THE SPECTRA OF THE UNITARY MATRIX OF A
2-TESSELLABLE STAGGERED QUANTUM WALK
ON A GRAPH

By

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Abstract. Recently, the staggered quantum walk (SQW) on a graph is discussed as a generalization of coined quantum walks on graphs and Szegedy walks. We present a formula for the characteristic polynomial of the time evolution matrix of a 2-tessellable SQW on a graph, and so directly give its spectra. Furthermore, we present a formula for the characteristic polynomial of the Szegedy matrix of a bipartite graph by the same method, and so give its spectra. As an application, we present a formula for the characteristic polynomial of the modified Szegedy matrix in the quantum search problem on a graph, and give its spectra.

1. Introduction

As a quantum counterpart of the classical random walk, the quantum walk has recently attracted much attention for various fields. The review and book on quantum walks are Ambainis [3], Kempe [8], Kendon [11], Konno [12], Venegas-Andraca [25], Manouchehri and Wang [15], Portugal [18], for examples.

Quantum walks of graphs were studied by many researchers. A discrete-time quantum walk on a line was proposed by Aharonov et al [1]. In [2], a discrete-time quantum walk on a regular graph was proposed. The Grover walk is a discrete-time quantum walk on a graph which originates from the Grover algorithm. The Grover algorithm which was introduced in [7] is a quantum search algorithm that performs quadratically faster than the best classical search algorithm. Using a different quantization procedure, Szegedy [24] proposed a new coinless discrete-time quantum walk, i.e., the Szegedy walk on a bipartite graph and provided a natural definition of quantum hitting time. Also, Szegedy developed quantum walk-based search algorithm, which can detect the presence of a marked vertex at a hitting time that is quadratically smaller than the classical average time on ergodic Markov chains. Portugal [19], [20], [21], defined the staggered quantum
walk (SQW) on a graph as a generalization of coined quantum walks on graphs and Szegedy walks. In [19], [20], Portugal studied the relation between SQW and coined quantum walks, Szegedy walks. In [21], Portugal presented some properties of 2-tessellable SQW on graphs by using several results of the graph theory.

Spectra of various quantum walk on a graph were computed by many researchers. Related to graph isomorphism problems, Emms et al. [4] presented spectra of the Grover matrix (the time evolution matrix of the Grover walk) on a graph and those of the positive supports of the Grover matrix and its square. Konno and Sato [13] computed the characteristic polynomials for the Grover matrix and its positive supports of a graph by using determinant expressions for several graph zeta functions, and so directly gave their spectra. Godsil and Guo [6] gave new proofs of the results of Emms et al. [4].

In the quantum search problem, the notion of hitting time in classical Markov chains is generalized to quantum hitting time. Kempe [9] provided two definitions and proved that a quantum walker hits the opposite corner of an $n$-hypercube in time $O(n)$. Krovi and Brun [14] provided a definition of average hitting time that requires a partial measurement of the position of the walker at each step. Kempe and Portugal [10] discussed the relation between hitting times and the walker’s group velocity. Szegedy [24] gave a definition of quantum hitting time that is a natural generalization of the classical definition of hitting time. Magniez et al [16] extended Szegedy’s work to non-symmetric ergodic Markov chains. Recently, Santos and Portugal [23] calculated analytically Szegedy’s hitting time and the probability of finding a set of marked vertices on the complete graph.

The rest of the paper is organized as follows. Section 2 states some definitions and notation on graph theory, and gives the definitions of the Grover walk, the Szegedy walk, the staggered quantum walk (SQW) on a graph and a short review on the quantum search problem on a graph. In Section 3, we give a key method to calculate the characteristic polynomials for the time evolution matrices of SQW and the Szegedy walk on a graph. In Section 4, we present a formula for the time evolution matrix of a 2-tessellable SQW on a graph, and so give its spectra. In Section 5, we present a formula for the Szegedy matrix of a bipartite graph, and so give its spectra. In Section 7, we present a formula for the modified time evolution matrix of the duplication of the modified digraph which is appeared in the quantum search problem on a graph, and so give its spectra.
2. Definition of several quantum walks on a graph

2.1 Definitions and notation

Graphs treated here are finite. Let \( G = (V(G), E(G)) \) be a connected graph (possibly multiple edges and loops) with the set \( V = V(G) \) of vertices and the set \( E = E(G) \) of unoriented edges \( uv \) joining two vertices \( u \) and \( v \). Two vertices \( u \) and \( v \) of \( G \) are adjacent if there exists an edge \( e \) joining \( u \) and \( v \) in \( G \). Furthermore, two vertices \( u \) and \( v \) of \( G \) are incident to \( e \). The degree \( \deg v = \deg_G v \) of a vertex \( v \) of \( G \) is the number of edges incident to \( v \). For a natural number \( k \), a graph \( G \) is called \( k \)-\textit{regular} if \( \deg_G v = k \) for each vertex \( v \) of \( G \).

For \( uv \in E(G) \), an arc \( (u, v) \) is the oriented edge from \( u \) to \( v \). Set \( D(G) = \{ (u, v), (v, u) \mid uv \in E(G) \} \). For \( a = (u, v) \in D(G) \), set \( u = o(a) \) and \( v = t(a) \). Furthermore, let \( a^{-1} = (v, u) \) be the inverse of \( a = (u, v) \). A \textit{path} \( P = (v_1, v_2, \ldots, v_{n+1}) \) of length \( n \) in \( G \) is a sequence of \( (n + 1) \) vertices such that \( v_i v_{i+1} \in E(G) \) for \( i = 1, \ldots, n \). Then \( P \) is called a \( (v_1, v_{n+1}) \)-\textit{path}. If \( e_i = v_i v_{i+1} \in E(G)(1 \leq i \leq n) \), then we write \( P = (e_1, \ldots, e_n) \).

A graph \( G \) is called a \textit{complete} if any two vertices of \( G \) are adjacent. We denote the complete graph with \( n \) vertices by \( K_n \). Furthermore, a graph \( G \) is called \textit{bipartite}, denoted by \( G = (V_1, V_2) \) if there exists a partition \( V(G) = V_1 \cup V_2 \) of \( V(G) \) such that the vertices in \( V_i \) are mutually nonadjacent for \( i = 1, 2 \). The subsets \( V_1, V_2 \) of \( V(G) \) is called the \textit{bipartite set} or the \textit{bipartition} of \( G \). A bipartite graph \( G = (V_1, V_2) \) is called \textit{complete} if any vertex of \( V_1 \) and any vertex of \( V_2 \) are adjacent. If \( |V_1| = m \) and \( |V_2| = n \), then we denote the complete bipartite with bipartition \( V_1, V_2 \) by \( K_{m,n} \).

Next, we define two operations of a graph. Let \( G \) be a connected graph. Then a subgraph \( H \) of \( G \) is called a \textit{clique} if \( H \) is a complete subgraph of \( G \). The \textit{clique graph} \( K(G) \) of \( G \) has the maximal cliques of \( G \) as its vertices, and two vertices are adjacent whenever they have some vertex of \( G \) in common. Furthermore, the \textit{line graph} \( L(G) \) of \( G \) has the edges of \( G \) as its vertices, and two vertices are adjacent whenever they have some vertex of \( G \) in common.

2.2 The Grover walk on a graph

A discrete-time quantum walk is a quantum analog of the classical random walk on a graph whose state vector is governed by a matrix called the transition matrix. Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges, \( V(G) = \{v_1, \ldots, v_n\} \) and \( D(G) = \{a_1, \ldots, a_m, a_1^{-1}, \ldots, a_m^{-1}\} \). Set \( d_j = d_{v_j} = \deg v_j \) for
The transition matrix \( U = U(G) = (U_{ab})_{a,b \in D(G)} \) of \( G \) is defined by

\[
U_{ab} = \begin{cases} 
\frac{2}{d_t(b)} (= 2/d_o(a)) & \text{if } t(b) = o(a) \text{ and } b \neq a^{-1}, \\
\frac{2}{d_t(b)} - 1 & \text{if } b = a^{-1}, \\
0 & \text{otherwise}.
\end{cases}
\]

The matrix \( U \) is called the Grover matrix of \( G \).

We introduce the positive support \( F^+ = (F^+_{ij}) \) of a real matrix \( F = (F_{ij}) \) as follows:

\[
F^+_{ij} = \begin{cases} 
1 & \text{if } F_{ij} > 0, \\
0 & \text{otherwise}.
\end{cases}
\]

Let \( G \) be a connected graph. If the degree of each vertex of \( G \) is not less than 2, i.e., \( \delta(G) \geq 2 \), then \( G \) is called an \( md2 \) graph.

The transition matrix of a discrete-time quantum walk in a graph is closely related to the Ihara zeta function of a graph. Ren et al. [22] gave a relationship between the discrete-time quantum walk and the Ihara zeta function of a graph.

Konno and Sato [13] obtained the following formula of the characteristic polynomial of \( U \) by using the determinant expression for the second weighted zeta function of a graph.

Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then the \( n \times n \) matrix \( T(G) = (T_{uv})_{u,v \in V(G)} \) is given as follows:

\[
T_{uv} = \begin{cases} 
1/\deg_G u & \text{if } (u, v) \in D(G), \\
0 & \text{otherwise}.
\end{cases}
\]

Note that the matrix \( T(G) \) is the transition matrix of the simple random walk on \( G \).

**Theorem 2.1.** (Konno and Sato [13]) Let \( G \) be a connected graph with \( n \) vertices \( v_1, \ldots, v_n \) and \( m \) edges. Then, for the transition matrix \( U \) of \( G \), we have

\[
\det(\lambda I_{2m} - U) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)I_n - 2\lambda T(G)) = (\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)D - 2\lambda A(G))
\]

\[
\frac{d_{v_1} \cdots d_{v_n}}{d_{u_1} \cdots d_{u_n}},
\]

where \( A(G) \) is the adjacency matrix of \( G \), and \( D = (d_{uv}) \) is the diagonal matrix given by \( d_{uu} = \deg u \) (\( u \in V(G) \)).

From this Theorem, the spectra of the Grover matrix on a graph is obtained by means of those of \( T(G) \) (see [4]). Let \( \text{Spec}(F) \) be the spectrum of a square matrix \( F \).
Corollary 2.2. (Emms, Hancock, Severini and Wilson [4]) Let $G$ be a connected graph with $n$ vertices and $m$ edges. The transition matrix $U$ has $2n$ eigenvalues of the form

$$\lambda = \lambda_T \pm i \sqrt{1 - \lambda_T^2},$$

where $\lambda_T$ is an eigenvalue of the matrix $T(G)$. The remaining $2(m - n)$ eigenvalues of $U$ are $\pm 1$ with equal multiplicities.

Emms et al. [4] determined the spectrum of the transition matrix $U$ by examining the elements of the transition matrix of a graph and using the properties of the eigenvector of a matrix. And now, we could explicitly obtain the spectrum of the transition matrix $U$ from its characteristic polynomial.

Next, we state about the positive support of the transition matrix of a graph.

Emms et al [4] expressed the spectrum of the positive support $U^+$ of the transition matrix of a regular graph $G$ by means of those of the adjacency matrix $A(G)$ of $G$.

Theorem 2.3. (Emms, Hancock, Severini and Wilson [4]) Let $G$ be a connected $k$-regular graph with $n$ vertices and $m$ edges, and $\delta(G) \geq 2$. The positive support $U^+$ has $2n$ eigenvalues of the form

$$\lambda = \frac{\lambda_A}{2} \pm i \frac{\sqrt{k - 1 - \lambda_A^2}}{4},$$

where $\lambda_A$ is an eigenvalue of the matrix $A(G)$. The remaining $2(m - n)$ eigenvalues of $U^+$ are $\pm 1$ with equal multiplicities.

Godsil and Guo [6] presented a new proof of Theorem by using linear algebraic technique.

