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A remark on zeta functions of finite graphs via quantum walks

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Abstract

From the viewpoint of quantum walks, the Ihara zeta function of a finite graph can be said to be closely related to its evolution matrix. In this note we introduce another kind of zeta function of a graph, which is closely related to, as to say, the square of the evolution matrix of a quantum walk. Then we give to such a function two types of determinant expressions and derive from it some geometric properties of a finite graph. As an application, we illustrate the distribution of poles of this function comparing with those of the usual Ihara zeta function.

Keywords: Quantum walk; Grover matrix; Positive support; Ihara zeta function

1 Introduction

As the classical random walk on a graph has important roles in various fields, the quantum walk, say QW, is expected to play such a role in the quantum field. In fact, we can find many studies on QW cover a wide research area from the basic theoretical mathematics to the application oriented fields. It has been shown, for example, that analyzing some spatial structure [2,27,39] as an extension of quantum speed-up algorithm [15,16], and application to a universal computation in quantum mechanical computers [6], expressing the energy transfer on the chromatographic network in the photosynthetic system [30] and so on are strongly influenced by its virtue. Besides, approximations of QWs describing physical processes are derived from Dirac and Schrödinger equations [5,37]. A QW model has been also shown to be useful for describing the fundamental dynamics of the quantum multi-level system which is irradiated by lasers [29]. The laser control technology of quantum system is expected to be applied for the industry as a highly-selective method for material separation, especially, isotope-selective excitation of diatomic molecules such as Cs133 and Cs135. Recently by the above theoretical evidences for the usefulness and activeness of the studies of QWs, experimental implementations of QWs are quite aggressively investigated. See [20,33,41], for example.

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Now we shall focus on mathematical research on QW. The starter creating studies of QW in earnest are considered as the QW on one dimensional lattice introduced by [2]: one of the most striking properties is the spreading property of the walker. Its standard deviation of the position grows linearly in time, quadratically faster than the classical random walk. The behaviour is clarified by a limit theorem characterized by a new density function named "f_K function" [22,23]. The review and book on QWs are J. Kempe [21] and N. Konno [24]. See also [1,28,40]. For a general graph, it is usual to consider some special but typical type of QWs: the *Grover walk* originated in [15,16] or the *Szegedy walk* in [39]. Roughly speaking, the former is induced by the simple random walk and the latter by more general random walk on a graph. In this context, the relationship between spectra of QW and that of the classical random walk is investigated in [9,18,25,34]. From now on we call the evolution matrices of the Grover walk and the Szegedy walk just the *Grover matrix* $\mathbf{U}$ and the *Szegedy matrix* $\mathbf{U}_{sz}$, respectively.

Recently there are some trials to apply QW to graph isomorphism problems [9-11,35]. For graph isomorphism problems, while spectra of the Grover matrix is considered to have almost same power as that of conventional operator, it is suggested that the method of $(\mathbf{U}^3)^+$, which is the *positive support* of the cube of the Grover matrix $\mathbf{U}^3$, outperforms the graph spectra methods, in particular, in distinguishing strongly regular graphs in [9]. What we emphasize is that not only the Grover matrix $\mathbf{U}$ itself but the *positive support* $(\mathbf{U}^n)^+$ of its n-th power is an

important operator of a graph. See also [13,18]. Meanwhile, in [25,32] the relationship between the Ihara zeta function and the positive support $(\mathbf{U})^+$ of the Grover matrix of a graph is discussed: a matrix $(\mathbf{U})^+$ derived from QW is essentially the same as the edge-matrix in [3,17] and the Perron-Frobenius operator in [26], both of which are important operators in characterizing that function. The Ihara zeta functions of graphs started for regular graphs by Y. Ihara [19] and is generalized to a general graph. Already various success related to graph spectra is obtained in [3,17,19,26,38].

This note is a sequel work to our previous work [18], therein we established a general relation between QW and the classical random walk; as its application, we recover the results in [9,13,25,34] of spectral relation between three matrices $\mathbf{U}, (\mathbf{U})^+, (\mathbf{U}^2)^+$ from QW and the adjacency matrix $\mathbf{A}_G$. Our main purpose in this note is to characterize another kind of zeta function with respect to $(\mathbf{U}^2)^+$, which is the positive support of the squared Grover matrix.

To state our result precisely, let us give our setting. A graph G is a pair of two sets $(V(G), E(G))$, where $V(G)$ stands for the set of its vertices and $E(G)$ the set of its unoriented edges. Assigning two orientations to each unoriented edge in $E(G)$, we introduce the set of all oriented edges and denote it by $D(G)$. For an oriented edge $e \in D(G)$, the origin of e, the terminus of e and the inverse edge of e are denoted by $o(e)$, $t(e)$ and e^{-1}, respectively. Furthermore the *degree* of $x \in V(G)$, $\deg_G x$, is defined as the number of oriented edges e such that $o(e) = x$; we denote $\min_{x \in V(G)} \deg_G x$ and $\max_{x \in V(G)} \deg_G x$ by $\delta(G)$ and $\Delta(G)$, respectively. A graph G here is basically assumed to be a connected finite graph with n vertices, m unoriented edges and $\delta(G) \geq 3$; it may have multiple edges or self-loops. For a natural number k, if $\deg_G v = k$ for each vertex $v \in V(G)$, then a graph G is called *k-regular*.

