= \sum_{a, b \in A(G^\pm)} \frac{1}{\sqrt{\deg x}} \frac{1}{\sqrt{\deg y}} e^{\theta(b)i} \delta_{a, b^{-1}}$$

$$= \sum_{a \in A(G^\pm)} \frac{1}{\sqrt{\deg x}} \frac{1}{\sqrt{\deg y}} e^{\theta(a^{-1})i}$$
\[
\frac{e^{i\theta(x,y)}}{\sqrt{\deg x \sqrt{\deg y}}} \quad \text{if } x \text{ is adjacent to } y \text{ on } G^+, \\
0 \\
\frac{1}{\sqrt{\deg x \sqrt{\deg y}}} \quad \text{if } (x, y) \in A(G) \cap A(G)^{-1}, \\
\frac{e^{i\theta}}{\sqrt{\deg x \sqrt{\deg y}}} \quad \text{if } (x, y) \in A(G) \setminus A(G)^{-1}, \\
\frac{e^{-i\theta}}{\sqrt{\deg x \sqrt{\deg y}}} \quad \text{if } (x, y) \in A(G)^{-1} \setminus A(G), \\
0
\]

Supplementing a property of the eigenvalues of the normalized \(\eta\)-Hermitian adjacency matrix, we complete this section. In general, it is revealed that the eigenvalues of the discriminant are in the closed interval \([-1, 1]\) (see the proof of Proposition 1 in [15]), but we give a proof of this fact from the viewpoint of spectral graph theory.

**Lemma 3.2** Let \(A \in M_n(\mathbb{C})\) be a complex matrix such that \(A^* = A\) and \(A^2 = A\). Then, \(\langle f, Af \rangle\) is a real number for any vector \(f \in \mathbb{C}^n\) and

\[\langle f, Af \rangle \leq \langle f, f \rangle\]

holds.

**Proof** Pick a vector \(f \in \mathbb{C}^n\). From \(A^* = A\) and \(A^2 = A\),

\[
||Af|| = \langle Af, Af \rangle = \langle f, A^*Af \rangle = \langle f, A^2f \rangle = \langle f, Af \rangle,
\]

so \(\langle f, Af \rangle\) is a real number. Since the eigenvalues of \(A\) are only 0, 1, we can write as \(f = g_0 + g_1\), where \(g_i\) is an eigenvector of \(i \in \{0, 1\}\). Then, we have

\[
\langle f, f \rangle - \langle f, Af \rangle = \langle g_0 + g_1, g_0 + g_1 \rangle - \langle g_0 + g_1, g_1 \rangle \\
= ||g_0||^2 + ||g_1||^2 - ||g_1||^2 \\
= ||g_0||^2 \geq 0.
\]

Remark that the matrix \(A\) satisfying the conditions \(A^2 = A\) and \(A^* = A\) is known as the orthogonal projection operator in the literature of the functional analysis.

**Proposition 3.3** Let \(\eta \in \mathbb{R}\) and \(G\) be a digraph. Then, for any eigenvalue \(\lambda\) of \(\tilde{\mathcal{H}}_\eta(G)\), we have \(|\lambda| \leq 1\).

**Proof** Let \(f\) be an eigenvector of \(\tilde{\mathcal{H}}_\eta = \tilde{\mathcal{H}}_\eta(G)\) of an eigenvalue \(\lambda\). Then,

\[|
\lambda|^2 ||f||^2 = ||\tilde{\mathcal{H}}_\eta f||^2 \]
\[ \langle KS_\theta K^* f, KS_\theta K^* f \rangle \leq \langle S_\theta K^* f, S_\theta K^* f \rangle \quad (\text{by Lemma 3.2}) \]
\[ = \langle f, K K^* f \rangle \quad (S_\theta \text{ is unitary}) \]
\[ = \langle f, f \rangle \quad (\text{by } KK^* = I) \]
\[ = ||f||^2, \]
so we have the desired inequality. \hfill \square

### 4 Spectral mapping theorem

The eigenvalues of the normalized \(\eta\)-Hermitian adjacency matrix are real, and they are in the closed interval \([-1, 1] \subseteq \mathbb{R}\) from Proposition 3.3. In fact, most eigenvalues of the transfer matrix \(U_\theta\) are values obtained by lifting the eigenvalues of \(\tilde{H}_\eta\) onto the unit circle in the complex plane. Such facts are often called spectral mapping theorems, and well studied in quantum walks on graphs (see, e.g., [20] and its references therein). In 2014, Higuchi, Konno, Sato and Segawa [15] introduced certain quantum walks, which are called twisted Szegedy walks and revealed a spectral mapping theorem derived from twisted random walks. In this section, we confirm that a spectral mapping theorem holds for our quantum walk via twisted Szegedy walks.

For a digraph \(G\), a path of \(G\) is a sequence of arcs \((a_1, a_2, \ldots, a_r)\) with \(t(a_j) = o(a_{j+1})\) for \(j = 1, \ldots, r-1\). If \(t(a_r) = o(a_1)\), then it is said to be closed. We denote the set of all closed paths of \(G\) by \(C(G)\). A function \(A(G^\pm) \rightarrow (0, 1]\) is called a transition probability if
\[ \sum_{a \in A(G^\pm)} p(a) = 1 \]
for all \(u \in V(G)\). A transition probability \(p\) is said to be reversible if there exists a positive valued function \(m : V(G) \rightarrow (0, \infty)\) such that
\[ m(o(a)) p(a) = m(t(a)) p(a^{-1}) \]
for all \(a \in A(G^\pm)\).

**Lemma 4.1** Let \(G\) be a digraph. Then, the transition probability \(p\) defined by
\[ p(a) = \frac{1}{\deg_{G^\pm} o(a)} \]
is reversible.
Table 2  The operators related to twisted Szegedy walks

| Notation | Name               | Indices of rows and columns | Definition                                                                 |
|----------|--------------------|------------------------------|----------------------------------------------------------------------------|
| $L$      | Boundary           | $V(G) \times A(G)$          | $L_{v,a} = w(a)\delta_{v,o(a)}$                                           |
| $C^{(w)}$| Coin               | $A(G) \times A(G)$          | $C^{(w)} = 2L^*L - I$                                                      |
| $S^{(\theta)}$ | Twisted shift     | $A(G) \times A(G)$          | $S_{ab}^{(\theta)} = e^{\theta(b,i)}\delta_{a,b}^{-1}$                    |
| $U^{(w,\theta)}$ | Time evolution    | $A(G) \times A(G)$          | $U^{(w,\theta)} = S^{(\theta)}C^{(w)}$                                    |
| $T^{(w,\theta)}$ | Discriminant      | $V(G) \times V(G)$          | $T^{(w,\theta)} = LS^{(\theta)}L^*$                                       |

**Proof** Considering the positive valued function $m$ defined by

$$m(u) = \deg_{G\pm u},$$

we can check $m(o(a))p(a) = 1 = m(t(a))p(a^{-1})$ for any $a \in A(G)^{\pm 1}$. $\square$

### 4.1 Twisted Szegedy walks

In this subsection, we review twisted Szegedy walks. Let $G$ be a finite simple and connected graph. A function $w : A(G) \to \mathbb{C} \setminus \{0\}$ is a *weight function* if

$$\sum_{a \in A(G), o(a) = x} |w(a)|^2 = 1$$

for any $x \in V(G)$. A function $\theta : A(G) \to \mathbb{R}$ is a *1-form function* if

$$\theta(a^{-1}) = -\theta(a)$$

for any $a \in A(G)$. The operators (matrices) related to twisted Szegedy walks are summarized in Table 2.