2.3 The Szegedy quantum walk on a bipartite graph

Let $G = (X \cup Y, E)$ be a connected bipartite graph with partite set $X$ and $Y$. Moreover, set $|V(G)| = \nu$, $|E| = |E(G)| = \epsilon$, $|X| = m$ and $|Y| = n$. Then we consider the Hilbert space $H = \ell^2(E) = \text{span}\{|e\rangle | e \in E\}$. Let $p : E \to [0, 1]$ and $q : E \to [0, 1]$ be the functions such that

$$\sum_{X(e) = x} p(e) = \sum_{Y(e) = y} q(e) = 1, \forall x \in X, \forall y \in Y,$$

where $X(e)$ and $Y(e)$ are the vertex of $e$ belonging to $X$ and $Y$, respectively.

For each $x \in X$ and $y \in Y$, let

$$|\phi_x\rangle = \sum_{X(e) = x} \sqrt{p(e)}|e\rangle \text{ and } |\psi_y\rangle = \sum_{Y(e) = y} \sqrt{q(e)}|e\rangle.$$
From these vectors, we construct two $\epsilon \times \epsilon$ matrices $R_0$ and $R_1$ as follows:

$$R_0 = 2 \sum_{x \in X} |\phi_x \rangle \langle \phi_x| - I, \quad R_1 = 2 \sum_{y \in Y} |\psi_y \rangle \langle \psi_y| - I.$$ 

Furthermore, we define an $\epsilon \times \epsilon$ matrix $W$ as follows:

$$W = R_1 R_0.$$ 

Note that two matrices $R_0$ and $R_1$ are unitary, and $R_0^2 = R_1^2 = I$.

The quantum walk on $G$ with $W$ as a time evolution matrix is called the Szegedy walk on $G$, and the matrix $W$ is called the Szegedy matrix of $G$.

2.4 The staggered quantum walk on a graph

Let $G$ be a connected graph with $\nu$ vertices and $\epsilon$ edges. Furthermore, let $H^\nu$ be the Hilbert space generated by the vertices of $G$. We take a standard basis as $\{|u\rangle \mid u \in V\}$. In general, a unitary and Hermitian operator $U$ on $H^\nu$ can be written by

$$U = \sum_x |\psi_x^+ \rangle \langle \psi_x^+| - \sum_y |\psi_y^- \rangle \langle \psi_y^-|,$$

where the set of vectors $|\psi_x^+ \rangle$ is a normal orthogonal basis of $(+1)$-eigenspace, and the set of vectors $|\psi_x^- \rangle$ is a normal orthogonal basis of $(-1)$-eigenspace. Since

$$\sum_x |\psi_x^+ \rangle \langle \psi_x^+| + \sum_y |\psi_y^- \rangle \langle \psi_y^-| = I,$$

we obtain

$$U = 2 \sum_x |\psi_x^+ \rangle \langle \psi_x^+| - I \cdots (\ast).$$

A unitary and Hermitian matrix $U$ in $H^\nu$ given by (\ast) is called an orthogonal reflection of $G$ if the set of the orthogonal set of $(+1)$-eigenvectors $\{|\psi_x^+ \rangle\}_x$ obeying the following properties:

1. If the $i$-th entry of $|\psi^+_x \rangle$ for a fixed $x$ is nonzero, the $i$-th entry of the other $(+1)$-eigenvectors are zero, that is, if $\langle i|\psi_x \rangle \neq 0$, then $\langle i|\psi_{x'} \rangle = 0$ for any $x' \neq x$;
2. The vector $\sum_x |\psi^+_x \rangle$ has no zero entries.

Next, a polygon of a graph $G$ induced by a vector $|\psi \rangle \in H^\nu$ is a clique. That is, two vertices of $G$ are adjacent if the corresponding entries of $|\psi \rangle$ in the basis associated with $G$ are nonzero. Thus if $\langle u|\psi \rangle \neq 0$ and $\langle v|\psi \rangle \neq 0$, then $u$ is
connected to $v$. A vertex belongs to the polygon if and only if it corresponding entry in $|\psi\rangle$ is nonzero. An edge belongs to the polygon if and only if the polygon contains the endpoints of the edge.

A tessellation induced by an orthogonal reflection $U$ of $G$ is the union of the polygons induced by the $(+1)$-eigenvectors $\{|\psi^+_x\rangle\}_{x}$ of $U$ described in the above. The staggered quantum walk (SQW) on $G$ associated with the Hilbert space $\mathcal{H}_G$ is driven by

$$U = U_1U_0,$$

where $U_0$ and $U_1$ are orthogonal reflections of $G$. The union of the tessellations $\alpha$ and $\beta$ induced by $U_0$ and $U_1$ must cover the edges of $G$. Furthermore, set $\alpha = \{\alpha_1, \ldots, \alpha_m\}$ and $\beta = \{\beta_1, \ldots, \beta_n\}$. Then $U_0$ and $U_1$ are given as follows:

$$U_0 = 2\sum_{k=1}^{m} |\alpha_k\rangle\langle\alpha_k| - I_\nu, \quad U_1 = 2\sum_{l=1}^{n} |\beta_l\rangle\langle\beta_l| - I_\nu,$$

where

$$|\alpha_k\rangle = \sum_{k' \in \alpha_k} a_{kk'} |k'\rangle \quad (1 \leq k \leq m), \quad |\beta_l\rangle = \sum_{l' \in \beta_l} b_{ll'} |l'\rangle \quad (1 \leq l \leq n),$$

and

$$\langle\alpha_k|\alpha_{k'}\rangle = \delta_{kk'} \quad (1 \leq k, k' \leq m), \quad \langle\beta_l|\beta_{l'}\rangle = \delta_{ll'} \quad (1 \leq l, l' \leq n),$$

$$a_{kk'} = \begin{cases} \text{nonzero} & \text{if } k' \in \alpha_k, \\ 0 & \text{otherwise}, \end{cases} \quad b_{ll'} = \begin{cases} \text{nonzero} & \text{if } l' \in \beta_l, \\ 0 & \text{otherwise}. \end{cases}$$

A graph $G$ is 2-tessellable if the following conditions holds:

$$V(\alpha_1) \sqcup \cdots \sqcup V(\alpha_m) = V(\beta_1) \sqcup \cdots \sqcup V(\beta_n) = V(G)$$

and

$$(E(\alpha_1) \sqcup \cdots \sqcup E(\alpha_m)) \cup (E(\beta_1) \sqcup \cdots \sqcup E(\beta_n)) = E(G),$$

where $U = U_1U_0$ is the unitary matrix of a SQW on $G$, and $\alpha = \{\alpha_1, \ldots, \alpha_m\}$ and $\beta = \{\beta_1, \ldots, \beta_n\}$ are tessellations of $U$ corresponding to $U_0$ and $U_1$, respectively. If $A$ and $B$ are disjoint subsets of a set $X$, then the union of $A$ and $B$ is denoted by $A \cup B$.

2.5 The quantum search problem on a graph

Let $G = (V, E)$ be a connected non-bipartite graph with $n$ vertices and $e$ edges which may have multiple edges and self loops. Let $E_H(u, v)$ be the subset of the edge set of a graph $H$ connecting between vertices $u$ and $v$. Furthermore,
for $S, T \subseteq V(H)$, set $E_H(S, T) = \{e \in E(H) \mid e = uv, u \in S, v \in T\}$. It holds $\bigcup_{e=uv \in E(H)} E_H(u, v) = E(H)$, where “$\bigcup$” means the disjoint union. We want to set the quantum search of an element of $M \subseteq V$ by the Szegedy walk. The Szegedy walk is defined by a bipartite graph. To this end, we construct the duplication of $G$. The duplication $G_2$ of $G$ is defined as follows: The duplication graph $G_2$ of $G$ is defined as follows. $V(G_2) = V \sqcup V'$, where $v'$ is the copy of $v \in V$, therefore $V' = \{v' \mid v \in V\}$. The edge set of $E(G_2)$ is denoted by $E_G(u, v) \subseteq E(G) \Leftrightarrow E_{G_2}(u, v') \subseteq E(G_2)$.

The end vertex of $e \in E(G_2)$ included in $V$ is denoted by $V(e)$, and one included in $V'$ is denoted by $V'(e)$. We consider two functions $p : E(G_2) \to [0, 1]$ and $q : E(G_2) \to [0, 1]$ be the functions such that

$$\{p(e) \mid e \in E_{G_2}(u, v')\} = \{q(e) \mid e \in E_{G_2}(u', v)\}$$

where

$$\sum_{V(e) = x} p(e) = \sum_{V'(e) = y} q(e) = 1, \forall x \in V, \forall y \in V'.$$

The $2n \times 2n$ stochastic matrix $P$ is denoted by

$$(P)_{u, v} = p_{uv} = \begin{cases} \sum_{V(e) = u, V'(e) = v} p(e) & \text{if } u \in V, v \in V', \\ \sum_{V'(e) = u} q(e) & \text{if } u \in V', v \in V, \\ 0 & \text{otherwise.} \end{cases}$$

Let $V(G) = \{v_1, \ldots, v_n\}$ and $M = \{v_{n-m+1}, \ldots, v_n\}$. The elements of $M$ are called marked vertices. Then define the modified digraph $\tilde{G}$ from $G$ as follows: The modified digraph $\tilde{G}$ with respect to $M$ is obtained from the symmetric digraph $D_G$ by converting all arcs leaving from the marked vertices into loops. In the duplication $G_2$, the set $M_2$ of marked vertices is

$$M_2 = M \cup \{u' \mid u \in M\}.$$ 

The modified bipartite digraph $\tilde{G}_2$ is obtained from the symmetric digraph of $G_2$ by deleting all arcs leaving from the marked vertices of $G_2$, but keeping the incoming arcs to the marked vertices of $G_2$ and all other arcs unchanged. Moreover, we add new $2m = 2|M|$ arcs $(u, u'), (u', u)$ for $u \in M$. Then the modified bipartite digraph $\tilde{G}_2$ is obtained by taking the duplication of $\tilde{G}$. More
precisely, let $A(G_2) = D(G_2)$ be the set of symmetric arcs naturally induced by
$E(G_2)$, then

$$V(\overline{G}_2) = V(G_2),$$

$$A(\overline{G}_2) = \{a \in A(G_2) \mid o(a) \notin M \cup M'\} \cup \{a, a^{-1} \mid o(a) = u, t(a) = u', u \in M\}.$$ 

Here $M' \subset V'$ is the copy of $M$. We put the first arcset in RHS by $A_2$, and the second one by $N_2$. The modified bipartite digraph $\overline{G}_2$ keeps the bipartiteness with $V$ and $V'$. Thus once a random walker steps in $M_2$, then she will be trapped in $M_2$ forever.

