1

A background in graph spectra

In Section 1.1 we introduce notation and terminology which will be used throughout the book. The limitations of the spectrum as a graph invariant are illustrated by the discussion of non-isomorphic cospectral graphs in Section 1.2. In Section 1.3 we describe the extent to which certain classes of graphs are characterized by spectral properties, and in Section 1.4 we discuss ways of extending the spectrum to a set of invariants which together are sufficient to characterize a graph.

1.1 Basic notions and results

A comprehensive treatment of the theory of graph spectra is given in the monograph [CvDS], while some of the underlying results from matrix theory are given in Appendix A. Here we present only those basic notions and further results which are needed frequently in other chapters. We recommend as general references the texts by Biggs [Big] and Harary [Har2].

The *adjacency matrix* of a (multi)(di)graph G, with vertex set $\{1, 2, \dots, n\}$, is the $n \times n$ matrix $A = (a_{ij})$ whose (i, j)-entry a_{ij} is equal to the number of edges, or arcs, originating at the vertex i and terminating at the vertex j. Two vertices of G are said to be *adjacent* if they are connected by an edge or arc. Unless we indicate otherwise we shall assume that G is an undirected graph without loops or multiple edges.

As an example, the adjacency matrix of a 4-cycle is illustrated in Fig. 1.1.

The characteristic polynomial $\det(xI - A)$ of the adjacency matrix A of G is called the *characteristic polynomial of* G and denoted by $P_G(x)$. The eigenvalues of A (i.e. the zeros of $\det(xI - A)$) and the spectrum of A (which consists of the n eigenvalues) are also called the *eigenvalues* and

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

G:

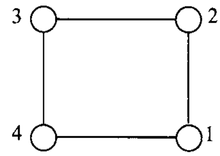

Fig. 1.1. A labelled graph G and its adjacency matrix A.

the *spectrum* of G, respectively. These notions are independent of vertex labelling because a reordering of vertices results in a similar adjacency matrix. The eigenvalues of G are usually denoted by $\lambda_1, \ldots, \lambda_n$; they are real because A is symmetric. Unless we indicate otherwise, we shall assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and use the notation $\lambda_i = \lambda_i(G)$ for $i = 1, 2, \ldots, n$. Clearly, isomorphic graphs have the same spectrum.

The eigenvalues of A are the numbers λ satisfying $A\mathbf{x} = \lambda\mathbf{x}$ for some non-zero vector $\mathbf{x} \in \mathbb{R}^n$. Each such vector $\mathbf{x}$ is called an *eigenvector* of the matrix A (or of the labelled graph G) belonging to the eigenvalue λ. The relation $A\mathbf{x} = \lambda\mathbf{x}$ can be interpreted in the following way: if $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ then $\lambda x_u = \sum_{v \sim u} x_v$ where the summation is over all neighbours v of the vertex u. If λ is an eigenvalue of A then the set $\{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \lambda\mathbf{x}\}$ is a subspace of $\mathbb{R}^n$, called the *eigenspace* of λ and denoted by $\mathscr{E}(\lambda)$ or $\mathscr{E}_A(\lambda)$. Such eigenspaces are called eigenspaces of G. Of course, relabelling of the vertices in G will result in a permutation of coordinates in eigenvectors (and eigenspaces).

For the eigenvalues λ of the graph in Fig. 1.1 we have

$$P_G(\lambda) = \begin{vmatrix} \lambda & -1 & 0 & -1 \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ -1 & 0 & -1 & \lambda \end{vmatrix} = \lambda^4 - 4\lambda^2 = 0.$$

The eigenvalues in non-increasing order are $\lambda_1 = 2$, $\lambda_2 = 0$, $\lambda_3 = 0$, $\lambda_4 = -2$ with eigenvectors $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, $\mathbf{x}_4$ where $\mathbf{x}_1 = (1, 1, 1, 1)^T$, $\mathbf{x}_2 = (1, 1, -1, -1)^T$, $\mathbf{x}_3 = (-1, 1, 1, -1)^T$, $\mathbf{x}_4 = (1, -1, 1, -1)^T$. We have $\mathscr{E}(2) = \langle \mathbf{x}_1 \rangle$, $\mathscr{E}(0) = \langle \mathbf{x}_2, \mathbf{x}_3 \rangle$ and $\mathscr{E}(-2) = \langle \mathbf{x}_4 \rangle$, where $\langle \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k \rangle$ denotes the subspace spanned by the vectors $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k$.

