TAIWANESE JOURNAL OF MATHEMATICS
Vol. 15, No. 1, pp. 129-139, February 2011
This paper is available online at http://www.tjm.nsysu.edu.tw/

A NOTE ON THE NORMALIZED LAPLACIAN SPECTRA

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Abstract. Let G be a connected graph and $\mathcal{L}$ be its normalized Laplacian matrix. Let λ_1 be the second smallest eigenvalue of $\mathcal{L}$. In this paper we studied the effect on the second smallest normalized Laplacian eigenvalue by grafting some pendant paths.

1. Introduction

Throughout this paper it is assumed that all graphs are simple and all matrices are real. We shall use the standard terminology of graph theory and matrix theory, as introduced in most textbooks. The transpose of A is denoted by A^T, and the identity matrix is denoted by I. The vector e will always mean the vector $(1, 1, \ldots, 1)^T$, with n ones.

Let G be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set E. Let d_v denote the degree of the vertex v. We first define the *Laplacian matrix* of G, denoted by $L(G)$, as

$$L_{uv} = \begin{cases} d_u & \text{if} \quad u = v, \\ -1 & \text{if} \quad uv \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Let D denote the diagonal matrix of vertex degrees with the $(u, u)-$entries d_u corresponding to the vertex u. The *normalized Laplacian matrix* of G is the matrix

Received January 27, 2008, accepted June 10, 2009.
Communicated by Hung-Lin Fu.
2000 *Mathematics Subject Classification*: Primary 05C50; Secondary 15A18.
Key words and phrases: Laplacian, Normalized Laplacian, Second smallest eigenvalue, Harmonic eigenfunction.
Supported by youth scientific funds of the Education Department of Jiangxi Province (No. GJJ09460), Natural Science Foundation of Jiangxi Normal University(No.2058), National Natural Science Foundation of China (No.10601001).

$\mathcal{L}(G)$ given by

$$\mathcal{L}_{uv} = \begin{cases} 1 & \text{if} \quad u = v, \\ -\frac{1}{\sqrt{d_u d_v}} & \text{if} \quad uv \in E, \\ 0 & \text{otherwise.} \end{cases}$$

We can write

$$\begin{aligned} \mathcal{L} &= D^{-1/2} L D^{-1/2} \\ &= I - D^{-1/2} A D^{-1/2} \end{aligned}$$

with the convention that $D^{-1}(u,u) = 0$ if $d_u = 0$, where A is the adjacency matrix of G. It is easy to see that $\mathcal{L}$ is a symmetric positive semidefinite matrix, so its eigenvalues are all real and nonnegative, and we can use the variational description of the eigenvalues of a real symmetric matrix. Let g denote an arbitrary real-valued function on the vertex set of G. We can view g as a column vector. Then

$$\begin{aligned} \frac{\langle g, \mathcal{L} g \rangle}{\langle g, g \rangle} &= \frac{\langle g, D^{-1/2} L D^{-1/2} g \rangle}{\langle g, g \rangle} = \frac{\langle f, Lf \rangle}{\langle D^{1/2} f, D^{1/2} f \rangle} \\ &= \frac{\sum\limits_{u \sim v} (f(u) - f(v))^2}{\sum\limits_{v} f(v)^2 d_v} \end{aligned} \tag{1.1}$$

where $f = D^{-1/2} g$ and $\sum_{u \sim v}$ denotes the sum over all unordered pairs $\{u, v\}$ for which u and v are adjacent. Here $\langle f, g \rangle = \sum_x f(x) g(x)$ denotes the standard inner product in $\mathbb{R}^n$.

From the definition $\mathcal{L} := D^{-1/2} L D^{-1/2}$ we readily check that $D^{1/2} e$ is an eigenfunction of $\mathcal{L}$ corresponding to 0. We denote the eigenvalues of $\mathcal{L}$ by $0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$. Furthermore,

$$\lambda_1 = \inf_{f \perp De} \frac{\sum\limits_{u \sim v} (f(u) - f(v))^2}{\sum\limits_{v} f(v)^2 d_v}. \tag{1.2}$$

We call the nonzero function f achieving (1.2) a *harmonic eigenfunction* of $\mathcal{L}(G)$. The corresponding eigenfunction is $g = D^{1/2} f$ as in (1.1).