We want to induce the Szegedy walk from this absorption picture into $M_2$ of $\overline{G}_2$. The Szegedy walk is denoted by non-directed edges of the bipartite graph. So we consider the support of $A(\overline{G}_2)$ by $E_2 := [A(\overline{G}_2)] := \{[a] \mid a \in A(\overline{G}_2)\}$. Here $[a]$ is the edge obtained by removing the direction of the arc $a$. Thus $E_2 = [A_2] \cup [N_2]$, and remark that $[N_2]$ describes the set of the matching between $m$ and $m'$ for $m \in M$. Taking the following modification to $p$ and $q$, the above absorption picture of a classical walk is preserved by the following random walk as follows. For $e \in E_2$,

$$p'(e) = \begin{cases} 
    p(e) & \text{if } V(e) \notin M, \\
    1 & \text{if } e \in [N_2], \\
    0 & \text{if } V(e) \in M \text{ and } V'(e) \notin M',
\end{cases}$$

$$q'(e) = \begin{cases} 
    q(e) & \text{if } V'(e) \notin M, \\
    1 & \text{if } e \in [N_2], \\
    0 & \text{if } V'(e) \in M' \text{ and } V(e) \notin M,
\end{cases}$$

The modified $2n \times 2n$ stochastic matrix $P'$ is given by changing $p$ and $q$ to $p'$ and $q'$ as follows:

$$(P')_{u,v} = p'_{uv} = \begin{cases} 
    \sum_{V'(e)=u, V(e)=u} p'(e) & \text{if } u \in V, v \in V', \\
    \sum_{V'(e)=u, V(e)=u} q'(e) & \text{if } u \in V', v \in V, \\
    0 & \text{otherwise.}
\end{cases}$$

If there exists a marked element connecting to another marked element in $G$, then such an edge is omitted by the procedure of the deformation to $\overline{G}_2$, thus $[A_2] \subset E(G_2)$, on the other hand, otherwise, $[A_2] = E(G_2)$. We set $F_2 = \{e \in E(G_2) \mid V(e), V'(e) \in M_2\}$. Now we are considering a quantum search setting without any connected information about marked elements, so we want to set the initial state as a usual way,

$$\psi_0 = \sum_{e \in E(G_2)} \sqrt{p(e)} |e).$$
However in the above situation, that is, \( F_2 \neq \emptyset \), since an original edge of \( G_2 \) is omitted, we cannot define this initial state. So we expand the considering edge set

\[
E_M := E_2 \cup F_2.
\]

We re-define \( p' \) and \( q' \) whose domain is changed to \( E_M \): for every \( e \in E_M \),

\[
p'(e) = \begin{cases} 
p(e) & \text{if } V(e) \not\subseteq M, \\
1 & \text{if } e \in [N_2], \\
0 & \text{otherwise} \end{cases}
\]

\[
q'(e) = \begin{cases} 
q(e) & \text{if } V'(e) \not\subseteq M, \\
1 & \text{if } e \in [N_2], \\
0 & \text{otherwise} \end{cases}
\]

Remark that the above “otherwise” in the definition of \( p' \) is equivalent to the situation of “\( V(e) \in M \) and \( V'(e) \not\subseteq M' \)” or “\( e \in F_2 \)”.

Now we are ready to give the setting of quantum search problem. Remark that \( E_M = 2^n + m \). For each \( x \in V \) and \( y \in V' \), let

\[
|\phi'_x\rangle = \sum_{V(e) = x} \sqrt{p'(e)} |e\rangle \quad \text{and} \quad |\psi'_y\rangle = \sum_{V'(f) = y} \sqrt{q'(f)} |f\rangle.
\]

From these unit vectors, we construct two \((2^n + m) \times (2^n + m)\) matrices \( R'_0 \) and \( R'_1 \) as follows:

\[
R'_0 = 2 \sum_{x \in V} |\phi'_x\rangle \langle \phi'_x| - I_{2^n + m}, \quad R'_1 = 2 \sum_{y \in V'} |\psi'_y\rangle \langle \psi'_y| - I_{2^n + m}
\]

Furthermore, we define an \((2^n + m) \times (2^n + m)\) matrix \( W' \) as follows:

\[
W' = R'_1 R'_0.
\]

Then \( W' \) is the time evolution matrix of the modified Szegedy walk on \( \ell^2(E_M) \).

The initial condition of the quantum walk is

\[
|\psi(0)\rangle = \frac{1}{\sqrt{n}} \sum_{e \in E(G)} \sqrt{p(e)} |e\rangle.
\]

Note that \( |\psi(0)\rangle \) is defined using a random walk on \( G \) determined by \( p \), and it is invariant under the action of \( W = R_1 R_0 \) associated with \( G \) (see [18]). We assume that \( p_{uv'} = p_{v'u}, u, v \in V(G) \) for the stochastic matrix \( P \). Then \( P \) is doubly stochastic. Let

\[
|\psi(t)\rangle = (W')^t |\psi(0)\rangle, \quad t = 0, 1, 2, \ldots
\]
and

\[ F(T) = \frac{1}{T + 1} \sum_{t=0}^{T} \|\psi(t) - \|\psi(0)||^2. \]

Then the quantum hitting time \( H_{P,M} \) of a quantum walk on \( G \) is defined as the smallest number of steps \( T \) such that

\[ F(T) \geq 1 - \frac{m}{n}, \]

where \( n = |V(G)| \) and \( m = |M| \). The quantum hitting time is evaluated by the square of the spectral gap of the \( n \times n \) matrix \( P_M \):

\[ (P_M)_{u,v} = \begin{cases} p_{u,v} & \text{if } u, v \notin M, \\ 0 & \text{otherwise}. \end{cases} \]

3. Key method

From now on, we will attempt three cases of the characteristic polynomials of the time evolution; “a 2-tessellable staggered quantum matrix”, “Szegedy matrix” and “modified Szegedy matrix of quantum search”. To this end, we provide the key lemma.

**Theorem 3.1.** Let \( A \) and \( B \) be \( N \times s \) and \( N \times t \) complex valued isometry matrices, that is,

\[ *AA = I_s, \text{ and } *BB = I_t, \]

where \( *Y \) is the conjugate and transpose of \( Y \). Putting \( U = UBUA \) with \( UB = (2B *B - I_N) \) and \( UA = (2A *A - I_N) \), we have

\[
\det(I_N - uU) = (1 - u)^{N-(s+t)}(1 + u)^{s-t} \det [(1 + u)^2I_t - 4u^*BA^*AB],
\]

\[ = (1 - u)^{N-(s+t)}(1 + u)^{t-s} \det [(1 + u)^2I_s - 4u^*AB^*BA]. \]

**Proof.** At first, we have

\[ \det(I_N - uU) = \det(I_N - uUBUA). \]

Therefore once we can show the first equality, then changing the variables by \( A \leftrightarrow B \) and \( t \leftrightarrow s \), we have the second equality.
Now we will show the first equality.

\[ \det(I_N - uU) = \det(I_N - uU_B U_A) \]
\[ = \det(I_N - u(2B \ast B - I_N)(2A \ast A - I_N)) \]
\[ = \det(I_N - 2uB \ast B(2A \ast A - I_N) + u(2A \ast A - I_N)) \]
\[ = \det((1 - u)I_N + 2uA \ast A - 2uB \ast B(2A \ast A - I_N)) \]
\[ = (1 - u)^N \det(I_N + \frac{2u}{1 - u}A \ast A - \frac{2u}{1 - u}B \ast B(2A \ast A - I_N)) \]
\[ = (1 - u)^N \det(I_N - \frac{2u}{1 - u}B(2A \ast A - I_N)(I_N + \frac{2u}{1 - u}A \ast A)^{-1}) \]
\[ \det(I_N + \frac{2u}{1 - u}A \ast A). \]

If \( A' \) and \( B' \)are a \( m \times n \) and \( n \times m \) matrices, respectively, then we have

\[ \det(I_m - A'B') = \det(I_n - B'A'). \]

Thus, we have

\[ \det(I_N + \frac{2u}{1 - u}A \ast A) = \det(I_s + \frac{2u}{1 - u}A A) \]
\[ = \det(I_s + \frac{2u}{1 - u}I_n) \]
\[ = (1 + \frac{2u}{1 - u})^s = \frac{(1 + u)^s}{(1 - u)^s}. \]

Furthermore, we have

\[ (I_N + \frac{2u}{1 - u}A \ast A)^{-1} \]
\[ = I_N - \frac{2u}{1 - u}A \ast A + \left( \frac{2u}{1 - u} \right)^2 A \ast AA \ast A - \left( \frac{2u}{1 - u} \right)^3 A \ast AA \ast AA \ast A + \cdots \]
\[ = I_N - \frac{2u}{1 - u}A \ast A + \left( \frac{2u}{1 - u} \right)^2 A \ast A - \left( \frac{2u}{1 - u} \right)^3 A \ast A + \cdots \]
\[ = I_N - \frac{2u}{1 - u}(1 - \frac{2u}{1 - u} + \left( \frac{2u}{1 - u} \right)^2 - \cdots)A \ast A \]
\[ = I_N - \frac{2u}{1 - u} / (1 + \frac{2u}{1 - u})A \ast A = I_N - \frac{2u}{1 + u}A \ast A. \]
Therefore, it follows that
\[
\det(I_N - uU) \\
= (1 - u)^N \det(I_N - \frac{2u}{1-u} B * B(2A * A - I_N)(I_N - \frac{2u}{1+u} A * A)) \frac{(1 + u)^s}{(1 - u)^s} \\
= (1 - u)^N s(1 + u)^s \det(I_N + \frac{2u}{1-u} B * B(I_N - \frac{2}{1+u} A * A)) \\
= (1 - u)^N s(1 + u)^s \det(I_N + \frac{2u}{1-u} * B - \frac{4u}{1-u^2} * B * AB) \\
= (1 - u)^N s(1 + u)^s \det(I_N + \frac{2u}{1-u} I_N - \frac{4u}{1-u^2} * B * AB) \\
= (1 - u)^N s(1 + u)^s \det((1 + u)^2 I_N - 4u * B * AB). \]

We put \( T_{BA} := *B \) and \( T_{AB} := *A \). Thus \( *T_{BA} = T_{AB} \).

**Lemma 3.2.** For any eigenvalue \( \lambda_q \) of \( T_{BA}T_{AB} \),
\[
0 \leq \lambda_q \leq 1.
\]

**Proof.** At first, we define the inner product in the Hilbert space \( \mathbb{C}^t \) as follows:
\[
\langle f, g \rangle = \sum_{i=1}^t f_i g_i,
\]
where \( f = \langle f_1 \ldots f_t \rangle, \ g = \langle g_1 \ldots g_t \rangle \in \mathbb{C}^t \). Furthermore, the norm of \( f \in \mathbb{C}^t \) is given by
\[
||f|| = \langle f, f \rangle.
\]

Next, let
\[
T_{BA}T_{AB}f = \lambda_q f.
\]
Then we have
\[
|\lambda_q|^2 ||f||^2 = ||*B*A*Bf||^2 = \langle *A*Bf, *A*Bf \rangle = \langle Bf, A*Bf \rangle \\
\leq \langle Bf, Bf \rangle = \langle f, *B*Bf \rangle = \langle f, f \rangle = ||f||.
\]
Thus,
\[
|\lambda_q| \leq 1.
\]
Since \( \langle g, T_{BA}T_{AB}g \rangle \geq 0 \) for every \( g \), we have \( 0 \leq \lambda_q \) holds. Therefore \( \lambda_q \in [0, 1] \).
**Remark 3.3.** Let \( s \geq t \). Then it holds
\[
\text{Spec}(T_{AB}T_{BA}) = \{0\}^{s-t} \cup \text{Spec}(T_{BA}T_{AB}),
\]
where \( \{0\}^{s-t} \) is the multi-set of \( s - t \). Thus \( 0 \leq \lambda_p \leq 1 \) for any \( \lambda_p \in \text{Spec}(T_{AB}T_{BA}) \).