The following remarks on matrices will serve to establish more notation.

Since A is a symmetric matrix with real entries there exists an orthogonal matrix U such that $U^T A U$ is a diagonal matrix, D say. Here $D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ (where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of A in some order), and the columns of U are corresponding eigenvectors which form an orthonormal basis of $\mathbb{R}^n$. If this basis is constructed by stringing together orthonormal bases of the eigenspaces of A then $D = \mu_1 E_1 + \cdots + \mu_m E_m$ where $\mu_1, \ldots, \mu_m$ are the distinct eigenvalues of A and each E_i has block diagonal form $\text{diag}(O, \ldots, O, I, O, \ldots O)$ $(i = 1, \ldots, m)$. Then A has the *spectral decomposition*

$$A = \mu_1 P_1 + \cdots + \mu_m P_m \tag{1.1.1}$$

where $P_i = UE_iU^T$ $(i = 1, \ldots, m)$. For fixed i, if $\mathscr{E}(\mu_i)$ has $\{\mathbf{x}_1, \ldots, \mathbf{x}_d\}$ as an orthonormal basis then

$$P_i = \mathbf{x}_1\mathbf{x}_1^T + \cdots + \mathbf{x}_d\mathbf{x}_d^T \tag{1.1.2}$$

and P_i represents the orthogonal projection of $\mathbb{R}^n$ onto $\mathscr{E}(\mu_i)$ with respect to the standard orthonormal basis of $\mathbb{R}^n$. Moreover $P_i^2 = P_i = P_i^T$ $(i = 1, \ldots, m)$ and $P_iP_j = O$ $(i \neq j)$. We shall assume throughout that $\mu_1 > \cdots > \mu_m$. We shall also need the observation that for any polynomial f, we have

$$f(A) = f(\mu_1)P_1 + \cdots + f(\mu_m)P_m.$$

In particular, P_i is a polynomial in A for each i; explicitly, $P_i = f_i(A)$ where

$$f_i(x) = \frac{\prod_{s \neq i}(x - \mu_s)}{\prod_{s \neq i}(\mu_i - \mu_s)}.$$

The largest eigenvalue $(\mu_1 = \lambda_1)$ of a graph G is called the *index* of G; since adjacency matrices are non-negative there is a corresponding eigenvector whose entries are all non-negative (see Theorem A.1 of Appendix A). The index is a simple eigenvalue if and only if G is connected, equivalently if and only if A is irreducible, and in this situation the corresponding eigenspace is spanned by a vector whose entries are all positive (see Theorem A.2 of Appendix A). The unique positive unit eigenvector corresponding to the index of a connected (labelled) graph G is called the *principal eigenvector* of G. We may extend this notion as follows to the case in which G is a graph with just one non-trivial component. Without loss of generality the adjacency matrix of G then has the form $\begin{pmatrix} A & O \\ O & O \end{pmatrix}$ where A is irreducible. Since $\mu_1 \neq 0$ we have

$$\begin{pmatrix} A & O \\ O & O \end{pmatrix}\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \mu_1 \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \text{ if and only if } A\mathbf{x} = \mu_1\mathbf{x} \text{ and } \mathbf{y} = \mathbf{0}.$$

Accordingly there is a unique non-negative unit eigenvector corresponding to μ_1, and its i-th entry is zero if and only if the i-th vertex is isolated. Now we call this eigenvector the principal eigenvector of the labelled graph G.

1.1.1 Definition *For any matrix $M = (\sigma_{i,j})_{m,n}$ we define a weighted bipartite (di)graph $K(M)$ with vertices $r_1, \ldots, r_m$ and $c_1, \ldots, c_n$ in the respective parts as follows: if $\sigma_{ij} \neq 0$, then the vertices r_i and c_j are joined by an edge (arc) whose weight is σ_{ij}. The (di)graph $K(M)$ is called the König (di)graph of the matrix M.*

Here, vertices $r_1, \ldots, r_m$ correspond to rows of M while vertices $c_1, \ldots, c_n$ correspond to the columns of M. The term 'König digraph' was introduced in [Cve11] in view of König's use of digraphs in investigating certain problems in matrix theory [Kön].