The normalized Laplacian eigenvalues of a graph were introduced by Fan Chung. These eigenvalues relate well to many graph invariants for general graphs in a way that other definitions (such as the eigenvalues of adjacency matrices) often fail to do. The advantages of this definition are perhaps due to the fact that it is consistent with the eigenvalues in spectral geometry and in stochastic processes. We refer the reader to [4] for the detail. More recent work on the normalized Laplacian can be found in [1, 2, 3, 7, 10].

We will need the following two results. The first result is simply the eigenvector equation of g, but expressed in terms of f.

Lemma 1.1. [4]. *Let f be a harmonic eigenfunction corresponding to λ_1. Then for any $v \in V$, we have*

$$\frac{1}{d_v}\sum_{u\sim v}(f(v)-f(u)) = \lambda_1 f(v).$$

Lemma 1.2. [3]. *Let G be a simple graph and let $H = G - e$ be the graph obtained from G with edge e removed. If $\lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$ and $\theta_0 \le \theta_1 \le \cdots \le \theta_{n-1}$ are the eigenvalues of $\mathcal{L}(G)$ and $\mathcal{L}(H)$ respectively, then*

$$\lambda_{i-1} \le \theta_i \le \lambda_{i+1}, i = 0, 1, \ldots, n-1,$$

where $\lambda_{-1} = 0$ and $\lambda_n = 2$.

The Laplacian eigenvalues of a graph play an important role in spectral graph theory, especially the second smallest eigenvalue of the Laplacian matrix, which Fiedler referred to as the algebraic connectivity. The eigenvector associated with the algebraic connectivity has often been called the Fiedler vector. Guo[8] in his PhD thesis investigated how the algebraic connectivity behaves when the graph is altered by grafting pendant paths. The definition of grafting is as follows: Let u and v be two different vertices of the connected graph G and let $H_{k,l}$ be the graph obtained from G by appending two disjoint paths $P : vv_kv_{k-1}\cdots v_1$ and $Q : uu_lu_{l-1}\cdots u_1$ at v and u,respectively. The graph $H'_{k+l} = H_{k,l} - vv_k + u_1v_k$ or $H''_{k+l} = H_{k,l} - uu_l + v_1u_l$ is said to be obtained from $H_{k,l}$ by grafting pendant paths. He obtained the following result.

Theorem 1.3. *Let u and v be two different vertices of the connected graph G and $H_{k,l}$ the graph obtained from G by appending two paths $P : vv_kv_{k-1}\cdots v_1$ and $Q : uu_lu_{l-1}\cdots u_1 (k \ge l \ge 1)$ at u and v,respectively. Let X be a Fiedler vector associated with algebraic connectivity $\alpha(H_{k,l})$ of $H_{k,l}$ and let*

$$H'_{k+l} = H_{k,l} - vv_k + u_1v_k$$

$$H''_{k+l} = H_{k,l} - uu_l + v_1u_l.$$

If $X(v_1)X(u_1) \ge 0$, we have

$$\alpha(H_{k,l}) \ge \alpha(H'_{k+l}) \quad or \quad \alpha(H_{k,l}) \ge \alpha(H''_{k+l}).$$

We are interested in a similar problem for the case of the normalized Laplacian matrix. In [11], we studied the effect on the second smallest eigenvalue of the normalized Laplacian of a graph by grafting pendant paths, in which the two paths are appended to the same vertex. In this paper we treat the problem for the case when the two paths are appended to different vertices.

2. Main RESULTS

First we give some preliminary results which can be found in [11].

Lemma 2.1. [11]. *Let G be a non-complete connected graph and f be the harmonic eigenfunction of $\mathcal{L}$ corresponding to the second smallest eigenvalue λ_1. Then for any $\alpha \geq 0$, the subgraph of G induced by $M(\alpha)$ is connected, where $M(\alpha) = \{v \in V | f(v) \leq \alpha\}$.*

In particular, we have the following corollary.

