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THE LAPLACIAN SPECTRUM OF A GRAPH*

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Abstract. Let G be a graph. The Laplacian matrix $L(G) = D(G) - A(G)$ is the difference of the diagonal matrix of vertex degrees and the 0-1 adjacency matrix. Various aspects of the spectrum of $L(G)$ are investigated. Particular attention is given to multiplicities of integer eigenvalues and to the effect on the spectrum of various modifications of G.

Key words. tree(s), eigenvalue(s), spectra, graph(s)

AMS(MOS) subject classifications. primary 05C05, 05C50; secondary 05C10, 05C25, 05C40

1. Introduction. Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \cdots, v_n\}$ and edge set $E = \{e_1, e_2, \cdots, e_m\}$. For each edge $e_j = \{v_i, v_k\}$, choose one of v_i, v_k to be the positive end of e_j and the other to be the negative end. We refer to this procedure by saying G has been given an *orientation*. The vertex-edge *incidence matrix* afforded by an orientation of G is the n-by-m matrix $Q = Q(G) = (q_{ij})$, where

$$q_{ij} = \begin{cases} +1, & \text{if } v_i \text{ is the positive end of } e_j, \\ -1, & \text{if it is the negative end,} \\ 0, & \text{otherwise.} \end{cases}$$

It turns out that $L(G) = QQ^t$ is independent of the orientation. In fact, $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees and $A(G)$ is the (symmetric) 0-1 adjacency matrix. Forsman [9] and Gutman [11] have shown how the connection between $L(G)$ and $K(G) = Q^tQ$ simultaneously explain the statistical and the dynamic properties of flexible branched polymer molecules. Indeed, since $L(G)$ and $K(G)$ share the same nonzero eigenvalues, it follows that for bipartite graphs the smallest eigenvalue of $A(G^*) \geqq -2$, where G^* is the line graph of G. This observation, first made by Hoffman, has led to a connection with the theory of root systems [2], [3]. Eichinger [5] has shown how the spectrum of $L(G)$ may be used to calculate the radius of gyration of a Gaussian molecule. Mohar [13] argues that, because of its importance in various physical and chemical theories, the spectrum of $L(G)$ is more natural and important than the more widely studied adjacency spectrum. In [1], Bien uses the smallest positive eigenvalue of $L(G)$ to estimate the "magnifying coefficient" of G.

It seems that $L(G)$ first occurred in the celebrated **Matrix-Tree Theorem:** If L_{ij} is the submatrix of $L(G)$ obtained by deleting its ith row and jth column, then $(-1)^{i+j} \det(L_{ij})$ is the number of different spanning trees in G. Since this result is attributed to G. Kirchhoff, $L(G)$ is sometimes called a *Kirchhoff matrix*. It is also known as a *matrix of admittance* (admittance = conductivity). Following [7], we will refer to $L(G)$ as a *Laplacian* matrix because it is a discrete analogue of the Laplace differential operator.

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We have suppressed the dependence of $L(G)$ on the ordering of V because our primary interest is with the characteristic polynomial $c_G(x) = \det(xI - L(G))$.

Example 1.1. Let $G = C_6$, the simple circuit on six vertices. Then

$$\begin{aligned} c_G(x) &= x(x-1)^2(x-3)^2(x-4) \\ &= x^6 - 12x^5 + \cdots - 36x. \end{aligned}$$

Of course, 12 is the sum of the vertex degrees and 36 is the sum of the six principal minors of $L(G)$ of order five. We can state each of these facts in another way. The sum of the vertex degrees is twice the number of edges. The sum of the minors is ($n =$) six times the number of spanning trees. Similar statements are available for the other coefficients [4, p. 38].

Example 1.2. Let $G = *_n$, the "star," i.e., $G = K_{1,n-1}$, the complete bipartite graph with $n - 1$ pendant (degree 1) vertices and one vertex of degree $n - 1$. Then $c_G(x) = x(x-n)(x-1)^{n-2}$. If the central vertex is listed last, then $(-1, -1, \cdots, n-1)$ is an eigenvector of $L(G)$ corresponding to n, while

$$\{(1,-1,0,\cdots,0),(0,1,-1,0,\cdots,0),\cdots,(0,0,\cdots,0,1,-1,0)\}$$

is a set of $n - 2$ linearly independent eigenvectors corresponding to one.

Denote the eigenvalues of $L(G)$ by $\lambda_1 \geqq \cdots \geqq \lambda_{n-1} \geqq 0 = \lambda_n$. From the Matrix-Tree Theorem (for example) we may deduce that $\lambda_{n-1} > 0$ if and only if G is connected. (In particular, $K(G)$ is nonsingular if and only if G is a tree.) Fiedler has called λ_{n-1} the *algebraic connectivity* of G [7], denoting it by $a(G)$.

2. Preliminary results. A vertex of degree one is called a pendant vertex. Denote by $p(G)$ the number of pendant vertices of G. A vertex is *quasipendant* if it is adjacent to a pendant vertex. Denote by $q(G)$ the number of quasipendant vertices of G. If T is a tree, it is known [4, p. 258] that

$$p(T) - q(T) \leqq \eta \leqq p(T) - 1, \tag{1}$$

where η is the multiplicity of zero as an eigenvalue of $A(T)$.

Denote by $m_G(\lambda)$ the multiplicity of λ as an eigenvalue of $L(G)$. Incidental to her work on permanental polynomials, Faria observed that

$$p(G) - q(G) \leqq m_G(1), \tag{2}$$

for any graph G [6].

THEOREM 2.1. *Suppose T is a tree on n vertices. If $\lambda > 1$ is an integer eigenvalue of $L(T)$ with corresponding eigenvector u, then*

(i) $\lambda \mid n$ (*i.e.*, λ *exactly divides* n),

(ii) $m_T(\lambda) = 1$,

(iii) *no coordinate of u is zero.*

Theorem 2.1 can fail totally for graphs that are not trees. (See Example 1.1.)

Proof. The characteristic polynomial of $L(T)$ is $xf(x)$, where $f(x)$ is an integer polynomial. Since T is a tree, $f(0) = n$ (as in Example 1.1). This proves (i). If $L(T)$ had two linearly independent eigenvectors corresponding to λ, we could produce a third eigenvector with zero in any prescribed coordinate. Hence, (iii) implies (ii).

Suppose u is an eigenvector of $L(T)$ afforded by λ. If some coordinate of u is zero, we may assume it is the last one, corresponding to vertex v_n. With $d = d_n$, the degree of v_n, $L(T)$ takes the form

$$L(T)=\begin{pmatrix} B_1 & 0\cdots 0 & * \\ 0 & B_2\cdots 0 & * \\ & \cdots & \\ 0 & 0\cdots B_d & * \\ * & *\cdots * & d \end{pmatrix}, \tag{3}$$

where $B_1, B_2, \cdots, B_d$ are the principal submatrices of $L(T)$ corresponding, respectively, to the branches $T_1, T_2, \cdots, T_d$ of T at v_n. If u is partitioned conformally as $u = (u_1, u_2, \cdots, u_d, 0)$, then $uL(T) = \lambda u$ implies $u_i B_i = \lambda u_i$, $1 \leqq i \leqq d$. Since at least one of these u_i's must be nonzero, λ is an eigenvalue of some B_i. We may assume it is B_1. Note that B_1 is not quite $L(T_1)$. One of its main diagonal entries is too large, the one corresponding to the vertex of T_1 that is adjacent (in T) to v_n. If we assume this vertex is v_1, then $B_1 = L(T_1) + E_{11}$, where E_{11} is the matrix whose only nonzero entry is a one in position $(1, 1)$. But then $\det B_1 = \det L(T_1) + \det L_{11}$, where L_{11} is the submatrix of $L(T_1)$ obtained by eliminating its first row and column. Now, $\det L(T_1) = 0$ while, by the Matrix-Tree Theorem, $\det L_{11} = 1$. Thus, λ is an eigenvalue of the unimodular matrix B_1, a contradiction. □

It seems surprising that for trees, $m_T(1)$ can be arbitrarily large while $m_T(2)$ can be at most one. It turns out that, integer or not, the largest eigenvalue of any bipartite graph is simple. This is a consequence of the following elementary observation.

PROPOSITION 2.2. *Let G be a bipartite graph. Then $B(G) = D(G) + A(G)$ and $D(G) - A(G) = L(G)$ are unitarily similar; in particular, the maximum eigenvalue of $L(G)$ is simple provided G is connected.*

If $G = K_n$, the complete graph, then $\lambda_1 = n$ and $m_G(\lambda_1) = n - 1$, i.e., the result can fail if G is not bipartite.

Proof. Since G is bipartite, the vertex set can be partitioned into two subsets V_1 and V_2 so that no two vertices in V_i are adjacent, for $i = 1, 2$.

Let $U = (u_{ij})$ be the diagonal matrix with

$$u_{ii} = \begin{cases} 1, & \text{if } v_i \in V_1, \\ -1, & \text{if } v_i \in V_2. \end{cases}$$

It is simple to verify that $UA(G)U^{-1} = -A(G)$ and that U commutes with $D(G)$. In case G is connected, the matrix $D(G) + A(G)$ is a nonnegative irreducible matrix and the second assertion is a consequence of the Perron–Frobenius theory. □

We now show that the upper-bound in (1) is a uniform upper bound on the multiplicity of any eigenvalue of $L(T)$.