Note that the twisted shift operator $S^{(\theta)}$ is unitary and self-adjoint.

Let $\varphi$ be a function from the unit circle $\{z \in \mathbb{C} \mid |z| = 1\}$ to the closed interval $[-1, 1] \subset \mathbb{R}$, where $\varphi(z) = (z + z^{-1})/2$.

**Theorem 4.2** ([15]) Let $G$ be a graph equipped with a weight function $w$ and a 1-form function $\theta$. Denote $m_{\pm 1}$ by the multiplicities of the eigenvalues $\pm 1$ of $T^{(w,\theta)}$, respectively. Then, we have

$$\text{Spec}(U^{(w,\theta)}) = \varphi^{-1}(\text{Spec}(T^{(w,\theta)})) \cup \{1\}^{M_1} \cup \{-1\}^{M_{-1}},$$

where $M_{\varepsilon} = \max\{0, |E(G)| - |V(G)| + m_\varepsilon\}$ for $\varepsilon \in \{\pm 1\}$. $\Box$
4.2 Spectral mapping theorem for our quantum walk

The function \( w_0 : A(G) \to \mathbb{C} \setminus \{0\} \) defined by

\[
w_0(a) = \frac{1}{\sqrt{\deg o(a)}}
\]

is clearly a weight function, and any \( \eta \)-function \( \theta \) is a 1-form function by (2.4).

**Theorem 4.3** Let \( G \) be a digraph equipped with an \( \eta \)-function \( \theta \) and \( U_{\theta} \) be the transfer matrix. Denote \( m_{\pm 1} \) by the multiplicities of the eigenvalues \( \pm 1 \) of \( \tilde{H}_\eta(G) \), respectively.

Then, we have

\[
\text{Spec}(U_{\theta}) = \phi^{-1}(\text{Spec}(\tilde{H}_\eta(G))) \cup \{1\}^{M_1} \cup \{-1\}^{M_{-1}},
\]

where \( M_\varepsilon = \max\{0, |E(G^\varepsilon)| - |V(G^\varepsilon)| + m_\varepsilon\} \) for \( \varepsilon \in \{\pm 1\} \).

**Proof** We consider the twisted Szegedy walk on \( G^\pm \) associated with \( w_0 \) and \( \theta \). By Theorem 4.2, it is enough to show that \( \tilde{H}_\eta(G) = T^{(w_0, \theta)} \) and \( U_{\theta} \) is similar to \( U^{(w_0, \theta)} \).

The following equalities can be checked immediately:

(i) \( L = K(G^\pm)S(G^\pm) \);
(ii) \( S^{(\theta)} = S_\theta(G^\pm) \);
(iii) \( S(G^\pm)S_\theta(G^\pm)S(G^\pm) = S_\theta(G^\pm) \).

Thus, as for the discriminant operators, we have

\[
T^{(w_0, \theta)} = LS^{(\theta)}L^* = K(G^\pm)S(G^\pm)S_\theta(G^\pm)S(G^\pm)K^*(G^\pm) \quad \text{(by (i) and (ii))}
\]
\[
= K(G^\pm)S_\theta(G^\pm)K^*(G^\pm) \quad \text{(by (iii))}
\]
\[
= \tilde{H}_\eta(G). \quad \text{(by Theorem 3.1)}
\]

In addition,

\[
2L^*L - I = 2S(G^\pm)K^*(G^\pm)K(G^\pm)S(G^\pm) - S(G^\pm)S(G^\pm) \quad \text{(by (i))}
\]
\[
= S(G^\pm)(2K^*(G^\pm)K(G^\pm) - I)S(G^\pm)
\]
\[
= S(G^\pm)C(G^\pm)S(G^\pm),
\]

so we have

\[
U^{(w_0, \theta)} = S^{(\theta)}(2L^*L - I) = S_\theta(G^\pm)S(G^\pm)C(G^\pm)S(G^\pm) \quad \text{(by (ii))}
\]
\[
= S(G^\pm)S_\theta(G^\pm)S(G^\pm)C(G^\pm)S(G^\pm) \quad \text{(by (iii))}
\]
We have the desired statement. □

Theorem 4.3 implies that all the spectral information of the normalized η-Hermitian adjacency matrix corresponding to a continuous-time random walks can be reproduced. Moreover, we will see that from the second and third terms of RHS of (4.1) in Theorem 4.3, a part of information of all the cycles in given graphs can be used for the identification of digraphs.

In [15], the values $m_{\pm 1}$ are also determined with a general weight function and a 1-form function. In the quantum walks we consider, the situations of case division can be summarized slightly simpler.

Fix a digraph $G$ with an η-function $\theta$. For a function $f : A(G^{\pm}) \to \mathbb{C}$ and a closed path $c = (a_1, \ldots, a_r)$, we define

$$\int_c \arg f = \sum_{j=1}^{r} \left\{ \arg(f(a_j)) - \arg(f(a_j^{-1})) \right\}.$$

In determining $m_{\pm 1}$, the value

$$\int_c \arg \tilde{w}$$

in [15] is the key. In our situation, the modified weight function $\tilde{w} : A(G^{\pm}) \to \mathbb{C}$ is nothing but the one defined by

$$\tilde{w}(a) = \frac{1}{\sqrt{\deg o(a)}} e^{i\theta(a)/2},$$

so for a closed path $c = (a_1, \ldots, a_r)$, we have

$$\int_c \arg \tilde{w} = \sum_{j=1}^{r} \left\{ \arg(\tilde{w}(a_j)) - \arg(\tilde{w}(a_j^{-1})) \right\}$$

$$= \sum_{j=1}^{r} \left\{ \frac{\theta(a_j)}{2} - \frac{\theta(a_j^{-1})}{2} \right\}$$

$$= \sum_{j=1}^{r} \theta(a_j).$$

Again, for a digraph $G$ equipped with an η-function $\theta$, we define the function $\mathcal{I} : \mathcal{C}(G^{\pm}) \to \mathbb{C}$ by

$$\mathcal{I}(c) = \sum_{j=1}^{r} \theta(a_j)$$
for a closed path $c = (a_1, \ldots, a_r)$. We consider four situations:

(i) $G^\pm$ is bipartite and $I(c) \in 2\pi\mathbb{Z}$ for any closed path $c$;
(ii) $G^\pm$ is non-bipartite and $I(c) \in 2\pi\mathbb{Z}$ for any closed path $c$;
(iii) $G^\pm$ is non-bipartite and for any closed path $c$,

$$I(c) \in \begin{cases} 2\pi\mathbb{Z} & \text{if } c \text{ is an even length closed path,} \\ 2\pi(\mathbb{Z} + \frac{1}{2}) & \text{if } c \text{ is an odd length closed path;} \end{cases}$$

(iv) otherwise.