Corollary 2.2. *Let G be a non-complete connected graph, f a harmonic eigenfunction. Then the subgraph induced by the vertex set consisting of all vertices v that satisfy $f(v) \leq 0$ is connected. Moreover, the subgraph induced by the vertex set consisting of all vertices v that satisfy $f(v) \geq 0$ is also connected.*

Since $-f$ is a harmonic eigenfunction of $\mathcal{L}$ whenever f is, the second half of the preceding corollary clearly follows from its first half.

Theorem 2.3. [11]. *Let $G = (V, E)$ be a connected graph and $\mathcal{L}$ be its normalized Laplacian matrix. Let f be a harmonic eigenfunction of $\mathcal{L}$. Let v be a cut vertex of G such that $G_0, G_1, \ldots, G_r$ are all the connected components of the graph $G - v$. Then:*

(1) *If $f(v) > 0$, then exactly one of the components G_i contains a vertex negatively valuated by f. For all vertices u in the remaining components $f(u) > f(v)$.*

(2) *If $f(v) = 0$ and there exists a component G_i containing both positively and negatively valuated vertices, then there is exactly one such component, all remaining components being zero valuated.*

(3) *If $f(v) = 0$ and no component contains both positively and negatively valuated vertices, then each component contains either only positively valuated, or negatively valuated, or zero valuated vertices.*

In the following we use the notation vol$G$ to denote the sum of degrees of all vertices in G.

Theorem 2.4. *Let G be a connected graph, u, v be two different vertices in G, and $H_{k,l}$ be the graph obtained from G by appending two paths $P : vv_kv_{k-1}\cdots v_1$ and $Q : uu_lu_{l-1}\cdots u_1$ of length k and l at u and v respectively, where $u_1, u_2, \ldots, u_l$ and $v_1, v_2, \ldots, v_k$ are distinct new vertices. Let f be a harmonic eigenfunction of $\mathcal{L}(H_{k,l})$ and let*

$$H'_{k,l} = H_{k,l} - vv_k + u_1v_k,$$

$$H''_{k,l} = H_{k,l} - uu_l + v_1u_l.$$

If $f(v_1)f(u_1) \geq 0$, then we have

$$\lambda_1(H_{k,l}) \geq \lambda_1(H'_{k,l}) \qquad or \qquad \lambda_1(H_{k,l}) \geq \lambda_1(H''_{k,l}).$$

Note that $f(v_1)f(u_1) \geq 0$ is equivalent to $g(v_1)g(u_1) \geq 0$.

Proof. Let $V(G) = \{u, v, w_1, w_2, \ldots, w_h\}$. Then the order of $H_{k,l}$ is $n = k + l + h + 2$. Let f' be the vector given by

$$\begin{cases} f'(v_i) = f(v_i) + f(u_1) - f(v), i = 1, \ldots, k, \\ f'(w) = f(w), w \neq v_i, i = 1, \ldots, k. \end{cases}$$

By a straightforward calculation, we have

$$\langle f', L(H'_{k,l})f'\rangle = \sum_{xy\in E(H'_{k,l})} (f'(x) - f'(y))^2$$
$$= \sum_{xy\in E(H_{k,l})} (f(x) - f(y))^2 = \langle f, L(H_{k,l})f\rangle.$$

Now we use d_x(respectively, d'_x) to denote the degree of x in $H_{k,l}$(respectively, $H'_{k,l}$), unless specified otherwise. Let D' denote the diagonal matrix of vertex degrees of $H'_{k,l}$. Then $d'_v = d_v - 1$, $d'_{u_1} = d_{u_1} + 1$ and $d'_w = d_w$ for $w \neq v, u_1$, we have

$$\langle f', D'e\rangle$$
$$= \sum_x f'(x)d'_x = \sum_{i=1}^{k} f'(v_i)d'_{v_i} + f'(u_1)d'_{u_1} + f'(v)d'_v + \sum_{w\neq u_1,v,v_1,\ldots,v_k} f'(w)d'_w$$
$$= \sum_{i=1}^{k}(f(v_i) + f(u_1) - f(v))d_{v_i} + f(u_1)(d_{u_1} + 1) + f(v)(d_v - 1)$$

$$+\sum_{w\neq u_1,v,v_1,\ldots,v_k} f(w)d_w$$
$$=\sum_x f(x)d_x+(f(u_1)-f(v))(1+2(k-1))+(f(u_1)-f(v))$$
$$=\langle f,De\rangle+2k(f(u_1)-f(v))=2k(f(u_1)-f(v)).$$