THEOREM 2.3. *Let λ be an eigenvalue of $L(T)$ for some tree T on $n \geqq 2$ vertices. Then $m_T(\lambda) \leqq p(T) - 1$.*

As we saw in Example 1.2, equality can occur. On the other hand, if G is not a tree, it may have no pendant vertices.

Proof. Suppose v_n is a pendant vertex of T. We may assume v_{n-1} is the quasipendant of T adjacent to v_n. Let $u = (u_1, \cdots, u_n)$ be an eigenvector of $L(T)$ corresponding to λ. Then $(1 - \lambda)u_n = u_{n-1}$. Consider the possibility that $u_n = 0$. In this case, $u_{n-1} = 0$ and, moreover, $u' = (u_1, \cdots, u_{n-1})$ is an eigenvector of $L(T')$ corresponding to λ, where T' is the tree obtained from T by deleting v_n from V and $\{v_{n-1}, v_n\}$ from E. It follows by induction that u cannot be zero in all coordinates corresponding to pendant vertices, or even in all but one of them! On the other hand, if the eigenspace W of $L(T)$ corresponding to λ were to have dimension greater than $p(T) - 1$, it would be possible to find a nonzero vector $w \in W$ that is zero on all but (at most) one of its coordinates corresponding to pendant vertices. □

In order to discuss the next result, the following notation will be convenient. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs with $V_1 \cap V_2 = \emptyset$. A *connected sum* of G_1 and G_2 is any graph $G = (V, E)$ where $V = V_1 \cup V_2$, and E differs from $E_1 \cup E_2$ by the addition of a single edge joining some (arbitrary) vertex of V_1 to some vertex of V_2. It will be useful to write $G = G_1 \# G_2$. Note that "#" is not a binary operation on graphs because it is not well defined. If $n_1 = o(V_1)$, the cardinality of V_1, and $n_2 = o(V_2)$, then $G_1 \# G_2$ may represent any of $n_1 n_2$ different graphs. In general, of course, some of these graphs will be isomorphic as the following example shows.

Example 2.4. Denote by P_n the path on n vertices (of length $n - 1$). If $G_1 = P_2$ and $G_3 = P_3$, then $G_1 \# G_2$ is isomorphic either to P_5 or the graph in Fig. 1.

THEOREM 2.5. *Let G be a (nonempty) graph on n vertices. Let $H = G \# *_k$ be a connected sum of G with the star on $k > 1$ vertices. Then $m_G(k) = m_H(k)$.*

Proof. Assume the vertices have been numbered so that $G \# *_k$ is obtained by joining the last vertex of G to the first vertex of $*_k$. If $L = L(G)$, $L_* = L(*_k)$, and $L_\# = L(H)$, then, with respect to the obvious ordering of vertices,

$$L_\# = (L \dotplus L_*) + A, \tag{4}$$

where $A = (a_{ij})$ is the $(n + k)$-by-$(n + k)$ matrix with

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in \{(n,n),(n+1,n+1)\}, \\ -1 & \text{if } (i,j) \in \{(n,n+1),(n+1,n)\}, \\ 0 & \text{otherwise.} \end{cases}$$

From Example 1.2, we may choose an eigenvector w for L_*, corresponding to k, whose first component is $w_1 = 1$. We will use w to produce a linear bijection $u \to u_\#$ from $\ker(L - kI_n)$ onto $\ker(L_\# - kI_{n+k})$. For $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^k$, denote their juxtaposition by $x \oplus y \in \mathbb{R}^{n+k}$. Then for any $u \in \mathbb{R}^n$, define $u_\# = u \oplus u_n w$. Clearly, $u \to u_\#$ is linear and one-to-one. Since the nth and $(n + 1)$st coordinates of $u_\#$ are equal, $Au_\# = 0$ and, hence, $L_\# u_\# = Lu \oplus u_n L_* w$. But, then $u_\#$ is an eigenvector of $L_\#$ corresponding to k whenever u is an eigenvector of L corresponding to k. It remains to prove that every eigenvector of $L_\#$ corresponding to k is of the form $u_\#$ for some $u \in \ker(L - kI_n)$. Suppose $x \in \mathbb{R}^n$, $y \in \mathbb{R}^k$ and $x \oplus y$ is an eigenvector for $L_\#$ corresponding to k. We first assert that y is a multiple of w. This is seen by considering two cases.

Case i. The first vertex of $*_k$ (the one being connected to G by the new edge) is a pendant vertex. In this case, we may assume the vertices of $*_k$ so ordered that the kth

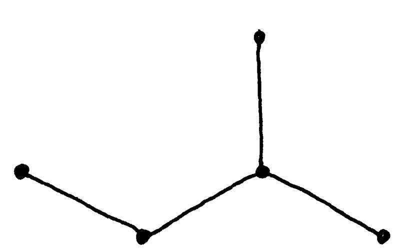

FIG. 1

vertex has degree $k-1$. Hence, $w=(1, 1, \cdots, 1, 1-k)$. (See Example 1.2.) We proceed to show that $y = y_1 w$. For $1 < i < k$ (when $k > 2$), we may conclude from the $(n+i)$th row of $L_{\#}(x \oplus y) = k(x \oplus y)$ that $y_k = (1-k)y_i$. Then, from the $(n+k)$th row, namely,

$$-y_1 - y_2 - \cdots - y_{k-1} + (k-1)y_k = ky_k,$$

it follows that $(1-k)y_1$ is also equal to y_k. In other words (since $k > 1$), $y = y_1 w$.

Case ii. The first vertex of $*_k$ has degree $k-1$. In this case, $w_1 = 1$ while $w_2 = \cdots = w_k = 1/(1-k)$. (When $k = 2$, the two cases coincide.) We use a similar argument to deduce that $(1-k)y_i = y_1$ for $i = 2, \cdots, k$. Thus, $y = y_2 w$.

We have shown that the typical vector in $\ker(L_{\#} - kI_{n+k})$ is of the form $x \oplus cw$. It remains only to show that $x_n = c$ and that $x \in \ker(L - kI_n)$. Now, by comparing $(n+1)$st rows of

$$\begin{aligned} k(x \oplus cw) &= L_{\#}(x \oplus cw) \\ &= (Lx \oplus kcw) + (0, \cdots, 0, x_n - c) \oplus (-x_n + c, 0, \cdots, 0), \end{aligned}$$

we see that $kc = kc - x_n + c$. Finally, compare the first n rows to deduce that $Lx = kx$. □

Theorem 2.5 is useful as a reduction device. Suppose, for example, that T is a tree and we want to know whether or not two is an eigenvalue. Then we may *prune* off P_2's without changing the answer to our question.

Example 2.6. Let G be the graph in Fig. 2. Then we may write $G = G' \# *_2$ in a variety of ways. For any of these, $m_G(2) = m_{G'}(2)$. But then G' can be written as $G'' \# *_2$, also in several ways. Indeed, we may eventually prune off six copies of $*_2$. (See Fig. 3.) The result is that $m_G(2) = m_{C_4}(2)$. The characteristic polynomial for the square is $x(x-2)^2(x-4)$, so $m_G(2) = 2$.

Example 2.7. As nice as the pruning process of Example 2.6 is, we eventually come to a "core" graph from which no P_2's may be pruned and for which it still may not be clear, even for trees, whether or not two is an eigenvalue. For the tree T in Fig. 4, $c_T(x) = x(x-1)^3(x-2)(x-5)(x^2-4x+1)^2$.

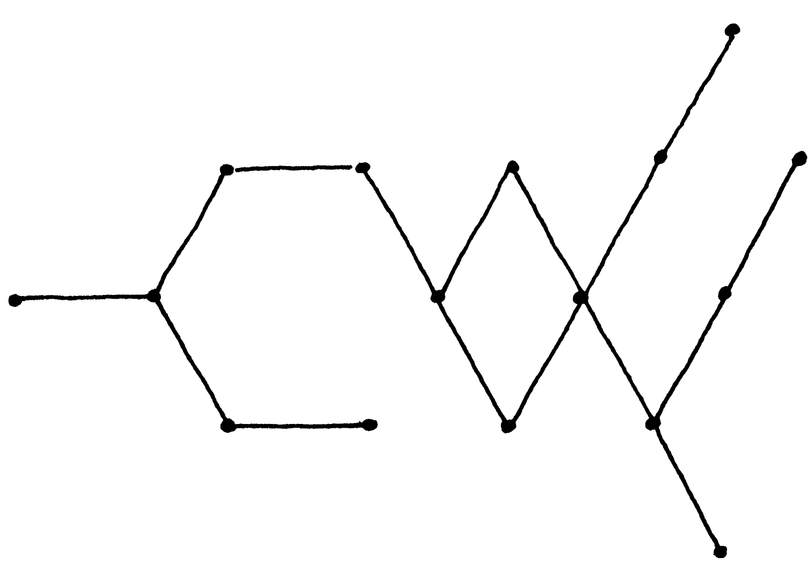

FIG. 2

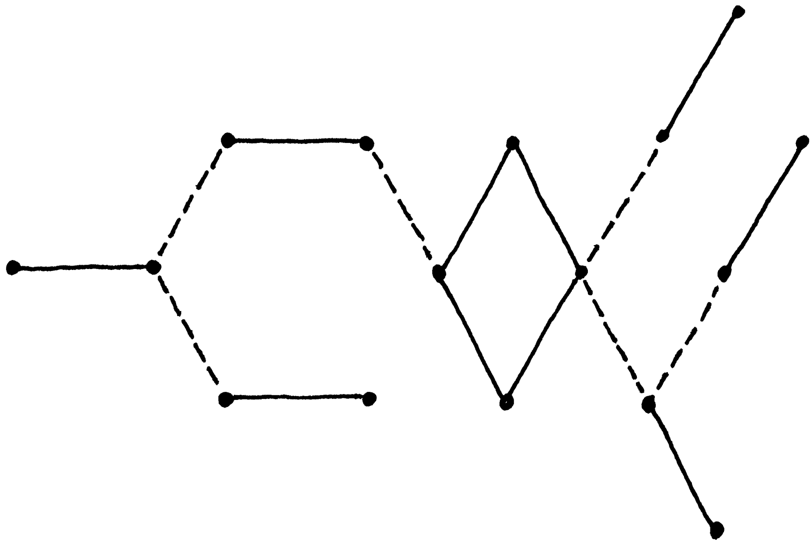

FIG. 3

COROLLARY 2.8. *Let $T = P_n$, the path on n vertices. Then*

(i) $$m_T(2) = \begin{cases} 1 & \text{if } 2 \mid n, \\ 0 & \text{otherwise.} \end{cases}$$

