

The Discrete-time Quaternionic Quantum Walk and the Second Weighted Zeta Function on a Graph

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We define the quaternionic quantum walk on a finite graph and investigate its properties. This walk can be considered as a natural quaternionic extension of the Grover walk on a graph. We explain the way to obtain all the right eigenvalues of a quaternionic matrix and a notable property derived from the unitarity condition for the quaternionic quantum walk. Our main results determine all the right eigenvalues of the quaternionic quantum walk by using complex eigenvalues of the quaternionic weighted matrix which is easily derivable from the walk. Since our derivation is owing to a quaternionic generalization of the determinant expression of the second weighted zeta function, we explain the second weighted zeta function and the relationship between the walk and the second weighted zeta function.

KEYWORDS: Quantum walk, Ihara zeta function, quaternion, quaternionic quantum walk

1. Introduction

The discrete-time quaternionic quantum walk on a graph is a quantum process on a graph which is governed by a unitary matrix. The study of quantum walks started in earnest as quantum versions of random walks around the end of the last century, and quantum walks have been developed rapidly for more than two decades in connection with various fields such as quantum information science and quantum physics. Detailed information on quantum walks can be found in several books at present, for example, Manouchehri and Wang [12], Portugal [13], Konno [8]. An important example of the quantum walk on a graph is the Grover walk which originates from Grover's algorithm. Grover's algorithm which was introduced in [5] is a quantum search algorithm that performs quadratically faster than the best classical search algorithm. Later various researchers investigated the Grover walk and developed the theory of discrete-time quantum walks intensively.

Recently, Konno [9] established a quaternionic extension of quantum walks, which can be viewed as quaternionic quantum dynamics. One of the important backgrounds of quaternionic quantum walk is quaternionic quantum mechanics. The origin of quaternionic quantum mechanics goes back to the axiomatization of quantum mechanics by Birkhoff and von Neumann in 1930s. After that, the subject was studied further by Finkelstein, Jauch, and Speiser [4], and more recently by Adler [1] and others. One significant motivation of studying quaternionic quantum mechanics is that physical reality might be described by quaternionic quantum system at the fundamental level, and this dynamics is described asymptotically by the (ordinary) quantum field theory at the level of all presently known physical phenomena. A detailed exposition of quaternionic quantum mechanics can be found in Adler [1].

On the other hand, Zeta functions of graphs have been investigated for half a century. Their origin is the Ihara zeta function which was defined by Ihara [7], and various extensions have appeared so far. Among them we focus on the second weighted zeta function of a graph. The second weighted zeta function proposed by Sato [14] is a kind of generalization of that in [2, 6]. This is a multi-weighted version of the Ihara zeta function, and has several applications in discrete-time quantum walks and quantum graphs. For example, the second weighted zeta function played essential roles in the concise proof of the spectral mapping theorem for the Grover walk on a graph in [11].

In this paper, we define the discrete-time quaternionic quantum walk on a graph as a quaternionic extension of the Grover walk on a finite graph, and discuss its right spectrum and the relationship between the walk and the second weighted zeta function of a graph. Our results can be viewed as a generalization of [10].

2. The Grover Walk on a Graph

Let $G = (V(G), E(G))$ be a finite connected graph with the set $V(G)$ of vertices and the set $E(G)$ of undirected edges uv joining two vertices u and v . We assume that G is finite connected and has neither loops nor multiple edges throughout. For $uv \in E(G)$, we mean by an arc (u, v) the directed edge from u to v . Let $D(G) = \{(u, v), (v, u) \mid uv \in E(G)\}$ and $|V(G)| = n, |E(G)| = m, |D(G)| = 2m$. For $e = (u, v) \in D(G)$, $o(e) = u$ and $t(e) = v$ denote the *origin* and the *terminus* of e , respectively. Furthermore, let $e^{-1} = (v, u)$ be the *inverse* of $e = (u, v)$. The *degree* $d_u = \deg u = \deg_G u$ of a vertex u of G is the number of edges incident to u . A *path* P of length ℓ in G is a sequence $P = (e_1, \dots, e_\ell)$ of ℓ arcs such that $e_i \in D(G)$ and $t(e_i) = o(e_{i+1})$ for $i \in \{1, \dots, \ell - 1\}$. We set $o(P) = o(e_1)$ and $t(P) = t(e_\ell)$. $|P|$ denotes the length of P . A path $P = (e_1, \dots, e_\ell)$ is said to be a *cycle* if $t(P) = o(P)$ and to have a *backtracking* if $e_{i+1} = e_i^{-1}$ for some $i(1 \leq i \leq \ell - 1)$. The *inverse* of a path $P = (e_1, \dots, e_\ell)$ is the path $(e_\ell^{-1}, \dots, e_1^{-1})$ and is denoted by P^{-1} .

We give a definition of the discrete-time quantum walk on G . Let $\mathcal{H} = \bigoplus_{e \in D(G)} \mathbb{C}|e\rangle$ be the finite dimensional Hilbert space spanned by arcs of G . The transition matrix \mathbf{U} of a discrete-time quantum walk consists of the following two consecutive operations $\mathbf{U} = \mathbf{S}\mathbf{C}$:

1. For each $u \in V$, we perform a unitary transformation \mathbf{C}_u on the states $|f\rangle$ that satisfy $t(f) = u$.
2. For all $e \in D(G)$, we perform the shift \mathbf{S} that is defined by $\mathbf{S}|e\rangle = |e^{-1}\rangle$.