Let us introduce the *Grover matrix* $\mathbf{U}_G = \mathbf{U}$, which is a special QW related to the simple random walk on G, and the *positive support* $\mathbf{F}^+$ for a real matrix $\mathbf{F}$.

Definition 1. *The Grover matrix* $\mathbf{U} = \left(U_{e,f}\right)_{e,f \in D(G)}$ *of G is a $2m \times 2m$ matrix defined by*

$$U_{ef} = \begin{cases} 2/\deg_G o(e), & \text{if } t(f) = o(e) \text{ and } f \neq e^{-1}, \\ 2/\deg_G o(e) - 1, & \text{if } f = e^{-1}, \\ 0, & \text{otherwise}, \end{cases}$$

and the positive support $\mathbf{F}^+ = \left(F_{i,j}^+\right)$ *of a real square matrix* $\mathbf{F} = (F_{i,j})$ *is defined by*

$$F_{i,j}^+ = \begin{cases} 1, & \text{if } F_{i,j} > 0, \\ 0, & \text{otherwise}. \end{cases}$$

Properties of the Grover matrix can be seen in [15,16]; see also [9,13,18,25,34]. The Szegedy matrix related to a general random walk on G is omitted since we do not use here; its definition and properties can be seen in [18,34,39], for instance. The spectra of the positive support $\mathbf{U}^+$ of the Grover matrix and $(\mathbf{U}^2)^+$ of its square on a regular graph G are expressed in [9], also in [13,18], by means of those of the *adjacency matrix* $\mathbf{A}_G$ of G, which is an important matrix also in this note and defined as follows: the *adjacency matrix* $\mathbf{A}_G = \left(a_{x,y}\right)_{x,y \in V(G)}$ is an $n \times n$-matrix such that $a_{x,y}$ coincides with the number of oriented edges such that $o(e) = x$ and $t(e) = y$.

Now let us consider the following function $\mathbf{Z}_G(u)$ of a graph G for $u \in \mathbb{C}$ with $|u|$ sufficiently small:

$$\mathbf{Z}_G(u) = \prod_{[C]} \left(1 - u^{|C|}\right)^{-1}. \tag{1}$$

In (1), if $[C]$ runs over all *equivalence classes of prime and reduced cycles* of G, then $\mathbf{Z}_G(u)$ becomes the well-known Ihara zeta function. Details will be seen Section 2, therein we give a brief summary on the Ihara zeta function. Roughly speaking, we will find two matrices $(\mathbf{U})^+$ and $\mathbf{A}_G$ control this function. On the other hand, if $[C]$ runs over all *equivalence class of prime 2-step-cycles* of G, then $\mathbf{Z}_G(u)$ becomes a *modified zeta function*, say $\tilde{\mathbf{Z}}_G(u)$, which is the main object in this note. Precise definitions around this can be seen in Section 3. Roughly speaking, we will find two matrices $(\mathbf{U}^2)^+$ and $\mathbf{A}_G$ control this function. Our main theorem in this note is as follows:

Theorem 1 (Main Theorem). *Let G be a simple connected graph with n vertices, m unoriented edges and $\delta(G) \geq 3$. Then*

$$\tilde{\mathbf{Z}}_G(u) = 1/\det\left(\mathbf{I}_{2m} - u\left(\mathbf{U}^2\right)^+\right),$$
$$= (1 - 2u)^{2(n-m)} \cdot (p_G(u))^{-1},$$

and $p_G(1/2) = 0$. If G is not bipartite, then the derivative at $u = 1/2$ of $p_G(u)$ is as follows:

$$p'_G(1/2) = \frac{m-n}{2^{2n-2}} \cdot \kappa(G) \cdot \iota(G),$$

where $\kappa(G)$ is the number of spanning trees in G and $\iota(G)$ is the following graph invariant:

$$\iota(G) = \sum_{H \in OUCF(G)} 4^{\omega(H)}.$$

Here $OUCF(G)$ stands for the set of all *odd-unicyclic factors* in G. On the other hand, if G is bipartite, then

$p'_G(1/2) = 0$ and the second derivative at $u = 1/2$ is as follows:

$$p''_G(1/2) = \frac{(m-n)^2}{2^{2n-5}}(\kappa(G))^2.$$

Furthermore $u = \rho$ is also a pole, whose order 2 or 1 if G is bipartite or not, respectively. Here ρ is the radius of convergence of (1).

Definitions not given here and details can be seen in Section 3, especially in Proposition 1, Theorems 4 and 5. Also the radius of convergence is discussed in Theorem 3.

The rest of the paper is organized as follows. In Section 2, we present a brief survey on the Ihara zeta function $\mathbf{Z}_G(u)$ of a graph, which is related to $(\mathbf{U})^+$. In Section 3, we introduce and discuss a modified zeta function $\tilde{\mathbf{Z}}_G(u)$ related to $(\mathbf{U}^2)^+$ on a graph G and present two types of determinant expressions, properties of poles and geometric information derived from $\tilde{\mathbf{Z}}_G(u)$. In Section 4, we illustrate the distribution of poles of $\tilde{\mathbf{Z}}_G(u)$ for a k-regular graph comparing with those of the Ihara zeta function.