(ii) $$m_T(3) = \begin{cases} 1 & \text{if } 3 \mid n, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. We know from Theorem 2.1 that $m_T(k)$ is at most one when $k > 1$ is an integer and T is a tree. Since $P_2 = *_2$ and $P_3 = *_3$, the result follows from Theorem 2.5 and the pruning process of Example 2.6. □

Example 2.9. The graph in Fig. 4 is just one of a class of examples. If $k \geqq 2$ is an integer, we define a tree Z_k on $(2k - 1)(k + 1) + 1$ vertices as follows. Start with $k + 1$

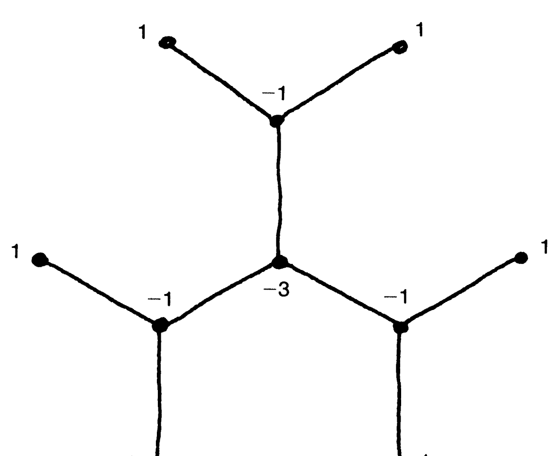

FIG. 4

copies of $*_{2k-1}$ and an additional vertex v. Then join the "center" of each star to v by an edge. It turns out that $m_{Z_k}(k) = 1$: that the multiplicity cannot be greater than one is assured by Theorem 2.1(ii). To see that the multiplicity is greater than zero, we may simply describe an eigenvector. The components of this eigenvector will be one in each of the $(2k-2)(k+1)$ coordinates corresponding to pendant vertices, $1-k$ in each of the $k+1$ coordinates corresponding to star centers, and $1-k^2$ in the coordinate corresponding to v. This explains the numbers in Fig. 4.

3. The multiplicity of $\lambda = 1$. We begin this section with an analogue of Theorem 2.5. We will be concerned with a slightly restricted version of the connected sum idea. By $G \vee P_3$ we mean (any) one of the graphs obtained from G and P_3 by joining some (arbitrary) vertex of G to a *pendant* vertex of P_3. (Of course, $P_3 = *_3$. We are using "$\vee$" here rather than "#" to indicate that it is now forbidden to join a vertex of G to the middle vertex of P_3. We will deal separately with this latter case in Proposition 3.14 below.)

THEOREM 3.1. *Let G be a (nonempty) graph on n vertices and suppose $H = G \vee P_3$. Then $m_G(1) = m_H(1)$.*

Proof. Let the second vertex of P_3 be the one of degree two. Then $w = (1, 0, -1)$ is an eigenvector of $L(P_3)$ corresponding to one. Number the vertices of G so that it is the last vertex that is joined to vertex one of P_3. Let L, L', and $\tilde{L}$ denote the Laplacian matrices of G, P_3, and H, respectively. Then, as in the proof of Theorem 2.5, $\tilde{L} = (L \dotplus L') + A$, where

$$A = 0_{n-1} \dotplus \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \dotplus 0_2.$$

Argue exactly as in Theorem 2.5 to show the map $u \to u \oplus u_n w$ is a linear injection of $\ker(L - I_n)$ into $\ker(\tilde{L} - I_{n+3})$. Conversely, if $x \oplus y$ is an eigenvector of $\tilde{L}$ corresponding to one, deduce that $y_2 = 0$ and that $y_3 = -y_1$. Proceed as in the proof of Theorem 2.5 to conclude that $y = x_n w$, so that $x \oplus y = x \oplus x_n w$ where $x \in \ker(L - I_n)$, as desired. □

Example 3.2. Let T be the tree in Fig. 5, with $k \geqq 2$. Then we may express T as $T' \vee P_3$ in a variety of ways; for any of these, $m_T(1) = m_{T'}(1)$. But, then $T' = T'' \vee P_3$, etc. Eventually, we see that $m_T(1) = m_S(1) = k - 1$, where $S = *_{k+1}$. It is instructive to compare this value with the Faria lower bound in (2), namely, $p(T) - q(T) = 0$. At the other extreme, the upper bound of Theorem 2.3 is $p(T) - 1 = k - 1$.

COROLLARY 3.3. *Let $T = P_n$. Then*

$$m_T(1) = \begin{cases} 1 & \textit{if } 3 \mid n, \\ 0 & \textit{otherwise}. \end{cases}$$

Proof. By Theorem 3.1, it suffices to consider $n = 1$, 2, or 3. The characteristic polynomials for P_1, P_2, and P_3 are, respectively, x, $x(x-2)$, and $x(x-1)(x-3)$. □

Example 3.4. Since $P_3 = *_3$, pruning of a path of length three affects neither $m_G(3)$ (Theorem 2.5) nor $m_G(1)$ (Theorem 3.1). If G is the graph in Fig. 6, we may prune off 5 P_3's and obtain the hexagon of Example 1.1. Thus, $m_G(3) = m_G(1) = 2$.

Example 3.5. As in Example 2.7, one may prune off only so many P_3's, even for trees. If T is the tree in Fig. 7, then

$$c_T(x) = x(x-1)(x^2-3x+1)^2(x^2-7x+11)(x^3-6x^2+8x-1).$$

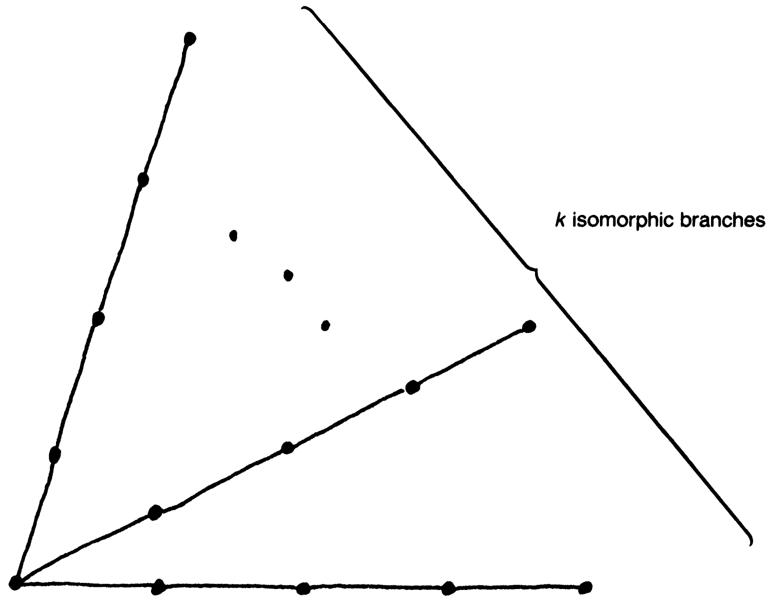

FIG. 5

We proceed now with a closer scrutiny of $m_G(1)$. Suppose G is a fixed but arbitrary graph on n vertices. Note that $u = (u_1, \cdots, u_n)$ is an eigenvector of $L(G)$ corresponding to $\lambda = 1$, if and only if

(5) $$\sum_{\{v_i,v_j\} \in E} u_j = (d_i - 1)u_i, \qquad 1 \leqq i \leqq n.$$

(In particular, if $uL(G) = u$, then $u_t = 0$ for all quasipendant vertices v_t.)