**Corollary 3.4.** For the unitary matrix \( U = U_B U_A \), we have
\[
\det(\lambda I_N - U) = (\lambda - 1)^{N-s-t}(\lambda + 1)^{s-t} \det((\lambda + 1)^2 I_t - 4\lambda T_{BA}T_{AB}).
\]

**Proof.** Let \( u = 1/\lambda \). Then, by Theorem 3.1, we have
\[
\det(I_N - \lambda U) = (1 - 1/\lambda)^{N-s-t}(1 + 1/\lambda)^{s-t} \det((1 + 1/\lambda)^2 I_t - 4/\lambda T_{BA}T_{AB}),
\]
and so,
\[
\det(\lambda I_N - U) = (\lambda - 1)^{N-s-t}(\lambda + 1)^{s-t} \det((\lambda + 1)^2 I_t - 4\lambda T_{BA}T_{AB}).
\]

**Corollary 3.5.** Set \( \text{Spec}(T_{BA}T_{AB}) = \{\lambda_{q,1}, \ldots, \lambda_{q,t}\} \) with \( 0 \leq \lambda_{q,1} \leq \cdots \leq \lambda_{q,t} \leq 1 \). Moreover the two solutions of
\[
\lambda^2 - 2(2\lambda_{q,j} - 1)\lambda + 1 = 0
\]
is denoted by \( \alpha_j^{(\pm)} \). Then \( N \) eigenvalues of \( U \) are described as follows:
1. \( |N - (s + t)| \)-multiple eigenvalue: 1;
2. \( |t - s| \)-multiple eigenvalue: \((-1)\);
3. \( 2(\text{Min}\{t, N - s\} - \text{Max}\{0, t - s\}) \) eigenvalues:
\[
\alpha_j^{(\pm)}, \ (j = \text{Max}\{1, t - s + 1\}, \ldots, \text{Min}\{t, N - s\}).
\]

Here an expression for \( \alpha_j^{(\pm)} \) is
\[
\alpha_j^{(\pm)} = e^{\pm 2\sqrt{-1} \arccos \sqrt{\lambda_{q,j}}}
\]

**Remark 3.6.** It holds
\[
|N - (s + t)| + |t - s| + 2(\text{Min}\{t, N - s\} - \text{Max}\{0, t - s\}) = N.
\]
In particular,
1. If \( t < s \), then \( \lambda_{q,1} = \cdots = \lambda_{q,s-t} = 0 \).
2. If \( N < t + s \), then \( \lambda_{q,N-s+1} = \cdots = \lambda_{q,t} = 1 \).
Corollary 3.7. Set $\text{Spec}(T_{AB}T_{BA}) = \{\lambda_{p,1}, \ldots, \lambda_{p,s}\}$ with $0 \leq \lambda_{p,1} \leq \cdots \leq \lambda_{p,s} \leq 1$. Moreover the two solutions of

$$\lambda^2 - 2(2\lambda_{p,j} - 1)\lambda + 1 = 0$$

is denoted by $\beta_j^{(\pm)}$. Then $N$ eigenvalues of $U$ are described as follows:

1. $|N - (s + t)|$-multiple eigenvalue: 1;
2. $|t - s|$-multiple eigenvalue: $(-1)$;
3. $2(\min\{s, N - t\} - \max\{0, s - t\})$ eigenvalues:

$$\beta_j^{(\pm)}, \ (j = \max\{1, s - t + 1\}, \ldots, \min\{s, N - t\}).$$

Here an expression for $\beta_j^{(\pm)}$ is

$$\beta_j^{(\pm)} = e^{\pm 2\sqrt{-1}\arccos \sqrt{\lambda_{p,j}}}.$$

Remark 3.8.

1. If $s < t$, then $\lambda_{p,1} = \cdots = \lambda_{p,t-s} = 0$.
2. If $N < t + s$, then $\lambda_{p,N-t+1} = \cdots = \lambda_{p,s} = 1$.

Once we show Corollary 3.5, then Corollary 3.7 automatically holds by Theorem 3.1. So in the following we give a proof of Corollary 3.5.

Proof of Corollary 3.5. By Corollary 3.4, we can rewrite the characteristic polynomial of $U$ by

$$\det(\lambda I_N - U) = (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{s-t}\prod_{j=1}^{t}((\lambda + 1)^2 - 4\lambda_{q,j}\lambda)$$

$$= (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{s-t}\prod_{j=1}^{t}(\lambda^2 - 2(2\lambda_{q,j} - 1)\lambda + 1).$$

We put the two solution of $\lambda^2 - 2(2\lambda_{q,j} - 1)\lambda + 1 = 0$ by $\alpha_j^{(\pm)}$. Then

$$\det(\lambda I_N - U) = (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{s-t}\prod_{j=1}^{t}(\lambda - \alpha_j^{(+)})(\lambda - \alpha_j^{(-)}).$$

Concerning that RHS is an $N$-th degree polynomial of $\lambda$, we consider the four cases with respect to the signes of $N - (s + t)$ and $s - t$. 

\[\begin{align*}
\end{align*}\]
1. \( N - (s + t) \geq 0, \ s - t \geq 0 \) case:
   we directly obtain \((N - s - t)\)-multiple eigenvalue 1, \((s - t)\)-multiple eigenvalue \(-1\) and 2\(t\) eigenvalues \(\alpha_{q,j}^{(z)} \ (j = 1, \ldots, t)\).

2. \( N - (s + t) \geq 0, \ s - t < 0 \) case:
   Since \( s - t < 0 \), \((\lambda + 1)^{s-t}\) is a negative power term. To cancel down it, 
   \(\{(\lambda - \alpha_{j}^{(+)}), (\lambda - \alpha_{j}^{(-)})\}_{j=1}^{t}\) must contain \((t - s)\) terms of \((\lambda + 1)\). Remark that if \( \lambda = -1 \), then \( \lambda_{q,j} = 0 \) from the above quadratic equation. So \( \lambda_{q,1} = \cdots = \lambda_{q,t-s} = 0 \). By the above consideration, the characteristic polynomial is expressed by
   \[
   \det(\lambda I_{N} - U) = (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{t-s} \prod_{j=t-s+1}^{t} (\lambda - \alpha_{j}^{(+)})(\lambda - \alpha_{j}^{(-)}). 
   \]
   Then we obtain \((N - s - t)\)-multiple eigenvalue 1, \((t - s)\)-multiple eigenvalue \(-1\) and 2\(s\) eigenvalues \(\alpha_{q,j}^{(z)} \ (j = t - s + 1, \ldots, t)\).

3. \( N - (s + t) < 0, \ s - t \geq 0 \) case:
   Since \( N - (s + t) < 0 \), \((\lambda - 1)^{N-(s+t)}\) is a negative power term. To cancel down it, 
   \(\{(\lambda - \alpha_{j}^{(+)}), (\lambda - \alpha_{j}^{(-)})\}_{j=1}^{t}\) must contain \((s + t) - N\) terms of \((\lambda - 1)\). Remark that if \( \lambda = 1 \), then \( \lambda_{q,j} = 1 \) from the above quadratic equation. So \( \lambda_{q,N-s+1} = \cdots = \lambda_{q,t} = 1 \). By the above consideration, the characteristic polynomial is expressed by
   \[
   \det(\lambda I_{N} - U) = (\lambda - 1)^{(s+t)-N}(\lambda + 1)^{s-t} \prod_{j=1}^{N-s} (\lambda - \alpha_{j}^{(+)})(\lambda - \alpha_{j}^{(-)}). 
   \]
   Then we obtain \((s+t-N)\)-multiple eigenvalue 1, \((s-t)\)-multiple eigenvalue \(-1\) and \(2(N - s)\) eigenvalues \(\alpha_{q,j}^{(z)} \ (j = 1, \ldots, N - s)\).

4. \( N - (s + t) < 0, \ s - t < 0 \) case:
   Since \( N - (s + t) < 0 \) and \( s - t < 0 \), both \((\lambda - 1)^{N-(s+t)}\) and \((\lambda + 1)^{s-t}\) are negative power terms. To cancel down it, 
   \(\{(\lambda - \alpha_{j}^{(+)}), (\lambda - \alpha_{j}^{(-)})\}_{j=1}^{t}\) must contain \((s + t) - N\) terms of \((\lambda - 1)\) and \(t - s\) terms of \((\lambda + 1)\). From the arguments of cases (2) and (3), we have \( \lambda_{q,N-s+1} = \cdots = \lambda_{q,t} = 1 \) and \( \lambda_{q,1} = \cdots = \lambda_{q,t-s} = 0 \). By the above consideration of the characteristic polynomial is expressed by
   \[
   \det(\lambda I_{N} - U) = (\lambda - 1)^{(s+t)-N}(\lambda + 1)^{t-s} \prod_{j=t-s+1}^{N-s} (\lambda - \alpha_{j}^{(+)})(\lambda - \alpha_{j}^{(-)}). 
   \]
   Then we obtain \((s+t-N)\)-multiple eigenvalue 1, \((t-s)\)-multiple eigenvalue \(-1\) and \(2(N - t)\) eigenvalues \(\alpha_{q,j}^{(z)} \ (j = t - s + 1, \ldots, N - s)\).

Compiling the four cases, we have the desired conclusion. \( \square \)
4. The characteristic polynomial of the unitary matrix of a 2-tessellable staggered quantum matrix

Let $G$ be a connected graph with $\nu$ vertices and $\epsilon$ edges, and let $U = U_1 U_0$ be the unitary matrix of a 2-tessellable SQW on $G$ such that both $U_0$ and $U_1$ are orthogonal reflections. Furthermore, let $\alpha$ and $\beta$ be tessellations of $U$ corresponding to $U_0$ and $U_1$, respectively. Set $\alpha = \{\alpha_1, \ldots, \alpha_m\}$ and $\beta = \{\beta_1, \ldots, \beta_n\}$. Then we have

$$|\alpha_k\rangle = \sum_{k' \in \alpha_k} a_{kk'}|k'\rangle \ (1 \leq k \leq m), \quad |\beta_l\rangle = \sum_{l' \in \beta_l} b_{ll'}|l'\rangle \ (1 \leq l \leq n),$$

$$U_0 = 2 \sum_{k=1}^m |\alpha_k\rangle\langle \alpha_k| - I_\nu, \quad U_1 = 2 \sum_{l=1}^n |\beta_l\rangle\langle \beta_l| - I_\nu.$$

Now, let $X$ be a finite nonempty set and $S = \{S_1, \ldots, S_r\}$ a family of subsets of $X$. Then the \textit{generalized intersection graph} $\Omega(S)$ is defined as follows: $V(\Omega(S)) = S = \{S_1, \ldots, S_r\}$; $S_i$ and $S_j$ are joined by $|S_i \cap S_j|$ edges in $\Omega(S)$.

Peterson [17] gave a necessary and sufficient condition for a graph to be 2-tessellable.

\textbf{Proposition 4.1. (Perterson)} A graph $G$ is 2-tessellable if and only if $G$ is the line graph of a bipartite graph.

\textbf{Sketch of proof} Let $G$ be a 2-tessellable graph with two tessellations $\alpha$ and $\beta$. Set $S = \alpha \cup \beta$ and $H = \Omega(S)$. Then $H$ is a graph with multi-bipartite partite set $\alpha$ and $\beta$. Furthermore, we have $G = L(\Omega(S))$.

Conversely, it is clear that the line graph of a bipartite graph is 2-tessellable. Q.E.D.

By Proposition 4.1, we can rewrite $|\alpha_k\rangle$ and $|\beta_l\rangle$. Let $H = \Omega(\alpha \cup \beta)$ be a bipartite graph with partition $X = \{x_1, \ldots, x_m\}$, $Y = \{y_1, \ldots, y_n\}$ such that $G = L(H)$. Furthermore, we set $\alpha_k = N(x_k)(1 \leq k \leq m)$ and $\beta_l = N(y_l)(1 \leq l \leq n)$, where $N(x) = \{e \in E(H) \mid x \in e\}$. Then we can write

$$|\alpha_k\rangle = \sum_{e \in N(x_k)} a_e|e\rangle \ (1 \leq k \leq m), \quad |\beta_l\rangle = \sum_{f \in N(y_l)} b_f|f\rangle \ (1 \leq l \leq n),$$

where $a_e$ (or $b_f$) corresponds to $a_{kk'}$ (or $b_{ll'}$) if $k'$ (or $l'$) $\in V(G)$ corresponds to an edge $e$ (or $f$) $\in E(H)$.

Now, we define an $m \times m$ matrix $\hat{A} = (a_{xx'})_{x,x' \in X}$ as follows:

$$a_{xx'} := \sum_{p = (e,f)} \bar{a}_e b_a \bar{a}_f \bar{b}_f,$$
where $P$ runs over all $(x, x')$-paths of length two in $H$.