The transition matrix \mathbf{U}^{Gro} of the Grover walk on G is defined by setting the Grover's diffusion matrix as \mathbf{C}_u :

$$\mathbf{C}_u = \begin{pmatrix} -1 + \frac{2}{d_u} & \frac{2}{d_u} & \cdots & \frac{2}{d_u} \\ \frac{2}{d_u} & -1 + \frac{2}{d_u} & \cdots & \frac{2}{d_u} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{2}{d_u} & \frac{2}{d_u} & \cdots & -1 + \frac{2}{d_u} \end{pmatrix}.$$

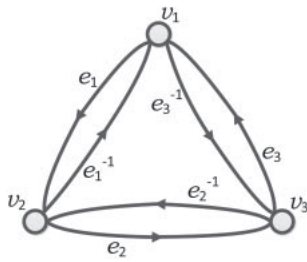
Then $\mathbf{U}^{\text{Gro}} = (\mathbf{U}_{ef}^{\text{Gro}})_{e, f \in D(G)}$ is given by

$$\mathbf{U}_{ef}^{\text{Gro}} = \begin{cases} 2/d_{o(e)} (= 2/d_{t(f)}) & \text{if } t(f) = o(e) \text{ and } f \neq e^{-1}, \\ 2/d_{o(e)} - 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

\mathbf{U}^{Gro} is called the *Grover matrix*.

We denote by $\text{Spec}(\mathbf{A})$ the multiset of eigenvalues of a complex square matrix \mathbf{A} counted with multiplicity. We shall give examples of Grover walks and their spectra.

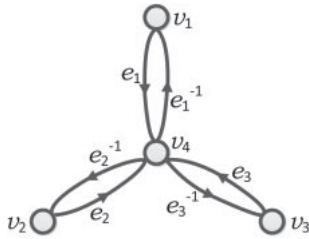
Example 2.1. $G = K_3$. Then $d_{o(e)} = 2$ for all $e \in D(G)$ and \mathbf{U}^{Gro} is given as follows:



$$\mathbf{U}^{\text{Gro}} = \begin{matrix} & e_1 & e_1^{-1} & e_2 & e_2^{-1} & e_3 & e_3^{-1} \\ \begin{matrix} e_1 \\ e_1^{-1} \\ e_2 \\ e_2^{-1} \\ e_3 \\ e_3^{-1} \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix}.$$

$$\text{Spec}(\mathbf{U}^{\text{Gro}}) = \{1, 1, \frac{-1 \pm \sqrt{3}i}{2}, \frac{-1 \pm \sqrt{3}i}{2}\}.$$

Example 2.2. $G = K_{1,3}$. Then $d_{o(e_1)} = d_{o(e_2)} = d_{o(e_3)} = 1, d_{o(e_1^{-1})} = d_{o(e_2^{-1})} = d_{o(e_3^{-1})} = 3$ and \mathbf{U}^{Gro} is given as follows:



$$\mathbf{U}^{\text{Gro}} = \begin{matrix} & e_1 & e_1^{-1} & e_2 & e_2^{-1} & e_3 & e_3^{-1} \\ \begin{matrix} e_1 \\ e_1^{-1} \\ e_2 \\ e_2^{-1} \\ e_3 \\ e_3^{-1} \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{2}{3} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ \frac{2}{3} & 0 & -\frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{2}{3} & 0 & \frac{2}{3} & 0 & -\frac{1}{3} & 0 \end{pmatrix} \end{matrix}.$$

$$\text{Spec}(\mathbf{U}^{\text{Gro}}) = \{\pm i, \pm i, 1, -1\}.$$

Let $\mathbf{T} = (\mathbf{T}_{uv})_{u, v \in V(G)}$ be the $n \times n$ matrix defined as follows:

$$\mathbf{T}_{uv} = \begin{cases} 1/d_u & \text{if } (u, v) \in D(G), \\ 0 & \text{otherwise.} \end{cases}$$

In [3], Emms *et al.* determined the spectrum of \mathbf{U}^{Gro} by using that of \mathbf{T} .

Theorem 2.3 (Emms, Hancock, Severini and Wilson [3]). *Let G be a connected graph with n vertices and m edges. The transition matrix \mathbf{U}^{Gro} has $2n$ eigenvalues of the form:*

$$\lambda = \lambda_{\mathbf{T}} \pm i\sqrt{1 - \lambda_{\mathbf{T}}^2},$$

where $\lambda_{\mathbf{T}}$ is an eigenvalue of the matrix \mathbf{T} . The remaining $2(m - n)$ eigenvalues of \mathbf{U}^{Gro} are ± 1 with equal multiplicities.

As stated in Section 1, Konno and Sato [11] gave a concise proof of Theorem 2.3 by using the second weighted zeta function of a graph.

3. A Quaternionic Extension of the Grover Walk on a Graph

In this section, we define a quaternionic extension of the Grover walk on G and discuss some of its properties. Beforehand, we give a brief account of quaternionic matrices and their right eigenvalues. Let \mathbb{H} be the set of quaternions. \mathbb{H} is a noncommutative associative algebra over \mathbb{R} , whose underlying real vector space has dimension 4 with a basis $1, i, j, k$ which satisfy the following relations:

$$i^2 = j^2 = k^2 = -1, \quad ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j.$$

For $x = x_0 + x_1i + x_2j + x_3k \in \mathbb{H}$, $x^* = x_0 - x_1i - x_2j - x_3k$ denotes the *conjugate* of x in \mathbb{H} . $|x| = \sqrt{xx^*} = \sqrt{x^*x} = \sqrt{x_0^2 + x_1^2 + x_2^2 + x_3^2}$ is called the *norm* of x . Since $x^{-1} = x^*/|x|^2$ for a nonzero element $x \in \mathbb{H}$, \mathbb{H} constitutes a skew field. Since quaternions do not mutually commute in general, we must treat left eigenvalues and right eigenvalues separately. In this paper, we concentrate only on right eigenvalues.