In terms of eigenvectors, it is easy to explain why $m_G(1) \geqq p(G) - q(G)$, a difference that Faria refers to as the "Star Degree" of G. Suppose $v_1, \cdots, v_t$ are the pendant vertices adjacent to the quasipendant v_{t+1}. Then it is easily seen that

$$u_i = (1, 0, \cdots, 0, -1, 0, \cdots, 0),$$

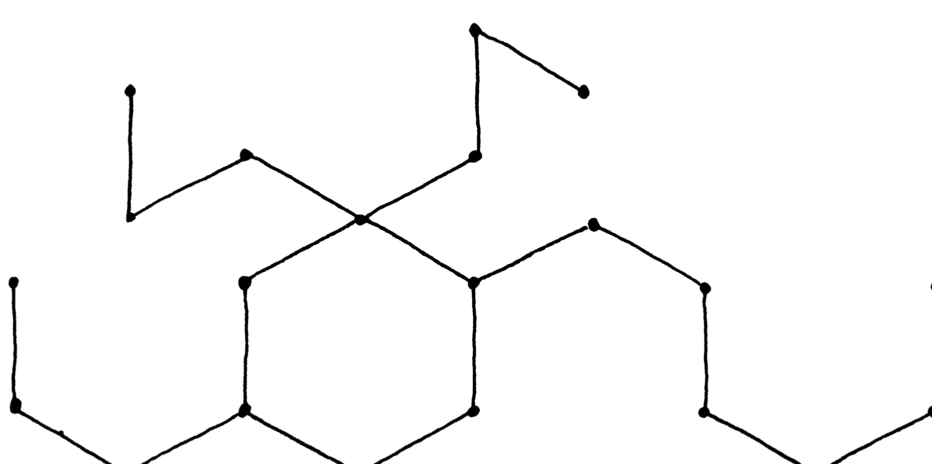

FIG. 6

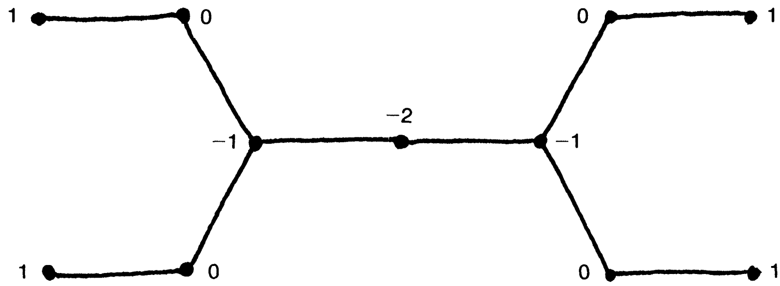

FIG. 7

with -1 in the ith coordinate, $2 \leqq i \leqq t$, is a set of $t-1$ linearly independent eigenvectors for $L(G)$ corresponding to $\lambda = 1$. We will call eigenvectors of this type *Faria vectors*. If the Faria vectors arising at each of the $q(G)$ quasipendant vertices are collected, the resulting $p(G) - q(G)$ set is a basis of what we call the *Faria space*. Thus, the Faria space accounts for the lower bound in (2). Our attention is naturally drawn to the excess or "spurious" multiplicity of one given by

$$s(G) = m_G(1) - p(G) + q(G), \tag{6}$$

i.e., the dimension of the space spanned by eigenvectors of $L(G)$ corresponding to one that are orthogonal to all the Faria vectors.

Let $p = p(G)$, $q = q(G)$, and $r = r(G)$, where $r(G) = n - p - q$ is the number of vertices of G that remain after the pendants and quasipendants have been accounted for. We will refer to these remaining vertices as *inner* vertices.

Assume the vertex set of G is ordered as $V = \{v_1, \cdots, v_n\}$, where $v_1, \cdots, v_r$ are the inner vertices, $v_{r+1}, \cdots, v_{r+q}$ are the quasipendants, and $v_{n-p+1}, \cdots, v_n$ are the pendant vertices. Assume further that $\{v_{r+i}, v_{n-p+i}\} \in E$, $1 \leqq i \leqq q$. It follows that $L(G)$ has the form

$$L(G) = \begin{pmatrix} A & X & 0 \\ X^t & Q & C \\ 0 & C^t & I_p \end{pmatrix},$$

where A is r-by-r and Q is q-by-q. Moreover, the submatrix of C occupying its first q columns is $-I_q$. Using this I_q submatrix (and its transpose in C^t) in elementary row and column operations, we may transform $L(G) - I_n$ to

$$\begin{pmatrix} L_R(G) & 0 & 0 \\ 0 & 0 & B \\ 0 & B^t & 0 \end{pmatrix}, \tag{7}$$

where $B = (-I_q 0)$, and $L_R(G) = A - I_r$ is the leading r-by-r principal submatrix of $L(G) - I_n$. Hence, from (7),

$$\begin{aligned} m_G(1) &= \text{nullity } [L(G) - I_n] \\ &= n - 2q - \text{rank } L_R(G) \\ &= p - q + \text{nullity } L_R(G). \end{aligned} \tag{8a}$$

(Note that the "$p - q$" in (8a) is the same "$p - q$" that arises as the dimension of the Faria space. The nullity of $L_R(G)$ corresponds to the eigenvectors for one that are orthogonal to the Faria vectors.) If we let $m_A(1)$ denote the multiplicity of one as an eigenvalue of A, then we may rewrite (8a) as

$$s(G) = \text{nullity } L_R(G) = m_A(1). \tag{8b}$$

We now proceed to estimate the nullity of $L_R(G)$ in two different ways, giving rise to two upper bounds for $s(G)$. Our first estimate involves the "point independence number" (PIN—also known as the "interior stability number" [2]) of a graph. A subset of vertices is *independent* if no two of them are adjacent. The PIN of G, $\alpha(G)$, is the maximum size of any independent set of vertices. Thus, e.g., $\alpha(K_n) = 1$ and $\alpha(K_{s,t}) = \max\{s, t\}$. If G has (exactly) k connected components $C_1, \cdots, C_k$, then $\alpha(G) = \sum \alpha(C_i)$. If R is the subgraph of G induced on the inner vertices, we will write $e(G) = \alpha(R)$.

THEOREM 3.6. *Suppose $G = (V, E)$ is a graph on n vertices. Then*

$$s(G) \leqq r(G) - e(G). \tag{9}$$

(The quantity $r(G) - e(G)$ is the *covering number* of R.)

Example 3.7. Let G be the graph in Fig. 8. Then $p = q = 2$, and the inner vertex graph R is the graph on $r = 4$ vertices having two components each consisting of a single edge. The matrix "A" is the direct sum of two copies of $3I_2 - J_2$, where J_2 is the 2-by-2 matrix each of whose entries is equal to one. Alternatively, $L_R(G)$ is the direct sum of $2I_2 - J_2$ with itself. In any case, $m_G(1) = s(G) = m_A(1) = \text{nullity } L_R(G) = 2$. On the other hand, $e(G) = 2$ and the upper bound in (9) is sharp. In fact,

$$c_G(x) = x(x-1)^2(x-2)(x-3)(x-4)(x^2-5x+2).$$

Proof of Theorem 3.6. Returning to (7)–(8), it suffices to show that

$$\text{rank } L_R(G) \geqq e = e(G).$$

By definition of e, $L_R(G)$ has a principal e-by-e diagonal submatrix. Since the degree (in G) of every vertex in R is at least two, this diagonal submatrix has full rank. □

The upper bound $r(G) - e(G) \geqq s(G)$ tends to be best when vertex degrees in the induced subgraph R are small. Our next result is a bound that tends to be best when vertex degrees are relatively large. We will say that a graph $G = (V, E)$ on n vertices is *rich* if $G = K_n$ or if $d_i + d_j \geqq n$ whenever $\{v_i, v_j\} \notin E$. (In particular, the "closure" of a rich graph is K_n.)

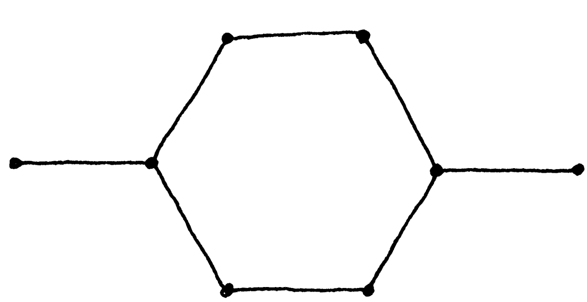

FIG. 8

THEOREM 3.8. *Suppose $G = (V, E)$ is a graph. Denote by R the subgraph of G induced on its inner vertices. If each of the k components of R is a rich graph, then $s(G) \leqq k$.*

In Example 3.7, R has two components, each of which is isomorphic to K_2. Since K_2 is rich, $s(G) \leqq 2$, and the upper bounds of Theorems 3.6 and 3.8 coincide. If, however, G were to be K_n, then $r(G) - e(G) = n - 1$, while the new upper bound is one. (In fact, of course, $m_{K_n}(1) = 0$.)

Proof. Observe that $L(G) + L(\bar{G}) = L(K_n) = nI_n - J_n$, where $\bar{G}$ is the complement of G and J_n is the n-by-n matrix each of whose entries is one. It follows that $\bar{\lambda}_{n-i} = n - \lambda_i$, $1 \leqq i < n$, where $\bar{\lambda}_1 \geqq \cdots \geqq \bar{\lambda}_n = 0$ are the eigenvalues of $L(\bar{G})$ and (as usual) $\lambda_1 \geqq \cdots \geqq \lambda_n = 0$ are the eigenvalues of $L(G)$. We next observe that

$$\lambda_1 \leqq \max_{\{v_i, v_j\} \in E} (d_i + d_j).$$

This follows immediately from the Geršgorin Circle Theorem applied to the edge version $K(G)$. (The circles are all centered at two and their radii are $d_i + d_j - 2$, $\{v_i, v_j\} \in E$.)