Next we present certain notation, definitions and results from graph theory.

As usual, K_n, C_n and P_n denote respectively the *complete graph*, the *cycle* and the *path* on n vertices. The *wheel* W_{n+1} is obtained from C_n by adding a vertex v and edges (*spokes*) joining v to each vertex of the n-cycle. Further, $K_{m,n}$ denotes the *complete bipartite* graph on $m+n$ vertices. More generally, $K_{n_1,n_2,\ldots,n_k}$ denotes the complete k-partite graph with parts of size $n_1, n_2, \ldots, n_k$. The *cocktail-party graph* $CP(n)$ is the unique regular graph with $2n$ vertices of degree $2n-2$; it is obtained from K_{2n} by deleting n mutually non-adjacent edges.

A connected graph with n vertices is said to be *unicyclic* if it has n edges, *bicyclic* if it has $n+1$ edges, and *tricyclic* if it has $n+2$ edges.

Any set of mutually non-adjacent edges in a graph G is called a *matching* of G. A matching of G is *perfect* if each vertex of G is the endvertex of an edge from the matching. The weight of a matching in a weighted graph is the sum of weights of edges contained in the matching.

The *complement* of a graph G is denoted by $\overline{G}$, while mG denotes the union of m disjoint copies of G. We write $V(G)$ for the vertex set of G, and $E(G)$ for the edge set of G.

If uv is an edge of G we write $G - uv$ for the graph obtained from G by deleting uv. For $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting the vertex v and all edges incident with v. More generally, for $U \subseteq V(G)$, $G - U$ is the subgraph of G induced by $V(G) \setminus U$.

The *join* $G \nabla H$ of (disjoint) graphs G and H is the graph obtained from G and H by joining each vertex of G with each vertex of H.

The *coalescence* $G \cdot H$ of (disjoint) rooted graphs G and H is the graph obtained from G and H by identifying the root of G with the root of H.

The *line graph* $L(H)$ of any graph H is defined as follows. The vertices of $L(H)$ are the edges of H and two vertices of $L(H)$ are adjacent whenever the corresponding edges of H have a vertex of H in common. Let N denote the vertex-edge $(0,1)$-incidence matrix of H. Then the $(0,1)$-adjacency matrices B of H and A of $L(H)$ satisfy

$$NN^T = D + B,\ N^TN = 2I + A, \tag{1.1.3}$$

where now D is the diagonal matrix whose diagonal entries are the vertex degrees of H.

A *generalized line graph* $L(H; a_1, \dots, a_n)$ is defined for graphs H with vertex set $\{1, \dots, n\}$ and non-negative integers $a_1, \dots, a_n$ by taking the graphs $L(H)$ and $CP(a_i)$ $(i = 1, \dots, n)$ and adding extra edges: a vertex e in $L(H)$ is joined to all vertices in $CP(a_i)$ if i is an endvertex of e as an edge of H. We include as special cases an ordinary line graph $(a_1 = a_2 = \cdots = a_n = 0)$ and the cocktail-party graph $CP(n)$ $(n = 1$ and $a_1 = n)$.

Given a subset U of vertices of the graph G, the graph G' obtained from G by *switching* with respect to U differs from G as follows: for $u \in U, v \notin U$ the vertices u, v are adjacent in G' if and only if they are non-adjacent in G. Note that switching with respect to U is the same as switching with respect to its complement. Switching is described easily in terms of the *Seidel matrix* S of G defined as follows: the (i,j)-entry of S is 0 if $i = j$, -1 if i is adjacent to j, and 1 otherwise. The Seidel matrix of G' is $D^{-1}SD$ where D is the (involutory) diagonal matrix whose i-th diagonal entry is 1 if $i \in U$, -1 if $i \notin U$. Now it is easy to see that switching with respect to U and then with respect to V is the same as switching with respect to $(U \setminus V) \cup (V \setminus U)$. It follows that switching determines an equivalence relation on graphs; moreover, switching-equivalent graphs have similar Seidel matrices and hence the same Seidel spectrum.