Let $\text{Mat}(m \times n, \mathbb{H})$ be the set of $m \times n$ quaternionic matrices and $\text{Mat}(n, \mathbb{H})$ the set of $n \times n$ quaternionic square matrices. For $\mathbf{M} \in \text{Mat}(m \times n, \mathbb{H})$, we can write $\mathbf{M} = \mathbf{M}^S + j\mathbf{M}^P$ uniquely where $\mathbf{M}^S, \mathbf{M}^P \in \text{Mat}(m \times n, \mathbb{C})$. Such an expression is called the *symplectic decomposition* of \mathbf{M} . \mathbf{M}^S and \mathbf{M}^P are called the *simplex part* and the *perplex part* of \mathbf{M} , respectively. The quaternionic conjugate \mathbf{M}^* of a quaternionic square matrix \mathbf{M} is obtained from \mathbf{M} by taking the transpose and then taking the quaternionic conjugate of each entry. A quaternionic square matrix \mathbf{M} is said to be *quaternionic unitary* if $\mathbf{M}^*\mathbf{M} = \mathbf{M}\mathbf{M}^* = \mathbf{I}$. We define ψ to be the map from $\text{Mat}(m \times n, \mathbb{H})$ to $\text{Mat}(2m \times 2n, \mathbb{C})$ as follows:

$$\psi : \text{Mat}(m \times n, \mathbb{H}) \longrightarrow \text{Mat}(2m \times 2n, \mathbb{C}) \quad \mathbf{M} \mapsto \begin{pmatrix} \mathbf{M}^S & -\overline{\mathbf{M}^P} \\ \mathbf{M}^P & \overline{\mathbf{M}^S} \end{pmatrix},$$

where $\overline{\mathbf{A}}$ is the complex conjugate of a matrix \mathbf{A} . Then ψ is an \mathbb{R} -linear map. We can easily check that

Lemma 3.1. *Let $\mathbf{M} \in \text{Mat}(m \times n, \mathbb{H})$ and $\mathbf{N} \in \text{Mat}(n \times m, \mathbb{H})$. Then*

$$\psi(\mathbf{M}\mathbf{N}) = \psi(\mathbf{M})\psi(\mathbf{N}).$$

Moreover, if $m = n$, then ψ is an injective \mathbb{R} -algebra homomorphism. We consider \mathbb{H}^n as a right vector space. $\lambda \in \mathbb{H}$ is said to be a right eigenvalue of \mathbf{M} and $\mathbf{v} \in \mathbb{H}^n$ a right eigenvector corresponding to λ if $\mathbf{M}\mathbf{v} = \mathbf{v}\lambda$ for $\mathbf{M} \in \text{Mat}(n, \mathbb{H})$. Now we state the facts about right eigenvalues of a quaternionic matrix as follows:

Theorem 3.2. *For any quaternionic matrix $\mathbf{M} \in \text{Mat}(n, \mathbb{H})$, there exist $2n$ complex right eigenvalues of \mathbf{M} counted with multiplicity, which can be obtained by solving $\det(\lambda\mathbf{I}_{2n} - \psi(\mathbf{M})) = 0$. They appear in complex conjugate pairs $\lambda_1, \overline{\lambda_1}, \dots, \lambda_n, \overline{\lambda_n}$. The set of right eigenvalues $\sigma_r(\mathbf{M})$ is given by $\sigma_r(\mathbf{M}) = \lambda_1^{\mathbb{H}^*} \cup \dots \cup \lambda_n^{\mathbb{H}^*}$ where $\lambda^{\mathbb{H}^*} = \{h^{-1}\lambda h \mid h \in \mathbb{H}^* = \mathbb{H} - \{0\}\}$.*

Remark 3.3. If $\mathbf{M}\mathbf{v} = \mathbf{v}\lambda$ then $\mathbf{M}\mathbf{v}q = \mathbf{v}q(q^{-1}\lambda q)$ for every $q \in \mathbb{H}^*$ and hence $\mathbf{v}q$ is a right eigenvector corresponding to the right eigenvalue $q^{-1}\lambda q$.

Example 3.4. $\mathbf{M} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$, $\det(\lambda\mathbf{I}_4 - \psi(\mathbf{M})) = \det \begin{pmatrix} \lambda - 1 & 0 & 0 & 0 \\ 0 & \lambda - i & 0 & 0 \\ 0 & 0 & \lambda - 1 & 0 \\ 0 & 0 & 0 & \lambda + i \end{pmatrix} = 0$

$$\Leftrightarrow \lambda = 1, \pm i, \sigma_r(\mathbf{M}) = \{1\} \cup i^{\mathbb{H}^*}.$$

Example 3.5. $\mathbf{M} = \begin{pmatrix} 1 & j \\ k & i \end{pmatrix}$, $\det(\lambda \mathbf{I}_4 - \psi(\mathbf{M})) = \det \begin{pmatrix} \lambda - 1 & 0 & 0 & 1 \\ 0 & \lambda - i & i & 0 \\ 0 & -1 & \lambda - 1 & 0 \\ i & 0 & 0 & \lambda + i \end{pmatrix} = 0$

$$\Leftrightarrow \lambda = \frac{1 + \sqrt{3}}{2} \pm \frac{1 - \sqrt{3}}{2}i, \frac{1 - \sqrt{3}}{2} \pm \frac{1 + \sqrt{3}}{2}i, \sigma_r(\mathbf{M}) = \left(\frac{1 + \sqrt{3}}{2} + \frac{1 - \sqrt{3}}{2}i \right)^{\mathbb{H}^*} \cup \left(\frac{1 - \sqrt{3}}{2} + \frac{1 + \sqrt{3}}{2}i \right)^{\mathbb{H}^*}.$$