Now, the matrix $L_R(G)$ is a direct sum, over the components C of R, of matrices $M(C) = L(C) - I + F(C)$, where $F(C)$ is a diagonal matrix with nonnegative integer entries, and I is an appropriately sized identity matrix. Let $\mu_1 \geqq \cdots \geqq \mu_t = 0$ be the eigenvalues of $L(C)$, and $\bar{\mu}_1 \geqq \cdots \geqq \bar{\mu}_t = 0$ the Laplacian eigenvalues of its complement. Denote by δ_i the degree, in C, of the ith vertex of C. Then, because C is rich,

$$\begin{aligned} \bar{\delta}_i + \bar{\delta}_j &= 2(t-1) - (\delta_i + \delta_j) \\ &\leqq t-2, \end{aligned}$$

for each pair (i, j) corresponding to an edge of $\bar{C}$. Consequently, by what we have just seen, $\bar{\mu}_1 \leqq t - 2$ so $\mu_{t-1} \geqq 2$. We deduce that one eigenvalue of $L(C) - I$ is -1 and the rest are not less than $+1$. Since $M(C) \geqq L(G) - I$, in the positive semidefinite sense, the contribution of $M(C)$ to the rank of $L_R(G)$ is at least $t - 1$. □

It should be remarked that Theorems 3.6 and 3.8 are most effective after paths of length three have been pruned off (see, e.g., Example 3.4). Moreover, it is possible to mix the techniques among the components of R.

In the subsequent discussion, it will be useful to describe eigenvectors of $L(G)$ by labeling the vertices of G with the corresponding components of the eigenvectors. If, e.g., G is the tree in Example 3.5, then $p(G) - q(G) = 0$ and $s(G) = 1$. An eigenvector affording $\lambda = 1$ is exhibited in Fig. 7. It is clear that this vector is something new. It differs from the Faria vectors, e.g., in being constant on the orbits of the automorphism group $\Gamma(G)$. Evidently, $(1, 2, 1)$ is a null vector of $L_R(G)$.

We define the *symmetric part* of the spectrum of $L(G)$ to be those eigenvalues, including appropriate multiplicities, that can be accounted for by eigenvectors that are constant on the orbits of $\Gamma(G)$. If, for example, $\Gamma(G)$ is trivial, then every eigenvalue is "symmetric." If, on the other hand, $\Gamma(G)$ acts transitively on the vertices, then $\lambda = 0$ is the only symmetric eigenvalue. In general, the number of symmetric eigenvalues of $L(G)$, multiplicities included, is equal to the number of orbits of $\Gamma(G)$.

We will say an eigenvalue is "alternating" or that it belongs to the *alternating part* of the spectrum if it is afforded by an eigenvector that (such as each of the Faria vectors) is orthogonal to the characteristic functions of the orbits. If T is the tree in Example 2.7, then $\lambda = 2$ is in the symmetric part and $\lambda = 1$ is in the alternating part. (Every eigenvector afforded by $\lambda = 1$ is in the Faria space.)

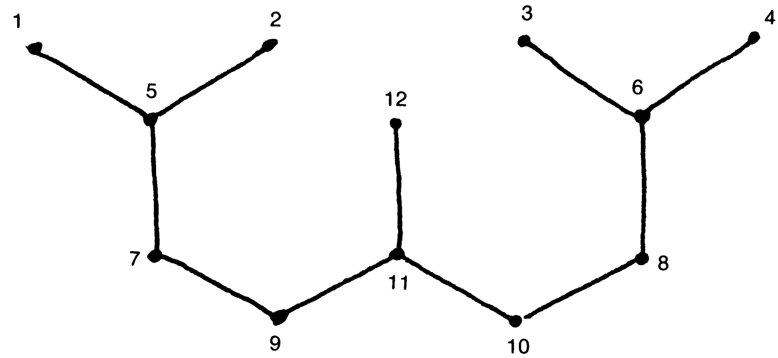

FIG. 9

Example 3.9. Let T be the tree in Fig. 9 with the vertices numbered as shown. Then, using (5), we may easily confirm that

$$u^{(1)}=(1,1,1,1,0,0,-2,-2,-2,-2,0,4),$$
$$u^{(2)}=(1,1,-1,-1,0,0,-2,2,-2,2,0,0),$$
$$u^{(3)}=(1,-1,0,0,0,0,0,0,0,0,0,0),$$

and

$$u^{(4)}=(0,0,1,-1,0,0,0,0,0,0,0,0),$$

are orthogonal eigenvectors corresponding to $\lambda = 1$. On the other hand (in the notation of Theorems 3.6 and 3.8), R consists of the subgraph induced on $\{v_i : 7 \leqq i \leqq 10\}$, both components of which are rich. (Alternatively, $\alpha(R) = 2$.) Thus,

$$\begin{aligned} m_T(1) &= P(T)-q(T)+s(T) \\ &= 4-2+s(T) \\ &\leqq 2+2=4. \end{aligned}$$

Observe that $u^{(1)}$ is symmetric, $u^{(3)}$ and $u^{(4)}$ are Faria vectors, whereas $u^{(2)}$ is a yet to be explained eigenvector that is alternating but not in the Faria space. (Note that both $u^{(1)}$ and $u^{(2)}$ arise from the null space of the matrix $L_R(G)$.)

It is a straightforward procedure to determine the symmetric part of the spectrum [10]. Any symmetric eigenvector must be in the space spanned by the characteristic functions of the orbits. The graph T in Fig. 9, for example, has six orbits. Hence, $c_T(x) = f(x)g(x)$, where $f(x)$ has degree six (accounting for the symmetric part of the spectrum) and $g(x)$ has degree $12 - 6 = 6$, accounting for the alternating part. Note that $f(x) = xf_1(x)$ since the eigenvector corresponding to $\lambda = 0$ is constant on *all* vertices. To obtain $f(x)$, we perform a similarity transformation of the following type. Suppose the m orbits of $\Gamma(G)$ have sizes $k_1, k_2, \cdots, k_m$ and characteristic functions $w_1, \cdots, w_m$. Then the vectors $u_j = k_j^{-1/2} w_j$, $1 \leqq j \leqq m$, are orthonormal. Let U be any orthogonal matrix having u_j in column j, $1 \leqq j \leqq m$. Then $U^t L(G) U$ is the direct sum of an m-by-m matrix A (affording the symmetric part of the spectrum) and an $(n-m)$-by-$(n-m)$ matrix B. We note that A can easily be obtained as follows. Order the vertices of G by orbits and partition $L(G)$ into m^2 blocks of sizes k_i-by-k_j. Then the (i,j)-element of A is obtained by summing the elements in the (i,j)-block of $L(G)$ and dividing by $(k_i k_j)^{1/2}$.

Example 3.10. Let T be the tree in Fig. 9. Then

$$L(T)=\left[\begin{array}{cccc|cc|cc|cc|c|c}
1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0\\ \hline
-1 & -1 & 0 & 0 & 3 & 0 & -1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & -1 & -1 & 0 & 3 & 0 & -1 & 0 & 0 & 0 & 0\\ \hline
0 & 0 & 0 & 0 & -1 & 0 & 2 & 0 & -1 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 2 & 0 & -1 & 0 & 0\\ \hline
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 2 & 0 & -1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 2 & -1 & 0\\ \hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1\\ \hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1
\end{array}\right].$$

Hence,

$$A=\begin{pmatrix}
1 & -\sqrt{2} & 0 & 0 & 0 & 0\\
-\sqrt{2} & 3 & -1 & 0 & 0 & 0\\
0 & -1 & 2 & -1 & 0 & 0\\
0 & 0 & -1 & 2 & -\sqrt{2} & 0\\
0 & 0 & 0 & -\sqrt{2} & 3 & -1\\
0 & 0 & 0 & 0 & -1 & 1
\end{pmatrix},$$

and $f(x) = \det(xI - A) = x(x-1)(x-4)(x^3 - 7x^2 + 12x - 3)$. It turns out that $g(x) = c_T(x)/f(x) = (x-1)^3(x^3 - 7x^2 + 12x - 1)$.

Returning to (6), we observe (since $r(G) \geqq s(G)$) that $n - m_G(1) \geqq 2q(G)$. We claim, in fact, that $m_G[0, 1) \geqq q(G)$ and $m_G(1, \infty) \geqq q(G)$, where $m_G(I)$ denotes the number of eigenvalues of $L(G)$, multiplicities included, belonging to the interval I.

THEOREM 3.11. *Let G be a graph. Then $m_G[0, 1) \geqq q(G)$ and $m_G(1, \infty) \geqq q(G)$.*

It follows from (2) and Theorem 3.11 that $m_G[0, 1] \geqq p(G) \leqq m_G[1, \infty)$. (This fact may also be proved by observing that I_p, $p = p(G)$, is a principal submatrix of $L(G)$, and using the Cauchy interlacing inequalities.) A result similar to Theorem 3.11 for $m_G(0, 2)$ and $m_G(2, \infty)$, when G is a tree, can be found in Corollary 4.3 below.

Before attempting a proof of Theorem 3.11 we require some background concerning the relationship of the sequence of leading principal subdeterminants of a symmetric matrix to the number of positive and negative eigenvalues of the matrix. Suppose that A is n-by-n, symmetric and nonsingular. Let $\alpha_0 = 1$ and let $\alpha_k = \det(A_k)$ where A_k is the leading principal k-by-k submatrix of A. It is well known (or easily proven by induction on n) that the number of negative eigenvalues of A is equal to the number of sign changes in the sequence $(\alpha_0, \alpha_1, \cdots, \alpha_n)$. We note that this sequence may contain intermediate zeros, in which case we can shorten the sequence by deleting the zeros and the theorem will still hold. As an immediate consequence we have the following lemma.

