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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

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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 exits 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-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 $D(G) = \{(u, v), (v, u) | uv \in E(G)\}$. 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 *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})*-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 *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 *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 *bipartite set* or the *bipartition* of G. A bipartite graph $G = (V_1, V_2)$ is called *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 *clique* if H is a complete subgraph of G. The *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 *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 $d_j = d_{u_j} = \deg v_j$ for

$i = 1, \ldots, n$. The *transition matrix* $\mathbf{U} = \mathbf{U}(G) = (U_{ab})_{a,b \in D(G)}$ of G is defined by

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

The matrix $\mathbf{U}$ is called the *Grover matrix* of G.

We introduce the *positive support* $\mathbf{F}^+ = (F^+_{ij})$ of a real matrix $\mathbf{F} = (F_{ij})$ 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 $\mathbf{U}$ 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 $\mathbf{T}(G) = (T_{uv})_{u,v \in V(G)}$ 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 $\mathbf{T}(G)$ 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 $\mathbf{U}$ of G, we have*

$$\begin{aligned} \det(\lambda \mathbf{I}_{2m} - \mathbf{U}) &= (\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{I}_n - 2\lambda \mathbf{T}(G)) \\ &= \frac{(\lambda^2 - 1)^{m-n} \det((\lambda^2 + 1)\mathbf{D} - 2\lambda \mathbf{A}(G))}{d_{v_1} \cdots d_{v_n}}, \end{aligned}$$

where $\mathbf{A}(G)$ is the adjacency matrix of G, and $\mathbf{D} = (d_{uv})$ 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 $\mathbf{T}(G)$ (see [4]). Let *Spec*$(\mathbf{F})$ be the spectrum of a square matrix $\mathbf{F}$.

COROLLARY 2.2. (Emms, Hancock, Severini and Wilson [4]) *Let G be a connected graph with n vertices and m edges. The transition matrix* $\mathbf{U}$ *has* $2n$ *eigenvalues of the form*

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

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

Emms et al. [4] determined the spectrum of the transition matrix $\mathbf{U}$ 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 $\mathbf{U}$ 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 $\mathbf{U}^+$ of the transition matrix of a regular graph G by means of those of the adjacency matrix $\mathbf{A}(G)$ 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* $\mathbf{U}^+$ *has* $2n$ *eigenvalues of the form*

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

where λ_A *is an eigenvalue of the matrix* $\mathbf{A}(G)$. *The remaining* $2(m-n)$ *eigenvalues of* $\mathbf{U}^+$ *are* ± 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 $G = (X \sqcup Y, E)$ 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 $\mathcal{H} = \ell^2(E) = span\{|e\rangle \mid e \in E\}$. 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.

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

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

From these vectors, we construct two $\epsilon \times \epsilon$ matrices $\mathbf{R}_0$ and $\mathbf{R}_1$ as follows:

$$\mathbf{R}_0 = 2\sum_{x\in X} |\phi_x\rangle\langle\phi_x| - \mathbf{I}_\epsilon,\ \mathbf{R}_1 = 2\sum_{y\in Y} |\psi_y\rangle\langle\psi_y| - \mathbf{I}_\epsilon$$

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

$$\mathbf{W} = \mathbf{R}_1\mathbf{R}_0.$$

Note that two matrices $\mathbf{R}_0$ and $\mathbf{R}_1$ are unitary, and $\mathbf{R}_0^2 = \mathbf{R}_1^2 = \mathbf{I}_\epsilon$.

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

2.4 The staggered quantum walk on a graph

Let G be a connected graph with ν vertices and ϵ edges. Furthermore, let $\mathcal{H}^\nu$ 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 $\mathbf{U}$ on $\mathcal{H}^\nu$ can be written by

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

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

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

we obtain

$$\mathbf{U} = 2\sum_x |\psi_x^+\rangle\langle\psi_x^+| - \mathbf{I} \cdots (*).$$

A unitary and Hermitian matrix $\mathbf{U}$ in $\mathcal{H}^\nu$ given by (*) 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 $|\psi\rangle \in \mathcal{H}^\nu$ 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 $\mathbf{U}$ of G is the union of the polygons induced by the (+1)-eigenvectors $\{|\psi_x^+\rangle\}_x$ of $\mathbf{U}$ described in the above. The *staggered quantum walk(SQW)* on G associated with the Hilbert space $\mathcal{H}^\nu$ is driven by

$$\mathbf{U} = \mathbf{U}_1\mathbf{U}_0,$$

where $\mathbf{U}_0$ and $\mathbf{U}_1$ are orthogonal reflections of G. The union of the tessellations α and β induced by $\mathbf{U}_0$ and $\mathbf{U}_1$ must cover the edges of G. Furthermore, set $\alpha = \{\alpha_1, \dots, \alpha_m\}$ and $\beta = \{\beta_1, \dots, \beta_n\}$. Then $\mathbf{U}_0$ and $\mathbf{U}_1$ are given as follows:

$$\mathbf{U}_0 = 2\sum_{k=1}^{m} |\alpha_k\rangle\langle\alpha_k| - \mathbf{I}_\nu,\ \mathbf{U}_1 = 2\sum_{l=1}^{n} |\beta_l\rangle\langle\beta_l| - \mathbf{I}_\nu,$$

where

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

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

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

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 $\mathbf{U} = \mathbf{U}_1\mathbf{U}_0$ is the unitary matrix of a SQW on G, and $\alpha = \{\alpha_1, \dots, \alpha_m\}$ and $\beta = \{\beta_1, \dots, \beta_n\}$ are tessellations of $\mathbf{U}$ corresponding to $\mathbf{U}_0$ and $\mathbf{U}_1$, respectively. If A and B are disjoint subsets of a set X, then the union of A and B is denoted by $A \sqcup B$.