Now, we give a quaternionic extension of the Grover walk on G . A discrete-time quaternionic quantum walk is a quantum process on G whose state vector, whose entries are quaternions, is governed by a quaternionic unitary matrix called the quaternionic transition matrix. Let G be a finite connected graph with n vertices and m edges. We define the state space to be the quaternionic right Hilbert space $\mathcal{H}_{\mathbb{H}} = \bigoplus_{e \in D(G)} |e\rangle \mathbb{H}$. We define the *quaternionic transition matrix* $\mathbf{U} = (\mathbf{U}_{ef})_{e, f \in D(G)}$ of G as follows:

$$\mathbf{U}_{ef} = \begin{cases} q(e) & \text{if } t(f) = o(e) \text{ and } f \neq e^{-1}, \\ q(e) - 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise,} \end{cases} \quad (3.1)$$

where q is a map from $D(G)$ to \mathbb{H} . \mathbf{U} can be viewed as the time evolution operator of a discrete-time quaternionic quantum system. In [10], we obtained the necessary and sufficient condition for \mathbf{U} to be quaternionic unitary as follows:

Theorem 3.6 (Konno-Mitsuhashi-Sato [10]).

\mathbf{U} is unitary $\Leftrightarrow q_0(e)^2 + q_1(e)^2 + q_2(e)^2 + q_3(e)^2 - \frac{2q_0(e)}{d_{o(e)}} = 0$, where $q(e) = q_0(e) + q_1(e)i + q_2(e)j + q_3(e)k$, and $q(e) = q(f)$ for any two arcs $e, f \in D(G)$ with $o(e) = o(f)$.

From Theorem 3.6, it follows that $q_0(e)$ must satisfy

$$0 \leq q_0(e) \leq \frac{2}{d_{o(e)}}.$$

Moreover, for every $u \in V(G)$, $|\sum_{e: o(e)=u} q(e) - 1| = 1$. Furthermore we can readily see if $q(e)$ is positive real for each $e \in D(G)$, then \mathbf{U} must be \mathbf{U}^{Gro} .

4. The Second Weighted Zeta Function of a Graph

In this section, we give a brief summary of the second weighted zeta functions of a graph. We introduce an equivalence relation between cycles in G . Two cycles $C_1 = (e_1, \dots, e_\ell)$ and $C_2 = (f_1, \dots, f_\ell)$ are said to be *equivalent* if there exists k such that $f_j = e_{j+k}$ for all j where indices are treated modulo ℓ . Let $[C]$ be the equivalence class which contains the cycle C . Let B^r be the cycle obtained by going r times around a cycle B . Such a cycle is called a *power* of B . A cycle C is said to be *reduced* if both C and C^2 have no backtracking. Furthermore, a cycle C is said to be *prime* if it is not a power of a strictly smaller cycle.

The *Ihara zeta function* of a graph G is a function of $t \in \mathbf{C}$ with $|t|$ sufficiently small, defined by

$$\mathbf{Z}(G, t) = \mathbf{Z}_G(t) = \prod_{[C]} (1 - t^{|C|})^{-1},$$

where $[C]$ runs over all equivalence classes of prime, reduced cycles of G .

$\mathbf{Z}(G, t)$ has two types of determinant expressions as explained below. Let $\mathbf{B} = (\mathbf{B}_{ef})_{e, f \in D(G)}$ and $\mathbf{J}_0 = (\mathbf{J}_{ef})_{e, f \in D(G)}$ be $2m \times 2m$ matrices defined as follows:

$$\mathbf{B}_{ef} = \begin{cases} 1 & \text{if } t(e) = o(f), \\ 0 & \text{otherwise,} \end{cases} \quad \mathbf{J}_{ef} = \begin{cases} 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases} \quad (4.1)$$

The matrix $\mathbf{B} - \mathbf{J}_0$ is called the *edge matrix* of G . Then we can state two determinant expressions of $\mathbf{Z}(G, t)$ as follows:

Theorem 4.1 (Hashimoto [6]; Bass [2]). *The reciprocal of the Ihara zeta function of G is given by*

$$\mathbf{Z}(G, t)^{-1} = \det(\mathbf{I}_{2m} - t(\mathbf{B} - \mathbf{J}_0)) = (1 - t^2)^{r-1} \det(\mathbf{I}_n - t\mathbf{A} + t^2(\mathbf{D} - \mathbf{I}_n)), \quad (4.2)$$

where r and \mathbf{A} are the Betti number and the adjacency matrix of G , respectively, and $\mathbf{D} = (\mathbf{D}_{uv})_{u, v \in V(G)}$ is the diagonal matrix with $\mathbf{D}_{uu} = \deg u$ for all $u \in V(G)$.

We call the middle formula of (4.2) the determinant expression of *Hashimoto type* and the right hand side the determinant expression of *Bass type*.

We shall define the second weighted zeta function by using a modification of the edge matrix. Consider an $n \times n$ complex matrix $\mathbf{W} = (\mathbf{W}_{uv})_{u, v \in V(G)}$ with (u, v) -entry equals 0 if $(u, v) \notin D(G)$. We call \mathbf{W} a *weighted matrix* of G . Let $w(u, v) = \mathbf{W}_{uv}$ for $u, v \in V(G)$ and $w(e) = w(u, v)$ if $e = (u, v) \in D(G)$. then \mathbf{W}_{uv} is given by

$$\mathbf{W}_{uv} = \begin{cases} w(e) & \text{if } e = (u, v) \in D(G), \\ 0 & \text{otherwise.} \end{cases} \quad (4.3)$$

For a weighted matrix \mathbf{W} of G , let $\mathbf{B}_w = (\mathbf{B}_{ef}^{(w)})_{e,f \in D(G)}$ be a $2m \times 2m$ complex matrix defined as follows:

$$\mathbf{B}_{ef}^{(w)} = \begin{cases} w(f) & \text{if } t(e) = o(f), \\ 0 & \text{otherwise.} \end{cases} \quad (4.4)$$