Then we obtain the following formula for the unitary matrix of a SQW on a 2-tessellable graph.

**Theorem 4.2.** Let $G$ be a connected 2-tessellable graph with $\nu$ vertices and $\epsilon$ edges, and let $U = U_1U_0$ be the unitary matrix of a 2-tessellable SQW on $G$ such that both $U_0$ and $U_1$ are orthogonal reflections. Furthermore, let $\alpha$ and $\beta$ be tessellations of $U$ corresponding to $U_0$ and $U_1$, respectively. Set $|\alpha| = m$ and $|\beta| = n$. Then, for the unitary matrix $U = U_1U_0$, we have

$$\det(I_\nu - uU) = (1 - u)^{\nu-m-n}(1 + u)^{n-m} \det((1 + u)^2I_m - 4u\hat{A}).$$

**Proof.** Let $\alpha = \{\alpha_1, \ldots, \alpha_m\}$ and $\beta = \{\beta_1, \ldots, \beta_n\}$. Then we have

$$|\alpha_k| = \sum_{k' \in \alpha_k} a_{kk'}|k'| \quad (1 \leq k \leq m), \quad |\beta_l| = \sum_{l' \in \beta} b_{l'l'} \quad (1 \leq l \leq n),$$

$$U_0 = 2\sum_{k=1}^m |\alpha_k\rangle \langle \alpha_k| - I_\nu, \quad U_1 = 2\sum_{l=1}^n |\beta_l\rangle \langle \beta_l| - I_\nu.$$  

Furthermore, $H = \Omega(\alpha \cup \beta)$ is expressed as follows:

$$V(H) = X \cup Y: \text{ a bipartition, } X = \{x_1, \ldots, x_m\}, \quad Y = \{y_1, \ldots, y_n\};$$

$$N(x_k) = \{e_k, \ldots, e_{d_k}\}, \quad d_k = \deg Hx_k \quad (1 \leq k \leq m);$$

$$N(y_l) = \{f_l, \ldots, e_{d_l}\}, \quad d_l = \deg Hy_l \quad (1 \leq l \leq n),$$

where $N(x) = \{e \in E(H) \mid x \in e\}, \quad x \in V(H)$ and $d_1 + \cdots + d_m = \overline{d}_1 + \cdots + \overline{d}_n = \nu$.

We consider $\alpha_k = N(x_k)\{1 \leq k \leq m\}$ and $\beta_l = N(y_l)\{1 \leq l \leq n\}$. By Proposition 4.1, we can write

$$|\alpha_k| = \sum_{e \in N(x_k)} a_e|e| \quad (1 \leq k \leq m), \quad |\beta_l| = \sum_{f \in N(y_l)} b_f|f| \quad (1 \leq l \leq n),$$

$$U_0 = 2\sum_{k=1}^m |\alpha_k\rangle \langle \alpha_k| - I_\nu, \quad U_1 = 2\sum_{l=1}^n |\beta_l\rangle \langle \beta_l| - I_\nu \quad \text{and} \quad U = U_1U_0.$$  

Now, let $x = x_1 \in X$, $d = d_x = \deg x$, and $N(x) = \{e_1, \ldots, e_d\}$. Set $\alpha_x = \alpha_i(x = x_i)$. Then the submatrix of $|\alpha_x\rangle \langle \alpha_x|$ corresponding to the $e_1, \ldots, e_d$ rows and the $e_1, \ldots, e_d$ columns is we have

$$\begin{bmatrix}
|a_{e_1}|^2 & a_{e_1} \overline{a}_{e_2} & \cdots & a_{e_1} \overline{a}_{e_d} \\
a_{e_2} \overline{a}_{e_1} & |a_{e_2}|^2 & \cdots & a_{e_2} \overline{a}_{e_d} \\
\vdots & \vdots & \ddots & \vdots \\
a_{e_d} \overline{a}_{e_1} & a_{e_d} \overline{a}_{e_2} & \cdots & |a_{e_d}|^2
\end{bmatrix}.$$
where $E(H) = \{e_1, \ldots, e_d, \ldots\}$. Thus, the submatrix of $U_0 = 2 \sum_{i=1}^{n} |\alpha_i\rangle \langle \alpha_i| - I_\nu$ corresponding to the $e_1, \ldots, e_d$ rows and the $e_1, \ldots, e_d$ columns is

$$
\begin{bmatrix}
2|a_{e_1}|^2 - 1 & 2a_{e_1} \bar{a}_{e_2} & \cdots & 2a_{e_1} \bar{a}_{e_d} \\
2a_{e_2} \bar{a}_{e_1} & 2|a_{e_2}|^2 - 1 & \cdots & 2a_{e_2} \bar{a}_{e_d} \\
\vdots & \vdots & \ddots & \vdots \\
2a_{e_d} \bar{a}_{e_1} & 2a_{e_d} \bar{a}_{e_2} & \cdots & 2|a_{e_d}|^2 - 1
\end{bmatrix}.
$$

Let $y = y_1, d' = d_y = \deg y$ and $N(y) = \{f_1, \ldots, f_{d'}\}$. Similarly to $U_0$, the submatrix of $U_1 = 2 \sum_{j=1}^{n} \langle \beta_j | \beta_j \rangle - I_\nu$ corresponding to the $f_1, \ldots, f_{d'}$ rows and the $f_1, \ldots, f_{d'}$ columns is we have

$$
\begin{bmatrix}
2|b_{f_1}|^2 - 1 & 2b_{f_1} \bar{b}_{f_2} & \cdots & 2b_{f_1} \bar{b}_{f_{d'}} \\
2b_{f_2} \bar{b}_{f_1} & 2|b_{f_2}|^2 - 1 & \cdots & 2b_{f_2} \bar{b}_{f_{d'}} \\
\vdots & \vdots & \ddots & \vdots \\
2b_{f_{d'}} \bar{b}_{f_1} & 2b_{f_{d'}} \bar{b}_{f_2} & \cdots & 2|b_{f_{d'}}|^2 - 1
\end{bmatrix}.
$$

Now, let $K = (K_{ex})_{e \in E(H); x \in X}$ be the $\nu \times m$ matrix defined as follows:

$$
K_{ex} := \begin{cases} 
a_e & \text{if } x \in e, \\
0 & \text{otherwise.}
\end{cases}
$$

Furthermore, we define the $\nu \times n$ matrix $L = (L_{ey})_{e \in E(H); y \in Y}$ as follows:

$$
L_{ey} := \begin{cases} 
b_e & \text{if } y \in e, \\
0 & \text{otherwise.}
\end{cases}
$$

Then we have

$$
K^*K = \sum_{k=1}^{m} |\alpha_k\rangle \langle \alpha_k|, \quad L^*L = \sum_{l=1}^{n} |\beta_l\rangle \langle \beta_l|.
$$

Furthermore, since

$$
\sum_{e \in N(x)} |a_e|^2 = \sum_{f \in N(y)} |b_f|^2 = 1 \text{ for each } x \in X \text{ and } y \in Y,
$$

we have

$$
^*KK = I_m \text{ and } ^*LL = I_n.
$$

Therefore, by Theorem 3.1, it follows that

$$
\det(I_\nu - uU) = (1 - u)^{\nu-m-n}(1 + u)^{n-m} \det((1 + u)^2 I_m - 4u \ ^*KL \ ^*K).
$$
But, we have

\((^{(\ast)\textbf{KL}})_{xy} = \overline{a_e} b_e \) for \( e = xy \in E(G) \).

Furthermore, we have

\(^{(\ast)\textbf{KL}} * \textbf{LK} = (^{(\ast)\textbf{KL}}) * (^{(\ast)\textbf{KL}}) \).

Thus, for \( x, x' \in X \),

\((^{(\ast)\textbf{KL}} * \textbf{LK})_{xx'} = \sum_{P=(e,f)} \overline{a_e} a_f \bar{b}_f \),

where \( P \) runs over all \((x, x')\)-paths of length two in \( H \). Thus, we have

\(^{\ast}\textbf{KL} * \textbf{LK} = \hat{A} \).

Hence,

\[ \det(I_\nu - u\textbf{U}) = (1 - u)^{\nu - m - n}(1 + u)^{n - m} \det((1 + u)^2\textbf{I}_m - 4u\hat{A}). \]

By Theorem 4.2 and Corollary 3.4, we obtain the following.

**Corollary 4.3.** Let \( G \) be a connected 2-tessellable graph with \( \nu \) vertices and \( \varepsilon \) edges, and let \( \textbf{U} = \textbf{U}_1\textbf{U}_0 \) be the unitary matrix of a 2-tessellable SQW on \( G \) such that both \( \textbf{U}_0 \) and \( \textbf{U}_1 \) are orthogonal reflections. Furthermore, let \( \alpha \) and \( \beta \) be tessellations of \( \textbf{U} \) corresponding to \( \textbf{U}_0 \) and \( \textbf{U}_1 \), respectively. Set \( |\alpha| = m \) and \( |\beta| = n \). Then, for the unitary matrix \( \textbf{U} = \textbf{U}_1\textbf{U}_0 \), we have

\[ \det(\lambda I_\nu - \textbf{U}) = (\lambda - 1)^{\nu - m - n}(\lambda + 1)^{n - m} \det((\lambda + 1)^2\textbf{I}_m - 4\lambda\hat{A}). \]

By Corollary 3.7, we obtain the spectrum of \( \textbf{U} \).

**Corollary 4.4.** Let \( G \) be a connected 2-tessellable graph with \( \nu \) vertices and \( \varepsilon \) edges, and let \( \textbf{U} = \textbf{U}_1\textbf{U}_0 \) be the unitary matrix of a 2-tessellable SQW on \( G \) such that both \( \textbf{U}_0 \) and \( \textbf{U}_1 \) are orthogonal reflections. Furthermore, let \( \alpha \) and \( \beta \) be tessellations of \( \textbf{U} \) corresponding to \( \textbf{U}_0 \) and \( \textbf{U}_1 \), respectively. Set \( |\alpha| = m \) and \( |\beta| = n \). Then the spectrum of the unitary matrix \( \textbf{U} = \textbf{U}_1\textbf{U}_0 \) are given as follows: Let 0 \( \leq \lambda_{p,1} \leq \cdots \leq \lambda_{p,m} \) be the eigenvalues of \( \hat{A} \).

1. 2(\( \max\{n, \nu - n\} - \max\{0, m - n\}\)) eigenvalues:

\[ \lambda = e^{\pm 2i\theta}, \]

\[ \cos^2\theta \in \{\lambda_{p,j} \in \text{Spec}(\hat{A}) \mid j = \max\{1, m - n + 1\}, \ldots, \max\{m, \nu - n\}\} \]
2. \(|\nu - m - n| \) eigenvalues: 1;
3. \(|n - m| \) eigenvalues: -1.

5. The characteristic polynomial of the Szegedy matrix

We present a formula for the characteristic polynomial of the Szegedy matrix of a bipartite graph. Let \( G = (X \sqcup Y, E) \) be a connected multi-bipartite graph with partite set \( X \) and \( Y \). Moreover, set \(|V(G)| = \nu, |E| = |E(G)| = \epsilon, |X| = m \) and \(|Y| = n \). Then we consider the Hilbert space \( \mathcal{H} = \ell^2(E) = \text{span}\{|e| \mid e \in E\} \).

Let \( p : E \to [0, 1] \) and \( q : E \to [0, 1] \) be the functions such that

\[
\sum_{X(e)=x} p(e) = \sum_{Y(e)=y} q(e) = 1, \forall x \in X, \forall y \in Y,
\]

where \( X(e) \) and \( Y(e) \) are the vertex of \( e \) belonging to \( X \) and \( Y \), respectively.