2.5 The quantum search problem on a graph

Let $G = (V, E)$ be a connected non-bipartite graph with n vertices and ϵ 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 $S, T \subset V(H)$, set $E_H(S,T) = \{e \in E(H) \mid e = uv, u \in S, v \in T\}$. It holds $\sqcup_{e=uv,\in E(H)} E_H(u,v) = E(H)$, where "$\sqcup$" means the disjoint union. We want to set the quantum search of an element of $M \subset V$ 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 $V' = \{v' : v \in V\}$. The edge set of $E(G_2)$ is denoted by

$$E_G(u,v) \subset E(G) \Leftrightarrow E_{G_2}(u,v') \subset E(G_2)$$

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 $\mathbf{P}$ is denoted by

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

Let $V(G) = \{v_1, \ldots, v_n\}$ and $M = \{v_{n-m+1}, \ldots, v_n\}$. The elements of M are called *marked verices*. Then define the *modified digraph* $\vec{G}$ from G as follows: The *modified digraph* $\vec{G}$ 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 $\vec{G}_2$ 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 $\vec{G}_2$ is obtained by taking the duplication of $\vec{G}$. More precisely, let $A(G_2) = D(G_2)$ be the set of symmetric arcs naturally induced by $E(G_2)$, then

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

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 $\vec{G}_2$ 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 $\vec{G}_2$. The Szegedy walk is denoted by non-directed edges of the bipartite graph. So we consider the support of $A(\overrightarrow{G}_2)$ by $E_2 := [A(\overrightarrow{G}_2)] := \{[a] \mid a \in A(\overrightarrow{G}_2)\}$. Here $[a]$ is the edge obtained by removing the direction of the arc a. Thus $E_2 = [A_2] \sqcup [N_2]$, 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 $\mathbf{P}'$ is given by changing p and q to p' and q' as follows:

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

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 $\vec{G}_2$, 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,

$$\psi_0 = \sum_{e \in E(G_2)} \sqrt{p(e)} |e\rangle.$$

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 $e \in E_M$.

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

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

Remark that the above "otherwise" in the definition of p' is equivalent to the situation of "$V(e) \in M$ and $V'(e) \notin M'$" or "$e \in F_2$".

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

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

From these unit vectors, we construct two $(2\epsilon + m) \times (2\epsilon + m)$ matrices $\mathbf{R}'_0$ and $\mathbf{R}'_1$ as follows:

$$\mathbf{R}'_0 = 2\sum_{x\in V} |\phi'_x\rangle\langle\phi'_x| - \mathbf{I}_{2\epsilon+m},\ \mathbf{R}'_1 = 2\sum_{y\in V'} |\psi'_y\rangle\langle\psi'_y| - \mathbf{I}_{2\epsilon+m}$$

Furthermore, we define an $(2\epsilon + m) \times (2\epsilon + m)$ matrix $\mathbf{W}'$ as follows:

$$\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0.$$

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

The initial condition of the quantum walk is

$$|\psi(0)\rangle = \frac{1}{\sqrt{n}} \sum_{e\in E(G_2)} \sqrt{p(e)}|e\rangle.$$

Note that $|\psi(0)\rangle$ is defined using a random walk on G determined by p, and it is invariant under the action of $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$ associated with G(see [18]). We assume that $p_{uv'} = p_{v'u}, u, v \in V(G)$ for the stochastic matrix $\mathbf{P}$. Then $\mathbf{P}$ is doubly stochastic. Let

$$|\psi(t)\rangle = (\mathbf{W}')^t|\psi(0)\rangle, t = 0, 1, 2, \ldots$$

and

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

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 $\mathbf{P}_M$:

$$(\mathbf{P}_M)_{u,v} = \begin{cases} p_{u,v'} & \text{if } u, v \notin M, \\ 0 & \text{otherwise.} \end{cases}$$

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* $\mathbf{A}$ *and* $\mathbf{B}$ *be* $N \times s$ *and* $N \times t$ *complex valued isometry matrices, that is,*

$${}^*\mathbf{A}\mathbf{A} = \mathbf{I}_s, \text{ and } {}^*\mathbf{B}\mathbf{B} = \mathbf{I}_t,$$

where ${}^*\mathbf{Y}$ *is the conjugate and transpose of* $\mathbf{Y}$. *Putting* $\mathbf{U} = \mathbf{U}_B\mathbf{U}_A$ *with* $\mathbf{U}_B = (2\mathbf{B}\,{}^*\mathbf{B} - \mathbf{I}_N)$ *and* $\mathbf{U}_A = (2\mathbf{A}\,{}^*\mathbf{A} - \mathbf{I}_N)$, *we have*

$$\begin{aligned}\det(\mathbf{I}_N - u\mathbf{U}) &= (1-u)^{N-(s+t)}(1+u)^{s-t}\det\left[(1+u)^2\mathbf{I}_t - 4u^*\mathbf{B}\mathbf{A}^*\mathbf{A}\mathbf{B}\right], \\ &= (1-u)^{N-(s+t)}(1+u)^{t-s}\det\left[(1+u)^2\mathbf{I}_s - 4u^*\mathbf{A}\mathbf{B}^*\mathbf{B}\mathbf{A}\right].\end{aligned}$$

Proof. At first, we have

$$\det(\mathbf{I}_N - u\mathbf{U}) = \det(\mathbf{I}_N - u\mathbf{U}_B\mathbf{U}_A).$$

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.

$$\det(\mathbf{I}_N - u\mathbf{U}) = \det(\mathbf{I}_N - u\mathbf{U}_B\mathbf{U}_A)$$
$$= \det(\mathbf{I}_N - u(2\mathbf{B}\ {}^*\mathbf{B} - \mathbf{I}_N)(2\mathbf{A}\ {}^t\mathbf{A} - \mathbf{I}_N))$$
$$= \det(\mathbf{I}_N - 2u\mathbf{B}\ {}^*\mathbf{B}(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N) + u(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N))$$
$$= \det((1-u)\mathbf{I}_N + 2u\mathbf{A}\ {}^*\mathbf{A} - 2u\mathbf{B}\ {}^*\mathbf{B}(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N))$$
$$= (1-u)^N \det(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A} - \frac{2u}{1-u}\mathbf{B}\ {}^*\mathbf{B}(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N))$$
$$= (1-u)^N \det(\mathbf{I}_N - \frac{2u}{1-u}\mathbf{B}\ {}^*\mathbf{B}(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N)(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A})^{-1})$$
$$\det(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A}).$$

If $\mathbf{A}'$ and $\mathbf{B}'$are a $m \times n$ and $n \times m$ matrices, respectively, then we have

$$\det(\mathbf{I}_m - \mathbf{A}'\mathbf{B}') = \det(\mathbf{I}_n - \mathbf{B}'\mathbf{A}').$$

Thus, we have

$$\det(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A}) = \det(\mathbf{I}_s + \frac{2u}{1-u}\ {}^*\mathbf{A}\mathbf{A})$$
$$= \det(\mathbf{I}_s + \frac{2u}{1-u}\mathbf{I}_n)$$
$$= (1 + \frac{2u}{1-u})^s = \frac{(1+u)^s}{(1-u)^s}.$$