LEMMA 3.12. *Suppose that $A = A^t$ is $2q$-by-$2q$ and that* $\det(A_{2k}) = (-1)^k$, $k = 1, \cdots, q$. *Then A has q positive and q negative eigenvalues.*

Another well-known fact we require relates the spectrum of a principal submatrix of symmetric A to the spectrum of A.

LEMMA 3.13. *Suppose that B is a principal submatrix of the symmetric matrix A and that α is real. Then the number of eigenvalues of B that are greater than (respectively, greater than or equal to, less than, less than or equal to) α is a lower bound for the* *number of eigenvalues of A that are greater than (respectively, greater than or equal to, less than, less than or equal to)* α.

Proof of Theorem 3.11. We may assume without loss of generality that the quasipendant vertices of G are numbered $1, 3, \cdots, 2q-1$, and that vertex $2k$ is a pendant vertex adjacent to vertex $2k-1$, for each $k = 1, \cdots, q$. Let B be the leading principal $2q$-by-$2q$ submatrix of $L(G)$. In view of Lemma 3.12, it will suffice to show that B has q eigenvalues greater than one and q eigenvalues less than one. To do this it will suffice to show that $A = B - I_{2q}$ satisfies the hypotheses of Lemma 3.12. Note that A has the form

$$\begin{pmatrix} (d_1-1) & -1 & * & 0 & \cdots & * & 0 \\ -1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ * & 0 & (d_3-1) & -1 & \cdots & * & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 \\ & \cdots & & & & & \\ * & 0 & * & 0 & \cdots & (d_{2q}-1) & -1 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 0 \end{pmatrix}$$

and that the even numbered rows (corresponding to pendants) of A have a single nonzero entry. We assume an inductive hypothesis on q, and hence it will suffice to prove that $\det(A) = (-1)^q$. If we use elementary row and column operations corresponding to adding multiples of even numbered rows and columns to other rows and columns, then A can be transformed into a direct sum of m copies of $-P$, where P is the 2-by-2 permutation matrix corresponding to a transposition. Hence $\det(A) = [\det(-P)]^q = (-1)^q$ and the proof is finished. □

In Theorem 3.1, we modified the connected sum idea from Theorem 2.5 and showed that $m_G(1) = m_H(1)$ when $H = G \vee P_3$, some graph obtained from G and P_3 by joining any vertex of G to a *pendant* vertex of P_3. Denote by $G \multimap P_3$ some graph obtained from G and P_3 by joining any vertex of G to the middle (quasipendant) vertex of P_3.

PROPOSITION 3.14. *Let G be a graph on n vertices and suppose* $H = G \multimap P_3$. *Then* $m_G(1) \leqq m_H(1) \leqq m_G(1) + 2$, *and each of the three possibilities for* $m_H(1)$ *can occur.*

Proof. Write $m_G(1) = m$. Assume the numbering of vertices to be such that the last vertex of G and the first vertex of P_3 have been joined to form H. Let M be an $(m-1)$-dimensional subspace of $\ker(L(G) - I_n)$ such that $v_n = 0$ for all $v \in M$. Then $\{v \oplus (0, a, -a) : v \in M, a \in R\}$ is an m-dimensional subspace of $\ker(L(H) - I_{n+3})$. Hence, $m \leqq m_H(1)$.

As in the proofs of Theorems 2.5 and 3.1, let $L = L(G)$, $L' = L(P_3)$, and $\tilde{L} = L(H)$. Then $\tilde{L} = (L \dotplus L') + A$, where A is the rank one matrix whose only nonzero entries amount to

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

in rows and columns n and $n+1$. Then

$$\begin{aligned} \operatorname{rank}(\tilde{L} - I_{n+3}) &= \operatorname{rank}([(L - I_n) \dotplus (L' - I_3)] + A) \\ &\geqq \operatorname{rank}[(L - I_n) \dotplus (L' - I_3)] - 1 \\ &= \operatorname{rank}(L - I_n) + 1, \end{aligned}$$

so

$$m_H(1) = \text{nullity}\,(\tilde{L} - I_{n+3}) \leqq n + 2 - \text{rank}\,(L - I_n) = m + 2.$$

The last assertion is demonstrated by the following examples: (1) Let $G = P_3$. Form $G \multimap P_3$ by joining a pendant vertex of G to the "middle" vertex of P_3. Then $P_3 = G$ can be pruned off as in Example 3.2 and $m_H(1) = m_G(1)$. (2) Let $G = P_2$. Then $m_G(1) = 0$ while the characteristic polynomial of $G \multimap P_3$ (pictured in Fig. 1) is $x(x-1)(x^3 - 7x^2 + 13x - 5)$. (3) Let G be the tree in Fig. 10. Form $G \multimap P_3$ by joining the open vertex to the middle of P_3. Then $G \multimap P_3$ is the tree in Fig. 9 (Example 3.9). In this case, $m_G(1) = 2$ and $m_H(1) = 4$.

We now return to the "spurious multiplicity" $s(G)$ in (6). We know that the multiplicity of $\lambda = 1$ in the symmetric part of the spectrum of $L(G)$ accounts for part but not (in general) all of $s(G)$. (See Example 3.9). In Theorems 3.6 and 3.8 we found upper bounds for $s(G)$. We conclude this section with a discussion of possible lower bounds when G is a tree. We begin by defining an equivalence relation on the set Q of quasipendants of a tree T. If $v_1, v_2 \in Q$, we say $v_1 \equiv v_2$ if the distance $d(v_1, v_2)$ from v_1 to v_2 is an (integer) multiple of three, and if the degree d_t of vertex v_t is two whenever v_t is on the unique path from v_1 to v_2 and $d(v_1, v_t) \equiv 0 \pmod 3$.

PROPOSITION 3.15. *Let Q be the set of quasipendants of a tree T. Suppose $C_1, \cdots, C_t$ are the equivalence classes of Q and that their respective cardinalities are $q_1, \cdots, q_t$. Then $s(T) \geqq (\sum q_i) - t$.*

The somewhat laborious proof of this result involves finding a principal submatrix of $L_R(G)$ (see (7)) of sufficiently large nullity. This submatrix turns out to be a direct sum of $2I_2 - J_2$ with itself several times. We omit the computational details.

Example 3.16. Let T be the tree in Fig. 9. Then Q consists of the vertices numbered 5, 6, and 11. In this case, Q consists of a single equivalence class of size $q_1 = q(G) = 3$, and Proposition 3.15 asserts that $s(T) \geqq 2$. Since $p(T) - q(T) = 5 - 3 = 2$, and $m_T(1) = 4$ (Example 3.9), we know that $s(T) = 2$. In other words, Proposition 3.15 is strong enough to capture the existence (but not the nature) of eigenvectors $u^{(1)}$ and $u^{(2)}$ in Example 3.9.

Example 3.17. The tree T in Fig. 11 is exhibited with an eigenvector affording $\lambda = 1$. Indeed, for this tree, $m_T(1) = 1 = s(T)$, $p(T) = q(T)$, the lower bound given by Proposition 3.15 is zero (no two quasipendants are equivalent), the upper bound given in (9) is two, and Theorem 3.8 does not apply. It is an abundance of such examples

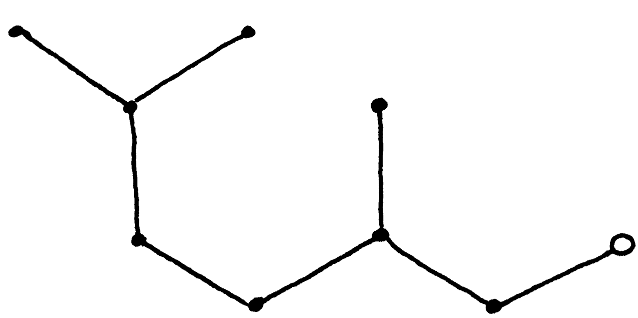

FIG. 10

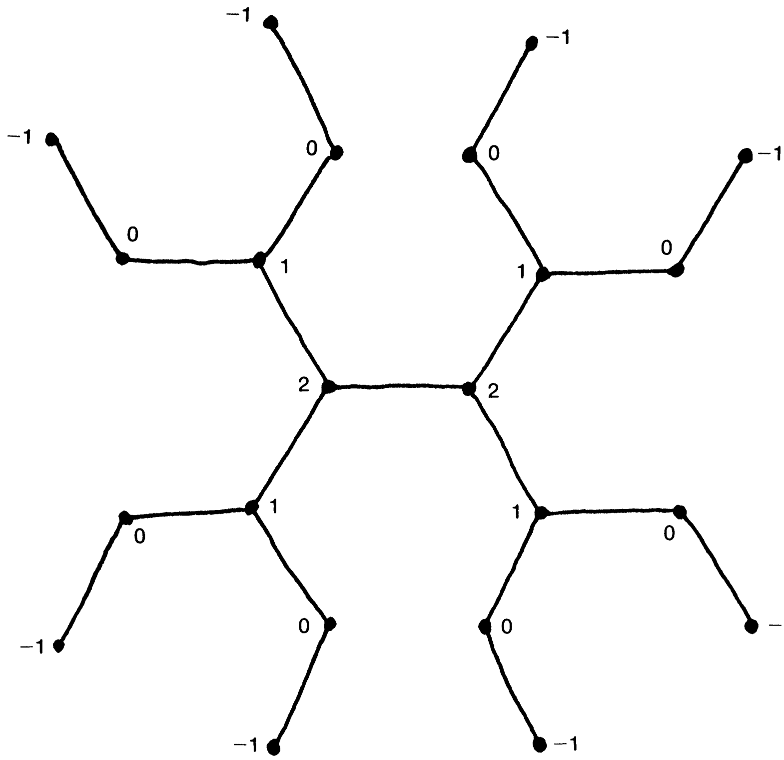

FIG. 11

that leads the authors to believe there can be no simple graph theoretic interpretation for $m_T(1)$.