1.1.2 Example Let S_1, S_2, S_3 be sets of vertices of $L(K_8)$ which induce subgraphs isomorphic to $4K_1$, $C_5 \cup C_3$ and C_8, respectively. The graphs Ch_1, Ch_2, Ch_3 obtained from $L(K_8)$ by switching with respect to S_1, S_2, S_3 respectively are called the *Chang graphs*. The graphs $L(K_8), Ch_1, Ch_2, Ch_3$ are regular of degree 12, cospectral and mutually non-isomorphic (see, for example, [BrCN], p. 105, and also [Sei2]).

If we switch $L(K_8)$ with respect to the set of neighbours of a vertex v, we obtain a graph H in which v is an isolated vertex. If we delete v from H we obtain a graph which is called the *Schläfli* graph. □

The *Laplacian* (or *admittance*) matrix L of G is the $n \times n$ matrix $D - A$ where A is the adjacency matrix of G and D is the diagonal matrix whose (i, i)-entry is the degree d_i of the i-th vertex ($i = 1, 2, \ldots, n$). In this book we are concerned primarily with the adjacency matrix A, but we note here one property of L. For any fixed orientation of the edges of G we may define the corresponding edge-vertex incidence matrix C as the matrix whose (e, i)-entry is 1 if i is the endvertex of the edge e, -1 if i is the initial vertex of e, and 0 otherwise. Note that always $L = C^T C$, and so $\mathbf{x}^T L\mathbf{x} = \|C\mathbf{x}\|^2 \geq 0$ for all $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$. Moreover $C\mathbf{j} = \mathbf{0}$ and if G is connected then conversely $x_1 = x_2 = \cdots = x_n$ whenever $C\mathbf{x} = \mathbf{0}$. It follows that the multiplicity of 0 as an eigenvalue of L is equal to the number of components of G. In particular, the second smallest eigenvalue λ is zero if and only if G is not connected.

1.2 The graph isomorphism problem and cospectral graphs

Since the spectrum of a graph is a graph invariant it is natural to ask whether the spectrum determines a graph to within isomorphism. This attractive but, in a sense, naive conjecture has appealed to many who have encountered graph spectra. If the conjecture were valid, it would provide a polynomial algorithm to decide whether two graphs are isomorphic and thereby solve the *graph isomorphism problem.* As is well known the graph isomorphism problem is not solved in so far as its algorithmic complexity is not known. It belongs to the class NP but it is not known whether it is NP-complete or belongs to the class P.

Graphs with the same spectrum are called *isospectral* or *cospectral* graphs. In this section we review what is known about cospectral graphs.

We first present early results (up to 1971) on cospectral graphs following the review given in [Cve7].

In [CoSi] Collatz and Sinogowitz had already noted that the spectrum of a graph does not determine the graph up to isomorphism. They gave an example of two isospectral trees with eight vertices and different sets of vertex degrees.

The term 'pair of isospectral non-isomorphic graphs' will be denoted by PING. The literature contains various examples of PINGs and a few of the constructions will be described in this section. The importance of PINGs lies in the following observations:

(1) For every pair of non-isomorphic graphs one can find a set of characteristic properties that are different for the two graphs. Therefore, every PING points to properties of graphs that are not uniquely determined by the spectrum.

(2) The existence of a PING rules out various possibilities in the search for families of graphs with the property that different graphs from the same family have different spectra.

We shall restrict our attention to undirected graphs without loops or multiple edges. (It is relatively easy to construct PINGs for other kinds of graphs. All digraphs without cycles have a spectrum containing only numbers equal to zero [Sed]. A further example consisting of directed graphs with seven vertices is cited in [Pon]; see also [Djo].)

In [Har1], Harary states that his conjecture, that isospectrality implies the isomorphism of graphs, was disproved by Bose, who described a PING with 16 vertices. According to [Har1], Bruck and Hoffman also found PINGs with 16 vertices.

There are no PINGs among the connected graphs with at most five vertices – see for example the table of spectra of graphs in [CvDS]. In [Bak2] Baker gives a PING consisting of connected graphs with six vertices, and so the number five above is the best bound possible.