Furthermore, we have

$$(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A})^{-1}$$
$$= \mathbf{I}_N - \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A} + (\frac{2u}{1-u})^2\mathbf{A}\ {}^*\mathbf{A}\mathbf{A}\ {}^*\mathbf{A} - (\frac{2u}{1-u})^3\mathbf{A}\ {}^*\mathbf{A}\mathbf{A}\ {}^*\mathbf{A}\mathbf{A}\ {}^*\mathbf{A} + \cdots$$
$$= \mathbf{I}_N - \frac{2u}{1-u}\mathbf{A}\ {}^*\mathbf{A} + (\frac{2u}{1-u})^2\mathbf{A}\ {}^*\mathbf{A} - (\frac{2u}{1-u})^3\mathbf{A}\ {}^*\mathbf{A} + \cdots$$
$$= \mathbf{I}_N - \frac{2u}{1-u}(1 - \frac{2u}{1-u} + (\frac{2u}{1-u})^2 - \cdots)\mathbf{A}\ {}^*\mathbf{A}$$
$$= \mathbf{I}_N - \frac{2u}{1-u}/(1 + \frac{2u}{1-u})\mathbf{A}\ {}^*\mathbf{A} = \mathbf{I}_N - \frac{2u}{1+u}\mathbf{A}\ {}^*\mathbf{A}.$$

Therefore, it follows that

$$
\begin{aligned}
&\det(\mathbf{I}_N - u\mathbf{U}) \\
&= (1-u)^N \det(\mathbf{I}_N - \frac{2u}{1-u}\mathbf{B}\ {}^*\mathbf{B}(2\mathbf{A}\ {}^*\mathbf{A} - \mathbf{I}_N)(\mathbf{I}_N - \frac{2u}{1+u}\mathbf{A}\ {}^*\mathbf{A}))\frac{(1+u)^s}{(1-u)^s} \\
&= (1-u)^{N-s}(1+u)^s \det(\mathbf{I}_N + \frac{2u}{1-u}\mathbf{B}\ {}^*\mathbf{B}(\mathbf{I}_N - \frac{2}{1+u}\mathbf{A}\ {}^*\mathbf{A})) \\
&= (1-u)^{N-s}(1+u)^s \det(\mathbf{I}_t + \frac{2u}{1-u}\ {}^*\mathbf{B}(\mathbf{I}_N - \frac{2}{1+u}\mathbf{A}\ {}^*\mathbf{A})\mathbf{B}) \\
&= (1-u)^{N-s}(1+u)^s \det(\mathbf{I}_t + \frac{2u}{1-u}\ {}^*\mathbf{B}\mathbf{B} - \frac{4u}{1-u^2}\ {}^*\mathbf{B}\mathbf{A}\ {}^*\mathbf{A}\mathbf{B}) \\
&= (1-u)^{N-s}(1+u)^s \det(\mathbf{I}_t + \frac{2u}{1-u}\mathbf{I}_t - \frac{4u}{1-u^2}\ {}^*\mathbf{B}\mathbf{A}\ {}^*\mathbf{A}\mathbf{B}) \\
&= (1-u)^{N-s}(1+u)^s \det(\frac{1+u}{1-u}\mathbf{I}_t - \frac{4u}{1-u^2}\ {}^*\mathbf{B}\mathbf{A}\ {}^*\mathbf{A}\mathbf{B}) \\
&= (1-u)^{N-s-t}(1+u)^{s-t} \det((1+u)^2\mathbf{I}_t - 4u\ {}^*\mathbf{B}\mathbf{A}\ {}^*\mathbf{A}\mathbf{B}).
\end{aligned}
$$

□

We put $\mathbf{T}_{BA} := {}^*\mathbf{B}\mathbf{A}$ and $\mathbf{T}_{AB} := {}^*\mathbf{A}\mathbf{B}$. Thus ${}^*\mathbf{T}_{BA} = \mathbf{T}_{AB}$.

Lemma 3.2. *For any eigenvalue λ_q of $\mathbf{T}_{BA}\mathbf{T}_{AB}$,*

$$0 \leq \lambda_q \leq 1.$$

Proof. At first, we define the inner product in the Hilbert space $\mathbf{C}^t$ as follows:

$$\langle f, g \rangle = \sum_{i=1}^{t} \overline{f}_i g_i,$$

where $f = {}^t(f_1 \dots f_t), g = {}^t(g_1 \dots g_t) \in \mathbf{C}^t$. Furthermore, the norm of $f \in \mathbf{C}^t$ is given by

$$||f|| = \langle f, f \rangle.$$

Next, let

$$\mathbf{T}_{BA}\mathbf{T}_{AB} f = \lambda_q f.$$

Then we have

$$
\begin{aligned}
|\lambda_q|^2 ||f||^2 = ||{}^*\mathbf{B}\mathbf{A}{}^*\mathbf{A}\mathbf{B}f||^2 &= \langle {}^*\mathbf{A}\mathbf{B}f, {}^*\mathbf{A}\mathbf{B}f \rangle = \langle \mathbf{B}f, \mathbf{A}{}^*\mathbf{A}\mathbf{B}f \rangle \\
&\leq \langle \mathbf{B}f, \mathbf{B}f \rangle = \langle f, {}^*\mathbf{B}\mathbf{B}f \rangle = \langle f, f \rangle = ||f||.
\end{aligned}
$$

Thus,

$$|\lambda_q| \leq 1.$$

Since $\langle g, \mathbf{T}_{BA}\mathbf{T}_{AB} g \rangle \geq 0$ 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

$$Spec(\mathbf{T}_{AB}\mathbf{T}_{BA}) = \{0\}^{s-t} \cup Spec(\mathbf{T}_{BA}\mathbf{T}_{AB}),$$

where $\{0\}^{s-t}$ is the multi-set of $s-t$ 0. Thus $0 \leq \lambda_p \leq 1$ for any $\lambda_p \in Spec(T_{AB}T_{BA})$.

COROLLARY 3.4. *For the unitary matrix* $\mathbf{U} = \mathbf{U}_B\mathbf{U}_A$*, we have*

$$\det(\lambda \mathbf{I}_N - \mathbf{U}) = (\lambda - 1)^{N-s-t}(\lambda + 1)^{s-t} \det((\lambda + 1)^2 \mathbf{I}_t - 4\lambda \mathbf{T}_{BA}\mathbf{T}_{AB}).$$

Proof. Let $u = 1/\lambda$. Then, by Theorem 3.1, we have

$$\det(\mathbf{I}_N - 1/\lambda \mathbf{U}) = (1 - 1/\lambda)^{N-s-t}(1 + 1/\lambda)^{s-t} \det((1 + 1/\lambda)^2 \mathbf{I}_t - 4/\lambda \mathbf{T}_{BA}\mathbf{T}_{AB}),$$

and so,

$$\det(\lambda \mathbf{I}_N - \mathbf{U}) = (\lambda - 1)^{N-s-t}(\lambda + 1)^{s-t} \det((\lambda + 1)^2 \mathbf{I}_t - 4\lambda \mathbf{T}_{BA}\mathbf{T}_{AB}).$$