2 The Ihara zeta function via QW
In this section, we shall summarize the results on the Ihara zeta function of a graph.

Let G be a connected graph. A *closed path* or *cycle* of length ℓ in G is a sequence $C = (e_0, \dots, e_{\ell-1})$ of ℓ oriented edges such that $e_i \in D(G)$ and $t(e_i) = o(e_{i+1})$ for each $i \in \mathbb{Z}/\ell\mathbb{Z}$. Such a cycle is often called an $o(e_0)$-cycle. We say that a path $P = (e_0, \cdots, e_{\ell-1})$ has a *backtracking* if $e_{i+1}^{-1} = e_i$ for some $i \in \mathbb{Z}/\ell\mathbb{Z}$. The *inverse cycle* of a cycle $C = (e_0, \cdots, e_{\ell-1})$ is the cycle $C^{-1} = \left(e_{\ell-1}^{-1}, \cdots, e_0^{-1}\right)$.

We introduce an equivalence relation between cycles. Two cycles C_1 and C_2 are said to be *equivalent* if C_1 can be obtained from C_2 by a cyclic permutation of oriented edges. Remark that the inverse cycle of C is in general not equivalent to C. Thus we write $[C]$ for the equivalence class which contains a cycle C. Let B^r be the cycle obtained by going r times around a cycle B: such a cycle is called a *power* of B. Furthermore, a cycle C is *prime* if it is not a power of a strictly smaller cycle. Besides, a cycle C is called *reduced* if C has no backtracking. Note that each equivalence class of prime and reduced cycles of a graph G corresponds to a unique conjugacy class of the fundamental group $\pi_1(G, v)$ of G at a vertex $v \in V(G)$.

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

$$\mathbf{Z}_G(u) = \prod_{[C]} \left(1 - u^{|C|}\right)^{-1},$$

where $[C]$ runs over all equivalence classes of prime and reduced cycles of G and $|C|$ is a length of a cycle C. This function $\mathbf{Z}_G(u)$ can be expressed as

$$\mathbf{Z}_G(u) = \exp\left(\sum_{k\geq 1} \frac{N_k}{k} u^k\right),$$

where N_k is the number of all reduced cycles of length k in G. A simple proof and an estimate for the radius of convergence for the power series in the above can be seen, for instance, in [26]. The following determinant expression is originally given in [17]; other proofs are seen in [3,26]. We should remark $^T(\mathbf{U})^+$, the transposed matrix of $(\mathbf{U})^+$, is essentially the same as the edge-matrix in [3,17] and the Perron-Frobenius operator in [26].

Theorem 2. ([17]; cf. [3,19,25,26,31,32]) Let G be a connected graph with n vertices and m unoriented edges. Then the reciprocal of the Ihara zeta function of G is given by

$$\mathbf{Z}_G(u)^{-1} = \det\left(\mathbf{I}_{2m} - u(\mathbf{U})^+\right)$$
$$= \left(1 - u^2\right)^{m-n} f_G(u).$$

Here we put

$$f_G(u) = \det\left(\mathbf{I}_n - u\mathbf{A}_G + u^2(\mathbf{D}_G - \mathbf{I}_n)\right),$$

where $\mathbf{A}_G$ is the adjacency matrix of G and $\mathbf{D}_G = (d_{x,y})_{x,y \in V(G)}$ is the *degree matrix* of G which is a diagonal matrix with $d_{x,x} = \deg_G x$ for $x \in V(G)$. In addition, $u = 1$ is a pole of $\mathbf{Z}_G(u)$ of order $m - n + 1$ and the derivative of $f_G(u)$ at $u = 1$ is expressed by a graph invariant $\kappa(G)$:

$$f'_G(1) = 2(m-n)\kappa(G),$$

where $\kappa(G)$ is the number of spanning trees in G.

The invariant $\kappa(G)$ is called the *complexity* of G and the complexities for various graphs are found in [4,7]. Seeing the determinant expression in the above, we may say the Ihara zeta function $\mathbf{Z}_G(u)$ of a graph is derived by the positive support $(\mathbf{U})^+$ of the Grover matrix $\mathbf{U}$.

3 A modified zeta function via QW
In this section, we will discuss a modified zeta function of a graph with respect to the positive support of the *square* of the Grover matrix.

First of all, let us introduce a new notion of cycle in a graph with respect to $(\mathbf{U}^2)^+$. For a connected graph G, a *2-step-cycle* $\tilde{C}$ of length ℓ in G is a sequence $\tilde{C} = (e_0, \cdots, e_{\ell-1})$ of ℓ oriented edges such that every ordered pair (e_i, e_{i+1}) is a *2-step-arc* or a *2-step-identity* for each $i \in \mathbb{Z}/\ell\mathbb{Z}$. Here a *2-step-arc* (e, f) is defined as follows: there exists an oriented edge $g(\neq e^{-1}, f^{-1})$ such that $o(g) = t(e)$ and $t(g) = o(f)$; a *2-step-identity* (e, f) is defined as $e = f$. Remark that a 2-step-cycle $\tilde{C}$ of length 1 exists if $\tilde{C} = (e)$. When G is a graph with $\delta(G) \geq 3$, it can

be easily checked that $\left({}^{T}(\mathbf{U}^2)^{+}\right)_{e,f}$ is positive if and only if (e,f) is a *2-step-arc* or a *2-step-identity*.