Let \( W = R_1R_0 \) be a Szegedy matrix of \( G \), where

\[
R_0 = 2 \sum_{x \in X} |\phi_x\rangle \langle \phi_x| - I_\epsilon, \quad R_1 = 2 \sum_{y \in Y} |\psi_y\rangle \langle \psi_y| - I_\epsilon,
\]

\[
|\phi_x\rangle = \sum_{X(e)=x} \sqrt{p(e)}|e\rangle \quad \text{and} \quad |\psi_y\rangle = \sum_{Y(e)=y} \sqrt{q(e)}|e\rangle.
\]

Then we define an \( m \times m \) matrix \( A_p = (a^{(p)}_{xx'})_{x,x' \in X} \) as follows:

\[
a^{(p)}_{xx'} := \sum_{P=(e,f)} \sqrt{p(e)p(f)}q(f),
\]

where \( P \) runs over all \((x, x')\)-paths of length two in \( G \). Note that

\[
a^{(p)}_{xx} = \sum_{e \in E} p(e)q(e), x \in X.
\]

Then a formula of the Szegedy matrix of a bipartite graph is given as follows.

**Theorem 5.1.** Let \( G = (X \sqcup Y, E) \) and \( W \) be as the above. Then, for the Szegedy matrix \( W = R_1R_0 \), we have

\[
\det(I_\epsilon - uW) = (1 - u)^{\nu - \nu'}(1 + u)^{n - m} \det((1 + u)^2I_m - 4uA_p).
\]

**Proof.** Let \( X = \{x_1, \ldots, x_m\} \) and \( Y = \{y_1, \ldots, y_n\} \). Let \( x \in X \) and \( y \in Y \). Then, let

\[
|\phi_x\rangle = \sum_{X(e)=x} \sqrt{p(e)}|e\rangle \quad \text{and} \quad |\psi_y\rangle = \sum_{Y(e)=y} \sqrt{q(e)}|e\rangle.
\]
Now, let $x \in X$, $d = d_x = \deg x$ and $N(x) = \{e_1, \ldots, e_d\}$. Moreover, set $e_j = xy_j$ and $p_{ej} = p(xy_j)$ for $j = 1, \ldots, d$. Then the submatrix of $|\phi_x\rangle\langle\phi_x|$ corresponding to the $e_1, \ldots, e_d$ rows and the $e_1, \ldots, e_d$ columns is

$$\begin{bmatrix}
    p_{x1} & \sqrt{p_{x1}p_{x2}} & \cdots & \sqrt{p_{x1}p_{xd}} \\
    \sqrt{p_{x2}p_{x1}} & p_{x2} & \cdots & \sqrt{p_{x2}p_{xd}} \\
    \vdots & \vdots & \ddots & \vdots \\
    \sqrt{p_{xd}p_{x1}} & \sqrt{p_{xd}p_{x2}} & \cdots & p_{xd}
\end{bmatrix}.$$  

Thus, the submatrix of $R_0 = 2\sum_{x \in X} |\phi_x\rangle\langle\phi_x| - I_e$ corresponding to the $e_1, \ldots, e_d$ rows and the $e_1, \ldots, e_d$ columns is

$$\begin{bmatrix}
    2p_{x1} - 1 & 2\sqrt{p_{x1}p_{x2}} & \cdots & 2\sqrt{p_{x1}p_{xd}} \\
    2\sqrt{p_{x2}p_{x1}} & 2p_{x2} - 1 & \cdots & 2\sqrt{p_{x2}p_{xd}} \\
    \vdots & \vdots & \ddots & \vdots \\
    2\sqrt{p_{xd}p_{x1}} & 2\sqrt{p_{xd}p_{x2}} & \cdots & 2p_{xd} - 1
\end{bmatrix}.$$  

Let $y \in Y$, $d' = d_y = \deg y$ and $N(y) = \{f_1, \ldots, f_{d'}\}$. Moreover, set $f_j = yx_{k_l}$ and $q_{yl} = q(yx_{k_l})$ for $l = 1, \ldots, d'$. Similarly to $R_0$, the submatrix of $R_1 = 2\sum_{x \in X} |\psi_y\rangle\langle\psi_y| - I_e$ corresponding to the $f_1, \ldots, f_{d'}$ rows and the $f_1, \ldots, f_{d'}$ columns is

$$\begin{bmatrix}
    2q_{y1} - 1 & 2\sqrt{q_{y1}q_{y2}} & \cdots & 2\sqrt{q_{y1}q_{yd'}} \\
    2\sqrt{q_{y2}q_{y1}} & 2q_{y2} - 1 & \cdots & 2\sqrt{q_{y2}q_{yd'}} \\
    \vdots & \vdots & \ddots & \vdots \\
    2\sqrt{q_{yd'}q_{y1}} & 2\sqrt{q_{yd'}q_{y2}} & \cdots & 2q_{yd'} - 1
\end{bmatrix}.$$  

Now, let $K = (K_{ex})_{e \in E(G); x \in X}$ be the $\epsilon \times m$ matrix defined as follows:

$$K_{ex} := \begin{cases}
\sqrt{p(e)} & \text{if } x \in e, \\
0 & \text{otherwise}.
\end{cases}$$

Furthermore, we define the $\epsilon \times n$ matrix $L = (L_{ey})_{e \in E(G); y \in Y}$ as follows:

$$L_{ey} := \begin{cases}
\sqrt{q(e)} & \text{if } y \in e, \\
0 & \text{otherwise}.
\end{cases}$$

Moreover, since

$$\sum_{X(e) = x} p(e) = \sum_{Y(e) = y} q(e) = 1, \forall x \in X, \forall y \in Y,$$

we have

$$^tKK = I_m \text{ and } ^tLL = I_n.$$
Thus, by Theorem 3.1, for $W = R_1 R_0$ and $|u| < 1$,
\[
\det(I - uW) = (1 - u)^{r - v}(1 + u)^{n - m} \det((1 + u)^2 I_m - 4u \KL \LK).
\]
But, we have
\[
(t KL)(xy) = \sum_{X(e) = x, Y(e) = y} \sqrt{p(e)q(e)}.
\]
Furthermore, we have
\[
\KL \LK = (t KL)^t (t KL).
\]
Thus, for $x, x' \in X(x \neq x')$,
\[
(t KL \LK)(xx') = \sum_{P = (e, f)} \sqrt{p(e)q(e)p(f)q(f)},
\]
where $P$ runs over all $(x, x')$-paths of length two in $G$. In the case of $x = x'$,
\[
(t KL \LK)(xx) = \sum_{X(e) = x} p_e q_e.
\]
Therefore, it follows that
\[
\KL \LK = A_p.
\]
Hence,
\[
\det(I - uW) = (1 - u)^{r - v}(1 + u)^{n - m} \det((1 + u)^2 I_m - 4u A_p).
\]
\[
\square
\]

By Theorem 5.1 and Corollary 3.4, we obtain the following.

**Corollary 5.2.** Let $G = (X \sqcup Y, E)$ and $W$ be as the above. Then, for the Szegedy matrix $W = R_1 R_0$, we have
\[
\det(\lambda I - W) = (\lambda - 1)^{r - v}(\lambda + 1)^{n - m} \det((\lambda + 1)^2 I_m - 4\lambda A_p).
\]
By Theorem 5.1 and Corollary 3.5, we obtain the spectrum of $W$, which is consistent with [24].

**Corollary 5.3.** Let $G = (X \sqcup Y, E)$ and $W$ be as the above. Suppose that $n \geq m$. Then, the spectra of the Szegedy matrix $W = R_1 R_0$ are given as follows:
If $G$ is not a tree, then
1. $2m$ eigenvalues:
\[
\lambda = e^{\pm 2i\theta}, \cos^2 \theta \in \text{Spec}(A_p);
\]
2. $\epsilon - \nu$ eigenvalues: 1;
3. $n - m$ eigenvalues: -1.

If $G$ is a tree, then
1. $2m - 2$ eigenvalues:
   \[
   \lambda = e^{\pm 2i\theta}, \quad \cos^2 \theta \in \text{Spec}(A_q \setminus \{1\});
   \]
2. one eigenvalue: 1;
3. $m - n$ eigenvalues: -1.

Similarly, if $n < m$, then the following result holds.

**Corollary 5.4.** Let $G = (X \sqcup Y, E)$ and $W$ be as the above. Suppose that $m \geq n$. Then we define an $n \times n$ matrix $A_q = (a_{y,y'}^{(q)})_{y,y' \in Y}$ as follows:
\[
a_{y,y'}^{(q)} := \sum_{Q=(e,f)} \sqrt{p(e)q(e)p(f)q(f)},
\]
where $Q$ runs over all $(y,y')$-paths of length two in $G$. Note that
\[
a_{xx}^{(q)} = \sum_{y \in e} p(e)q(e), y \in Y.
\]

Then, the spectrum of the Szegedy matrix $W = R_qR_0$ are given as follows:

If $G$ is not a tree, then
1. $2n$ eigenvalues:
   \[
   \lambda = e^{\pm 2i\theta}, \quad \cos^2 \theta \in \text{Spec}(A_q);
   \]
2. $\epsilon - \nu$ eigenvalues: 1;
3. $m - n$ eigenvalues: -1.

If $G$ is a tree, then
1. $2n - 2$ eigenvalues:
   \[
   \lambda = e^{\pm 2i\theta}, \quad \cos^2 \theta \in \text{Spec}(A_q \setminus \{1\});
   \]
2. one eigenvalue: 1;
3. $m - n$ eigenvalues: -1.

6. An example of the Szegedy walk

Let $G = K_{2,2}$ be the complete bipartite graph with partite set $X = \{a, b\}, Y = \{c, d\}$. Then we arrange edges of $G$ as follows:
\[
e_1 = ac, \ e_2 = ad, \ e_3 = bc, \ e_4 = bd.
\]
Furthermore, we consider the following two functions $p : E \to [0, 1]$ and $q : E \to [0, 1]$ such that

$$p(e_1) = p(e_2) = p(e_3) = p(e_4) = 1/2 \text{ and } q(e_1) = q(e_2) = q(e_3) = q(e_4) = 1/2.$$ 

Now, we have

$$|\phi\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}, \quad |\phi\rangle = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}, \quad |\psi\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \quad |\psi\rangle = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}.$$ 

Thus, we have

$$K = \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} \end{bmatrix}, \quad L = \begin{bmatrix} 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} \end{bmatrix}.$$ 

Therefore, it follows that

$$K^tK = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & 1/2 \end{bmatrix},$$

$$L^tL = \begin{bmatrix} 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \end{bmatrix}.$$ 

Hence,

$$R_0 = 2 \sum_{x \in X} |\phi_x\rangle \langle \phi_x| - I_4 = \begin{bmatrix} J_0 & 0 \\ 0 & J_0 \end{bmatrix},$$

$$R_1 = 2 \sum_{y \in Y} |\psi_y\rangle \langle \psi_y| - I_4 = \begin{bmatrix} 0 & I_2 \\ I_2 & 0 \end{bmatrix},$$

where

$$J_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$
Thus,
\[ W = R_1 R_0 = \begin{bmatrix} 0 & J_0 \\ J_0 & 0 \end{bmatrix}. \]

But,
\[ A_p = KL'K = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}. \]
Thus,
\[ \det(\lambda I_2 - A_p) = (\lambda - 1/2)^2 - 1/4 = \lambda(\lambda - 1). \]
Therefore, it follows that
\[ \text{Spec}(A_p) = \{1, 0\}. \]
Furthermore, since \( m = n = 2 \), we have \( mn - m - n = n - m = 0 \). By Corollary 5.3, the eigenvalues of \( W \) are
\[ \lambda = 1, 1, -1, -1. \]

These are eigenvalues induced from \( A_p \).