□

COROLLARY 3.5. *Set* $Spec(\mathbf{T}_{BA}\mathbf{T}_{AB}) = \{\lambda_{q,1}, \ldots, \lambda_{q,t}\}$ *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* $\mathbf{U}$ *are described as follows:*

1. $|N - (s + t)|$*-multiple eigenvalue:* 1*;*
2. $|t - s|$*-multiple eigenvalue:* (-1)*;*
3. $2(\mathrm{Min}\{t, N - s\} - \mathrm{Max}\{0, t - s\})$ *eigenvalues:*

$$\alpha_j^{(\pm)},\ (j = \mathrm{Max}\{1, t - s + 1\}, \cdots, \mathrm{Min}\{t, N - s\}).$$

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

$$|N - (s + t)| + |t - s| + 2(\mathrm{Min}\{t, N - s\} - \mathrm{Max}\{0, t - s\}) = N.$$

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 Spec*$(\mathbf{T}_{AB}\mathbf{T}_{BA}) = \{\lambda_{p,1}, \ldots, \lambda_{p,s}\}$ *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* $\mathbf{U}$ *are described as follows:*

1. $|N - (s+t)|$*-multiple eigenvalue:* 1;
2. $|t - s|$*-multiple eigenvalue:* (-1);
3. $2(\mathrm{Min}\{s, N-t\} - \mathrm{Max}\{0, s-t\})$ *eigenvalues:*

$$\beta_j^{(\pm)}, \ (j = \mathrm{Max}\{1, s-t+1\}, \cdots, \mathrm{Min}\{s, N-t\}).$$

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 $\mathbf{U}$ by

$$\begin{aligned}
&\det(\lambda \mathbf{I}_N - \mathbf{U}) \\
&= (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{s-t}\prod_{j=1}^{t}((\lambda+1)^2 - 4\lambda_{q,j}\lambda) \\
&= (\lambda - 1)^{N-(s+t)}(\lambda + 1)^{s-t}\prod_{j=1}^{t}(\lambda^2 - 2(2\lambda_{q,j} - 1)\lambda + 1).
\end{aligned}$$

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

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

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

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 $2t$ eigenvalues $\alpha_{q,j}^{(\pm)}$ $(j=1,\dots,t)$.
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
   $$\det(\lambda \mathbf{I}_N - \mathbf{U}) = (\lambda-1)^{N-(s+t)}(\lambda+1)^{t-s}\prod_{j=t-s+1}^{t}(\lambda-\alpha_j^{(+)})(\lambda-\alpha_j^{(-)}).$$
   Then we obtain $(N-s-t)$-multiple eigenvalue 1, $(t-s)$-multiple eigenvalue -1 and $2s$ eigenvalues $\alpha_{q,j}^{(\pm)}$ $(j=t-s+1,\dots,t)$.
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
   $$\det(\lambda \mathbf{I}_N - \mathbf{U}) = (\lambda-1)^{(s+t)-N}(\lambda+1)^{s-t}\prod_{j=1}^{N-s}(\lambda-\alpha_j^{(+)})(\lambda-\alpha_j^{(-)}).$$
   Then we obtain $(s+t-N)$-multiple eigenvalue 1, $(s-t)$-multiple eigenvalue -1 and $2(N-s)$ eigenvalues $\alpha_{q,j}^{(\pm)}$ $(j=1,\dots,N-s)$.
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
   $$\det(\lambda \mathbf{I}_N - \mathbf{U}) = (\lambda-1)^{(s+t)-N}(\lambda+1)^{t-s}\prod_{j=t-s+1}^{N-s}(\lambda-\alpha_j^{(+)})(\lambda-\alpha_j^{(-)}).$$
   Then we obtain $(s+t-N)$-multiple eigenvalue 1, $(t-s)$-multiple eigenvalue -1 and $2(N-t)$ eigenvalues $\alpha_{q,j}^{(\pm)}$ $(j=t-s+1,\dots,N-s)$.

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 ν vertices and ϵ edges, and let $\mathbf{U} = \mathbf{U}_1\mathbf{U}_0$ be the unitary matrix of a 2-tessellable SQW on G such that both $\mathbf{U}_0$ and $\mathbf{U}_1$ are orthogonal reflections. Furthermore, let α and β be tessellations of $\mathbf{U}$ corresponding to $\mathbf{U}_0$ and $\mathbf{U}_1$, respectively. Set $\alpha = \{\alpha_1, \dots, \alpha_m\}$ and $\beta = \{\beta_1, \dots, \beta_n\}$. Then we have

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

$$\mathbf{U}_0 = 2\sum_{k=1}^{m} |\alpha_k\rangle\langle\alpha_k| - \mathbf{I}_\nu,\ \mathbf{U}_1 = 2\sum_{l=1}^{n} |\beta_l\rangle\langle\beta_l| - \mathbf{I}_\nu.$$

Now, let X be a finite nonempty set and $S = \{S_1, \dots, S_r\}$ a family of subsets of X. Then the *generalized intersection graph* $\Omega(S)$ is defined as follows: $V(\Omega(S)) = S = \{S_1, \dots, S_r\}$; 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.

Proposition 4.1. (Perterson) *A graph G is 2-tessellable if and only if G is the line graph of a bipartite graph.*

Sketch of proof Let G be a 2-tessellable graph with two tessellations α and β. Set $S = \alpha \cup \beta$ and $H = \Omega(S)$. Then H is a graph with multi-bipartite partite set α and β. 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 bipartition $X = \{x_1, \dots, x_m\}$, $Y = \{y_1, \dots, y_n\}$ 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

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

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 $\hat{\mathbf{A}} = (a_{xx'})_{x,x' \in X}$ as follows:

$$a_{xx'} := \sum_{P=(e,f)} \overline{a}_e b_e a_f \overline{b}_f,$$

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 ν vertices and ϵ edges, and let $\mathbf{U} = \mathbf{U}_1\mathbf{U}_0$ be the unitary matrix of a 2-tessellable SQW on G such that both $\mathbf{U}_0$ and $\mathbf{U}_1$ are orthogonal reflections. Furthermore, let α and β be tessellations of $\mathbf{U}$ corresponding to $\mathbf{U}_0$ and $\mathbf{U}_1$, respectively. Set $|\alpha| = m$ and $|\beta| = n$. Then, for the unitary matrix $\mathbf{U} = \mathbf{U}_1\mathbf{U}_0$, we have*

$$\det(\mathbf{I}_\nu - u\mathbf{U}) = (1-u)^{\nu-m-n}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m - 4u\hat{\mathbf{A}}).$$

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

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

$$\mathbf{U}_0 = 2\sum_{k=1}^{m} |\alpha_k\rangle\langle\alpha_k| - \mathbf{I}_\nu, \ \mathbf{U}_1 = 2\sum_{l=1}^{n} |\beta_l\rangle\langle\beta_l| - \mathbf{I}_\nu.$$