Similarly to the case of usual cycles in Section 2, we give an equivalence relation between 2-step cycles. Two cycles $\tilde{C}_1$ and $\tilde{C}_2$ are said to be *equivalent* if $\tilde{C}_1$ can be obtained from $\tilde{C}_2$ by a cyclic permutation of oriented edges. Thus we write $[\tilde{C}]$ for the equivalence class which contains a 2-step-cycle $\tilde{C}$. Let $\tilde{B}^r$ be the 2-step-cycle obtained by going r times around some 2-step-cycle B; a 2-step-cycle $\tilde{C}$ is *prime* if it is not a multiple of a strictly smaller 2-step-cycle.

Let G be a connected graph with n vertices, m unoriented edges and $\delta(G) \geq 3$. Now let us define another kind of zeta function of a graph related to $(\mathbf{U}^2)^{+}$.

Definition 2. *The modified zeta function of a graph G is a function of $u \in \mathbb{C}$ with $|u|$ sufficiently small, defined by*

$$\tilde{\mathbf{Z}}_G(u) = \prod_{[\tilde{C}]} \left(1 - u^{|\tilde{C}|}\right)^{-1},$$

where $[\tilde{C}]$ is the equivalence class of prime 2-step-cycles and $|\tilde{C}|$ is the length of a 2-step-cycle $\tilde{C}$.

From the definitions of a *2-step-cycle* and an equivalence class, applying the usual method, which can be seen in [26,36] for instance, we can give the exponential expression and a determinant expression for the modified zeta function $\tilde{\mathbf{Z}}_G(u)$:

Proposition 1. Let G be a connected graph with n vertices and m unoriented edges. Suppose that $\delta(G) \geq 3$. Then

$$\tilde{\mathbf{Z}}_G(u) = \exp\left(\sum_{r \geq 1} \frac{\tilde{N}_r}{r} u^r\right) \qquad (2)$$

$$= 1/\det\left(\mathbf{I}_{2m} - u\left(\mathbf{U}^2\right)^{+}\right),$$

where $\tilde{N}_r$ is the number of all 2-step-cycles of length r.

Now let us give estimation of the radius of convergence ρ of the power series in the above. Naturally, ρ is also the singular point of $\tilde{\mathbf{Z}}_G(u)$ nearest to the origin. Recall $\delta(G)$ and $\Delta(G)$ stand for $\min_{x \in V(G)} \deg_G x$ and $\max_{x \in V(G)} \deg_G x$, respectively.

Theorem 3. Let G be a connected graph with $\delta(G) \geq 3$. The radius of convergence ρ of the power series in Proposition 1 (2) is $\rho = 1/\alpha$, where α is the maximal eigenvalue of $(\mathbf{U}^2)^{+}$; it holds that

$$1/\left((\delta(G) - 1)^2 + 1\right) \leq \rho \leq 1/((\Delta(G) - 1)^2 + 1).$$

In particular, $\tilde{\mathbf{Z}}_G(u)$ is a rational function of u with a pole ρ whose order is 2 or 1 if G is bipartite or not, respectively.

Proof. As is seen above, $(\mathbf{U}^2)^{+}$ is nonnegative, that is, all elements are nonnegative, and $\left((\mathbf{U}^2)^{+}\right)_{e,f}$ is positive if and only if (f,e) is a 2-step-arc or a 2-step-identity. To apply the Perron-Frobenius theorem, let us discuss the irreducibility of $(\mathbf{U}^2)^{+}$. A matrix M is called *irreducible* if, for each two indices i and j, there exists a positive integer k such that $(M^k)_{i,j} \neq 0$. For the matrix $(\mathbf{U}^2)^{+}$, it is sufficient to see whether, for any two oriented edges $e, f \in D(G)$, e is reachable or not from f by an *admissible* sequence of 2-step-arcs and 2-step-identities, that is, a sequence of oriented edges $(e_0, e_1, e_2, \ldots, e_{s-1}, e_s)$ such that $e_0 = f$, $e_s = e$ and (e_k, e_{k+1}) is a 2-step-arc or a 2-step-identity for $i = 0, \ldots, s-1$. It is easily checked that such an admissible sequence from f to e exists if and only if there exists a reduced path from f to e of odd length in G say an *admissible odd path*. Recall that a reduced path from e_1 to e_ℓ of length ℓ in G is a sequence $P = (e_1, \ldots, e_\ell)$ of ℓ oriented edges such that $t(e_i) = o(e_{i+1})$ and $e_{i+1}^{-1} \neq e_i$ for each $i = 1, \ldots, \ell - 1$. Since a graph G is finite and connected with $\delta(G) \geq 3$, G has at least two *unoriented cycles*. The terminology *unoriented cycle* used here is the same as "cycle" in usual graph theory, that is, if C is an unoriented cycle of length ℓ, then $V(C) = \{v_1, \ldots, v_\ell\}$ whose elements are mutually distinct, $v_i v_{i+1} \in E(G)$ for $i = 1, \ldots, \ell - 1$ and $v_\ell v_1 \in E(G)$. For two vertices $x, y \in V(G)$, we denote by $dist(x, y)$ the length of the shortest path from x to y.