Let $h=f'-ae$, where $a=\frac{2k(f(u_1)-f(v))}{volH_{k,l}}$. Then

$$\langle h,D'e\rangle=\langle f',D'e\rangle-\langle ae,D'e\rangle=2k(f(u_1)-f(v))-avolH_{k,l}=0,$$

and

$$\langle f,L(H_{k,l})f\rangle=\langle f',L(H'_{k,l})f'\rangle=\langle h+ae,L(H'_{k,l})(h+ae)\rangle$$
$$=\langle h,L(H'_{k,l})(h+ae)\rangle+\langle ae,L(H'_{k,l})f'\rangle=\langle h,L(H'_{k,l})h\rangle$$

where the last equality holds as $L(H'_{k,l})e=0$.

$$\begin{aligned}\langle h,D'h\rangle &=\langle h,D'f'\rangle-a\langle h,D'e\rangle=\langle h,D'f'\rangle=\langle f',D'f'\rangle-a\langle e,D'f'\rangle\\ &=\langle f',D'f'\rangle-a\langle f',D'e\rangle\\ &=\sum_{x\in V(H'_{k,l})} d'_x f'^2(x)-\frac{4k^2(f(u_1)-f(v))^2}{volH_{k,l}}\\ &=\sum_{x\in V(H_{k,l})} d_x f^2(x)+f^2(u_1)-f^2(v)+\sum_{i=1}^{k} d_{v_i}((f(u_1)-f(v))^2 \qquad (2.1)\\ &\quad +2f(v_i)(f(u_1)-f(v)))-\frac{4k^2(f(u_1)-f(v))^2}{volH_{k,l}}\\ &=\langle f,Df\rangle+(f(u_1)-f(v))(f(u_1)+f(v)+2\sum_{i=1}^{k} f(v_i)d_{v_i})\\ &\quad +(2k-\frac{4k^2}{volH_{k,l}}-1)(f(u_1)-f(v))^2.\end{aligned}$$

Since $volH_{k,l}>2k+4$, in the last line we always have $2k-\frac{4k^2}{volH_{k,l}}-1>2k-1-\frac{2k^2}{k+2}>0$.

Now in the same way we can construct a vector g corresponding to $H''_{k,l}$ satisfying

$$\langle g,D''e\rangle=0,\langle f,L(H_{k,l})f\rangle=\langle g,L(H''_{k,l})g\rangle$$

where D'' denotes the diagonal matrix of vertex degrees of $H''_{k,l}$, and

$$\begin{aligned}\langle g, D''g\rangle &= \langle f, Df\rangle + (f(v_1) - f(u))(f(v_1) + f(u) + 2\sum_{i=1}^{l} f(u_i)d_{u_i}) \\ &+(2l - \frac{4l^2}{volH_{k,l}} - 1)(f(v_1) - f(u))^2.\end{aligned} \tag{2.2}$$

We may assume that $f(u_1) \geq 0$ and $f(v_1) \geq 0$, replacing f by $-f$, if necessary. Note that the graph $H_{k,l}$ is non-complete. By Corollary 2.2 the subgraph H induced by subset of vertices w such that $f(w) \geq 0$ is connected. But P and Q are pendant paths of G at u and v respectively, so $u, u_1 \ldots, u_l, v, v_1, \ldots, v_k$ are vertices of H. Hence we have

$$\begin{cases} f(u_i) \geq 0 (i = 2, \ldots, l), f(u) \geq 0, \\ f(v_i) \geq 0 (i = 2, \ldots, k), f(v) \geq 0. \end{cases} \tag{2.3}$$

If $f(u) > 0$ then by Theorem 2.3(1)(with the cut vertex taken to be u), $f(u_j) > f(u)$ for $j = 1, 2, \ldots, l$.