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

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

$$N(x_k) = \{e_{k1}, \dots, e_{kd_k}\}, \ d_k = \deg_H x_k \ (1 \le k \le m);$$

$$N(y_l) = \{f_{l1}, \dots, e_{l\overline{d}_l}\}, \ \overline{d}_l = \deg_H y_l \ (1 \le l \le n),$$

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

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

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

$$\mathbf{U}_0 = 2\sum_{k=1}^{m} |\alpha_k\rangle\langle\alpha_k| - \mathbf{I}_\nu, \ \mathbf{U}_1 = 2\sum_{l=1}^{n} |\beta_l\rangle\langle\beta_l| - \mathbf{I}_\nu \textit{ and } \mathbf{U} = \mathbf{U}_1\mathbf{U}_0.$$

Now, let $x = x_1 \in X$, $d = d_x = \deg x$ and $N(x) = \{e_1, \dots, e_d\}$. Set $\alpha_x = \alpha_i(x = x_i)$. Then the submatrix of $|\alpha_x\rangle\langle\alpha_x|$ corresponding to the $e_1, \dots, e_d$ rows and the $e_1, \dots, e_d$ 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 $E(H)=\{e_1,\dots,e_d,\dots\}$. Thus, the submatrix of $\mathbf{U}_0=2\sum_{i=1}^{m}|\alpha_i\rangle\langle\alpha_i|-\mathbf{I}_\nu$ corresponding to the $e_1,\dots,e_d$ rows and the $e_1,\dots,e_d$ columns is

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

Let $y=y_1$, $d'=d_y=\deg y$ and $N(y)=\{f_1,\dots,f_{d'}\}$. Similarly to $\mathbf{U}_0$, the submatrix of $\mathbf{U}_1=2\sum_{j=1}^{n}|\beta_j\rangle\langle\beta_j|-\mathbf{I}_\nu$ corresponding to the $f_1,\dots,f_{d'}$ rows and the $f_1,\dots,f_{d'}$ columns is we have

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

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

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

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

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

Then we have

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

Furthermore, since

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

we have

$${}^*\mathbf{K}\mathbf{K}=\mathbf{I}_m\ and\ {}^*\mathbf{L}\mathbf{L}=\mathbf{I}_n.$$

Therefore, by Theorem 3.1, it follows that

$$\det(\mathbf{I}_\nu-u\mathbf{U})=(1-u)^{\nu-m-n}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m-4u\ {}^*\mathbf{K}\mathbf{L}\ {}^*\mathbf{L}\mathbf{K}).$$

But, we have

$$({}^*\mathbf{KL})_{xy} = \overline{a}_e b_e \ for\ e = xy \in E(G).$$

Furthermore, we have

$${}^*\mathbf{KL}\ {}^*\mathbf{LK} = ({}^*\mathbf{KL})\ {}^*({}^*\mathbf{KL}).$$

Thus, for $x, x' \in X$,

$$({}^*\mathbf{KL}\ {}^*\mathbf{LK})_{xx'} = \sum_{P=(e,f)} \overline{a}_e b_e a_f \overline{b}_f,$$

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

$${}^*\mathbf{KL}\ {}^*\mathbf{LK} = \hat{\mathbf{A}}.$$

Hence,

$$\det(\mathbf{I}_\nu - u\mathbf{U}) = (1-u)^{\nu-m-n}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m - 4u\hat{\mathbf{A}}).$$

□

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

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

$$\det(\lambda\mathbf{I}_\nu - \mathbf{U}) = (\lambda-1)^{\nu-m-n}(\lambda+1)^{n-m}\det((\lambda+1)^2\mathbf{I}_m - 4\lambda\hat{\mathbf{A}}).$$

By Corollary 3.7, we obtain the spectrum of $\mathbf{U}$.

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

1. $2(\mathrm{Max}\{n, \nu - n\} - \mathrm{Max}\{0, m-n\})$ *eigenvalues:*

$$\lambda = e^{\pm 2i\theta},$$
$$\cos^2\theta \in \{\lambda_{p,j} \in Spec(\hat{\mathbf{A}}) \mid j = \mathrm{Max}\{1, m-n+1\}, \ldots, \mathrm{Max}\{m, \nu - n\}\},$$

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 $\mathcal{H} = \ell^2(E) = span\{|e\rangle \mid e \in E\}$. 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 $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$ be a Szegedy matrix of G, where

$$\mathbf{R}_0 = 2\sum_{x\in X} |\phi_x\rangle\langle\phi_x| - \mathbf{I}_\epsilon,\ \mathbf{R}_1 = 2\sum_{y\in Y} |\psi_y\rangle\langle\psi_y| - \mathbf{I}_\epsilon,$$

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

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

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

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

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

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 $\mathbf{W}$ be as the above. Then, for the Szegedy matrix $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$, we have*

$$\det(\mathbf{I}_\epsilon - u\mathbf{W}) = (1-u)^{\epsilon-\nu}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m - 4u\mathbf{A}_p).$$

Proof. Let $X = \{x_1, \dots, x_m\}$ and $Y = \{y_1, \dots, y_n\}$. Let $x \in X$ and $y \in Y$. Then, let

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

Now, let $x \in X$, $d = d_x = \deg x$ and $N(x) = \{e_1, \dots, e_d\}$. Moreover, set $e_j = xy_{k_j}$ and $p_{xj} = p(xy_{k_j})$ for $j = 1, \dots, d$. Then the submatrix of $|\phi_x\rangle\langle\phi_x|$ corresponding to the $e_1, \dots, e_d$ rows and the $e_1, \dots, e_d$ 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 $\mathbf{R}_0 = 2\sum_{x \in X} |\phi_x\rangle\langle\phi_x| - \mathbf{I}_\epsilon$ corresponding to the $e_1, \dots, e_d$ rows and the $e_1, \dots, e_d$ 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 $N(y) = \{f_1, \dots, f_{d'}\}$. Moreover, set $f_j = yx_{k_l}$ and $q_{yl} = q(yx_{k_l})$ for $l = 1, \dots, d'$. Similarly to $\mathbf{R}_0$, the submatrix of $\mathbf{R}_1 = 2\sum_{x \in X} |\psi_y\rangle\langle\psi_y| - \mathbf{I}_\epsilon$ corresponding to the $f_1, \dots, f_{d'}$ rows and the $f_1, \dots, f_{d'}$ columns is

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

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

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

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

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

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

$${}^t\mathbf{K}\mathbf{K} = \mathbf{I}_m \textit{ and } {}^t\mathbf{L}\mathbf{L} = \mathbf{I}_n.$$