Then the *second weighted zeta function* of G is defined by

$$\mathbf{Z}_1(G, w, t) = \det(\mathbf{I}_{2m} - t(\mathbf{B}_w - \mathbf{J}_0))^{-1}. \quad (4.5)$$

One can consider (4.5) as a multi-parametrized deformation of the determinant expression of Hashimoto type for $\mathbf{Z}(G, t)$. If $w(e) = 1$ for all $e \in D(G)$, then the second weighted zeta function of G coincides with $\mathbf{Z}(G, t)$. In [14], Sato obtained the determinant expression of Bass type for $\mathbf{Z}_1(G, w, t)$ as follows:

Theorem 4.2 (Sato [14]).

$$\mathbf{Z}_1(G, w, t)^{-1} = (1 - t^2)^{m-n} \det(\mathbf{I}_n - t\mathbf{W} + t^2(\mathbf{D}_w - \mathbf{I}_n)),$$

where $n = |V(G)|$, $m = |E(G)|$ and $\mathbf{D}_w = (\mathbf{D}_{uv}^{(w)})_{u,v \in V(G)}$ is the diagonal matrix defined by

$$\mathbf{D}_{uu}^{(w)} = \sum_{e: o(e)=u} w(e) \quad (4.6)$$

for all $u \in V(G)$.

Remark 4.3. We mention that taking transpose, the following equation also holds:

$$\det(\mathbf{I}_{2m} - t({}^T\mathbf{B}_w - \mathbf{J}_0)) = (1 - t^2)^{m-n} \det(\mathbf{I}_n - t{}^T\mathbf{W} + t^2(\mathbf{D}_w - \mathbf{I}_n)), \quad (4.7)$$

where ${}^T\mathbf{M}$ denotes the transpose of \mathbf{M} . We will show a quaternionic generalization of (4.7) and apply it to the spectral problem for our quaternionic quantum walk on G in later sections.

5. A Quaternionic Generalization of the Determinant Expressions

In this section, we shall give a quaternionic generalization of (4.7). Assume that $w(e)$ is in \mathbb{H} for every $e \in D(G)$ in (4.3), (4.4) and (4.6). Let $\mathbf{K} = (\mathbf{K}_{ev})_{e \in D(G), v \in V(G)}$ and $\mathbf{L} = (\mathbf{L}_{ev})_{e \in D(G), v \in V(G)}$ be $2m \times n$ matrices defined as follows:

$$\mathbf{K}_{ev} = \begin{cases} w(e) & \text{if } o(e) = v, \\ 0 & \text{otherwise,} \end{cases} \quad \mathbf{L}_{ev} = \begin{cases} 1 & \text{if } t(e) = v, \\ 0 & \text{otherwise,} \end{cases}$$

where column index and row index are ordered by fixed sequences v_1, \dots, v_n and e_1, \dots, e_{2m} such that $e_{2r} = e_{2r-1}^{-1}$ for $r = 1, \dots, m$, respectively. Then we can readily see that ${}^T\mathbf{B}_w = \mathbf{K}{}^T\mathbf{L}$, ${}^T\mathbf{W} = {}^T\mathbf{L}\mathbf{K}$ and ${}^T\mathbf{L}\mathbf{J}_0\mathbf{K} = {}^T\mathbf{D}_w$.

Theorem 5.1. *Let t be a complex variable. Then*

$$\det(\mathbf{I}_{4m} - t\psi({}^T\mathbf{B}_w - \mathbf{J}_0)) = (1 - t^2)^{2m-2n} \det(\mathbf{I}_{2n} - t\psi({}^T\mathbf{W}) + t^2(\psi(\mathbf{D}_w) - \mathbf{I}_{2n})).$$

Proof. Using Lemma 3.1, we can show that

$$\begin{aligned} \det(\mathbf{I}_{4m} - t\psi({}^T\mathbf{B}_w - \mathbf{J}_0)) &= \det(\mathbf{I}_{4m} - t\psi(\mathbf{K}{}^T\mathbf{L} - \mathbf{J}_0)) \\ &= \det(\mathbf{I}_{4m} - t\psi(\mathbf{K})\psi({}^T\mathbf{L}) + t\psi(\mathbf{J}_0)) \\ &= \det(\mathbf{I}_{4m} - t\psi(\mathbf{K})\psi({}^T\mathbf{L})(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0))^{-1}) \det(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0)) \\ &= (1 - t^2)^{2m} \det(\mathbf{I}_{4m} - t\psi(\mathbf{K})\psi({}^T\mathbf{L})(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0))^{-1}) \\ &= (1 - t^2)^{2m} \det(\mathbf{I}_{2n} - t\psi({}^T\mathbf{L})(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0))^{-1}) \psi(\mathbf{K}). \end{aligned} \quad (5.1)$$

Since the following holds:

$$(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0))^{-1} = \frac{1}{1 - t^2} (\mathbf{I}_{4m} - t\psi(\mathbf{J}_0)),$$

we have

$$\begin{aligned} \psi({}^T\mathbf{L})(\mathbf{I}_{4m} + t\psi(\mathbf{J}_0))^{-1} \psi(\mathbf{K}) &= \frac{1}{1 - t^2} \psi({}^T\mathbf{L})(\mathbf{I}_{4m} - t\psi(\mathbf{J}_0)) \psi(\mathbf{K}) \\ &= \frac{1}{1 - t^2} \psi({}^T\mathbf{L}) \psi(\mathbf{K}) - \frac{t}{1 - t^2} \psi({}^T\mathbf{L}) \psi(\mathbf{J}_0) \psi(\mathbf{K}) \\ &= \frac{1}{1 - t^2} \psi({}^T\mathbf{L}\mathbf{K}) - \frac{t}{1 - t^2} \psi({}^T\mathbf{L}\mathbf{J}_0\mathbf{K}) \\ &= \frac{1}{1 - t^2} \psi({}^T\mathbf{W}) - \frac{t}{1 - t^2} \psi({}^T\mathbf{D}_w). \end{aligned} \quad (5.2)$$