For two oriented edges $e, f \in D(G)$ such that $dist(t(f), o(e))$ is odd, we can find an admissible odd path from f to e. In particular, if G is not bipartite, then G has at least one *unoriented cycle* of odd length and of even length, respectively. Hence G turns out to have an admissible odd path between e and f for any $e, f \in D(G)$; this implies $(\mathbf{U}^2)^{+}$ is irreducible. Next we assume G is bipartite; the length of any cycle in G is even. So we set the bipartition V_0 and V_1: $V(G) = V_0 \sqcup V_1$. It is obvious that an admissible odd path between e and f exists if and only if both $o(e)$ and $o(f)$ are in the same set of bipartition, that is, $o(e), o(f) \in V_0$ or $o(e), o(f) \in V_1$. Thus $(\mathbf{U}^2)^{+}$ is not irreducible and we may express, after rearranging rows and columns if necessary,

$$(\mathbf{U}^2)^{+} = \left(\begin{array}{c|c} \mathbf{M}_0 & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{M}_1 \end{array}\right),$$

where $\mathbf{M}_0$ and $\mathbf{M}_1$ are $m \times m$ irreducible submatrices of $(\mathbf{U}^2)^{+}$ induced by $D_0 = \{e \in D(G); o(e) \in V_0\}$ and $D_1 = \{e \in D(G); o(e) \in V_1\}$, respectively. Remark that $e \in D_0$ if and only if $e^{-1} \in D_1$ and that an admissible sequence from f to e exists if and only if that from e^{-1} to f^{-1} does. Thus the characteristic polynomials of $\mathbf{M}_0$ and $\mathbf{M}_1$ coincide.

Now let us apply the Perron-Frobenius Theorem on irreducible nonnegative matrices(see [12,14]). If G is not bipartite, then $(\mathbf{U}^2)^+$ has at least one positive eigenvalue and the maximal positive eigenvalue α is simple. If G is bipartite, then each of $\mathbf{M}_0$ and $\mathbf{M}_1$ has at least one positive eigenvalue and simple maximal eigenvalue. This implies the maximal eigenvalues of $\mathbf{M}_0$ and $\mathbf{M}_1$ coincide, say α. Hence $(\mathbf{U}^2)^+$ has the maximal eigenvalue which is positive and whose multiplicity is 2 when G is bipartite. In either case, the maximal eigenvalue α is estimated as follows:

$$\min_{e \in D(G)} \sum_{f \in D(G)} \left((\mathbf{U}^2)^+ \right)_{e,f} \leq \alpha \leq \max_{e \in D(G)} \sum_{f \in D(G)} \left((\mathbf{U}^2)^+ \right)_{e,f}.$$

It should be noted that the value $\sum_{f \in D(G)} \left((\mathbf{U}^2)^+ \right)_{e,f}$ is equal to the number of f such that (f, e) is a 2-step-arc or a 2-step-identity for e. Then we have

$$(\delta(G) - 1)^2 + 1 \leq \alpha \leq (\Delta(G) - 1)^2 + 1.$$

It is obvious to see the power series (2) in Proposition 1 converges absolutely in $|u| < 1/\alpha = \rho$ since $\tilde{N}_r = \text{trace}\left[\left((\mathbf{U}^2)^+ \right)^r \right]$. $\qquad\square$

Corresponding to Theorem 2, another determinant expression for this zeta function $\tilde{\mathbf{Z}}_G(u)$ can be obtained. Here and hereafter we assume G is *simple*, that is, G has no multiple edges and no self-loops. Firstly we set the following two functions $h_G(u)$ and $l_G(u)$:

$$h_G(u) = \det \left(\mathbf{I}_n - \sqrt{u(1-u)}\mathbf{A}_G + u(\mathbf{D}_G - 2\mathbf{I}_n) \right),$$
$$l_G(u) = \det \left(\mathbf{I}_n + \sqrt{u(1-u)}\mathbf{A}_G + u(\mathbf{D}_G - 2\mathbf{I}_n) \right), \quad (3)$$

where we choose the branch such that $\sqrt{u(1-u)} > 0$ for $0 < u < 1$. Here $\mathbf{A}_G$ and $\mathbf{D}_G$ are, as are seen in Theorem 2, the adjacency and degree matrices, respectively.