Thus, by Theorem 3.1, for $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$ and $|u| < 1$,

$$\det(\mathbf{I}_\epsilon - u\mathbf{W}) = (1-u)^{\epsilon-\nu}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m - 4u\ {}^t\mathbf{KL}\ {}^t\mathbf{LK}).$$

But, we have

$$({}^t\mathbf{KL})_{xy} = \sum_{X(e)=x, Y(e)=y} \sqrt{p(e)q(e)}.$$

Furthermore, we have

$${}^t\mathbf{KL}\ {}^t\mathbf{LK} = ({}^t\mathbf{KL})\ {}^t({}^t\mathbf{KL}).$$

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

$$({}^t\mathbf{KL}\ {}^t\mathbf{LK})_{xx'} = \sum_{P=(e,f)} \sqrt{p(e)q(e)p(f)q(f)},$$

where P runs over all (x, x')-paths of length two in G. In the case of $x = x'$,

$$({}^t\mathbf{KL}\ {}^t\mathbf{LK})_{xx} = \sum_{X(e)=x} p_e q_e.$$

Therefore, it follows that

$${}^t\mathbf{KL}\ {}^t\mathbf{LK} = \mathbf{A}_p.$$

Hence,

$$\det(\mathbf{I}_\epsilon - u\mathbf{W}) = (1-u)^{\epsilon-\nu}(1+u)^{n-m}\det((1+u)^2\mathbf{I}_m - 4u\mathbf{A}_p).$$

□

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

Corollary 5.2. *Let $G = (X \sqcup Y, E)$ and $\mathbf{W}$ be as the above. Then, for the Szegedy matrix $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$, we have*

$$\det(\lambda\mathbf{I}_\epsilon - \mathbf{W}) = (\lambda-1)^{\epsilon-\nu}(\lambda+1)^{n-m}\det((\lambda+1)^2\mathbf{I}_m - 4\lambda\mathbf{A}_p).$$

By Theorem 5.1 and Corollary 3.5, we obtain the spectrum of $\mathbf{W}$, which is consistent with [24].

Corollary 5.3. *Let $G = (X \sqcup Y, E)$ and $\mathbf{W}$ be as the above. Suppose that $n \geq m$. Then, the spectra of the Szegedy matrix $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$ are given as follows: If G is not a tree, then*

1. *$2m$ eigenvalues:*

$$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\mathbf{A}_p);$$

2. $\epsilon - \nu$ *eigenvalues: 1;*
3. $n - m$ *eigenvalues: -1.*

If G is a tree, then

1. $2m - 2$ *eigenvalues:*

$$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\mathbf{A}_p \setminus \{1\});$$

2. *one eigenvalue: 1;*
3. $n - m$ *eigenvalues: -1.*

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

Corollary 5.4. *Let $G = (X \sqcup Y, E)$ and $\mathbf{W}$ be as the above. Suppose that $m \geq n$. Then we define an $n \times n$ matrix $\mathbf{A}_q = (a^{(q)}_{yy'})_{y,y' \in Y}$ as follows:*

$$a^{(q)}_{yy'} := \sum_{Q=(e,f)} \sqrt{p(e)q(e)p(f)q(f)},$$

where Q runs over all (y, y')-paths of length two in G. Note that

$$a^{(q)}_{xx} = \sum_{y \in e} p(e)q(e), y \in Y.$$

Then, the spectrum of the Szegedy matrix $\mathbf{W} = \mathbf{R}_1\mathbf{R}_0$ are given as follows: If G is not a tree, then

1. $2n$ *eigenvalues:*

$$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\mathbf{A}_q);$$

2. $\epsilon - \nu$ *eigenvalues: 1;*
3. $m - n$ *eigenvalues: -1.*

If G is a tree, then

1. $2n - 2$ *eigenvalues:*

$$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\mathbf{A}_q \setminus \{1\});$$

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

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

Now, we have

$$|\phi_a\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}, |\phi_b\rangle = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}, |\psi_c\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, |\psi_d\rangle = \begin{bmatrix} 0 \\ 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{bmatrix}.$$

Thus, we have

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

Therefore, it follows that

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

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

Hence,

$$\mathbf{R}_0 = 2\sum_{x \in X} |\phi_x\rangle\langle\phi_x| - \mathbf{I}_4 = \begin{bmatrix} \mathbf{J}_0 & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_0 \end{bmatrix},$$

$$\mathbf{R}_1 = 2\sum_{y \in Y} |\psi_y\rangle\langle\psi_y| - \mathbf{I}_4 = \begin{bmatrix} \mathbf{0} & \mathbf{I}_2 \\ \mathbf{I}_2 & \mathbf{0} \end{bmatrix},$$

where

$$\mathbf{J}_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Thus,

$$\mathbf{W} = \mathbf{R}_1\mathbf{R}_0 = \begin{bmatrix} \mathbf{0} & \mathbf{J}_0 \\ \mathbf{J}_0 & \mathbf{0} \end{bmatrix}.$$

But,

$$\mathbf{A}_p = {}^t\mathbf{K}\mathbf{L}\,{}^t\mathbf{L}\mathbf{K} = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}.$$

Thus,

$$\det(\lambda \mathbf{I}_2 - \mathbf{A}_p) = (\lambda - 1/2)^2 - 1/4 = \lambda(\lambda - 1).$$

Therefore, it follows that

$$Spec(\mathbf{A}_p) = \{1, 0\}.$$

Furthermore, since $m = n = 2$, we have $mn - m - n = n - m = 0$. By Corollary 5.3, the eigenvalues of $\mathbf{W}$ are

$$\lambda = 1, 1, -1, -1.$$

These are eigenvalues induced from $\mathbf{A}_p$.

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 ϵ edges which may have multiple edges and self loops, and the duplication graph be G_2. We set $p, q : E(G_2) \rightarrow [0, 1]$ 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 $\mathbf{P}$ is denoted by

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

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

$$M_2 = M \cup M' \ (M' = \{v' \mid v \in M\})$$

be denoted by $\vec{G}_2$. Let $\mathbf{W}' = \mathbf{R}_1'\mathbf{R}_0'$ 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 $2\epsilon{+}m$. Under the setting of $\mathbf{W}'$, 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 $\mathbf{P}'$ is given by changing p and q to p' and q' as follows:

