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GRAPH ANGLES AND ISOSPECTRAL MOLECULES

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Various constructions for cospectral graphs, used in the investigation of isospectral molecules, are explained in terms of certain geometrical invariants of eutactic stars associated with a graph.

1. INTRODUCTION

This note is prompted by a recent paper in theoretical chemistry [**6**], where various rules for the construction of cospectral graphs are justified by means of second-order approximations in perturbation theory. The context is the representation of certain molecules by finite undirected graphs (without loops or multiple edges): vertices represent atoms, and edges represent bonds between atoms. For details the reader is referred to [**7**]. Suffice it to say here that, according to Hückel's theory of molecular orbitals, the energy levels of a generalized wave function associated with a hydrocarbon molecule are determined by the eigenvalues of a $(0,1)$-adjacency matrix of an underlying graph. Such a matrix is regarded as a matrix with real entries, and two graphs are said to be *cospectral* if they have adjacency matrices with the same spectrum; if the two graphs are non-isomorphic then the corresponding molecules are said to be *isospectral.*

The construction of cospectral graphs has been investigated not only in the context of perturbations of eigenvectors of an adjacency matrix [**5**], [**6**] but also in the context of self-returning walks [**8**], [**13**]. Further, various formulae of Heilbronner [**4**] and others [**9**], [**12**] may be used to construct cospectral graphs from a graph G which has distinct vertices u, v such that the graphs $G-u$, $G-v$ are cospectral. (Here $G-u$ is obtained from G by deleting vertex u and all edges containing u.) In this situation, u and v are said to be *cospectral* vertices (or *isospectral points* [**6**]): this concept was introduced in [**9**], while a first characterization of cospectral vertices in terms of eigenvectors appears in [**5**].

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The main purpose of this paper is to substantiate the claim that the notion central to all of the above themes is that of graph angles. The angles most commonly considered are those between coordinate axes and the eigenspaces of an adjacency matrix of a graph. If the n-vertex graph G has an adjacency matrix A with distinct eigenvalues $\mu_1, \dots, \mu_m$, and if $\mathbf{e}_1, \dots, \mathbf{e}_n$ comprise the standard orthonormal basis of R^n then we write β_{ij} for the angle $\left(0 \le \beta_{ij} \le \frac{\pi}{2}\right)$ between $\mathbf{e}_j$ and the eigenspace $\mathcal{E}(\mu_i)$. (Note that since similar matrices are cospectral, the eigenvalues of A are independent of the ordering of the vertices of the graph.) In the literature the numbers $\alpha_{ij} = \cos\beta_{ij}$ are customarily referred to as the angles of G, abusing terminology. Note that $\alpha_{ij} = |P_i\mathbf{e}_j|$, where P_i represents the orthogonal projection onto $\mathcal{E}(\mu_i)$.

The connection between angles and perturbations is explained in [**10**]. The connection between graph angles and eigenvectors is immediate since $P_i\mathbf{e}_j \in \mathcal{E}(\mu_i)$. A characterization of cospectral vertices in terms of the vectors $P_i\mathbf{e}_j$ is given in Proposition 2.2.

The connection between graph angles and self-returning walks is clear from the spectral decomposition $A^k = \sum_{i=1}^{m} \mu_i^k P_i$ $(k \ge 0)$ since on equating (j,j)-entries we see that the number $N_j^{(k)}$ of walks of length k beginning and ending at the j-th vertex is $\sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^k$. (This appears in [**2**, Section 5] where it is also noted that in the Hückel theory, $\sum\left\{\alpha_{ij}^2 \colon \mu_i > 0\right\}$ is essentially the probability of finding an electron at the j-th atom of the corresponding molecule.) Given $\mu_1, \dots, \mu_m$, knowledge of the angles α_{ij} $(i = 1, \dots, m;\ j = 1, \dots, n)$ is equivalent to knowledge of the numbers $N_j^{(k)}$ $(j = 1, \dots, n;\ k \in \mathrm{N})$.

Here we use graph angles independently of perturbations to establish with minimal effort the rules for the construction of cospectral graphs and isospectral molecules discussed in [**6**]. Some of the rules were propounded earlier [**1**], [**5**], [**14**], and some of the proofs are implicit in previous papers on the characteristic polynomial of a graph (that is, $\det(xI - A)$ in the notation above): see [**2**] and references therein. One new result here relates to the construction of cospectral graphs from a graph with so-called isospectral pairs of vertices, defined as follows. Let u, v be non-adjacent vertices of a graph G, and let $G(u,v)$ be the graph obtained from G by adding a new vertex w of degree 2 adjacent to u and v. The vertex w is called a *bridging vertex;* and the pairs $\{u,v\}$, $\{u',v'\}$ of non-adjacent vertices are called *isospectral* if the graphs $G(u,v)$, $G(u',v')$ are cospectral. Equation (2.5) below provides a formula for the characteristic polynomial of a graph modified by the addition of a bridging vertex.