If $f(u) = 0$ then applying Theorem 2.3, again with u as the cut vertex, we can conclude that either $f(u_j) = 0$ for $j = 1, 2, \ldots, l$ or they are all positive.

Similar remarks can be said for what happens when $f(v) > 0$ or $f(v) = 0$. Then we shall show that $f(u_1) > f(v)$ or $f(v_1) > f(u)$ if one of the following happens:

(i) $f(u) > 0$ and $f(v) > 0$;
(ii) $f(v) = 0$ and $f(u_j) > 0$ for $j = 1, 2, \ldots, l$;
(iii) $f(u) = 0$ and $f(v_j) > 0$ for $j = 1, 2, \ldots, k$.

In case (i), apply Theorem 2.3 to $H_{k,l}$ with u as the cut vertex. Since $f(u) > 0$, $u_1, \ldots, u_l$ are the vertices of the same component of $H_{k,l} - u$ and we have already shown that $f(u_i) \geq 0$ for $i = 1, \ldots, l$, by Theorem 2.3(1) we have $f(u_1) > f(u)$. Similarly, we also obtain $f(v_1) > f(v)$. Hence, we have either $f(u_1) > f(v)$ or $f(v_1) > f(u)$. In case (ii), obviously we have $f(u_1) > f(v)$. In case (iii), $f(v_1) > f(u)$.

If $f(u_1) > f(v)$, applying (2.1), we obtain $\langle h, D'h\rangle > \langle f, Df\rangle$ and consequently

$$\lambda_1(H_{k,l}) = \frac{\langle f, L(H_{k,l})f\rangle}{\langle f, Df\rangle} > \frac{\langle h, L(H'_{k,l})h\rangle}{\langle h, D'h\rangle} \geq \lambda_1(H'_{k,l}),$$

in view of the fact $\langle h, D'e\rangle = 0$ and $\langle f, L(H_{k,l})f\rangle = \langle h, L(H'_{k,l})h\rangle$.

Similarly, in the case $f(v_1) > f(u)$, using (2.2) we get $\lambda_1(H_{k,l}) > \lambda_1(H''_{k,l})$.

What remains to consider is the case:

(iv) $f(u) = f(v) = f(u_1) = \ldots = f(u_l) = f(v_1) = \ldots = f(v_k) = 0.$

In this case, in view of (2.1),$\langle f, Df\rangle = \langle h, D'h\rangle$. So we have

$$\lambda_1(H_{k,l}) = \frac{\langle f, L(H_{k,l})f\rangle}{\langle f, Df\rangle} = \frac{\langle h, L(H'_{k,l})h\rangle}{\langle h, D'h\rangle} \geq \lambda_1(H'_{k,l}).$$

By symmetry, we also obtain $\lambda_1(H_{k,l}) \geq \lambda_1(H''_{k,l})$. ■

Based on newGRAPH and Matlab, we generate some graphs which are given in Fig. 1. The real numbers attached to vertices in each graphs are the valuations by the harmonic eigenfuction of the graph. In graph G_1, g denotes the harmonic eigenfunction of the graph $G = G_1 - \{v_1, u_1, u_2, u_3\}$.

From the proof of Theorem 2.4, one can find that if $f(v_1)f(u_1) > 0$ then $\lambda_1(H_{k,l})$ is strictly greater than $\lambda_1(H'_{k,l})$ or $\lambda_1(H''_{k,l})$. The graph G_1 serves to illustrate that in Theorem 2.4 if $f(v_1)f(u_1) = 0$, it is possible that both inequalities become equalities. Here we take $H_{k,l}$ to be G_1(with $G = G_1 - \{v_1, u_1, u_2, u_3\}$), $\lambda_1(G_1 - \{v_1, u_1, u_2, u_3\}) = \lambda_1(G) = \lambda_1(G_1) = \lambda_1(G_1 - vv_1 + u_1v_1) = \lambda_1(G_1 - uu_3 + v_1u_3)$. More information can be found in our next proposition.