Consequently, we obtain the following equation from (5.1) and (5.2) as desired.

$$\begin{aligned} \det(\mathbf{I}_{4m} - t\psi({}^T\mathbf{B}_w - \mathbf{J}_0)) &= (1 - t^2)^{2m} \det\left(\mathbf{I}_{2n} - \frac{t}{1 - t^2} \psi({}^T\mathbf{W}) + \frac{t^2}{1 - t^2} \psi(\mathbf{D}_w)\right) \\ &= (1 - t^2)^{2m-2n} \det((1 - t^2)\mathbf{I}_{2n} - t\psi({}^T\mathbf{W}) + t^2\psi(\mathbf{D}_w)) \\ &= (1 - t^2)^{2m-2n} \det(\mathbf{I}_{2n} - t\psi({}^T\mathbf{W}) + t^2(\psi(\mathbf{D}_w) - \mathbf{I}_{2n})). \end{aligned}$$

□

6. The Right Spectrum of the Quaternionic Quantum Walk on a Graph

In this section, we derive the set of right eigenvalues of the quaternionic transition matrix \mathbf{U} by using eigenvalues of a complex matrix which can be easily derived from the map $q : D(G) \rightarrow \mathbb{H}$ given in (3.1). Putting $t = 1/\lambda$ in Theorem 5.1, we obtain

$$\det(\lambda\mathbf{I}_{4m} - \psi({}^T\mathbf{B}_w - \mathbf{J}_0)) = (\lambda^2 - 1)^{2m-2n} \det(\lambda^2\mathbf{I}_{2n} - \lambda\psi({}^T\mathbf{W}) + \psi(\mathbf{D}_w) - \mathbf{I}_{2n}). \quad (6.1)$$

Setting $w(e) = q(e)$ and comparing (3.1), (4.1) and (4.4), we readily see $\mathbf{U} = {}^T\mathbf{B}_w - \mathbf{J}_0$. Thus applying (6.1), we obtain

$$\det(\lambda\mathbf{I}_{4m} - \psi(\mathbf{U})) = (\lambda^2 - 1)^{2m-2n} \det(\lambda^2\mathbf{I}_{2n} - \lambda\psi({}^T\mathbf{W}) + \psi(\mathbf{D}_w) - \mathbf{I}_{2n}). \quad (6.2)$$

If $\psi({}^T\mathbf{W})$ and $\psi(\mathbf{D}_w)$ are simultaneously triangularizable, namely, there exists a regular matrix $\mathbf{P} \in \text{Mat}(2n, \mathbb{C})$ such that

$$\mathbf{P}^{-1}\psi({}^T\mathbf{W})\mathbf{P} = \begin{pmatrix} \mu_1 & 0 & \cdots & 0 \\ * & \mu_2 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ * & \cdots & * & \mu_{2n} \end{pmatrix}, \quad \mathbf{P}^{-1}\psi(\mathbf{D}_w)\mathbf{P} = \begin{pmatrix} \xi_1 & 0 & \cdots & 0 \\ * & \xi_2 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ * & \cdots & * & \xi_{2n} \end{pmatrix}, \quad (6.3)$$

then by (6.2) the characteristic equation of $\psi(\mathbf{U})$ turns out to be

$$\begin{aligned} \det(\lambda\mathbf{I}_{4m} - \psi(\mathbf{U})) &= (\lambda^2 - 1)^{2m-2n} \det(\lambda^2\mathbf{I}_{2n} - \lambda\mathbf{P}^{-1}\psi({}^T\mathbf{W})\mathbf{P} + \mathbf{P}^{-1}\psi(\mathbf{D}_w)\mathbf{P} - \mathbf{I}_{2n}). \\ &= (\lambda^2 - 1)^{2m-2n} \prod_{r=1}^{2n} (\lambda^2 - \lambda\mu_r + \xi_r - 1) = 0. \end{aligned} \quad (6.4)$$

We notice if (μ_r, μ_s) ($r \neq s$) is a complex conjugate pair as stated in Theorem 3.2 then so is (ξ_r, ξ_s) . Observing that $\det(\lambda\mathbf{I}_{4m} - \psi(\mathbf{U}))$ is a polynomial of λ , we obtain by solving (6.4) that

Theorem 6.1. $|\text{Spec}(\psi(\mathbf{U}))| = 4m$. Suppose that $\psi({}^T\mathbf{W})$ and $\psi(\mathbf{D}_w)$ are simultaneously triangularizable. If G is not a tree, then $4n$ of them are

$$\lambda = \frac{\mu_r \pm \sqrt{\mu_r^2 - 4(\xi_r - 1)}}{2} \quad (r = 1, \dots, 2n),$$

where $\mu_r \in \text{Spec}(\psi({}^T\mathbf{W}))$, $\xi_r \in \text{Spec}(\psi(\mathbf{D}_w))$ as presented in (6.3). The remaining $4(m - n)$ are ± 1 with equal multiplicities. If G is a tree, then

$$\text{Spec}(\psi(\mathbf{U})) = \left\{ \frac{\mu_r \pm \sqrt{\mu_r^2 - 4(\xi_r - 1)}}{2} \mid r = 1, \dots, 2n \right\} - \{1, 1, -1, -1\}.$$

$$\sigma_r(\mathbf{U}) = \bigcup_{\lambda \in \text{Spec}(\psi(\mathbf{U}))} \lambda^{\mathbb{H}^*}$$

Finally, we discuss quaternionic quantum walks which satisfy the following condition on $q(e)$:

$$\sum_{e:o(e)=u} q(e) \text{ does not depend on } u. \quad (6.5)$$

We have investigated this case in [10]. In short, this condition says that the sum of the entries in each column of \mathbf{U} does not depend on the column. Quaternionic quantum walks need not satisfy (6.5) in general, however, the Grover walk satisfies (6.5) by definition. Hence we can consider this condition is inherited from the Grover walk.