4. Surgery on graphs. Techniques that allow one graph to be transformed into another with predictable effects on the eigenvalues have already proved useful. (See, e.g., Examples 2.6 and 3.2.) The main purpose of this section is to examine the influence of "moving an edge" in the geometric senses of (i) removing it without affecting its endpoints, (ii) removing it and identifying its endpoints, (iii) disconnecting one pair of vertices and joining some other pair. (Note that we have already addressed, to some small extent, the removal of a pendant edge and *both* of its endpoints. See Example 2.6.) Our first result is part of the "Laplacian Folklore."

THEOREM 4.1. *Let $\tilde{G}$ be a graph on n vertices. Suppose G is a (spanning) edge subgraph of $\tilde{G}$ obtained by removing just one of its edges. Then the $(n-1)$ largest eigenvalues of $L(G)$ interlace the eigenvalues of $L(\tilde{G})$.*

Proof. It suffices to prove that the nonzero eigenvalues interlace and for this we may consider the edge version $K(G)$. The result follows from the Cauchy interlacing inequalities because $K(G)$ is a principal submatrix of $K(\tilde{G})$. □

Note that if a pendant edge of $\tilde{G}$ is removed in Theorem 4.1, then $L(G)$ is a direct sum of $L(G')$ and (0), where G' is obtained from $\tilde{G}$ by removing both the pendant edge and vertex. Thus, the nonzero eigenvalues of $L(G)$ and $L(G')$ are the same. We have proved the following corollary.

COROLLARY 4.2. *Suppose v is a pendant vertex of the graph $\tilde{G}$. Let G be the graph obtained from $\tilde{G}$ by removing v (and its edge). Then the eigenvalues of $L(G)$ interlace the eigenvalues of $L(\tilde{G})$.*

We can use Corollary 4.2 to obtain a result similar to Theorem 3.11. Reviving the notation there, recall that $m_G(I)$ denotes the number of eigenvalues of $L(G)$, multiplicities included, belonging to the interval I.

COROLLARY 4.3. *If T is a tree with diameter d, then*

$$m_T(0,2) \geqq [d/2] \leqq m_T(2,\infty),$$

where square brackets indicate the greatest integer function.

Proof. First consider the case that $T = P_{d+1}$. We can easily show that $K(T) = 2I_d + A(T^*)$, where $T^* = P_d$ is the line graph of T. Since the spectrum of $A(T^*)$ is symmetric about the origin, the spectrum of $K(T)$ is symmetric about two, i.e., the nonzero spectrum of $L(T)$ is symmetric about two. (Together with Theorem 2.1(ii), this gives another proof of Corollary 2.8(i).) Since $m_T(2) \leqq 1$, the result is established in this case. Now, any tree T with diameter d contains P_{d+1} as a subtree. Thus, T can be reduced to P_{d+1} by a sequential removal of pendant vertices. The result follows from the interlacing established in Corollary 4.2. (See Lemma 3.13.) □

This seems an appropriate place to recall a striking result of Fiedler [8, p. 612]: Suppose two is an eigenvalue of $L(T)$ for some tree $T = (V, E)$. Let u be an eigenvector of $L(T)$ corresponding to two. Then the number of eigenvalues of $L(T)$ greater than two is equal to the number of edges $\{v_i, v_j\} \in E$ such that $u_i u_j > 0$, whereas the number of eigenvalues of $L(T)$ less than two is equal to the number of edges such that $u_i u_j < 0$. (Note that Theorem 2.1(iii) guarantees $u_i \neq 0$ for all i.) If, for example, T is the tree in Fig. 4 (with u exhibited), the six pendant edges are all of the type $u_i u_j < 0$, while the remaining three edges all yield $u_i u_j > 0$. Thus, exactly six eigenvalues of $L(T)$ are less than two, whereas exactly three are greater than two. In this case, $d = 4$ and $[d/2] = 2$.

In another pioneering paper [7], Fiedler introduced the algebraic connectivity $a(G) = \lambda_{n-1}$ of G. He proved that the algebraic connectivity of a path,

$$a(P_n) = 2(1 - \cos(\pi/n)),$$

is a lower bound for $a(G)$ for any connected graph G on n vertices. As another application of Corollary 4.2, we recover a related upper bound stated in the context of $A(G^*)$ by Doob [4, p. 187].

COROLLARY 4.4. *Let T be a tree on n vertices with diameter d. Then*

$$a(T) \leqq 2(1 - \cos(\pi/(d+1))).$$

Proof. Observe that T can be built up from P_{d+1} by attaching pendant vertices. It is seen from Corollary 4.2 that this building process does not increase the algebraic connectivity. □

COROLLARY 4.5. *Let T be a tree on $n \geqq 6$ vertices. If $T \neq *_n$, then $a(T) < 0.49$.*

Proof. As in the proof of Corollary 4.4, we may build T on the foundation of P_4. After attaching two pendant vertices, we arrive at a (possibly intermediate) stage of a tree T_2 with six vertices. Moreover, $T_2 \neq *_6$. There are only five possibilities for T_2. The one with maximum algebraic connectivity is the "near star" in Fig. 12(b) with algebraic connectivity $= 0.485\cdots$. Repeated applications of Corollary 4.2, as more pendant vertices are attached, proves that $a(T) \leqq a(T_2)$. □

Our next result is reminiscent of popular newspaper accounts of the recombinant techniques of molecular genetics.

THEOREM 4.6. *Let $G_1 = (V, E_1)$ be a graph and $G_2 = (V, E_2)$ a graph obtained from G_1 by removing an edge and adding a new edge that was not there before. Suppose $\alpha_1 \geqq \cdots \geqq \alpha_n$ are the eigenvalues of $L(G_1)$ and $\beta_1 \geqq \cdots \geqq \beta_n$ are the eigenvalues of $L(G_2)$. Then $\alpha_i \geqq \beta_{i+1}$ and $\beta_i \geqq \alpha_{i+1}$, $1 \leqq i < n$.*

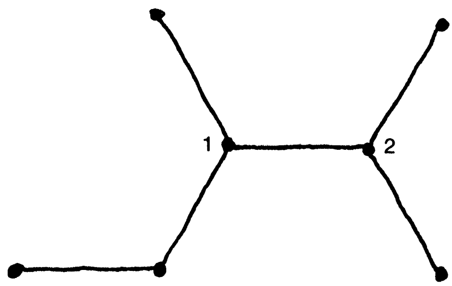

FIG. 12(a)

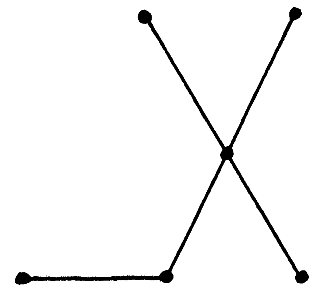

FIG. 12(b)

Proof. From the perspective of the edge version, $K(G_1)$ and $K(G_2)$ share an $(m-1)$-by-$(m-1)$ principal submatrix, where $m = o(E_1) = o(E_2)$ is the common cardinality of the two edge sets. Once again, the result is immediate from Cauchy interlacing. □

We now come to a less trivial situation in which the vertices at the ends of an edge are identified, in the process of which the edge is "collapsed" (or "contracted") and disappears (without producing a loop). In fact, Corollary 4.2 can be redrafted as a special case of this procedure, the case in which a pendant edge is collapsed. Our next result is a consequence of the Monotonicity Theorem [12].

LEMMA 4.7. *Let A, B, and C be n-by-n Hermitian matrices satisfying $A = B + C$. Denote the eigenvalues of A and B by $\alpha_1 \geqq \cdots \geqq \alpha_n$ and $\beta_1 \geqq \cdots \geqq \beta_n$, respectively. If C has exactly t positive eigenvalues, then $\beta_k \geqq \alpha_{k+t}$, $1 \leqq k \leqq n-t$.*

COROLLARY 4.8. *Let A, B, and C be n-by-n Hermitian matrices satisfying $A = B + C$. Denote the eigenvalues of A and B by $\alpha_1 \geqq \cdots \geqq \alpha_n$ and $\beta_1 \geqq \cdots \geqq \beta_n$, respectively. If C has exactly one positive eigenvalue and exactly one negative eigenvalue (so that rank $C = 2$), then $\alpha_k \geqq \beta_{k+1}$ and $\beta_k \geqq \alpha_{k+1}$, $1 \leqq k < n$.*

THEOREM 4.9. *Let $\tilde{G} = (\tilde{V}, \tilde{E})$ be a graph with $\tilde{e} = \{\tilde{v}_1, \tilde{v}_2\} \in \tilde{E}$. Suppose $\tilde{e}$ does not lie on a circuit of length three. Let $G = (V, E)$ be the graph obtained from $\tilde{G}$ by deleting (i.e., "collapsing") $\tilde{e}$ and identifying vertices $\tilde{v}_1$ and $\tilde{v}_2$. If $\tilde{\lambda}_1 \geqq \cdots \geqq \tilde{\lambda}_{n+1} = 0$ are the eigenvalues of $\tilde{L} = L(\tilde{G})$ and $\lambda_1 \geqq \cdots \geqq \lambda_n = 0$ are the eigenvalues of $L = L(G)$, then*

(i) $\lambda_i \geqq \tilde{\lambda}_{i+1}$, $1 \leqq i \leqq n$, *and*

(ii) $\tilde{\lambda}_i \geqq \lambda_{i+1}$, $1 \leqq i < n$.