Then, Lemma 2 in [15] can be rewritten as follows:

**Proposition 4.4** Let $G$ be a digraph equipped with an $\eta$-function $\theta$. Denote $m_{\pm 1}$ by the multiplicities of eigenvalues $\pm 1$ of $\tilde{H}_\eta(G)$, respectively. Then, we have

$$(m_1, m_{-1}) = \begin{cases} (1, 1) & \text{case (i)}, \\ (1, 0) & \text{case (ii)}, \\ (0, 1) & \text{case (iii)}, \\ (0, 0) & \text{case (iv)}. \end{cases}$$

In our quantum walk, we consider the transition probability $p$ defined by $p(e) = 1/\deg_{G^\pm} o(e)$, but $p$ is reversible by Lemma 4.1, so the condition on reversibility of Lemma 2 in [15] vanishes.

As a consequence of this proposition, a necessary and sufficient condition for the Hermitian adjacency matrix of a $k$-regular digraph to have eigenvalues $\pm k$ is clarified. This may be interesting also from the viewpoint of spectral graph theory.

**Corollary 4.5** Let $G$ be a weakly connected $k$-regular digraph equipped with the $\frac{\pi}{2}$-function $\theta$. Then, the Hermitian adjacency matrix $H = H_{\frac{\pi}{2}}(G)$ has at most one eigenvalue $\pm k$, respectively. In addition,

1. $H$ has an eigenvalue $k$ if and only if $I(c) \in 2\pi\mathbb{Z}$ for any closed path $c$ on $G^\pm$.
2. $H$ has an eigenvalue $-k$ if and only if $G$ is in the case (i) or (iii).

**Proof** Since $G$ is $k$-regular, we have $\tilde{H}_{\frac{\pi}{2}}(G) = \frac{1}{k}H$. Thus, the statement follows from Proposition 4.4. \qed

## 5 Guo–Mohar’s $H$-cospectral mates for $K_n$

Let $\eta \in \mathbb{R}$ and let $G$ and $G'$ be digraphs. $G'$ is $H_\eta$-cospectral for $G$ if $\text{Spec}(H_\eta(G)) = \text{Spec}(H_\eta(G'))$. Guo and Mohar [12] determined all $H$-cospectral mates for the complete graph $K_n$. They are the following graphs. Let $a \in \{0, 1, \ldots, n\}$. The digraph $Y_{a,n-a}$ is defined by

$$V(Y_{a,n-a}) = \{1, 2, \ldots, a\} \sqcup \{a + 1, a + 2, \ldots, n\} = \{1, 2, \ldots, n\},$$
\[ A(Y_{a,n-a}) = \{ (x, y) \mid x, y \in [a], x \neq y \} \]
\[ \cup \{ (x, y) \mid x, y \in [n] \setminus [a], x \neq y \} \]
\[ \cup \{ (x, y) \mid x \in [a], y \in [n] \setminus [a] \}, \]
where \([n] = \{1, 2, \ldots, n\}\). For convenience, we call the first \(a\) vertices the upper vertices and the last \(n-a\) vertices the lower vertices. Roughly speaking, this digraph is the two complete graphs \(K_a\) and \(K_{n-a}\) with all possible arcs from \(K_a\) to \(K_{n-a}\). Note that \(Y_{n,0} = Y_{0,n} = K_n\).

**Proposition 5.1** (Proposition 8.6 in [12]) For each \(n\), there are precisely \(n\) non-isomorphic \(H\)-cospectral digraphs for \(K_n\). These are the digraphs \(Y_{a,n-a}\) for \(a \in \{0, \ldots, n-1\}\).

This digraphs \(Y_{a,n-a}\) can be obtained from \(K_n\) by the following deformation. Let \(G\) be a digraph and \(S \subset V(G)\). Define \(\delta(S) = \{ (x, y) \in A(G) \mid |\{x, y\} \cap S| = 1\}\). If \(\delta(S)\) contains only digons, then \(G\) and the digraphs obtained by replacing each digon \(\{x, y\}\) with \(x \notin S\) and \(y \in S\) by the arc \((x, y)\) have the same spectrum in the sense of the \(\eta\)-Hermitian adjacency matrix (Proposition 8.3 in [12]). This can be generalized to the \(\eta\)-Hermitian adjacency matrix for any \(\eta \in \mathbb{R}\).

**Proposition 5.2** Fix \(\eta \in \mathbb{R}\). Let \(G\) be a digraph and \(S \subset V(G)\) such that \(\delta(S)\) contains only digons. Then, \(G\) and the digraphs obtained by replacing each digon \(\{x, y\}\) with \(x \notin S\) and \(y \in S\) by the arc \((x, y)\) have the same spectrum in the sense of the \(\eta\)-Hermitian adjacency matrix.

**Proof** We denote \(G'\) by the digraph obtained by the above deformation. Define the diagonal matrix \(M\) indexed by \(V(G)\) by

\[ M_{uu} = \begin{cases} e^{\eta i} & u \in S, \\ 1 & u \notin S. \end{cases} \]

Clearly, \(M^{-1} = M^*\). Since \(\delta(S)\) contains only digons, \(M^*H_\eta M\) is again \([0, 1, e^{\pm \eta i}]\)-matrix and this is nothing but the \(\eta\)-Hermitian adjacency matrix of \(G'\). Thus, \(G\) and \(G'\) are \(H_\eta\)-cospectral. \(\square\)

Moreover, we can also see the following. Recall that the function \(\varphi\) is defined by \(\varphi(z) = (z + z^{-1})/2\).

**Lemma 5.3** Suppose \(n \geq 3\). Let \(G\) be a digraph \(Y_{a,n-a}\) equipped with an \(\eta\)-function \(\theta\) for \(a \in \{0, 1, \ldots, n-1\}\). Then, the spectrum of \(U_\theta = U_\theta(G)\) is

\[ \text{Spec}(U_\theta) = \left\{ \frac{1}{n(n-1)/2-n+2}, -\frac{1}{n(n-1)/2-n}, \varphi^{-1}\left(\left\{ \frac{1}{n-1} \right\}^{(n-1)}\right) \right\}. \]

In particular, the digraphs \(Y_{a,n-a}\) are \(U_\theta\)-cospectral for \(K_n\).
Proof The $H_\eta$-spectrum of $K_n$ is $\{n - 1^{(1)}, -1^{(n-1)}\}$. By Proposition 5.2, the $H_\eta$-spectrum of $Y_{a,n-a}$ is also $\{n - 1^{(1)}, -1^{(n-1)}\}$. Since $Y_{a,n-a}$ is $(n-1)$-regular, we have $\text{Spec}(\tilde{H}_\eta(Y_{a,n-a})) = \{1^{(1)}, -1^{(n-1)}\}$. Considering the inverse image of $\phi$, a set of eigenvalues \[
abla \{1^{(1)}, \phi^{-1}\left(-\frac{1}{n-1}\right)^{(n-1)}\}\ (5.1)\]
of $U_\theta(Y_{a,n-a})$ is inherited from $\tilde{H}_\eta(Y_{a,n-a})$. In order to determine the multiplicity of the eigenvalues $\pm 1$, we next investigate the value $I(c)$ for any closed path $c$ on $Y_{a,n-a}$.