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

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

$$\mathbf{R}_0' = 2\sum_{v\in V} |\phi_v'\rangle\langle\phi_v'| - \mathbf{I}_{2\epsilon+m},$$
$$\mathbf{R}_1' = 2\sum_{u\in V'} |\psi_u'\rangle\langle\psi_u'| - \mathbf{I}_{2\epsilon+m},$$

where $\phi_v' = \sum_{V(e)=v} \sqrt{p'(e)}|e\rangle$, $\psi_v' = \sum_{V'(e)=v} \sqrt{q'(e)}|e\rangle$. 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 $(2\epsilon + m) \times n$ matrices as follows, where $2\epsilon = |E(G_2)|$:

$$K = \sum_{v\in V(e)} |\phi_v'\rangle\langle v|,$$
$$L = \sum_{u'\in V'(e)} |\psi_{u'}'\rangle\langle u|,$$

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,

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

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

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

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 $\vec{G}_2$ from G. By the definitions of $\mathbf{R}'_0$ and $\mathbf{R}'_1$, $\mathbf{K}\ {}^t\mathbf{K}$ is equal to $\sum_{x\in X} |\phi'_x\rangle\langle\phi'_x|$, and $\mathbf{L}\ {}^t\mathbf{L}$ is equal to $\sum_{y\in Y} |\psi'_y\rangle\langle\psi'_y|$. Thus,

$$\mathbf{R}'_0 = 2\sum_{x\in X} |\phi'_x\rangle\langle\phi'_x| - \mathbf{I}_{2\epsilon+m} = 2\mathbf{K}\ {}^t\mathbf{K} - \mathbf{I}_{2\epsilon+m},$$

$$\mathbf{R}'_1 = 2\sum_{y\in Y} |\psi'_y\rangle\langle\psi'_y| - \mathbf{I}_{2\epsilon+m} = 2\mathbf{L}\ {}^t\mathbf{L} - \mathbf{I}_{2\epsilon+m}.$$

Now, let $\mathbf{K}_1$ be the $\epsilon' \times n$ submatrix of $\mathbf{K}$ with respect to the rows corresponding to the edges of E'_M and the columns corresponding to the vertices of V. Furthermore, let $\mathbf{L}_1$ be the $\epsilon' \times n$ submatrix of $\mathbf{L}$ 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 $\hat{\mathbf{A}}'_p$ as follows:

$$\hat{\mathbf{A}}'_p = {}^t\mathbf{K}_1\mathbf{L}_1\ {}^t\mathbf{L}_1\mathbf{K}_1,$$

Remark that q is determined by p and so as p' and q'. The v, u element of this symmetric matrix $\hat{\mathbf{A}}'_p$ is computed as follows: ${}^t\mathbf{LK}$ is expressed by

$$
{}^t\mathbf{LK} = \begin{bmatrix} \langle \psi'_{v'_1}| \\ \vdots \\ \langle \psi'_{v'_n}| \end{bmatrix} \begin{bmatrix} |\phi'_{v_1}\rangle & \cdots & |\phi'_{v_n}\rangle \end{bmatrix}
$$

$$
= \begin{bmatrix} \langle \psi'_{v'_1}|\phi'_{v_1}\rangle & \cdots & \langle \psi'_{v'_1}|\phi'_{v_n}\rangle \\ \vdots & \ddots & \vdots \\ \langle \psi'_{v'_n}|\phi'_{v_1}\rangle & \cdots & \langle \psi'_{v'_n}|\phi'_{v_n}\rangle \end{bmatrix}
$$

Thus

$$
\begin{aligned}
({}^t\mathbf{LK})_{u,v} &= \langle \psi'_u|\phi'_v\rangle = \sum_{e\in E_M} \overline{\psi'_u(e)}\phi'_v(e) \\
&= \sum_{V(e)=v,\ V'(e)=u} \sqrt{p'(e)q'(e)},
\end{aligned}
$$

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

$$
({}^t\mathbf{KL}\ {}^t\mathbf{LK})_{u,v} = \sum_{(e,f):(u,v)-\text{path in } G_2} \sqrt{p'(e)q'(e)p'(f)q'(f)},
$$

where $u, v \in V$.

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

$$
({}^t\mathbf{KL}\ {}^t\mathbf{LK})_{u,v} = \begin{cases} \sum_{(e,f)\in Q_2} \sqrt{p(e)q(e)p(f)q(f)} & \text{if } u, v \in V \setminus M, \\ \delta_{u,v} & \text{if } u, v \in M, \\ 0 & \text{otherwise.} \end{cases}
$$

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,

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

if $u, v \notin M$.

If the following condition holds, we say p, q satisfies the detailed balanced condition: there exists $\pi : V \sqcup V' \to \mathbb{R}_{\geqslant 0}$ 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 $u \in (V \setminus M) \sqcup (V' \setminus M')$. 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

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

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

$$({}^t\mathbf{KL}\ {}^t\mathbf{LK})_{u,v} = \begin{cases} \sqrt{\pi(u)/\pi(v)} \sum_{(e,f)\in Q_2} p(e)q(f) & \text{if } u, v \notin M, \\ \delta_{u,v} & \text{if } u, v \in M \\ 0 & \text{otherwise,} \end{cases}$$

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

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

Thus

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

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 ϵ edges which may have multiple edges and self loops. Let $\mathbf{W}' = \mathbf{R}'_1 \mathbf{R}'_0$ 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 $\mathbf{W}'$, we have

$$\det(\mathbf{I}_{2\epsilon+m} - u\mathbf{W}') = (1 - u)^{2(\epsilon-n)+m} \det((1 + u)^2 \mathbf{I}_n - 4u\hat{\mathbf{A}}'_p).$$

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

$$\det(\mathbf{I}_{2\epsilon+m} - u\mathbf{W}') = (1 - u)^{2(\epsilon-n)+3m} \det((1 + u)^2 \mathbf{I}_{n-m} - 4u\mathbf{P}_M^2).$$

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

$$(\mathbf{K}\ {}^t\mathbf{K})_{e,f} = \sum_{v\in V}\langle e|\phi'_v\rangle\langle\phi'_v|f\rangle = 0,$$
$$(\mathbf{L}\ {}^t\mathbf{L})_{e,f} = \sum_{v\in V}\langle e|\psi'_v\rangle\langle\psi'_v|f\rangle = 0$$

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

$$\begin{aligned}\mathbf{R}'_0 &= 2\mathbf{K}\ {}^t\mathbf{K} - \mathbf{I}_{2\epsilon+m}\\ &= (2\mathbf{K}_1\ {}^t\mathbf{K}_1 - \mathbf{I}_{\epsilon'}) \oplus (-\mathbf{I}_{2\epsilon+m-\epsilon'})\\ \mathbf{R}'_1 &= 2\mathbf{L}\ {}^t\mathbf{L} - \mathbf{I}_{2\epsilon+m}\\ &= (2\mathbf{L}_1\ {}^t\mathbf{L}_1 - \mathbf{I}_{\epsilon'}) \oplus (-\mathbf{I}_{2\epsilon+m-\epsilon'})\end{aligned}$$