Since ψ is injective, ${}^T\mathbf{W}\mathbf{D}_w = \mathbf{D}_w{}^T\mathbf{W}$ is equivalent to $\psi({}^T\mathbf{W})\psi(\mathbf{D}_w) = \psi(\mathbf{D}_w)\psi({}^T\mathbf{W})$. In this case, $\psi({}^T\mathbf{W})$ and $\psi(\mathbf{D}_w)$ are simultaneously triangularizable.

Proposition 6.2. (6.5) implies ${}^T\mathbf{W}\mathbf{D}_w = \mathbf{D}_w{}^T\mathbf{W}$. Moreover, if $w(e) \neq 0$ for every $e \in D(G)$, then (6.5) $\Leftrightarrow {}^T\mathbf{W}\mathbf{D}_w = \mathbf{D}_w{}^T\mathbf{W}$.

Proof. If $(v, u) \in D(G)$, then by Theorem 3.6 we have

$$\begin{aligned} ({}^T\mathbf{W}\mathbf{D}_w)_{uv} &= w((v, u)) \sum_{\substack{e \in D(G) \\ o(e)=v}} w(e) = d_v w((v, u)) w((v, u)), \\ (\mathbf{D}_w {}^T\mathbf{W})_{uv} &= \sum_{\substack{e \in D(G) \\ o(e)=u}} w(e) w((v, u)) = d_u w((u, v)) w((v, u)). \end{aligned}$$

Therefore (6.5) implies $d_v w((v, u)) w((v, u)) = d_u w((u, v)) w((v, u))$ for all $(v, u) \in D(G)$ and thereby ${}^T\mathbf{W}\mathbf{D}_w = \mathbf{D}_w {}^T\mathbf{W}$. If $w(e) \neq 0$ for every $e \in D(G)$, then $d_v w((v, u)) w((v, u)) = d_u w((u, v)) w((v, u))$ implies $d_v w((v, u)) = d_u w((u, v))$. Hence $\sum_{e \in D(G), o(e)=v} w(e) = \sum_{e \in D(G), o(e)=u} w(e)$ for $u, v \in V(G)$ with $(v, u) \in D(G)$. Since G is connected, the equation just before holds for every pair of vertices and thereby (6.5) holds. \square

Hence one can view Theorem 6.1 as a generalization of [10]. By (6.5), we may put $\alpha = \sum_{e: o(e)=u} q(e)$ independently of u . Then we immediately see that $q(e) = \alpha/d_{o(e)}$ for every $e \in D(G)$. For $\alpha \in \mathbb{H} - \mathbb{R}$, it is known that there exist nonzero quaternions $h_{\pm} \in \mathbb{H}^*$ such that $h_{\pm}^{-1} \alpha h_{\pm} = \alpha_{\pm}$ are complex numbers which are complex conjugate with each other. (For the details, see [10]) Then we readily see

$$\mathbf{U}_{\pm} = h_{\pm}^{-1} \mathbf{U} h_{\pm} = ((\mathbf{U}_{\pm})_{ef})_{e, f \in D(G)} \in \text{Mat}(2m, \mathbb{C}), \quad \text{where } (\mathbf{U}_{\pm})_{ef} = \begin{cases} \frac{\alpha_{\pm}}{d_{o(e)}} & \text{if } t(f) = o(e) \text{ and } f \neq e^{-1}, \\ \frac{\alpha_{\pm}}{d_{o(e)}} - 1 & \text{if } f = e^{-1}, \\ 0 & \text{otherwise.} \end{cases}$$

It follows that

$$\begin{aligned} \det(\lambda \mathbf{I}_{4m} - \psi(\mathbf{U})) &= \det(\psi(h_+ \mathbf{I}_{2m})^{-1} (\lambda \mathbf{I}_{4m} - \psi(\mathbf{U})) \psi(h_+ \mathbf{I}_{2m})) = \det(\lambda \mathbf{I}_{4m} - \psi(h_+ \mathbf{I}_{2m})^{-1} \psi(\mathbf{U}) \psi(h_+ \mathbf{I}_{2m})) \\ &= \det(\lambda \mathbf{I}_{4m} - \psi(h_+^{-1} \mathbf{U} h_+)) = \det(\lambda \mathbf{I}_{4m} - \psi(\mathbf{U}_+)) = \begin{vmatrix} \lambda \mathbf{I}_{2m} - \mathbf{U}_+ & 0 \\ 0 & \lambda \mathbf{I}_{2m} - \mathbf{U}_- \end{vmatrix} \\ &= \det(\lambda \mathbf{I}_{2m} - \mathbf{U}_+) \det(\lambda \mathbf{I}_{2m} - \mathbf{U}_-) = \det(\lambda \mathbf{I}_{2m} - \mathbf{U}_+) \det(\lambda \mathbf{I}_{2m} - \overline{\mathbf{U}_+}). \end{aligned}$$