Since $c$ is a closed path, the number of arcs from an upper vertex to a lower vertex and the one from a lower vertex to an upper vertex have to be the same. This implies that $I(c)$ is always zero. Thus, $Y_{a,n-a}$ is always in the case (ii) of Proposition 4.4, so we have $(m_1, m_{-1}) = (1, 0)$. Therefore, a set of eigenvalues \[
abla \{1^{(n(n-1)/2-n+1)}, -1^{(n(n-1)/2-n)}\}\ (5.2)\]
of $U_\theta(Y_{a,n-a})$ is born. Combining (5.1) and (5.2), we have the statement.

We summarize this section. By Proposition 5.2, we see that the $H$-cospectral mates $Y_{a,n-a}$ for $K_n$ constructed by Guo and Mohar are actually $H_\eta$-cospectral for $K_n$. Moreover, they have the same spectrum in the sense of the transfer matrix $U_\theta$ with any $\eta$-function $\theta$ by Lemma 5.3. In the next section, we suggest a positive support of $U_\theta$ in a sense. This enables us to partially distinguish the digraphs $Y_{a,n-a}$ by their spectrum.

6 The positive and negative supports

As Emms, Hancock, Severini and Wilson [5] attempted to distinguish strongly regular graphs by the spectrum of matrices coming from quantum walks, we also want to define new matrices similar to the positive support of the Grover transfer matrix and consider the isomorphism problem of graphs from the viewpoint of quantum walks.

6.1 The positive support of the Grover transfer matrix

For a real matrix $M$, the positive support of $M$, denoted by $M^+$, is the $\{0, 1\}$-matrix obtained from $M$ as follows:

\[(M^+)^{xy} = \begin{cases} 
1 & \text{if } M_{xy} > 0, \\
0 & \text{otherwise}.
\end{cases}\]

Also, we define the negative support $M^-$ of $M$ by swapping the orientation of the inequality sign. The following is a basic formula on the positive support of the Grover transfer matrix.
Lemma 6.1 ([5]) Let $G$ be an undirected connected $k$-regular graph and $U = U(G)$ be the Grover transfer matrix. Then, we have

$$U^+ = kSK^*K - S.$$  

Consideration of the positive support of the $n$-th power has been done in various papers. Godsil and Guo [9] revealed a clear formula on the positive support $(U^2)^+$ of the square of $U$, which is that

$$(U^2)^+ = (U^+)^2 + I$$

holds for $k$-regular graphs with $k \geq 3$. In addition, consideration of $(U^3)^+$ was carried out in [8, 14]. More generally, $(U^n)^+$ has been investigated in [20]. On the other hand, those consideration always has assumptions on regularity or a condition on girth, and it seems that it has not been investigated much in general situation so far.

6.2 Our transfer matrix

Let $G$ be a digraph equipped with an $\eta$-function $\theta$. Define the diagonal matrix $D_\theta$ indexed by $A(G^\pm)$, where

$$(D_\theta)_{ab} = e^{\theta(a)i} \delta_{ab}.$$  

Now, we want to define the positive support of our transfer matrix $U_\theta = U_\theta(G)$, but this is a complex matrix, so we have to consider how to define its positive support. Considering the similarity to the one on undirected graphs, we propose the following definition.

Definition 6.2 Let $G$ be a digraph equipped with an $\eta$-function $\theta$. For a positive integer $n$, we define the positive support of the $n$-th power of the transfer matrix, denoted by $U^{(n,+)}_\theta = U_\theta(G)^{(n,+)}$, which is indexed by $A(G^\pm)$, where

$$(U^{(n,+)}_\theta)_{ab} = \begin{cases} 1 & \text{if } \text{Re}(D_\theta U^n_\theta)_{ab} > 0, \\ 0 & \text{otherwise}. \end{cases}$$

We will also consider the negative support of $U_\theta$. Define $U^{(n,-)}_\theta$ by swapping the orientation of the inequality sign.

If $G$ is an undirected graph, then $\theta$ is the zero function, so $D_\theta = I$ and $U_\theta(G) = U(G)$, where $U(G)$ is the Grover transfer matrix of the undirected graph $G$. Then, $D_\theta U^n_\theta = U(G)^n$, so we have $U_\theta(G)^{(n,+)} = (U(G)^n)^+$ for any positive integer $n$.

In the discussion below, our quantum walk on a digraph $G$ and the Grover walk on $G^\pm$ are intermixed, so we need to read cautiously.

Lemma 6.3 Let $G$ be a digraph equipped with an $\eta$-function $\theta$. Then, we have

(i) $D_\theta S_\theta = S(G^\pm)$;
(ii) \( D_\theta U_\theta = U(G^\pm) \).

**Proof**
(i) This statement can be checked by calculating the components of both sides.
(ii) Remarking that \( C = C(G) = C(G^\pm) \), we have

\[
D_\theta U_\theta = D_\theta S_\theta C = S(G^\pm)C = U(G^\pm).
\]

\( \Box \)

By this lemma, we see that the positive support of the first power of our transfer matrix is the same as the one of the Grover transfer matrix as follows. The reason for giving Definition 6.2 is to make this equality hold.

**Proposition 6.4** Let \( G \) be a digraph equipped with an \( \eta \)-function \( \theta \). For \( \varepsilon \in \{ +, - \} \), we have

\[
U^{(1, \varepsilon)}_\theta = U^\varepsilon,
\]

where \( U = U(G^\pm) \). If \( G \) is \( k \)-regular,

\[
U^{(1, +)}_\theta = kSK^*K - S
\]

holds, where \( S = S(G^\pm) \).

**Proof** By (ii) of Lemma 6.3, we have

\[
\text{Re}(D_\theta U_\theta)_{ab} > 0 \iff U(G^\pm)_{ab} > 0
\]

for any arcs \( a, b \in A(G^\pm) \). Considering the negative support as well, we see that the first statement follows. If \( G \) is \( k \)-regular, then \( G^\pm \) is also \( k \)-regular, so we have the second statement by Lemma 6.1.

\( \Box \)

**6.3 The negative support of the Grover transfer matrix**

Before discussing the positive support \( U^{(2, +)}_\theta \) of the square, we have to consider the negative support of \( U \) for undirected graphs. Actually, we will see that \( U^{(2, \varepsilon)}_\theta \) can be expressed by not only the positive also negative supports of \( U^2 \).

Let \( G \) be a \( k \)-regular undirected graph and \( U = U(G) \). Recalling that

\[
U_{ab} = \frac{2}{k} \delta_{t(b), o(a)} - \delta_{a^{-1}, b},
\]

we see that \( U_{ab} < 0 \) if and only if \( \delta_{a^{-1}, b} = 1 \). Thus, we have the following.

\( \Box \) Springer
Proposition 6.5 Let $G$ be a $k$-regular undirected graph with $k \geq 3$ and $U$ be the Grover transfer matrix of $G$. Then, we have

$$U^\ast = S.$$ 

Next, we discuss the negative support $(U^2)^\ast$ of the square. For general description, digraphs are assumed. Let $G = (V, A)$ be a $k$-regular digraph equipped with an $\eta$-function $\theta$ and $U = U(G^\pm)$ be the Grover transfer matrix of $G^\pm$. For arcs $a, b \in A^\pm$, define the set $\mathcal{A}(a, b)$ as follows:

$$\mathcal{A}(a, b) = \left\{ z \in A^\pm \mid e^{-\theta(z)} U_{az} U_{zb} \neq 0 \right\}.$$ 

Classification of arcs $a, b \in A^\pm$ to give $|\mathcal{A}(a, b)| = 1$ is the key to determine the positive and negative supports of the square.