If we consider graphs without the assumption of connectedness, then there exists a PING with five vertices, namely $K_{1,4}$ and $C_4 \cup K_1$. This example has been generalized in [Cve7] as follows. The graph having as components s isolated vertices and one complete bipartite graph K_{n_1,n_2} has eigenvalues $\sqrt{n_1 n_2}, -\sqrt{n_1 n_2}$ and $n_1 + n_2 - 2 + s$ numbers equal to 0. Now consider a graph with spectrum $\sqrt{m}, -\sqrt{m}$ and $n-2$ numbers equal to 0 (m a natural number). This spectrum belongs to each graph of the above type whose parameters n_1, n_2, s satisfy the equations $n_1 + n_2 + s = n,\ n_1 n_2 = m$.

From these examples we see that in general we cannot determine from the spectrum whether or not a graph is connected. If however we consider the narrower class of regular graphs then this information can be extracted from the spectrum (see Theorem 1.3.13). In this case, knowledge of the spectrum is equivalent to knowledge of the Laplacian spectrum, and we recall from Section 1.1 that the Laplacian spectrum of a graph does tell us whether or not the graph is connected.

Turner [Turn2] gives a PING consisting of 12-vertex trees which have the same vertex degree sequence. The author expresses his pessimism concerning the possibility of distinguishing even graphs of restricted type by means of their spectra.

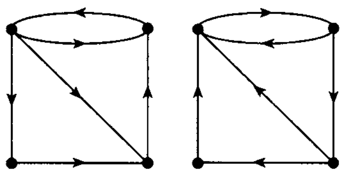

Fig. 1.2. A pair of cospectral digraphs.

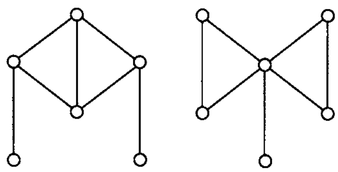

Fig. 1.3. A pair of cospectral graphs.

Fisher, who encountered the graph isospectrality problem when investigating the vibration of membranes [Fis], has considered graphs with the following restrictions (among others): (1) the graph does not contain a vertex of degree 1, (2) the graph is planar. He constructed an infinite sequence of PINGs with $5n$ vertices ($n = 3, 4, \ldots$) satisfying conditions (1) and (2). An infinite sequence of sets of mutually non-isomorphic isospectral graphs was also given by Bruck in [Bruc]. It seems that PINGs with a large number of vertices are a common occurrence, and some statistical data are given by Baker in [Bak2].

PINGs can also be found in the family of regular graphs. They can arise from switching-equivalent connected regular graphs of the same degree: examples are provided by the graphs having 16, 28 and 64 vertices which occur as exceptions in Theorems 1.3.5, 1.3.6 and 1.3.27. Further examples arise in the context of Theorems 1.3.9, 1.3.10 and 1.3.11.

If a PING with n vertices is known, then a PING with m vertices ($m > n$) can easily be constructed by adding an arbitrary graph with $m - n$ vertices as a new component in each of the two graphs. Also, from a PING consisting of regular graphs of degree greater than 2, we can construct another PING with more vertices by taking the line graphs of the graphs in question (cf. Theorem 1.3.17).

Another review of cospectral graphs appeared in 1971, written by Harary, King, Mowshowitz and Read [HaKMR]. Among other things they construct the smallest cospectral strongly connected digraphs which are not self-converse (Fig. 1.2), the smallest pair of connected cospectral graphs (Fig. 1.3) and the smallest triplet of connected cospectral graphs (Fig. 1.4).

A third review of cospectral graphs in 1971 appeared in the paper [BaHa], which repeats some of the examples mentioned earlier, and which gives a PING consisting of trees on 12 vertices with the same degrees, the maximal degree being 4. Since these trees are relevant to chemistry the authors justify in this way the main message of the paper, expressed

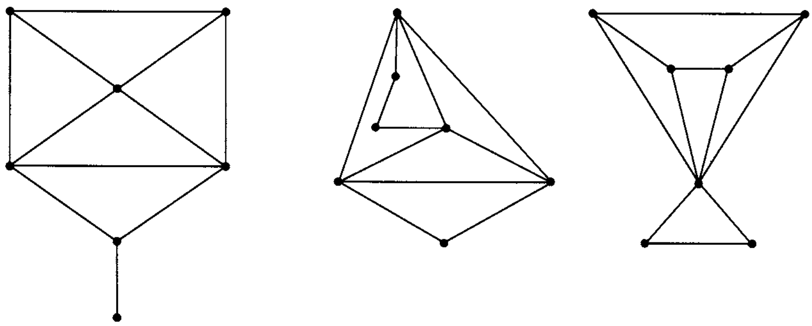

Fig. 1.4. Three cospectral graphs.