7. The characteristic polynomial of the modified time evolution matrix of the duplication of the modified digraph

Let \( G \) be a connected non-bipartite graph with \( n \) vertices and \( \epsilon \) edges which may have multiple edges and self loops, and the duplication graph be \( G_2 \). We set \( p, q : E(G_2) \to [0, 1] \) so that \( \sum_{V(e) = v} p(e) = \sum_{V'(e') = v'} q(e') = 1 \) with
\[ \{ p(e) \mid e \in E_{G_2}(v, u') \} = \{ q(f) \mid f \in E_{G_2}(v', u) \} \]
for any \( v \in V \) and \( u' \in V' \). Thus \( q \) is determined by \( p \). The \( 2n \times 2n \) stochastic matrix \( P \) is denoted by
\[ (P)_{u,v} = p_{uv} = \begin{cases} \sum_{V(e) = u, V'(e) = v} p(e) & \text{if } u \in V, v \in V', \\ \sum_{V'(e') = u, V(e) = v} q(e) & \text{if } u \in V', v \in V, \\ 0 & \text{otherwise}. \end{cases} \]

Furthermore, let \( M \) be a set of \( m \) marked vertices in \( G \), and the modified bipartite digraph of the duplication graph \( G_2 \) with the marked element
\[ M_2 = M \cup M' \quad (M' = \{ v' \mid v \in M \}) \]
be denoted by $\tilde{G}_2$. Let $W' = R'_i R'_0$ be the modified time evolution matrix of the modified Szegedy walk on $\ell^2(E_M)$. Here $E_M = E(G_2) \cup [N_2]$, where $[N_2]$ is set of the matching edges between marked elements and its copies, that is, $[N_2] = \{mm' \mid m \in M\}$. Furthermore, let $E'_M = E_M \setminus E_{G_2}(M, M')$. Thus the cardinality of $\ell^2(E_M)$ is $2\varepsilon + m$. Under the setting of $W'$, we took the modification of $p$ and $q$ as follows. Let $p', q' : E_M \to [0, 1]$ be

\[
p'(e) := \begin{cases} p(e) & \text{if } V(e) \notin M, \\ 1 & \text{if } e \in [N_2], \\ 0 & \text{otherwise}, \end{cases} \]

\[
q'(f) := \begin{cases} q(f) & \text{if } V'(f) \notin M', \\ 1 & \text{if } f \in [N_2], \\ 0 & \text{otherwise}, \end{cases} \]

where

\[
\sum_{V(e) = x} p'(e) = \sum_{V'(e) = y} q'(e) = 1, \forall x \in V, \forall y \in V'.
\]

The modified $2n \times 2n$ stochastic matrix $P'$ is given by changing $p$ and $q$ to $p'$ and $q'$ as follows:

\[
(P')_{u,v} = p'_{uv} = \begin{cases} \sum_{V(e) = u, V'(e) = v} p'(e) & \text{if } u \in V, v \in V', \\ \sum_{V'(e) = u, V(e) = v} q'(e) & \text{if } u \in V', v \in V, \\ 0 & \text{otherwise}. \end{cases}
\]

The reflection operators $R'_0$ and $R'_1$ are described by $\{\phi'_{v}\}_{v \in V}$ and $\{\psi'_{u}\}_{u \in V'}$ as follows:

\[
R'_0 = 2 \sum_{v \in V} |\phi'_{v}\rangle \langle \phi'_{v}| - I_{2\varepsilon + m},
\]

\[
R'_1 = 2 \sum_{u \in V'} |\psi'_{u}\rangle \langle \psi'_{u}| - I_{2\varepsilon + m},
\]

where $\phi'_{v} = \sum_{V(e) = v} \sqrt{p'(e)} |e\rangle$, $\psi'_{u} = \sum_{V'(e) = u} \sqrt{q'(e)} |e\rangle$. See Sect. 2.5 for more detailed this setting. Let $\{|v\rangle\}_{v \in V}$ be the standard basis of $\mathbb{C}^n$, that is, $(|v\rangle)_u = 1$ if $v = u$, $(|v\rangle)_u = 0$ otherwise, where $n = |V|$. We define $(2\varepsilon + m) \times n$ matrices as follows, where $2\varepsilon = |E(G_2)|$:

\[
K = \sum_{v \in V(e)} |\phi'_{v}\rangle \langle v|,
\]

\[
L = \sum_{u' \in V'(e)} |\psi'_{u'}\rangle \langle u'|,
\]
that is,

\[
K_{ev} := \begin{cases} 
\sqrt{p'(e)} & \text{if } V(e) = v, \\
0 & \text{otherwise},
\end{cases}
\]

\[
L_{ev} := \begin{cases} 
\sqrt{q'(e)} & \text{if } V'(e) = v, \\
0 & \text{otherwise}.
\end{cases}
\]

Let \( r \) be the number of edges connecting non-marked elements and its copies, that is,

\[
r = |\{ e \in E_M | V(e) \notin M, V'(e) \notin M' \}|.
\]

Let \( s \) be the number of edges connecting non-marked elements and copies of marked elements, that is,

\[
s = |\{ e \in E_M | V(e) \notin M, V'(e) \in M' \}|.
\]

We set \( \epsilon' = r + 2s + m \). Remark that if there is no marked element connecting to another marked element in the original graph \( G \), then \( \epsilon' = 2\epsilon + m \), on the other hand, if not, \( \epsilon' < 2\epsilon + m \) since such an edge connecting marked element in \( G \) is omitted in the procedure making \( \tilde{G}_2 \) from \( G \). By the definitions of \( R'_0 \) and \( R'_1 \), \( K'K \) is equal to \( \sum_{x \in X} |\phi'_x \rangle \langle \phi'_x| \), and \( L'L \) is equal to \( \sum_{y \in Y} |\psi'_y \rangle \langle \psi'_y| \). Thus,

\[
R'_0 = 2 \sum_{x \in X} |\phi'_x \rangle \langle \phi'_x| - I_{2\epsilon + m} = 2K'K - I_{2\epsilon + m},
\]

\[
R'_1 = 2 \sum_{y \in Y} |\psi'_y \rangle \langle \psi'_y| - I_{2\epsilon + m} = 2L'L - I_{2\epsilon + m}.
\]

Now, let \( K_1 \) be the \( \epsilon' \times n \) submatrix of \( K \) with respect to the rows corresponding to the edges of \( E_M' \) and the columns corresponding to the vertices of \( V \). Furthermore, let \( L_1 \) be the \( \epsilon' \times n \) submatrix of \( L \) with respect to the rows corresponding to the edges of \( E_M' \) and the columns corresponding to the vertices of \( V' \). Then we define an \( n \times n \) matrix \( \hat{A'}_p \) as follows:

\[
\hat{A'}_p = \ell K_1 L_1 \ell L_1 K_1,
\]

Remark that \( q \) is determined by \( p \) and so as \( p' \) and \( q' \). The \( v, u \) element of this
symmetric matrix $\hat{A}'_p$ is computed as follows: $\hat{L}K$ is expressed by

$$\hat{L}K = \begin{bmatrix}
\langle \psi'_{v_1} | & | \phi'_{v_1} \\ \vdots & \ddots & \vdots \\ \langle \psi'_{v_n} | & | \phi'_{v_n} 
\end{bmatrix}
\begin{bmatrix}
| & \phi'_{v_1} & \cdots & | \phi'_{v_n} \\
| & \vdots & \ddots & \vdots \\
| & \phi'_{v_1} & \cdots & \phi'_{v_n}
\end{bmatrix}
$$

Thus

$$\langle \hat{L}K \rangle_{u,v} = \langle \psi'_{u} | \phi'_{v} \rangle = \sum_{e \in \hat{E}_M} \overline{\psi'_{u}(e)} \phi'_{v}(e)$$

which is the summation of a real valued weight over all the path from $u \in V'$ to $v \in V$. Therefore

$$\langle \hat{K}L \hat{L}K \rangle_{u,v} = \sum_{(e,f) \text{-(path in } G_2)} \sqrt{p'(e)q'(f)p(f)q(f)}$$

where $u, v \in V$.

Since $p'(e) = 0, q'(f) = 0$ for every "$V(e) \in M, V'(e) \notin M'$" and "$V'(f) \in M', V(f) \notin M"$.

$$\langle \hat{K}L \hat{L}K \rangle_{u,v} = \begin{cases}
\sum_{(e,f) \in Q_2} \sqrt{p(e)q(e)p(f)q(f)} & \text{if } u, v \in V \setminus M, \\
\delta_{u,v} & \text{if } u, v \in M, \\
0 & \text{otherwise.}
\end{cases}$$

Here the summation $Q_2$ is over all the 2-length path in $G_2$ from $u \in V$ to $v \in V$ never going into $M$ and $M'$. Hence,

$$\langle \hat{A}'_p \rangle_{u,v} = \sum_{(e,f) \in Q_2} \sqrt{p(e)q(e)p(f)q(f)}$$

if $u, v \notin M$.

If the following condition holds, we say $p, q$ satisfies the detailed balanced condition: there exists $\pi : V \sqcup V' \to \mathbb{R}_{\geq 0}$ such that

$$p'(e)\pi(V(e)) = q'(e)\pi(V'(e))$$
for every $e \in E_M$ with $V(e) \notin M$ and $V'(e) \notin M'$, and $\pi(u) = 1$ if $u \in M \sqcup M'$. A typical setting of $p(e) = 1/\deg(V(e))$ and $q(e) = 1/\deg(V'(e))$ satisfies the detailed balanced condition by $\pi(u) = \deg(u)$ for every $u \in (V \setminus M) \cup (V' \setminus M')$. If the detailed balanced condition holds, since the values $q(e)$ and $p(f)$, where $(e, f)$ is $(u, v)$-path of length two in $G_2$, are equivalent to

$$q(e) = \frac{\pi(V(e))}{\pi(V'(e))}p(e) = \frac{\pi(u)}{\pi(V'(e))}p(e), \quad p(f) = \frac{\pi(V'(f))}{\pi(V(f))}q(f) = \frac{\pi(V'(f))}{\pi(v)}q(f),$$

we have

$$\sqrt{p(e)q(e)p(f)q(f)} = \sqrt{\pi(u)/\pi(v)p(e)q(f)}.$$

Then it is expressed by

$$(\hat{A}_p')_{u,v} = \begin{cases} \sqrt{\pi(u)/\pi(v)} \sum_{(e,f) \in Q_2} p(e)q(f) & \text{if } u, v \notin M, \\ \delta_{u,v} & \text{if } u, v \in M \\ 0 & \text{otherwise,} \end{cases}$$

Thus, $(\hat{A}_p')_{u,v} = \sqrt{\pi(u)/\pi(v)} \sum_{(e,f) \in Q_2} p(e)q(f)$ if $u, v \notin M$. Therefore if the detailed balanced condition holds, $\hat{A}_p'$ is unitary equivalent to the square of $P_M' := P_M \oplus I_m$, where $P_M$ is an $(n-m) \times (n-m)$ matrix describing the random walk with the Dirichlet boundary condition at $M$: for $u, v \notin M$,

$$(P_M)_{u,v} = \sum_{e \in E(G_2) \text{ with } V(e) = u, V'(e) = v'} p(e).$$

Thus

$$(P_M')_{u,v} = \begin{cases} (P_M)_{u,v} & \text{if } u, v \notin M, \\ \delta_{u,v} & \text{if } u, v \in M, \\ 0 & \text{otherwise.} \end{cases}$$

Now we are in the place to give the following formula for the modified time evolution matrix of the modified Szegedy walk on $\ell^2(E_M)$.

**Theorem 7.1.** Let $G$ be a connected graph with $n$ vertices and $e$ edges which may have multiple edges and self loops. Let $W' = R'_1 R'_0$ be the modified time evolution matrix of the modified Szegedy walk on $\ell^2(E_M)$ induced by random walk $p : E(G_2) \to [0, 1]$ and the set $M$ of marked elements with $|M| = m$.