Therefore if $F_M \neq \emptyset$, then

$$\mathbf{W}' = (2\mathbf{L}_1\ {}^t\mathbf{L}_1 - \mathbf{I}_{\epsilon'})(2\mathbf{K}_1\ {}^\mathbf{t}\mathbf{K}_1 - \mathbf{I}_{\epsilon'}) \oplus \mathbf{I}_{2\epsilon+m-\epsilon'}.$$

Therefore, if $F_M \neq \emptyset$, then at least $|F_M|$-multiple eigenvalue 1 of $\mathbf{W}'$ 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 $2\mathbf{K}\ {}^\mathbf{t}\mathbf{K} - \mathbf{I}_{\epsilon'} = \mathbf{R}'_0$, $2\mathbf{L}\ {}^\mathbf{t}\mathbf{L} - \mathbf{I}_{\epsilon'} = \mathbf{R}'_1$ and $\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0$. Since

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

we have

$${}^t\mathbf{K}\mathbf{K} = {}^t\mathbf{L}\mathbf{L} = \mathbf{I}_n.$$

Therefore, by Theorem 3.1, it follows that

$$\det(\mathbf{I}_{\epsilon'} - u\mathbf{W}') = (1-u)^{\epsilon'-2n}\det((1+u)^2\mathbf{I}_n - 4u\ {}^t\mathbf{K}_1\mathbf{L}_1\ {}^t\mathbf{L}_1\mathbf{K}_1).$$

But,

$$\hat{\mathbf{A}}'_p = {}^t\mathbf{K}_1\mathbf{L}_1\ {}^t\mathbf{L}_1\mathbf{K}_1.$$

Hence, If $F_M = \emptyset$, then

$$\det(\mathbf{I}_{\epsilon'} - u\mathbf{W}') = (1-u)^{\epsilon'-2n}\det((1+u)^2\mathbf{I}_n - 4u\hat{\mathbf{A}}'_p).$$

Therefore if $F_M \neq \emptyset$, then

$$\det(\mathbf{I}_{2\epsilon+m} - u\mathbf{W}') = (1-u)^{2\epsilon+m-\epsilon'} \times (1-u)^{\epsilon'-2n} \det((1+u)^2\mathbf{I}_n - 4u\hat{\mathbf{A}}'_p)$$
$$= (1-u)^{2(\epsilon-n)+m} \det((1+u)^2\mathbf{I}_n - 4u\hat{\mathbf{A}}'_p)$$

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, $\hat{\mathbf{A}}'_p = (\mathbf{D} \oplus \mathbf{I}_m){\mathbf{P}'_M}^2(\mathbf{D}^{-1} \oplus \mathbf{I}_m)$, $\mathbf{D}$ is an $(n-m)\times(n-m)$ diagonal matrix diag$[\sqrt{\pi(u)} \mid u \notin M]$, that is, $(\mathbf{D} \oplus \mathbf{I}_m)|u\rangle = \sqrt{\pi(u)}$ if $u \notin M$, $(\mathbf{D} \oplus \mathbf{I}_m)|u\rangle = |u\rangle$ if $u \in M$. □

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 ϵ edges which may have multiple edges and self loops. Let $\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0$ 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 marked element M with $|M| = m$. Then, for the $\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0$, we have*

$$\det(\lambda\mathbf{I}_{2\epsilon+m} - \mathbf{W}') = (\lambda-1)^{2(\epsilon-n)+m} \det((\lambda+1)^2\mathbf{I}_n - 4\lambda\hat{\mathbf{A}}'_p).$$

By Theorem 7.1 and Corollary 3.5, we obtain the eigenvalues of $\mathbf{W}'$.

Corollary 7.3. *Let G be a connected graph with n vertices and ϵ edges which may have multiple edges and self loops. Let $\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0$ 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 the spectrum of the unitary matrix $\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0$ 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:*
   $$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\hat{\mathbf{A}}'_p);$$
   (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:*
   $$\lambda = e^{\pm 2i\theta},\ \cos^2\theta \in Spec(\hat{\mathbf{A}}'_p) \setminus \{1\};$$
   (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,

$$\det(\lambda\mathbf{I}_{2\epsilon+m} - \mathbf{W}') = (\lambda-1)^{2(\epsilon-n)+m} \prod_{j=1}^{n}(\lambda - \alpha_j^{(+)})(\lambda - \alpha_j^{(-)})$$

holds, where $\alpha_j^{(\pm)}$ are the solutions of $\lambda^2-2(2\mu-1)\lambda+1=0$ with $\mu \in Spec(\hat{\mathbf{A}}'_p)$. 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. □

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 $\mathbf{P}=(p_{uv})_{u,v\in V(G)}$ the following stochastic matrix of G:

$$\mathbf{P}=\frac{1}{2}\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

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 $\mathbf{P}'=(p'_{uv})_{u,v\in V(G_2)}$ derived from $\mathbf{P}$ with $M=\{v_3\}$ is given as follows:

$$\mathbf{P}'=\begin{bmatrix} 0 & 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

which means

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

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 7×3 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:

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

Furthermore, the 7×3 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:

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

Thus, we have

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

and

$$\mathbf{L}\ {}^t\mathbf{L}=\sum_{y\in Y}|\psi_y\rangle\langle\psi_y|=\begin{bmatrix} 1/2 & 0 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 1/2 & 0 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Therefore, it follows that

$$\mathbf{R}'_0 = 2\mathbf{K}\,{}^t\mathbf{K} - \mathbf{I}_7 = \begin{bmatrix} 0 & 0 & 1 & 0 & & 0 \\ 0 & 0 & 0 & 1 & & \\ 1 & 0 & 0 & 0 & & \\ 0 & 1 & 0 & 0 & & \\ & & & & -\mathbf{I}_2 & \\ & & & & & 1 \end{bmatrix}$$

and

$$\mathbf{R}'_1 = 2\mathbf{L}\,{}^t\mathbf{L} - \mathbf{I}_7 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Hence,

$$\mathbf{W}' = \mathbf{R}'_1\mathbf{R}'_0 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Now, we have

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

Thus, we have

$$\hat{\mathbf{A}}'_p = {}^t\mathbf{K}\mathbf{L}\,{}^t\mathbf{L}\mathbf{K} = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/4 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Thus,

$$\det(\lambda\mathbf{I}_2 - \hat{\mathbf{A}}'_p) = (\lambda - 1)(\lambda - 1/4)^2.$$

Therefore, it follows that

$$Spec(\hat{\mathbf{A}}'_p) = \{1, 1/4\}.$$

Furthermore, since $n = 3$, we have $\epsilon' - 2n = 7 - 6 = 1$. By Corollary 7.3, the eigenvalues of $\mathbf{W}'$ are

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

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