Lemma 6.6 Suppose $k \geq 3$. Let $G$ be a $k$-regular digraph equipped with an $\eta$-function $\theta$. For arcs $a, b \in A(G)^\pm$, we have $|\mathcal{A}(a, b)| \leq 1$, and the equality holds if and only if either of the following happens.

(i) $a = b$;
(ii) $o(a) = o(b)$ and $a \neq b$;
(iii) $t(a) = t(b)$ and $a \neq b$;
(iv) $t(b) \sim o(a)$ in $G^\pm$, but the arcs $a, b$ are neither in (i), (ii) nor (iii).

Proof Suppose there exists an arc $z \in \mathcal{A}(a, b)$. Then, we have

$$\frac{2}{k} \delta_{t(z), o(a)} - \delta_{a, z^{-1}} \neq 0 \quad (6.1)$$

and

$$\frac{2}{k} \delta_{t(b), o(z)} - \delta_{z, b^{-1}} \neq 0. \quad (6.2)$$

Remarking that $(\delta_{t(z), o(a)}, \delta_{a, z^{-1}}) = (0, 1)$ does not happen, Equality (6.1) is equivalent to $(\delta_{t(z), o(a)}, \delta_{a, z^{-1}}) = (1, 0), (1, 1)$. Dealing with (6.2) similarly, there are precisely $2 \times 2$ cases which we have to consider. In each case, we have $\delta_{t(z), o(a)} = \delta_{t(b), o(z)} = 1$, so $z$ is determined to be the arc $(t(b), o(a))$. This implies that $|\mathcal{A}(a, b)| \leq 1$. Moreover, the $2 \times 2$ cases are nothing but the ones of (i), (ii), (iii), (iv) in our statement. \hfill $\Box$

Corollary 6.7 Let $G$ be a $k$-regular undirected graph and $U = U(G)$ be the Grover transfer matrix. For arcs $a, b \in A(G)$, $(U^2)_{ab} > 0$ if and only if $(a, b)$ is in either (i) or (iv) of Lemma 6.6, and $(U^2)_{ab} < 0$ if and only if $(a, b)$ is in either (ii) or (iii) of Lemma 6.6.

Proof By Lemma 6.6, we see that $(U^2)_{ab} \neq 0$ if and only if $|\mathcal{A}(a, b)| = 1$. From this, we have $(U^2)_{ab} > 0$ if $(a, b)$ is in either (i) or (iv), and $(U^2)_{ab} < 0$ if $(a, b)$ is in either (ii) or (iii). \hfill $\Box$
By this corollary, we are interested in the cases (ii) and (iii) to find \((U^2)^-\). In order to describe these situations in matrix, we introduce the following matrices.

Let \(G\) be a digraph. We define the two matrices \(F_t\) and \(F_o\) whose rows are indexed by \(V(G)\) and columns are indexed by \(A(G)^\pm\), respectively, where

\[
(F_t)_{x,a} = \delta_{x,t(a)}
\]

and

\[
(F_o)_{x,a} = \delta_{x,o(a)}.
\]

**Lemma 6.8** Let \(G\) be a digraph equipped with an \(\eta\)-function \(\theta\). Then, we have

(i) \((F_o^T F_t)_{ab} = \delta_{t(b),o(a)}\);

(ii) \(S F_t^T = F_o^T F_t - S\),

where \(S = S(G^\pm)\).

**Proof** Proven by direct calculation. \(\square\)

On regular digraphs, we have the following.

**Lemma 6.9** Suppose \(k \geq 3\). Let \(G\) be a \(k\)-regular digraph equipped with an \(\eta\)-function \(\theta\). Then, we have

(i) \(U_\theta = D_\theta^{-1}(\frac{2}{k} F_o^T F_t - S)\);

(ii) \(U_\theta^{(1,+)} = F_o^T F_t - S\),

where \(S = S(G^\pm)\).

**Proof** In order to prove (i), we first state

\[
U(G^\pm) = \frac{2}{k} F_o^T F_t - S.
\]  

(6.3)

This is proven by

\[
U(G^\pm)_{ab} = \frac{2}{k} \delta_{t(b), o(a)} - \delta_{a, b}^{-1}
\]

(by (2.1))

\[
= \frac{2}{k} (F_o^T F_t)_{ab} - S_{ab}
\]

(by (i) of Lemma 6.8)

\[
= \left(\frac{2}{k} F_o^T F_t - S\right)_{ab}.
\]

Therefore, we have

\[
U_\theta = D_\theta^{-1} U(G^\pm)
\]

(by (ii) of Lemma 6.3)

\[
= D_\theta^{-1} \left(\frac{2}{k} F_o^T F_t - S\right).
\]  

(by (6.3))
We next prove (ii). Remark that \( U^{(1, +)}_\theta = U(G^{\pm})^+ \) by Proposition 6.4. From (2.1) and \( k \geq 3 \), we have

\[
(U^{(1, +)}_\theta)_{ab} = \begin{cases} 
1 & \text{if } o(a) = t(b) \text{ and } a \neq b^{-1}, \\
0 & \text{otherwise}.
\end{cases}
\]

\[
= \delta_{o(a), t(b)} (1 - \delta_{a, b^{-1}})
\]

\[
= \delta_{o(a), t(b)} - \delta_{o(a), t(b)} \delta_{a, b^{-1}}
\]

\[
= \delta_{o(a), t(b)} - \delta_{a, b^{-1}}
\]

\[
= (F_o^\top F_t - S)_{ab}
\]

(by (i) of Lemma 6.8).

\[\square\]

Now, we give the structure of \((U^2)^-\).

**Proposition 6.10** Suppose \( k \geq 3 \). Let \( G \) be a \( k \)-regular undirected graph and \( U \) be the Grover transfer matrix of \( G \). Then, we have

\[
(U^2)^- = SU^+ + U^+ S.
\]

**Proof** For \( \varepsilon \in \{o, t\} \), we can confirm that

\[
(F_\varepsilon^\top F_\varepsilon - I)_{ab} = \delta_{\varepsilon(a), \varepsilon(b)} - \delta_{a, b} = \begin{cases} 
1 & \text{if } \varepsilon(a) = \varepsilon(b) \text{ and } a \neq b, \\
0 & \text{otherwise},
\end{cases}
\]

so by Corollary 6.7, we have

\[
(U^2)^- = F_t^\top F_t - I + F_o^\top F_o - I
\]

\[
= SF_o^\top F_t + F_o^\top F_t S - 2I \quad \text{(by (ii) of Lemma 6.8)}
\]

\[
= S(U^+ + S) + (U^+ + S)S - 2I \quad \text{(by (ii) of Lemma 6.9)}
\]

\[
= SU^+ + U^+ S.
\]

\[\square\]

### 6.4 The positive and negative supports of the square of our transfer matrix

In this subsection, we discuss the positive and negative supports of the square of transfer matrices. Let \( \varepsilon \in \{+, -\} \). In the case of \( U^{(2, \varepsilon)}_\theta \), the argument must be divided by the value of \( \eta \).