Example 4.10. Let $\tilde{G}$ be the graph in Fig. 12(a) with spectrum (approximately)

$$4.63 > 3.23 > 2.14 > 1.00 > 0.68 > 0.32 > 0.00.$$

If the 1-2 edge is collapsed, the result is the graph G in Figure 12(b) with spectrum

$$5.09 > 2.43 > 1.00 = 1.00 > 0.49 > 0.00.$$

Proof of Theorem 4.9. Let $L_0 = (0) \dotplus L$. Then $\tilde{L} = L_0 + A$, where $A = (A_{ij})$ is a 3-by-3 block partitioned matrix:

$$A_{11} = \begin{pmatrix} k+1 & -1 \\ -1 & 1-k \end{pmatrix},$$

where $k+1$ is the degree (in $\tilde{G}$) of $\tilde{v}_1$; A_{12} is the 2-by-k matrix whose first row consists entirely of -1's and whose second row is all $+1$'s; $A_{21} = A_{12}^t$, and the other blocks are appropriately sized zero matrices. (In particular, A_{22} and A_{33} are square blocks, whereas

A_{23} is k-by-$(n-k-1)$.) Suppose first that $k > 0$. Then it suffices to prove that the inertia of A is $(1, 1, n-1)$, and invoke Corollary 4.8. Let X be the $(n+1)$-square matrix

$$X = \begin{pmatrix} -k-1 & 0 & 1 & 1 & 1 & \cdots & 1 \\ 1 & -k & 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & k & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & k & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & k & \cdots & 0 \\ & & \cdot & \cdot & \cdot & & \\ 1 & 1 & 0 & 0 & 0 & \cdots & k \end{pmatrix}.$$

Then we may confirm that each column of X is an eigenvector for A. More particularly, X^1, the first column, corresponds to the eigenvalue $\lambda = k+2$; X^2 corresponds to $\lambda = -k$; and $X^3, \cdots, X^{n+1}$ all correspond to $\lambda = 0$.

The degenerate case $k = 0$ has already been established in Corollary 4.2. In fact, we can recover that stronger result here too since, in this case, $A \geqq 0$ (in the positive semi-definite sense) and rank $A = 1$. In this case, (i) is proved by appealing to Lemma 4.7, and $\tilde{\lambda}_i \geqq \lambda_i$, $1 \leqq i \leqq n$, because $\tilde{L} \geqq L_0$. □

It is clear from Example 4.10 that the strong inequalities $\tilde{\lambda}_i \geqq \lambda_i$, $1 \leqq i \leqq n$, may not hold for a general edge collapse, even for trees. Indeed, as the next result shows, Example 4.10 is not an isolated example.

THEOREM 4.11. *Let $\tilde{T}$ be a tree. Suppose $\tilde{e}$ is an edge of $\tilde{T}$ each of whose endpoints has degree at least three. If T is obtained from $\tilde{T}$ by collapsing $\tilde{e}$, then $\lambda_1 > \tilde{\lambda}_1$.*

Proof. It is somewhat more convenient to deal with the matrix $B(T) = D(T) + A(T)$ that, in view of Proposition 2.2 affords the same spectrum as $L(T)$. Let $\tilde{u}$ be the positive Perron eigenvector of $B(\tilde{T})$, normalized so that $\|\tilde{u}\| = 1$. The theorem will be proved by producing a unit vector u of size n such that $(B(T)u, u) > \tilde{\lambda}_1$.

Assume $\tilde{e} = \{\tilde{v}_n, \tilde{v}_{n+1}\}$ and write $a = \tilde{u}_n$ and $b = \tilde{u}_{n+1}$. Then $\tilde{e}$ and its immediate neighbors are pictured in Fig. 13, where the labels represent corresponding coordinates of $\tilde{u}$. Define $u \in \mathbb{R}^n$ by $u_i = \tilde{u}_i$, $1 \leqq i < n$ and $u_n = \alpha$, where $\alpha = (a^2+b^2)^{1/2}$. Note that u is a unit vector. Observe also that

$$(B(T)u, u) = \sum (u_i + u_j)^2,$$

where the sum extends over those pairs (i, j) such that $\{v_i, v_j\}$ is an edge of T. Note that many of the terms in $\tilde{\lambda}_1 = (B(\tilde{T})\tilde{u}, \tilde{u})$ and $(B(T)u, u)$ are the same. Denote the sum of these common terms by c. Then

$$\begin{aligned} \tilde{\lambda}_1 &= (B(\tilde{T})\tilde{u}, \tilde{u}) \\ &= c + \sum_{i=1}^{j} (p_i + a)^2 + (a+b)^2 + \sum_{i=1}^{k} (b + x_i)^2 \end{aligned}$$

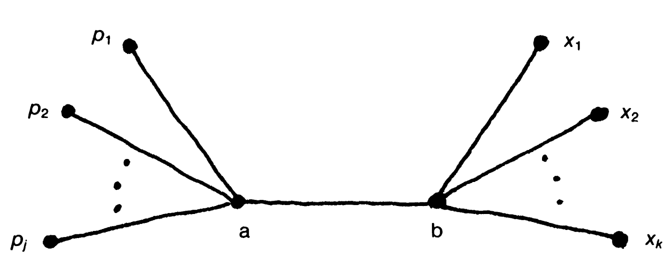

FIG. 13

while

$$(B(T)u,u)=c+\sum_{i=1}^{j}(p_i+\alpha)^2+\sum_{i=1}^{k}(\alpha+x_i)^2.$$

To show $(B(T)u, u) > \tilde{\lambda}_1$, we take their difference

$$2\sum_{i=1}^{j}p_i(\alpha-a)+2\sum_{i=1}^{k}x_i(\alpha-b)+(a-b)^2+(k-2)a^2+(j-2)b^2$$

and observe that $j+1=\tilde{d}_n$, the degree of $\tilde{v}_n$, while $k+1=\tilde{d}_{n+1}\geqq 3$. Hence, every term is nonnegative, and the first $j+k$ terms are all positive. □

It should be noted that the same reasoning will prove a slightly more general assertion: Let $\tilde{T}$ be a tree. Suppose $\tilde{v}_1$ and $\tilde{v}_2$ are vertices each of degree at least three. Suppose the unique path from $\tilde{v}_1$ to $\tilde{v}_2$ is homeomorphic to an edge (i.e., apart from the endpoints, each vertex on the path has degree two). Let T be the tree obtained by collapsing the entire path. Then $\lambda_1 > \tilde{\lambda}_1$. (Of course, if $\tilde{v}_1$ were a pendant vertex, we could have deduced $\lambda_1 \leqq \tilde{\lambda}_1$.)

Conjecture 4.12. Let $\tilde{T}$ be a tree with (Laplacian) spectrum $\tilde{\lambda}_1 \geqq \cdots \geqq \tilde{\lambda}_n > \tilde{\lambda}_{n+1}=0$. Let T be a tree obtained from $\tilde{T}$ by collapsing an edge. Then $\tilde{\lambda}_{n-1}\geqq\lambda_{n-1}=a(T)$, the algebraic connectivity of T.

Example 4.13. Let $\tilde{G}=C_4$ with spectrum $(4, 2, 2, 0)$. If an edge of $\tilde{G}$ is collapsed, the result is $G=C_3$ with spectrum $(3, 3, 0)$. In this case, $n=3$ and $\tilde{\lambda}_2=2<\lambda_2=3$. Thus, Conjecture 4.12 fails, even for a bipartite $\tilde{G}$ with a circuit.

For general edge collapsing in trees, empirical evidence suggests that departure from interlacing occurs "near the top." We conclude by showing that $\lambda_1 \in [\tilde{\lambda}_2, 2\tilde{\lambda}_1]$.

PROPOSITION 4.14. *Let T be the tree obtained from $\tilde{T}$ by collapsing an edge $\tilde{e}=\{\tilde{v}_1, \tilde{v}_2\}$. Let $\tilde{d}$ be the minimum of the degrees $\tilde{d}_1$ and $\tilde{d}_2$. Then $|\lambda_1-\tilde{\lambda}_1|\leqq\tilde{d}+1\leqq\tilde{\lambda}_1$. Consequently, $\lambda_1\leqq 2\tilde{\lambda}_1$.*

Proof. We revive the notation used in the proof of Theorem 4.9, with $\tilde{d}=k+1$. Then

$$\begin{aligned}|\tilde{\lambda}_1-\lambda_1| &= |\,\|\tilde{L}\|-\|L_0\|\,| \\ &\leqq \|\tilde{L}-L_0\| \\ &= \|A\| = k+2.\end{aligned}$$

Now, $\tilde{\lambda}_1$ is bounded below by the largest main diagonal entry of $L(\tilde{T})$. This is at least $\tilde{d}+1$ unless $\tilde{d}$ is the largest degree of any vertex of $\tilde{T}$. If it is, then $\tilde{d}_1=\tilde{d}_2=k+1$, and

$$B=\begin{pmatrix}k+1 & -1\\ -1 & k+1\end{pmatrix}$$

is a principal submatrix of $L(\tilde{T})$. But, the eigenvalues of B are k and $k+2$. Thus, by Cauchy interlacing, $\tilde{\lambda}_1\geqq k+2=\tilde{d}+1$. □

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