For explicit examples of the constructions described in Section 2 the reader is referred to [**6**]. As in that paper the question of isomorphism of cospectral graphs is not considered in this note.

2. CHARACTERISTIC POLYNOMIALS

We first describe a well-known means of constructing cospectral graphs from a graph with cospectral vertices. The characteristic polynomial of a graph G is denoted by $\phi_G(x)$.

Proposition 2.1. *Let H, K be graphs and let w be a fixed vertex of K. For any vertex u of H, let G^u be the graph obtained from $H \cup K$ by identifying u and w. If u, v are cospectral vertices of H then the graphs G^u, G^v are cospectral.*

Proof. The graph G^u is the union of two graphs which have just one vertex in common. Accordingly, by [**12**, Corollary 2b], the characteristic polynomial of G^u is

$$\phi_{H-u}(x)\phi_K(x) + \phi_H(u)\phi_{K-w}(x) - x\phi_{H-u}(x)\phi_{K-w}(x).$$

Thus if $\phi_{H-u}(x) = \phi_{H-v}(x)$ then G^u, G^v are cospectral. ¤

The relation between vertex-deleted subgraphs and angles was established in [**3**] by expressing in two ways a diagonal entry of the matrix generating function $\sum_{k=0}^{\infty} x^{-k}A^k$. Here A is the adjacency matrix of a graph G whose vertices are labelled $1, 2, \ldots, n$. In the notation of Section 1, the (j, j)-entry of $\sum_{k=0}^{\infty} x^{-k}A^k$ is $\sum_{k=0}^{\infty} x^{-k} \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^k$, or $\sum_{i=1}^{m} \frac{\alpha_{ij}^2}{1-x^{-1}\mu_i}$ when $x > \max\{|\mu_1|, \ldots, |\mu_m|\}$. On the other hand, $\sum_{k=0}^{\infty} x^{-k}A^k = (I - x^{-1}A)^{-1}$ with (j, j)-entry $\frac{x\phi_{G-j}(x)}{\phi_G(x)}$, and it follows that

$$\phi_{G-j}(x) = \phi_G(x) \sum_{i=1}^{m} \frac{\alpha_{ij}^2}{x - \mu_i}. \tag{2.1}$$

Consequently we have the following characterization of cospectral vertices.

Proposition 2.2. *Vertices u, v of a graph are cospectral if and only if the angles at u coincide with the angles at v, that is, $\alpha_{iu} = \alpha_{iv}$ $(i = 1, \ldots, m)$.*

If μ_i is a simple eigenvalue then to within sign α_{iu} is the u-th entry of a unit vector which spans $\mathcal{E}(\mu_i)$: hence the remark in [**5**, p. 101] that cospectral vertices "must have identical absolute values of eigenvectors in every non-degenerate eigenlevel". In the general case, let $\mathbf{x}_1, \ldots, \mathbf{x}_d$ comprise an orthonormal basis for $\mathcal{E}(\mu_i)$, say $\mathbf{x}_k = (x_{1k}, x_{2k}, \ldots, x_{nk})^{\mathrm{T}}$ $(k = 1, 2, \ldots, d)$. Then $P_i = \mathbf{x}_1\mathbf{x}_1^{\mathrm{T}} + \cdots + \mathbf{x}_d\mathbf{x}_d^{\mathrm{T}}$ and so $\alpha_{ij}^2 = x_{j1}^2 + \cdots + x_{jd}^2$: hence the remark in [**6**, p. 25] that "the sum-over-degenerate-eigenvalues of squares of coefficients at isospectral points must be equal".

The next result concerns the construction in [**6**] of a family of graphs with cospectral vertices from a given graph H with cospectral vertices u, v. A third vertex t of H is said to be an *unrestricted substitution vertex* with respect to u, v if for any graph K, the vertices u, v remain cospectral in the graph obtained from $H \cup K$ by identifying t with a vertex of K.

Proposition 2.3. *Let u, v be cospectral vertices of the graph H and let t be a third vertex of H. Then t is an unrestricted substitution vertex with respect to u, v if and only if u, v are cospectral vertices of $H - t$.*

Proof. Let G be the graph obtained from $H \cup K$ by identifying t with a vertex w of K. By [**12**, Corollary 2b] we have $\phi_{G-u}(x) = \phi_{H-t-u}(x)\phi_K(x) + \phi_{H-u}(x)\phi_{K-w}(x) - x\phi_{H-t-u}(x)\phi_{K-w}(x)$, together with a similar expression for $\phi_{G-v}(x)$. Since $\phi_{H-u}(x) = \phi_{H-v}(x)$, it follows that u, v are cospectral in G if and only if

$$\big(\phi_{H-t-u}(x) - \phi_{H-t-v}(x)\big) \cdot \big(\phi_K(x) - x\phi_{K-w}(x)\big) = 0. \tag{2.2}$$