The graph G_2(also G_3) serves to illustrate that when the condition $f(v_1)f(u_1) \geq 0$ is not met it is still possible that we have $\lambda_1(H_{k,l}) > \lambda_1(H'_{k,l})$ and $\lambda_1(H_{k,l}) > \lambda_1(H''_{k,l})$. This leads us to suspect that the conclusion of Theorem 2.4 always holds and the "or" in the conclusion may be replaced by "and".

Proposition 2.5. *Let G be a graph and v be a vertex of G. Let H be the graph obtained from G by adding a pendant edge $e = vu$ at v and let f be a harmonic eigenfunction of H. If $f(v) = f(u) = 0$, then the restriction of f to G is a harmonic eigenfuction of G and so $\lambda_1(H) = \lambda_1(G)$.*

Proof. Set $\lambda_1 = \lambda_1(H)$. Define a function g on $V(G)$ as follows: $g(w) = f(w)$, for any $w \in V(G)$. Then for any $w \in V(G) - v$,

$$(1 - \lambda_1)d'_w g(w) = (1 - \lambda_1)d_w f(w) = \sum_{x\sim w} f(x) = \sum_{x\sim w} g(x);$$

(Here and in the following d'_x stands for the degree of the vertex x in G) and

$$(1 - \lambda_1)d'_v g(v) = 0 = (1 - \lambda_1)d_v f(v) = \sum_{v_j\sim v} f(v_j) = \sum_{v_j\sim v, v_j\neq u} f(v_j) + f(u)$$
$$= \sum_{v_j\sim v, v_j\neq u} f(v_j) = \sum_{v_j\sim v, v_j\in V(G)} g(v_j).$$