Theorem 4. Let G be a simple connected graph with n vertices and m unoriented edges. Suppose that $\delta(G) \geq 3$. Then the reciprocal of the modified zeta function of G is given by

$$\tilde{\mathbf{Z}}_G(u)^{-1} = (1 - 2u)^{2(m-n)} \cdot h_G(u) \cdot l_G(u).$$

Proof. It is easy to see that

$$(\mathbf{U}^2)^+ = (\mathbf{U}^+)^2 + \mathbf{I}_{2m}$$

for any simple graph G with $\delta(G) \geq 3$; this equality is discussed also in [13,18]. Then we have

$$\det \left(\mathbf{I}_{2m} - u (\mathbf{U}^2)^+ \right) = u^{2m} \cdot \det \left(\frac{1-u}{u} \mathbf{I}_{2m} - (\mathbf{U}^+)^2 \right).$$

Corollary 2.3 in our previous paper [18] says that, for any G with $\delta(G) \geq 2$, the following holds:

$$\varphi(\lambda) = \det \left(\lambda \mathbf{I}_{2m} - \mathbf{U}^+ \right)$$
$$= \left(\lambda^2 - 1 \right)^{m-n} \det \left(\left(\lambda^2 - 1 \right) \mathbf{I}_n - \lambda \mathbf{A}_G + \mathbf{D}_G \right).$$

Also refer to [9,13,25]. It is easy to check

$$\det \left(\mathbf{I}_{2m} - u (\mathbf{U}^2)^+ \right)$$
$$= u^{2m} \cdot \varphi \left(\sqrt{(1-u)/u} \right) \cdot \varphi \left(-\sqrt{(1-u)/u} \right)$$

and

$$u^n \cdot \varphi \left(\sqrt{(1-u)/u} \right) = ((1-2u)/u)^{m-n} \cdot h_G(u),$$
$$u^n \cdot \varphi \left(-\sqrt{(1-u)/u} \right) = ((1-2u)/u)^{m-n} \cdot l_G(u).$$

Combining the above, we can obtain the desired expression. $\qquad\square$

Let us give information on a pole $u = 1/2$, which is a final analogous part in Theorem 2 for the usual Ihara zeta function.

Before stating the result, we introduce another kind of spanning graph in G discussed in [8]: a spanning subgraph H of G is called an *odd-unicyclic factor* if each connected component of H contains just one unoriented cycle of odd length and $V(H) = V(G)$. Here H may not be connected, so we denote the number of components of H by $\omega(H)$. The terminology *unoriented cycle* here is the same as in Proof of Theorem 3. Moreover we write $OUCF(G)$ for the set of all odd-unicyclic factors in G.

Theorem 5. Let G be a simple connected graph with n vertices, m unoriented edges and $\delta(G) \geq 3$. Set $p_G(u) = h_G(u) \cdot l_G(u)$ for $h_G(u)$ and $l_G(u)$ defined in (3). Then $p_G(1/2) = 0$. If G is not bipartite, then the derivative at $u = 1/2$ of $p_G(u)$ is as follows:

$$p'_G(1/2) = \frac{m-n}{2^{2n-2}} \cdot \kappa(G) \cdot \iota(G),$$

where $\kappa(G)$ is the complexity of G which is same as in Theorem 2 and $\iota(G)$ is the following graph invariant:

$$\iota(G) = \sum_{H \in OUCF(G)} 4^{\omega(H)}.$$

On the other hand, if G is bipartite, then $p'_G(1/2) = 0$ and the second derivative at $u = 1/2$ is as follows:

$$p''_G(1/2) = \frac{(m-n)^2}{2^{2n-5}} (\kappa(G))^2.$$

The following corollary is a direct consequence of Theorem 5.

Corollary 1. Let G be a simple connected graph with n vertices, m unoriented edges and $\delta(G) \geq 3$. Then $u = 1/2$

is a pole of the modified zeta function $\tilde{\mathbf{Z}}_G(u)$ whose order is $2(m - n + 1)$ if G is bipartite; $2(m - n) + 1$ otherwise.

Before proving Theorem 5, we give some lemmas.

Lemma 1. If G is bipartite, then $h_G(u) = l_G(u)$.

Proof. It is well known that A_G and $-A_G$ are unitarily equivalent if G is bipartite. In fact, let V_1 and V_2 be the bipartition of $V(G)$: $V(G) = V_1 \sqcup V_2$. Then we put a diagonal matrix T such that an (i, i)-element $T_{ii} = 1$ if $v_i \in V_1$; otherwise $T_{ii} = -1$. It is easy to check that $A_G = T^{-1}(-A_G)T$. Therefore $h_G(u) = l_G(u)$ if G is bipartite. $\square$

Lemma 2. Let G be a simple connected graph with n vertices. Then it holds that $h_G(1/2) = 0$; $l_G(1/2) = 0$ if G is bipartite. Moreover, if G is not bipartite, then $l_G(1/2) = 2^{-n}\iota(G)$.

Proof. We can see that $h_G(1/2) = 2^{-n}\det(\mathbf{D}_G - \mathbf{A}_G)$ and $l_G(1/2) = 2^{-n}\det(\mathbf{D}_G + \mathbf{A}_G)$. It is well known that $\mathbf{D}_G - \mathbf{A}_G$ is a discrete Laplacian and has 0-eigenvalues. Thus $h_G(1/2) = 0$. If G is bipartite, it follows from Lemma 1 that $l_G(1/2) = 0$. Theorem 4.4 in [8] tells us $\det(\mathbf{D}_G + \mathbf{A}_G) = \iota(G)$. $\square$