Then, for $W'$, we have

$$\det(I_{2e+m} - uW') = (1 - u)^{2(e-n)+m} \det((1 + u)^2 I_n - 4u\hat{A}_p').$$

In particular, if $p$ satisfies the detailed balanced condition, then

$$\det(I_{2e+m} - uW') = (1 - u)^{2(e-n)+3m} \det((1 + u)^2 I_{n-m} - 4u P_M^2).$$
Proof. The subset of edges connecting marked elements and its copies in $E_M$ denotes $F_M$, that is,

$$F_M = \{ e \in E_M \mid V(e) \in M, V'(e) \in M' \}.$$ 

The cardinality of $F_M = 2e + m - \epsilon'$. The definitions of $p'$ and $q'$ give $p'(e) = q'(e) = 0$ for $e \in F_M$, which implies $\langle e | \phi'_u \rangle = \langle e | \psi'_v \rangle = 0$ for any $u, v \in V$. Thus

$$(K^\dagger K)_{e,f} = \sum_{v \in V} \langle e | \phi'_u \rangle \langle \phi'_u | f \rangle = 0,$$

$$(L^\dagger L)_{e,f} = \sum_{v \in V} \langle e | \psi'_v \rangle \langle \psi'_v | f \rangle = 0$$

for every $e, f \in F_M$. Concerning the above, it holds that

$$R'_0 = 2K^\dagger K - I_{2e+m} = (2K_1^\dagger K_1 - I_{\epsilon'}) \oplus (-I_{2e+m-\epsilon'})$$

$$R'_1 = 2L^\dagger L - I_{2e+m} = (2L_1^\dagger L_1 - I_{\epsilon'}) \oplus (-I_{2e+m-\epsilon'})$$

Therefore if $F_M \neq \emptyset$, then

$$W' = (2L_1^\dagger L_1 - I_{\epsilon'}) (2K_1^\dagger K_1 - I_{\epsilon'}) \oplus I_{2e+m-\epsilon'}.$$ 

Therefore, if $F_M \neq \emptyset$, then at least $|F_M|$-multiple eigenvalue 1 of $W'$ exists.

From now on we consider the first term of the above RHS. To this end, it is not a loss of generality that we take the assumption that $F_M = \emptyset$ putting $2K^\dagger K - L_\epsilon = R'_0$, $2L^\dagger L - L_\epsilon = R'_1$ and $W' = R'_1 R'_0$. Since

$$\sum_{V(e) = x} p'(e) = \sum_{V'(e) = y} q'(e) = 1, \forall x \in X, \forall y \in Y,$$

we have

$${\dagger} K K = {\dagger} L L = I_n.$$ 

Therefore, by Theorem 3.1, it follows that

$$\det(I_{\epsilon'} - u W') = (1 - u)^{\epsilon'-2n} \det((1 + u)^2 I_n - 4u K_1 L_1^\dagger L_1 K_1).$$

But,

$${\hat A}'_p = K_1 L_1^\dagger L_1 K_1.$$ 

Hence, If $F_M = \emptyset$, then

$$\det(I_{\epsilon'} - u W') = (1 - u)^{\epsilon'-2n} \det((1 + u)^2 I_n - 4u {\hat A}'_p).$$
Therefore if \( F_M \neq \emptyset \), then
\[
\det(I_{2\epsilon+m} - uW') = (1-u)^{2\epsilon+m-\epsilon'} \times (1-u)^{\epsilon'-2n} \det((1+u)^2I_n - 4u\hat{A}'_p) \\
= (1-u)^{2(\epsilon-n)+m} \det((1+u)^2I_n - 4u\hat{A}'_p)
\]
Concerning the fact that \( F_M = \emptyset \) if and only if \( \epsilon' = 2\epsilon + m \), then we have obtained the desired conclusion. If the detailed balanced condition holds, \( \hat{A}'_p = (D \oplus I_m)P_M^2(D^{-1} \oplus I_m) \), \( D \) is an \((n-m) \times (n-m)\) diagonal matrix \( \text{diag}([\sqrt{\pi(u)} \mid u \notin M]) \), that is, \( (D \oplus I_m)|u\rangle = \sqrt{\pi(u)} \) if \( u \notin M \), \( (D \oplus I_m)|u\rangle = |u\rangle \) if \( u \in M \). \( \square \)

By Theorem 7.1 and Corollary 3.4, we have obtain following.

**COROLLARY 7.2.** Let \( G \) be a connected graph with \( n \) vertices and \( \epsilon \) edges which may have multiple edges and self loops. Let \( W' = R'_1R'_0 \) be the modified time evolution matrix of the modified Szegedy walk on \( \ell^2(E_M) \) induced by random walk \( p : E(G_2) \rightarrow [0,1] \) and the marked element \( M \) with \( |M| = m \). Then, for the \( W' = R'_1R'_0 \), we have
\[
\det(\lambda I_{2\epsilon+m} - W') = (\lambda - 1)^{2(\epsilon-n)+m} \det((\lambda + 1)^2I_n - 4\lambda\hat{A}'_p).
\]
By Theorem 7.1 and Corollary 3.5, we obtain the eigenvalues of \( W' \).

**COROLLARY 7.3.** Let \( G \) be a connected graph with \( n \) vertices and \( \epsilon \) edges which may have multiple edges and self loops. Let \( W' = R'_1R'_0 \) be the modified time evolution matrix of the modified Szegedy walk on \( \ell^2(E_M) \) induced by random walk \( p : E(G_2) \rightarrow [0,1] \) and the set \( M \) of marked elements with \( |M| = m \). Then the spectrum of the unitary matrix \( W' = R'_1R'_0 \) are given as follows:

1. If \( 2(\epsilon - n) + m \geq 0 \), that is, \( "G \) is not a tree" or \( "m > 1" \), then
   (a) 2n eigenvalues:
   \[
   \lambda = e^{\pm 2i\theta}, \quad \cos^2 \theta \in \text{Spec}(\hat{A}'_p);
   \]
   (b) \( 2(\epsilon - n) + m \) eigenvalues: 1.
2. otherwise, that is, \( G \) is a tree and \( m \in \{0,1\} \), then
   (a) \( 2(n-1) \) eigenvalues:
   \[
   \lambda = e^{\pm 2i\theta}, \quad \cos^2 \theta \in \text{Spec}(\hat{A}'_p) \setminus \{1\};
   \]
   (b) \( m \)-multiple eigenvalue 1.

**Proof.** Since \( \epsilon - n < 0 \) if and only if \( G \) is a tree, thus \( 2(\epsilon - n) + m < 0 \) if and only if \( G \) is a tree and \( m \in \{0,1\} \). By Corollary 7.2,
\[
\det(\lambda I_{2\epsilon+m} - W') = (\lambda - 1)^{2(\epsilon-n)+m} \prod_{j=1}^{n}(\lambda - \alpha_{j}^{(+)})\langle \lambda - \alpha_{j}^{(-)}\rangle
\]
holds, where $\alpha_j^{(\pm)}$ are the solutions of $\lambda^2 - 2(2\mu - 1)\lambda + 1 = 0$ with $\mu \in Spec(\tilde{\mathbf{A}}'_p)$. The second term has $2n = 2\epsilon + 2$ solutions while the dimension of the total space is now $2\epsilon + m$. But in this situation since $2(\epsilon - n) + m = -2 + m < 0$, then the power of the first term $(1 - \lambda)^{2(\epsilon - n) + m}$ is negative. Thus the second term should include the $(\lambda - 1)^{(2 - m)}$ term counteracted by the first term. The result follows.

\[\square\]

8. An example of the duplication of the modified digraph

Let $G = K_3$ be the complete graph with three vertices $v_1, v_2, v_3$, and $P = (p_{uv})_{u,v \in V(G)}$ the following stochastic matrix of $G$:

\[
P = \frac{1}{2} \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.
\]

Furthermore, let $M = \{v_3\}$ be a set of $m = 1$ marked vertices in $G$. Thus we set $E_M$ by

\[
\{e_1, e_2, f_1, f_2, f'_1, f'_2, g\}
\]

where $e_1 = \{v_1, v'_2\}$, $e_2 = \{v_2, v'_1\}$, $f_1 = \{v_1, v'_3\}$, $f_2 = \{v_2, v'_3\}$, $f'_1 = \{v_3, v'_2\}$, $f'_2 = \{v_3, v'_1\}$ and $g = \{v_3, v'_3\}$. The duplication graph of $G$ is denoted by $G_2$. $E_M$ is the union of $E(G_2)$ and $\{g\}$. The modified stochastic matrix $P' = (p'_{uv})_{u,v \in V(G_2)}$ derived from $P$ with $M = \{v_3\}$ is given as follows:

\[
P' = \begin{bmatrix} 0 & 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}
\]

which means

$p'(e_1) = p'(e_2) = p'(f_1) = p'(f_2) = 1/2$, $p'(f'_1) = p'(f'_2) = 0$, $p'(g) = 1$ and $q'(e_1) = q'(e_2) = q'(f'_1) = q'(f'_2) = 1/2$, $q'(f_1) = q'(f_2) = 0$, $q'(g) = 1$

Then the dimension of the total state space is

\[
|E_M| = 2\epsilon + m = \epsilon' = 2 + 2 \cdot 2 + 1 = 7.
\]
We put $X = \{v_1, v_2, v_3\}$ and its copy $X' = \{v'_1, v'_2, v'_3\}$. The $7 \times 3$ matrix $K$ is an incidence matrix between 7 edges $e_1, e_2, f_1, f_2, f'_1, f'_2, g$ and $X$ as follows:

$$
K = \begin{bmatrix}
\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1
\end{bmatrix}.
$$

Furthermore, the $7 \times 3$ matrix $L$ is an incidence matrix between 7 edges $e_1, e_2, f_1, f_2, f'_1, f'_2, g$ and $Y$ as follows:

$$
L = \begin{bmatrix}
0 & \frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 1
\end{bmatrix}.
$$

Thus, we have

$$
K^\dagger K = \sum_{x \in X} |\phi_x\rangle \langle \phi_x| = \begin{bmatrix}
1/2 & 0 & 1/2 & 0 & 0 \\
0 & 1/2 & 0 & 1/2 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
0 & 1/2 & 0 & 1/2 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1
\end{bmatrix}
$$

and

$$
L^\dagger L = \sum_{y \in Y} |\psi_y\rangle \langle \psi_y| = \begin{bmatrix}
1/2 & 0 & 0 & 0 & 0 & 1/2 & 0 \\
0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 \\
1/2 & 0 & 0 & 0 & 0 & 1/2 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1
\end{bmatrix}.
$$
Therefore, it follows that

\[
R_0 = 2K^tK - I_7 = \begin{bmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

and

\[
R_1 = 2L^tL - I_7 = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\]

Hence,

\[
W' = R_1R_0 = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
-1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\]

Now, we have

\[
^tKL = \begin{bmatrix}
0 & 1/2 & 0 \\
1/2 & 0 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\]

Thus, we have

\[
\hat{A}_p = ^tKL^tLK = \begin{bmatrix}
1/4 & 0 & 0 \\
0 & 1/4 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\]

Thus,

\[
\det(\lambda I_2 - \hat{A}_p) = (\lambda - 1)(\lambda - 1/4)^2.
\]

Therefore, it follows that

\[
\text{Spec}(\hat{A}_p) = \{1, 1/4\}.
\]
Furthermore, since \( n = 3 \), we have \( \epsilon' - 2n = 7 - 6 = 1 \). By Corollary 7.3, the eigenvalues of \( W' \) are

\[
\lambda = 1, 1, 1, -\frac{1 \pm i\sqrt{3}}{2}, -\frac{1 \pm i\sqrt{3}}{2}.
\]

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