Therefore, we can calculate all right eigenvalues of \mathbf{U} by calculating eigenvalues of \mathbf{U}_+ since eigenvalues of $\mathbf{U}_- = \overline{\mathbf{U}_+}$ are complex conjugates of those of \mathbf{U}_+ . Accordingly, $\mathbf{W}_{\pm} = h_{\pm}^{-1} \mathbf{W} h_{\pm}$ and $\mathbf{B}_{w_{\pm}} = h_{\pm}^{-1} \mathbf{B}_w h_{\pm} = (\mathbf{B}^{(w_{\pm})})_{ef}$ are given by

$$(\mathbf{W}_{\pm})_{uv} = \begin{cases} \frac{\alpha_{\pm}}{d_u} & \text{if } (u, v) \in D(G), \\ 0 & \text{otherwise,} \end{cases} \quad \mathbf{B}_{ef}^{(w_{\pm})} = \begin{cases} \frac{\alpha_{\pm}}{d_{o(f)}} & \text{if } t(e) = o(f), \\ 0 & \text{otherwise.} \end{cases}$$

In this case, we can apply (4.7) to obtain the next theorem which is a special case of Theorem 6.1.

Theorem 6.3 (Konno-Mitsuhashi-Sato [10]). $|\text{Spec}(\psi(\mathbf{U}))| = 4m$. Suppose that (6.5) holds. If G is not a tree, then $4n$ of them are

$$\lambda = \frac{\mu_+ \pm \sqrt{\mu_+^2 - 4(\alpha_+ - 1)}}{2}, \quad \frac{\mu_- \pm \sqrt{\mu_-^2 - 4(\alpha_- - 1)}}{2},$$

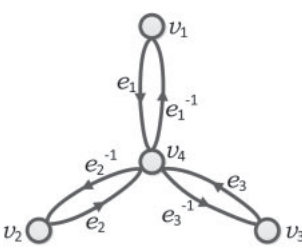
where $\mu_{\pm} \in \text{Spec}({}^T\mathbf{W}_{\pm})$. The remaining $4(m - n)$ are ± 1 with equal multiplicities. If G is a tree, then

$$\text{Spec}(\psi(\mathbf{U})) = \left\{ \frac{\mu_+ \pm \sqrt{\mu_+^2 - 4(\alpha_+ - 1)}}{2}, \frac{\mu_- \pm \sqrt{\mu_-^2 - 4(\alpha_- - 1)}}{2} \mid \mu_{\pm} \in \text{Spec}({}^T\mathbf{W}_{\pm}) \right\} - \{1, 1, -1, -1\}.$$

$$\sigma_r(\mathbf{U}) = \bigcup_{\lambda \in \text{Spec}(\mathbf{U}_+)} \lambda^{\mathbb{H}^*}$$

We will show an example which does not satisfy (6.5) but do the assumption in Theorem 6.1.

Example 6.4. $G = K_{1,3}$. Let $w(e_1) = 1 + i, w(e_2) = 1 - j, w(e_3) = 2, w(e_1^{-1}) = w(e_2^{-1}) = w(e_3^{-1}) = 0$.



$${}^T\mathbf{W} = \begin{matrix} & v_1 & v_2 & v_3 & v_4 \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1+i & 1-j & 2 & 0 \end{pmatrix} \end{matrix}, \quad \psi({}^T\mathbf{W}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1+i & 1 & 2 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1-i & 1 & 2 & 0 \end{pmatrix}.$$

Then \mathbf{U} , \mathbf{D}_w and $\psi(\mathbf{D}_w)$ are given by

$$\mathbf{U} = \begin{pmatrix} 0 & i & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -j & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}, \mathbf{D}_w = \begin{pmatrix} 1+i & 0 & 0 & 0 \\ 0 & 1-j & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\psi(\mathbf{D}_w) = \begin{pmatrix} 1+i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-i & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Let \mathbf{P} be defined by

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & i & -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then

$$\mathbf{P}^{-1}\psi(\mathbf{W})\mathbf{P} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1+i & 1+i & 1-i & 0 & 2 & 0 & 0 & 0 \\ 0 & -1+i & -1-i & 1-i & 0 & 2 & 0 & 0 \end{pmatrix},$$

$$\mathbf{P}^{-1}\psi(\mathbf{D}_w)\mathbf{P} = \begin{pmatrix} 1+i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1+i & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Hence it follows that $\text{Spec}(\psi(\mathbf{W})) = \{\mu_1, \mu_2, \dots, \mu_8\} = \{0, 0, 0, 0, 0, 0, 0, 0\}$, $\text{Spec}(\psi(\mathbf{D}_w)) = \{\xi_1, \xi_2, \dots, \xi_8\} = \{1+i, 1+i, 1-i, 1-i, 2, 2, 0, 0\}$. Applying Theorem 6.1, we obtain

$$\begin{aligned} \text{Spec}(\psi(\mathbf{U})) &= \{\pm\sqrt{-i}, \pm\sqrt{-i}, \pm\sqrt{i}, \pm\sqrt{i}, \pm\sqrt{-1}, \pm\sqrt{-1}, \pm 1, \pm 1\} - \{1, 1, -1, -1\} \\ &= \left\{ \pm \frac{1-i}{\sqrt{2}}, \pm \frac{1-i}{\sqrt{2}}, \pm \frac{1+i}{\sqrt{2}}, \pm \frac{1+i}{\sqrt{2}}, \pm i, \pm i \right\}. \end{aligned}$$

Since $-i = j^{-1}ij \in i^{\mathbb{H}^*}$, an eigenvalue and its complex conjugate belong to the same set of all quaternionic conjugations of the eigenvalue. Thus $\sigma_r(\mathbf{U}) = i^{\mathbb{H}^*} \cup \left(\frac{1+i}{\sqrt{2}}\right)^{\mathbb{H}^*} \cup \left(-\frac{1+i}{\sqrt{2}}\right)^{\mathbb{H}^*}$.

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