Proof of Theorem 5. For $p_G(u) = h_G(u)l_G(u)$, using Lemmas 1 and 2, we easily observe that, if G is bipartite,

$$p'(1/2) = 2 \cdot h_G(1/2) \cdot h'_G(1/2) = 0$$

and

$$p''(1/2) = 2 \cdot (h'_G(1/2))^2. \tag{4}$$

On the other hand, if G is non-bipartite,

$$p'(1/2) = h'_G(1/2) \cdot l_G(1/2) + h_G(1/2) \cdot l'_G(1/2)$$
$$= 2^{-n}\iota(G) \cdot h'_G(1/2). \tag{5}$$

Thus let us concentrate our attention on the computation on $h'_G(1/2)$. For $V(G) = \{v_1, \cdots, v_n\}$, we write $a_{i,j}$ for (i, j)-element of $\mathbf{A}_G$ and the matrix $M(u)$ for

$$\mathbf{I}_n - \sqrt{u(1-u)}\mathbf{A}_G + u(\mathbf{D}_G - 2\mathbf{I}_n).$$

In addition, let us denote the derivative of the (i, j)-element of $M(u)$ by $m'_{i,j}(u)$ and the (i, j)-cofactor of $M(u)$ by $M_{i,j}(u)$. Here we remark that $M_{i,j}(1/2)$ coincides with the (i, j)-cofactor of $(1/2)(\mathbf{D}_G - \mathbf{A}_G)$; by the Matrix-Tree Theorem ([4,7], for instance), we have

$$M_{i,j}(1/2) = \frac{1}{2^{n-1}}\kappa(G).$$

Furthermore, remarking that

$$m'_{i,j}(u) = -\frac{1-2u}{2\sqrt{u(1-u)}}a_{i,j} + (\deg v_i - 2)\delta_{i,j},$$

we easily obtain

$$h'_G(1/2) = \sum_{i,j} m'_{i,j}(1/2)M_{i,j}(1/2) \tag{6}$$

$$= \frac{1}{2^{n-1}}\kappa(G)\sum_i(\deg v_i - 2) = \frac{m-n}{2^{n-2}}\kappa(G).$$

This completes the proof of Theorem 5.

4 Example: distribution of poles of the modified zeta function

Throughout this section, we assume a graph G is k-regular with n vertices and m unoriented edges: $2m = kn$. Suppose further $k \geq 3$.

For regular graphs, Theorem 2 was originally obtained by [19] in the context of a p-adic analogue of the Selberg zeta function. The concrete form in an analytic continuation from Theorem 2 is as follows: for a k-regular connected graph G with n vertices,

$$\mathbf{Z}_G(u) = (1 - u^2)^{n - kn/2}\det\left(\mathbf{I}_n - u\mathbf{A}_G + (k-1)u^2\mathbf{I}_n\right)^{-1}. \tag{7}$$

Thus, in terms of eigenvalues of the adjacency matrix $\mathbf{A}_G$, we know the distribution of poles of $\mathbf{Z}_G(u)$. See [3,17,19,38]. Consequently, all of the real poles u satisfy $1/(k-1) \leq |u| \leq 1$ and all of the imaginary poles u lie on the circle whose center is the origin and radius is $1/\sqrt{k-1}$. Moreover it is concluded that $u = 1/(k-1)$ is a simple pole and $u = -1/(k-1)$ is also a simple pole if and only if G is bipartite. As is stated in Theorem 2, $u = 1$ is a pole of order $(kn-2n+2)/2$. Usually the pole with $u = \pm 1$ or $\pm 1/(k-1)$ is called a *trivial pole*. If G is a *Ramanujan graph*, that is, any nontrivial eigenvalue $\lambda \neq \pm k$ of $\mathbf{A}_G$ satisfies $|\lambda| \leq 2\sqrt{k-1}$, then any real pole is only *trivial pole* and any other poles lie on the circle above. In this sense, we say that the analogue of the Riemann hypothesis of the Ihara zeta function holds for a regular graph G if and only if G is a Ramanujan graph.

We shall investigate the distribution of poles of the modified zeta function $\tilde{\mathbf{Z}}_G(u)$ for k-regular graphs. Also in this case, in terms of eigenvalues of the adjacency matrix $\mathbf{A}_G$, we know the distribution of poles of $\tilde{\mathbf{Z}}_G(u)$. In particular, the eigenvalues of $(\mathbf{U}^2)^+$ are expressed by means of those of the adjacency matrix $\mathbf{A}_G$ of G in [9,13,18] as follows:

Theorem 6. ([9]) Let G be a simple connected k-regular graph with n vertices and m unoriented edges. Suppose that $k \geq 3$. The positive support $(\mathbf{U}^2)^+$ has $2n$ eigenvalues λ_{2+} of the form