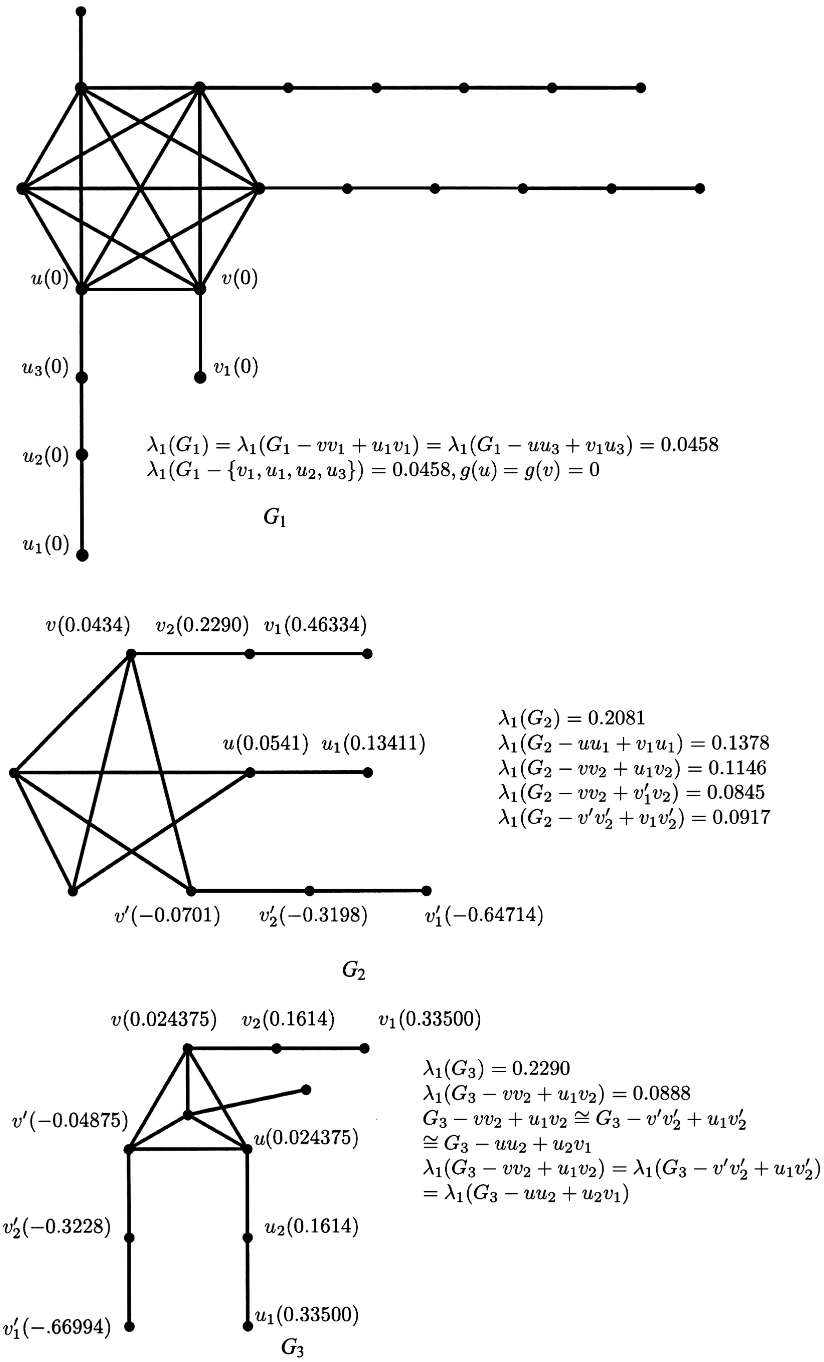
u(0)
v(0)
u3(0)
v1(0)
u2(0)
u1(0)
λ1(G1) = λ1(G1 − vv1 + u1v1) = λ1(G1 − uu3 + v1u3) = 0.0458
λ1(G1 − {v1, u1, u2, u3}) = 0.0458, g(u) = g(v) = 0
G1
v(0.0434)
v2(0.2290)
v1(0.46334)
u(0.0541)
u1(0.13411)
v′(−0.0701)
v′2(−0.3198)
v′1(−0.64714)
λ1(G2) = 0.2081
λ1(G2 − uu1 + v1u1) = 0.1378
λ1(G2 − vv2 + u1v2) = 0.1146
λ1(G2 − vv2 + v′1v2) = 0.0845
λ1(G2 − v′v′2 + v1v′2) = 0.0917
G2
v(0.024375)
v2(0.1614)
v1(0.33500)
v′(−0.04875)
u(0.024375)
v′2(−0.3228)
u2(0.1614)
v′1(−.66994)
u1(0.33500)
λ1(G3) = 0.2290
λ1(G3 − vv2 + u1v2) = 0.0888
G3 − vv2 + u1v2 ≅ G3 − v′v′2 + u1v′2
≅ G3 − uu2 + u2v1
λ1(G3 − vv2 + u1v2) = λ1(G3 − v′v′2 + u1v′2)
= λ1(G3 − uu2 + u2v1)
G3

Fig. 1.

So we conclude that for any $w \in V(G)$, $(1-\lambda_1)d'_w g(w) = \sum_{v_i \sim w} g(v_i)$. That is, $D^{-1}Lg = \lambda_1 g$, where D and L denote the diagonal matrix and Laplacian matrix of G, respectively. Thus λ_1 is an eigenvalue of $D^{-1}L$ and so an eigenvalue of $\mathcal{L}(G)$. By Lemma 1.2, we have that

$$\lambda_1(H) \leq \lambda_2(H-e) = \lambda_1(G).$$

So $\lambda_1(H) = \lambda_1(G)$ and g is a harmonic eigenfunction of G with $g(v) = 0$ as desired. ■

If case (iv) happens, i.e., if $f(u) = f(v) = f(u_1) = \ldots = f(u_l) = f(v_1) = \ldots = f(v_k) = 0$, then by applying Proposition 2.5 repeatedly we can conclude that $\lambda_1(H_{k,l}) = \lambda_1(G)$ and the harmonic eigenfunction g of G satisfies $g(u) = g(v) = 0$.

Acknowledgments

The first author is indebted to Professor Bit-Shun Tam whose comments have led to a better presentation.

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