Let \( G = (V, A) \) be a digraph. Then, the digraph \( G^{-1} = (V, A^{-1}) \) is so-called the transpose graph of \( G \). Also, when \( G \) is equipped with an \( \eta \)-function \( \theta \), we sometimes write as \( \theta = \theta_G \). For an \( \eta \)-function \( \theta \), we define a function \(-\theta\) by \((-\theta)(a) = -\theta(a)\) for any arc \( a \in A(G^{\pm}) \). Clearly,

\[
-\theta_G = \theta_G^{-1} \quad \text{(6.4)}
\]
follows. First, we state the following.

**Proposition 6.11** Let $G$ be a digraph equipped with an $\eta$-function $\theta$. Then, we have

$$U^{(2,\varepsilon)}_{\theta}(G) = U^{(2,\varepsilon)}_{\theta}(G^{-1})$$

for $\varepsilon \in \{+, -\}$.

**Proof** It is enough to show that

$$\text{Re}(D_{\theta}(G)U_{\theta}(G)^{2})_{ab} = \text{Re}(D_{\theta}(G^{-1})U_{\theta}(G^{-1})^{2})_{ab}$$

holds for any arcs $a, b \in A(G^{\pm})$. Writing as $U = U(G^{\pm})$, we can calculate as follows:

$$\text{Re}(D_{\theta}(G)U_{\theta}(G)^{2})_{ab} = \text{Re}(UD_{\theta}(G)U_{\theta}(G^{-1})^{2})_{ab}$$

(by (ii) of Lemma 6.3)

$$= \sum_{z \in A(G^{\pm})} \text{Re}\left(e^{-\theta_{G}(z)}U_{az}U_{zb}\right)$$

$$= \sum_{z \in A(G^{\pm})} \text{Re}\left(e^{-\theta_{G}(z)}U_{az}U_{zb}\right)$$

(by (6.4))

$$= \sum_{z \in A(G^{\pm})} \text{Re}\left(e^{-(\theta_{G}(z)-1)}U_{az}U_{zb}\right)$$

$$= \text{Re}(UD_{\theta}(G^{-1})^{-1}U)_{ab}$$

$$= \text{Re}(D_{\theta}(G^{-1})U_{\theta}(G^{-1})^{2})_{ab}.$$ 

$\square$

From the above proposition, we unfortunately cannot distinguish $G$ and $G^{-1}$ by $U^{(2,\varepsilon)}_{\theta}$. 

**Lemma 6.12** Let $G$ be a digraph equipped with an $\eta$-function $\theta$. Then, we have

$$U_{-\theta}(G) = U_{\theta}(G^{-1}).$$

**Proof** By (6.4), we have

$$(S_{-\theta}(G))_{ab} = e^{(-\theta_{G})(b)i}\delta_{a,b^{-1}}$$

$$= e^{\theta_{G^{-1}}(b)i}\delta_{a,b^{-1}}$$

$$= (S_{\theta}(G^{-1}))_{ab},$$

so $U_{-\theta}(G) = S_{-\theta}(G)C = S_{\theta}(G^{-1})C = U_{\theta}(G^{-1}).$ 

$\square$

For an $\eta$-function $\theta$, the function $-\theta$ is nothing but the $(-\eta)$-function. By Lemma 6.12, we need to consider only the range $0 \leq \eta \leq \pi$ since we consider $\eta$ to be the rotation angle.
Now, we determine the structure of $U^{(2,\varepsilon)}_{\theta}$ for $\varepsilon \in \{+, -\}$. For two arcs $a, b$, we define the ordered pair $m(a, b) = (t(b), o(a))$. Remark that $m(a, b)$ does not necessarily belong to the arc set. Let $G$ be a $k$-regular digraph equipped with an $\eta$-function $\theta$ and $U = U(G^{\pm})$. Observe that

$$(D_{\theta}U^{2}_{\theta})_{ab} = \sum_{z \in A(G^{\pm})} e^{-\theta(z)\varepsilon}U_{az}U_{zb}$$

and by Lemma 6.6, if the contents of the sum appear, it is just one and it is nothing but $z = m(a, b)$. Then,

$$(D_{\theta}U^{2}_{\theta})_{ab} = e^{-\theta(m(a,b))\varepsilon}(U^{2})_{ab}, \quad (6.5)$$

so the value of $(D_{\theta}U^{2}_{\theta})_{ab}$ is, roughly speaking, either rotated $U^{2}_{ab}$ or non-rotated $U^{2}_{ab}$, and it depends on whether $m(a, b) \in A(G) \cap A(G)^{-1}$ or not. Therefore, we define the following matrix $R$, which is indexed by $A(G^{\pm})$, such that

$$R_{ab} = \begin{cases} 
1 & \text{if } m(a, b) \in A(G) \cap A(G)^{-1}, \\
0 & \text{otherwise}.
\end{cases}$$

By using this matrix, $U^{(2,\varepsilon)}_{\theta}$ can be described depending on the value of $\eta$ as follows: For $\varepsilon \in \{+, -\}$, we denote the element of $\{+, -\} \setminus \{\varepsilon\}$ by $-\varepsilon$.

**Theorem 6.13** Let $G$ be a digraph equipped with an $\eta$-function $\theta$ and $U = U(G^{\pm})$ be the Grover transfer matrix of $G^{\pm}$. For $\varepsilon \in \{+, -\}$, we have

$$U^{(2,\varepsilon)}_{\theta} = \begin{cases} 
(U^{2})_{\varepsilon} & \text{if } 0 \leq \eta < \frac{\pi}{2}, \\
(U^{2})_{\varepsilon} \circ R & \text{if } \eta = \frac{\pi}{2}, \\
(U^{2})_{\varepsilon} \circ R + (U^{2})^{\varepsilon} \circ (J - R) & \text{if } \frac{\pi}{2} < \eta \leq \pi,
\end{cases}$$

where $A \circ B$ is the Hadamard product of $A$ and $B$, which is defined by $(A \circ B)_{xy} = A_{xy}B_{xy}$.

**Proof** We only provide a proof in the case of $\varepsilon = +$. Fix arcs $a, b \in A(G^{\pm})$. If $m(a, b) \notin A(G^{\pm})$, then $(D_{\theta}U^{2}_{\theta})_{ab} = 0$ by Lemma 6.6. From (6.5),

$$(D_{\theta}U^{2}_{\theta})_{ab} = \begin{cases} 
(U^{2})_{ab} & \text{if } m(a, b) \in A(G) \cap A(G)^{-1}, \\
e^{-\theta}(U^{2})_{ab} & \text{if } m(a, b) \in A(G^{\pm}) \setminus (A(G) \cap A(G^{-1})), \\
0 & \text{otherwise}.
\end{cases} \quad (6.6)$$

Suppose $0 \leq \eta < \frac{\pi}{2}$. By (6.6), we have $\text{Re}(D_{\theta}U^{2}_{\theta})_{ab} = \text{Re}(U^{2})_{ab}$, so $U^{(2,+)}_{\theta} = (U^{2})^{+}$ holds.

In the case of $\eta = \frac{\pi}{2}$, we see that $\text{Re}(D_{\theta}U^{2}_{\theta})_{ab} > 0$ if and only if $(U^{2})_{ab} > 0$ and $m(a, b) \in A(G) \cap A(G)^{-1}$ by (6.6). This implies $(U^{(2,+)}_{\theta})_{ab} = ((U^{2})^{+})_{ab}R_{ab}$. 