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

where λ_A is an eigenvalue of the adjacent matrix $\mathbf{A}_G$. The remaining $2(m - n)$ eigenvalues of $(\mathbf{U}^2)^+$ are 2.
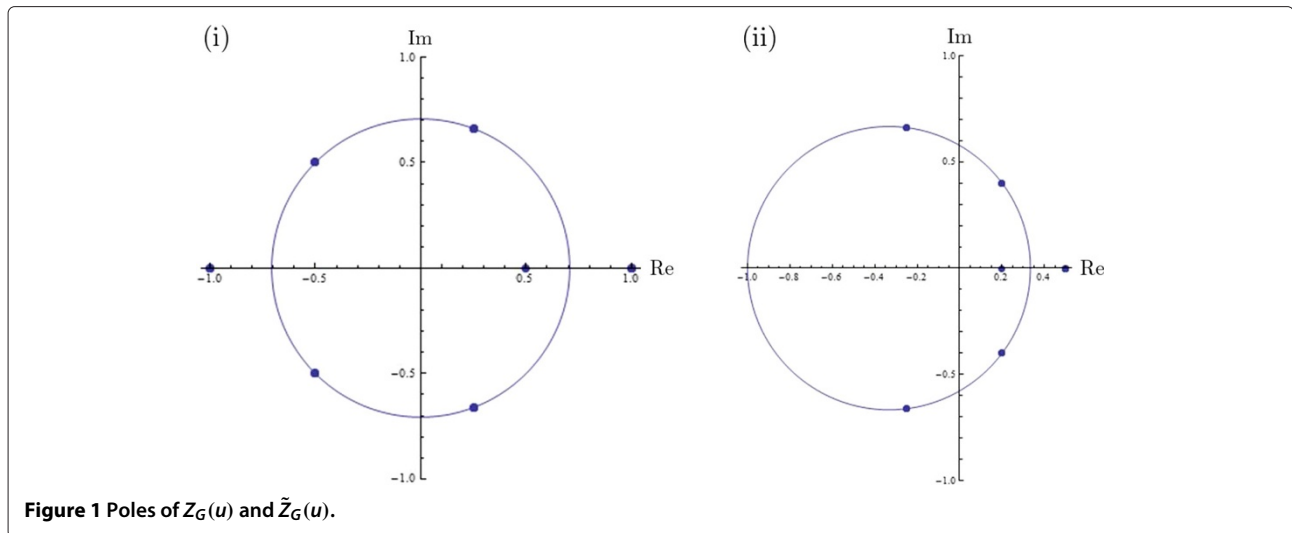
Figure 1 Poles of $Z_G(u)$ and $\tilde{Z}_G(u)$.

By Proposition 1, an analytic continuation $\tilde{Z}_G(u)$ has the following determinant expression:

$$\tilde{Z}_G(u) = 1/\det\left(I_{2m} - u\left(U^2\right)^+\right)$$
$$= \prod_{\lambda \in Spec\left((U^2)^+\right)} (1 - u\lambda)^{-1};$$

the poles of $\tilde{Z}_G(u)$ is given by $1/\lambda$ for $\lambda \in Spec\left(\left(U^2\right)^+\right)$. Using Theorem 6, we see the pole u corresponding to λ_A has the following form:

$$u = \frac{\lambda_A^2 - 2k + 4 \pm \sqrt{-1}\lambda_A\sqrt{4k - 4 - \lambda_A^2}}{2\left(\lambda_A^2 + (k-2)^2\right)}. \tag{8}$$

Remarking that $u = 1/(k^2 - 2k + 2), 1/2$, say *trivial poles*, if $\lambda_A = \pm k$ and $u = -1/(k-2)$ if $\lambda_A = 0$, we can see the real poles $u \in [1/(k^2 - 2k + 2), 1/2] \cup \{-1/(k-2)\}$. Moreover it can be easily checked that any imaginary pole $u = p + q\sqrt{-1} \ (p, q \in \mathbb{R})$ satisfies that

$$\left(p + \frac{1}{k^2 - 2k}\right)^2 + q^2 = \left(\frac{k-1}{k^2 - 2k}\right)^2.$$

Let us summarize the above.

Example 1. Let G be a simple connected k-regular graph with n vertices. Suppose that $k \geq 3$. Then the pole of the modified zeta function $\tilde{Z}_G(u)$ has the form as in (8) with an eigenvalue λ_A of the adjacency matrix A_G. In particular, all of the real poles u satisfy

$$\frac{1}{k^2 - 2k + 2} \leq u \leq \frac{1}{2}$$

and, if $0 \in Spec(A_G)$, $u = -1/(k-2)$; all of the imaginary poles u lie on the circle whose center is $-1/(k^2 - 2k)$ and radius is $(k-1)/(k^2 - 2k)$.

Of course, we have already known in Theorem 3 and Corollary 1 $u = 1/(k^2 - 2k + 2)$ is a pole whose order is 2 or 1 if G is bipartite or not, respectively; $u = 1/2$ is a pole and its order is $(k-2)n + 2$ or $(k-2)n + 1$ if G is bipartite or not, respectively. We should remark, for this modified zeta function $\tilde{Z}_G(u)$, all poles except *trivial poles* lie on the circle above if G is a *Ramanujan graph*. In this sense, we can say $\tilde{Z}_G(u)$ also has a property of the analogue of the *Riemann hypothesis*. We close this note with illustrating some figures of poles. The dots in (i) and (ii) of Figure 1 are the poles of $Z_G(u)$ and $\tilde{Z}_G(u)$ of the Petersen graph, which is 3-regular with 10 vertices, respectively. The circles in (i) and (ii) of Figure 1 are $p^2 + q^2 = 1/(k-1)$ and $(p + 1/(k^2 - 2k))^2 + q^2 = ((k-1)/(k^2 - 2k))^2$ for $k = 3$, respectively. Since the Petersen graph is a Ramanujan graph, all poles except trivial poles lie on the circles.

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