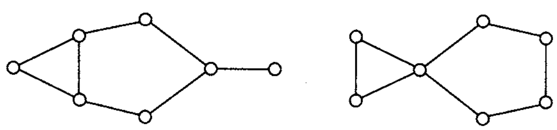

Fig. 1.5. Cospectral graphs with cospectral complements.

by its title: *the characteristic polynomial does not uniquely determine the topology of a molecule.*

The expository article [GoHMK] contains a list of smallest PINGs in various classes of graphs. In addition to the above results the paper gives the smallest cospectral graphs with cospectral complements (Fig. 1.5), the smallest cospectral forests ($K_{1,3} \cup K_2$ and $P_5 \cup K_1$), smallest cospectral regular graphs (two pairs of degree 4 on ten vertices and their complementary pairs; see Fig. 4.1) and some others.

The paper [GoMK1] presents the results of a computational study of spectra of graphs. Characteristic polynomials of all graphs up to nine vertices are computed and the cospectral graphs identified. Statistics are given for cospectral graphs in various classes of graphs.

We quote a theorem which provides a construction for cospectral trees with cospectral complements.

1.2.1 Theorem [GoMK1] *Let G be an arbitrary rooted graph. Let S and T be rooted trees as shown in Fig. 1.6. Then $G \cdot S$ and $G \cdot T$ are not isomorphic (unless the root of G is isolated) but are cospectral and have cospectral complements.*

Recall that $G \cdot H$ denotes the coalescence of rooted graphs G and H. The proof of Theorem 1.2.1 is based partly on a formula for the

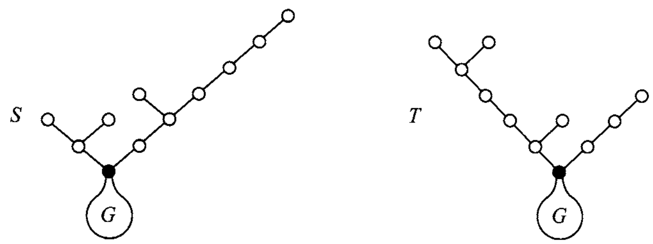

Fig. 1.6. The construction for Theorem 1.2.1.

characteristic polynomial of $G \cdot H$ given in Chapter 4: see equation (4.3.4).

An important result of Schwenk [Sch1] states that almost all trees have a cospectral mate. This result is described in some detail in Section 5.1. In order to formulate some extensions of this result, we define matrix functions called immanants. If χ is an irreducible character of the symmetric group S_n, if $A = (a_{ij})$ is a square matrix of order n, and if $d_\chi(A) = \sum_{\pi \in S_n} \chi(\pi) a_{1\pi(1)} a_{2\pi(2)} \cdots a_{n\pi(n)}$ then $d_\chi(A)$ is called an *immanant* of A. If $\chi(\pi) = 1$ for all $\pi \in S_n$ then $d_\chi(A)$ is the *permanent* of A, while the alternating character yields the *determinant* of A. If A is the adjacency matrix of a graph G and χ a fixed character then $d_\chi(xI - A)$ is the corresponding *immanantal polynomial* of G. As a generalization of a result in [Mer1], it is shown in [BotMe] that almost every tree has a co-immanantal mate, that is, a tree which shares the same immanantal polynomials $d_\chi(xI - A)$ for all χ. Indeed the authors prove a stronger theorem which includes the corresponding result for the Laplacian matrix $L = D - A$: in the above statement, the set of one-variable functions $d_\chi(xI - A)$ may be replaced by the set of three-variable functions $d_\chi(xI - yD - zA)$.

Schwenk [Sch1] found a construction of cospectral graphs which uses the concept of *cospectral vertices*. This construction will be described in Section 5.1, along with the notion of *unrestricted vertices*. Both concepts feature in the general procedures for constructing PINGs described in [HeEl2]. This paper describes methods for constructing graphs with such vertices, and discusses cospectral graphs with cospectral complements.

Graphs with cospectral vertices are called *endospectral* graphs [Ran2]. Hence the study of endospectral graphs is closely related to the study of procedures for constructing cospectral graphs. Some constructions of