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Similarly, in the case of $\frac{\pi}{2} < \eta \leq \pi$, \(\text{Re}(D_\theta U^2_\theta)_{ab} > 0\) if and only if
\[
(U^2)_{ab} > 0 \quad \text{and} \quad m(a, b) \in A(G) \cap A(G)^{-1},
\]
or
\[
(U^2)_{ab} < 0 \quad \text{and} \quad m(a, b) \in A(G^\pm) \setminus (A(G) \cap A(G^{-1}))
\]
by (6.6). This implies \((U^{\(2,+)\}_\theta)_{ab} = ((U^2)^{\ +}_{ab} R_{ab} + ((U^2)^{\ -}_{ab}(1 - R_{ab})). Summarizing the above, we have the statement. \(\square\)

By this theorem, we see that the structure of \(U^{\(2,+)\}(G)\) is determined by the under-lying graph \(G^\pm\) if \(0 \leq \eta < \frac{\pi}{2}\). On the other hand, if \(\frac{\pi}{2} \leq \eta \leq \pi\), the information of digraphs lives. However, if a digraph \(G\) does not have any digons, \(R\) is determined to be the zero matrix, so we have
\[
U^{\(2,+)\}_\theta = \begin{cases} 
(U^2)^{\ +} & \text{if } 0 \leq \eta < \frac{\pi}{2}, \\
O & \text{if } \eta = \frac{\pi}{2}, \\
(U^2)^{\ -} & \text{if } \frac{\pi}{2} < \eta \leq \pi.
\end{cases}
\]
In any case, it may be interesting that the structure of \(U^{\(2,+)\}_\theta\) is represented by the positive and negative supports of the underlying graph and it moreover changes by the value of \(\eta\).

### 7 Counting digons

In this section, we find the number of digons via \(U^{\(2,+)\}_\theta\). As a consequence, we show that Guo–Mohar’s digraphs \(Y_{a,n-a}\) which could not be identified by eigenvalues of \(H, H_\eta, U_\theta, U^{\(1,+)\}_\theta\) can be half identified by \(U^{\(2,+)\}_\theta\).

**Proposition 7.1** Let \(G\) be a digraph equipped with an \(\eta\)-function \(\theta\). We denote the number of digons in \(G\) by \(d\). Then, we have
\[
\text{Tr}(U^{\(2,+)\}_\theta) = \begin{cases} 
2|E(G^\pm)| & \text{if } 0 \leq \eta < \frac{\pi}{2}, \\
2d & \text{if } \frac{\pi}{2} \leq \eta \leq \pi.
\end{cases}
\]

**Proof** Let \(U = U(G^\pm)\). For any arc \(a \in A(G^\pm)\), the pair of arcs \((a, a)\) is in (i) of Lemma 6.6, so \(((U^2)^{\ +}_{aa} = 1\) by Corollary 6.7. Suppose \(0 \leq \eta < \frac{\pi}{2}\). By Theorem 6.13, we have
\[
\text{Tr}(U^{\(2,+)\}_\theta) = \text{Tr}((U^2)^{\ +}) = \sum_{a \in A(G^\pm)} ((U^2)^{\ +}_{aa} = |A(G^\pm)| = 2|E(G^\pm)|.
\]

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Suppose \( \frac{\pi}{2} \leq \eta \leq \pi \). Since \( R_{aa} = 1 \) if and only if \( a \in A(G) \cap A(G)^{-1} \),
\[
\text{Tr}(U^{(2,+)}_\theta) = \text{Tr}((U^2)^+ \circ R) \quad \text{(by Theorem 6.13)}
\]
\[
= \sum_{a \in A(G^+)} ((U^2)^+)_{aa} R_{aa}
\]
\[
= \sum_{a \in A(G) \cap A(G)^{-1}} 1
\]
\[
= 2d.
\]

Using this, we see that Guo–Mohar’s digraphs \( Y_{a,n-a} \) can be half identified by eigenvalues of \( U^{(2,+)}_\theta \).

**Corollary 7.2** Let \( \frac{\pi}{2} \leq \eta \leq \pi \) and we consider the \( \eta \)-function \( \theta \). Suppose \( a \geq n - a \) and \( b \geq n - b \), i.e., \( a, b \geq \frac{n}{2} \). If \( a \neq b \), then
\[
\Phi(U^{(2,+)}_\theta(Y_{a,n-a})) \neq \Phi(U^{(2,+)}_\theta(Y_{b,n-b})),
\]
where \( \Phi(M) \) denotes the characteristic polynomial of a matrix \( M \).

**Proof** We denote the number of digons in the digraph \( Y_{k,n-k} \) by \( d(k) \). Then,
\[
d(k) = \frac{k(k-1)}{2} + \frac{(n-k)(n-k-1)}{2}.
\]
Without loss of generality, we can assume \( a > b \). Since \( a + b > n \), we have
\[
d(a) - d(b) = (a - b)(a + b - n) > 0.
\]
In particular, \( d(a) \neq d(b) \). By (ii) of Proposition 7.1, it can be seen that the coefficients of the characteristic polynomials are different.

Note that we have \( d(a) = d(n-a) \), but \( Y_{a,n-a} \) and \( Y_{n-a,a} \) are not isomorphic to each other unless \( a \in \{0, n\} \). However, \( Y_{n-a,a}^{-1} = Y_{a,n-a} \), so we unfortunately have \( \Phi(U^{(2,+)}_\theta(Y_{a,n-a})) = \Phi(U^{(2,+)}_\theta(Y_{n-a,a})) \) by Proposition 6.11. The two digraphs \( Y_{a,n-a} \) and \( Y_{n-a,a} \) cannot be identified by the spectrum of \( U^{(2,+)}_\theta \).

**8 Tables**

Up to the previous section, we have obtained several new matrices defined by digraphs. In this section, using computer, we observe the behavior that small digraphs can be identified by eigenvalues of these matrices with how much. Here, we made the
Table 3  The adjacency matrix spectra of small digraphs

| Order | 2   | 3   | 4   | 5   | 6   |
|-------|-----|-----|-----|-----|-----|
| Number of digraphs | 3   | 16  | 218 | 9608| 1540944|
| Number of distinct characteristic polynomials | 2   | 7   | 46  | 718 | 35237|
| Maximum size of a $A$-cospectral class | 2   | 6   | 42  | 592 | 15842|
| Number of digraphs determined by $A$-spectrum | 1   | 5   | 23  | 166 | 2314|
| Number of $A$-cospectral classes containing: |     |     |     |     |     |
| (a) No graphs | 0   | 3   | 35  | 685 | 35086|
| (b) Only graphs | 1   | 2   | 5   | 15  | 69  |
| (c) At least one graph and a digraph | 1   | 2   | 6   | 18  | 82  |

Table 4  The $H_\eta$-spectra of small digraphs with $\eta = \frac{\pi}{\lambda}$

| Order | 2   | 3   | 4   | 5   | 6   |
|-------|-----|-----|-----|-----|-----|
| Number of digraphs | 3   | 16  | 218 | 9608| 1540944|
| Number of distinct characteristic polynomials | 2   | 7   | 41  | 765 | 81175|
| Maximum size of a $H_\eta$-cospectral class | 2   | 6   | 18  | 84  | 888 |
| Number of digraphs determined by $H_\eta$-spectrum | 1   | 3   | 9   | 82  | 1559|
| Number of $H_\eta$-cospectral classes containing: |     |     |     |     |     |
| (a) No graphs | 0   | 3   | 30  | 732 | 81024|
| (b) Only graphs | 1   | 1   | 1   | 1   | 1   |
| (c) At least one graph and a digraph | 1   | 3   | 10  | 32  | 150 |

following tables similar to the one for adjacency matrices and Hermitian adjacency matrices made by Guo and Mohar [12].