Hence $\phi_{G-u}(x) = \phi_{G-v}(x)$ for all choices of K if and only if $\phi_{H-t-u}(x) = \phi_{H-t-v}(x)$. ¤

Remark. It follows from Equation (2.2) that if $\phi_{G-u}(x) = \phi_{G-v}(x)$ for just one choice of K in which w is not isolated then t is an unrestricted substitution vertex; for if $\phi_K(x) = x\phi_{K-w}(x)$ then w is an isolated vertex. To see this we apply Proposition 2.1 to K: taking $\mu_1 = 0$ we have $\alpha_{1w} = 1$ and $\alpha_{iw} = 0$ $(i > 1)$, whence $\mathbf{e}_w = P_i\mathbf{e}_w \in \mathcal{E}(\mu_1)$ and $A\mathbf{e}_w = \mathbf{0}$. ¤

We now turn our attention to the characterization of isospectral pairs of vertices. First note that the introduction of a bridging vertex between non-adjacent vertices u, v of a graph G is equivalent to adding the edge uv and then subdividing uv. A formula for the characteristic polynomial of a graph with a subdivided edge is derived from a deletion-contraction algorithm in [**9**, Proposition 1.7]. If we apply this to the graph $G + uv$ we obtain

$$\phi_{G(u,v)}(x) = \phi_{G+uv}(x) + (x-1)\phi_G(x) - \phi_{G-u}(x) - \phi_{G-v}(x) + \phi_{G-u-v}(x). \tag{2.3}$$

Now [**10**, Equation (6)] provides an expression for $\phi_{G+uv}(x)$ involving further angles associated with a graph, namely the angles $\cos^{-1}\gamma_{uv}^{[i]}$ between $P_i\mathbf{e}_u$ and $P_i\mathbf{e}_v$ (defined when $P_i\mathbf{e}_u$, $P_i\mathbf{e}_v$ are non-zero). For our purposes, we write this expression in the form

$$\phi_{G+uv}(x) = \phi_G(x)\left\{1 - 2\sum_{i=1}^{m}\frac{P_i\mathbf{e}_u \cdot P_i\mathbf{e}_v}{x - \mu_i}\right\} - \phi_{G-u-v}(x). \tag{2.4}$$

Thus is proved in [**10**] by first expressing in two ways the (u, v)-entry of the matrix generating function $\sum_{k=0}^{\infty} x^{-k}A^k$ (cf. the derivation of Equation (2.1)). If we eliminate $\phi_{G+uv}(x) + \phi_{G-u-v}(x)$ from Equations (2.3) and (2.4) we obtain

$$\phi_{G(u,v)}(x) = \phi_G(x)\left\{x - 2\sum_{i=1}^{m}\frac{P_i\mathbf{e}_u \cdot P_i\mathbf{e}_v}{x-\mu_i}\right\} - \phi_{G-u}(x) - \phi_{G-v}(x).$$

If we now express $\phi_{G-u}(x)$ and $\phi_{G-v}(x)$ in the form of Equation (2.1), we obtain

$$\phi_{G(u,v)}(x) = x\phi_G(x) - \phi_G(x)\sum_{i=1}^{m}\frac{|P_i\mathbf{e}_u + P_i\mathbf{e}_v|^2}{x-\mu_i}. \tag{2.5}$$

This yields the following "absolute value sum rule for isospectral pairs" conjectured in [**1**] and justified in [**6**] by means of second-order approximations in perturbation theory.

Proposition 2.4. *Let $\{u,v\}$, $\{u',v'\}$ be pairs of non-adjacent vertices in the graph G. Then $\{u,v\}$, $\{u',v'\}$ are isospectral pairs in G if and only if*

$$|P_i\mathbf{e}_u + P_i\mathbf{e}_v| = |P_i\mathbf{e}_{u'} + P_i\mathbf{e}_{v'}| \qquad (i = 1,2,\ldots,m).$$

3. REMARKS

Let $\mathcal{V}$ be an inner product space, $\mathcal{U}$ a subspace of $\mathcal{V}$. A *eutactic star* in $\mathcal{U}$ is defined in [**15**] essentially as the orthogonal projection onto $\mathcal{U}$ of an orthonormal set of vectors in $\mathcal{V}$. Thus in the notation of the previous sections, for each $i \in \{1,2,\ldots,m\}$ the vectors $P_i\mathbf{e}_1,\ldots,P_i\mathbf{e}_n$ comprise a eutactic star $\mathcal{S}_i$ in $\mathcal{E}(\mu_i)$. The angles α_{ij} $(j = 1,\ldots,n)$ are the lengths of the vectors (or arms) of $\mathcal{S}_i$, while $\cos^{-1}\gamma_{uv}^{[i]}$ is the angle between the arms $P_i\mathbf{e}_u$ and $P_i\mathbf{e}_v$. Thus the invariants which determine cospectrality in the various constructions discussed in Section 2 are just invariants of the geometries of the eutactic stars $\mathcal{S}_1,\ldots,\mathcal{S}_m$.

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