Let $E_n = (\{1, 2, \ldots, n\}, \emptyset)$ be the empty graph with $n$ vertices. We give tables on $U_\theta^{(2, +)}$, but the transfer matrix cannot be defined from $E_n$, so this graph is excluded from the following tables.

8.1 Discussion on the tables

Characterizing graphs by eigenvalues is one of the interesting research topics in spectral graph theory. In the case of undirected graphs, there are many studies that characterize graphs by eigenvalues, while there are many studies that construct cospectral graphs, which are non-isomorphic graphs with the same eigenvalues. For example, [3,11,18] can be cited as references. Chapter 14 of the first one is on spectral characterization and the other two are on constructing cospectral graphs.

In fact, it is extremely difficult to find a matrix to characterize all graphs by eigenvalues. Digraphs are even more difficult. First, we compare Tables 3 and 5. Table 3 is obtained using the adjacency matrix, and Table 5 is obtained using the Hermitian adjacency matrix. There are 1540944 digraphs with 6 vertices, from which only 35237 distinct characteristic polynomials can be obtained. In Table 5, there are 10920 distinct
characteristic polynomials. On the other hand, according to the maximum size of a cospectral class (on 6 vertices) in both tables, Table 3 has 15842 and Table 5 has 1338. This shows that Hermitian adjacency matrices more easily find a specific digraph from digraphs with the same eigenvalues. In this way, the size of a cospectral class is also an important index for evaluating the goodness of matrices. Such as $H_\eta$ and $U_{\theta}^{(n,+)}$, we defined many matrices induced by digraphs. Tables 4, 6, 7 and 8 are the tables obtained from $H_{\pi^3}$, $H_{\frac{\pi}{2} \pi}$, $U_{\theta}^{(2,+)}$ with $\eta = \frac{\pi}{2}$, and $U_{\theta}^{(2,+)}$ with $\frac{\pi}{2} < \eta \leq \pi$, respectively. Among these, $H_{\frac{\pi}{2}}$ of Table 4 is relatively good, but $U_{\theta}^{(2,+)}$ is unexpectedly bad for any $\eta$. It is worth investigating in the future how $\eta$ plays a role in distinguishing digraphs. Note that the information of digraphs completely disappears when $0 \leq \eta < \frac{\pi}{2}$ by Theorem 6.13. However, as for the transfer matrix, there is still room for further consideration because $U_{\theta}^{(n,+)}$ can be considered for any $n \in \mathbb{N}$.

### 9 Summaries and remarks

In this paper, we proposed a quantum walk defined by digraphs and stated that the transfer matrix relates to Hermitian adjacency matrices. Our quantum walk is a generalization of the Grover walk, and there is an arbitrariness of perturbation. If $\eta = 0$, this is nothing but the Grover walk on the underlying graph. In Sect. 6, we defined the positive and negative supports of the transfer matrix to the $n$-th power, and clarified the structure for the case of $n = 2$. Theorem 6.13 states that the structure of $U_{\theta}^{(2,\varepsilon)}$ discretely changes depending on $\eta$. However, the values in Tables 7 and 8 are by no means good. Considerations for $n \geq 3$ should be done as our future tasks. Finding an explicit formula on $U_{\theta}^{(n,\varepsilon)}$ is also interesting.

On the other hand, the eigenvalues of our transfer matrix are roughly determined from those of Hermitian adjacency matrices (Theorem 4.3). Therefore, eigenvalue analysis of Hermitian adjacency matrices themselves seems to be important in order to study properties of the quantum walk brought by features that each digraph has. For example, research to determine periodic digraphs while establishing a method for eigenvalue analysis of Hermitian adjacency matrices may be interesting. Also,
Table 6  The $H_\eta$-spectra of small digraphs with $\eta = \frac{2}{3} \pi$

| Order | 2   | 3   | 4   | 5   | 6   |
|-------|-----|-----|-----|-----|-----|
| Number of digraphs | 3   | 16  | 218 | 9608| 1540944 |
| Number of distinct characteristic polynomials | 2   | 5   | 20  | 150 | 3698  |
| Maximum size of a $H_\eta$-cospectral class | 2   | 6   | 27  | 243 | 2430  |
| Number of digraphs determined by $H_\eta$-spectrum | 1   | 1   | 1   | 1   | 1     |
| Number of $H_\eta$-cospectral classes containing: |     |     |     |     |       |
| (a) No graphs | 0   | 1   | 9   | 117 | 3547  |
| (b) Only graphs | 1   | 1   | 1   | 1   | 1     |
| (c) At least one graph and a digraph | 1   | 3   | 10  | 32  | 150   |

Table 7  The $U(2,+)_\eta$-spectra of small digraphs except $E_n$ with $\eta = \frac{\pi}{2}$

| Order | 2   | 3   | 4   | 5   | 6   |
|-------|-----|-----|-----|-----|-----|
| Number of digraphs | 3   | 16  | 218 | 9608| 1540944 |
| Number of distinct characteristic polynomials | 2   | 6   | 34  | 371 | 11748 |
| Maximum size of a $U(2,+)_\eta$-cospectral class | 1   | 6   | 53  | 700 | 37013 |
| Number of digraphs determined by $U(2,+)_\eta$-spectrum | 2   | 4   | 13  | 50  | 284   |
| Number of $U(2,+)_\eta$-cospectral classes containing: |     |     |     |     |       |
| (a) No graphs | 1   | 3   | 25  | 339 | 11598 |
| (b) Only graphs | 1   | 3   | 9   | 32  | 150   |
| (c) At least one graph and a digraph | 0   | 0   | 0   | 0   | 0     |

Table 8  The $U(2,+)_\eta$-spectra of small digraphs except $E_n$ with $\frac{\pi}{2} < \eta \leq \pi$

| Order | 2   | 3   | 4   | 5   | 6   |
|-------|-----|-----|-----|-----|-----|
| Number of digraphs | 3   | 16  | 218 | 9608| 1540944 |
| Number of distinct characteristic polynomials | 2   | 6   | 45  | 601 | 20306 |
| Maximum size of a $U(2,+)_\eta$-cospectral class | 1   | 6   | 22  | 204 | 5120  |
| Number of digraphs determined by $U(2,+)_\eta$-spectrum | 2   | 4   | 13  | 47  | 280   |
| Number of $U(2,+)_\eta$-cospectral classes containing: |     |     |     |     |       |
| (a) No graphs | 1   | 3   | 36  | 569 | 20156 |
| (b) Only graphs | 1   | 3   | 9   | 27  | 135   |
| (c) At least one graph and a digraph | 0   | 0   | 0   | 5   | 15     |
researching matrices associated with quantum walks to determine or estimate invariants of digraphs may be worthwhile.

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