A Group-Theoretical Bound for the Number of Main Eigenvalues of a Graph

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An eigenvalue of a graph is called main if the corresponding eigenspace contains an eigenvector in which the sum of coordinates is different from zero. It is proved that the number of main eigenvalues does not exceed the number of orbits (sets of vertices equivalent under the group of automorphisms of the graph).

1. INTRODUCTION

Qualitative theories of electronic structure of unsaturated π systems are essentially graph-theoretical in nature. In particular, the diagonalization of adjacency matrices leads to eigenvectors and eigenvalues that give direct information on the form of the π orbitals and their relative energies within the simple Hückel model.[1] Systematic rules for stability and reactivity of π systems can be obtained from properties of adjacency matrices for special classes of graphs, and much work has been done by both chemists and mathematicians on symmetry-based methods for obtaining all or part of the eigenvalue spectrum.[1−3]

Recent mathematical work has explored the extra information that can be obtained if the graph angles (see below) as well as the eigenvalues are taken into account. In certain classes of graph, the angles allow full reconstruction of the graph; in graphs that represent π systems, the charges and bond orders can be obtained as functions of the angles.[4] Particular interest is attached to those eigenvalues in the spectrum that have nonzero angles with the vector that has a unit component on all n vertices of the graph. Several theorems have been proved about the properties of these *main* eigenvalues, and the present paper shows how "chemical" methods of point-group theory can be used to give a bound on the number of main eigenvalues of any graph. With the translation "adjacency matrix" → "Hückel Hamiltonian matrix", this becomes a result about π systems.

We describe first the notation and basic definitions, before stating our results.

Eigenvalues, *eigenvectors*, the *spectrum* and the *characteristic polynomial* of a graph G are eigenvalues, eigenvectors, the spectrum, and the characteristic polynomial of the adjacency matrix of G. An eigenvalue is called *degenerate* if its multiplicity is greater than 1.

The n-dimensional vector $j = (1, 1, ..., 1)$ is called the *main vector* (in the corresponding space $\mathbf{R}^n$). The direction spanned by the main vector is called the *main direction*. An eigenvalue of a graph is called *main* if the corresponding eigenspace contains an eigenvector x which is not orthogonal to j. This implies that the sum of coordinates of such an eigenvector, called a *main* eigenvector, is different from 0. The *main angle* of an eigenvalue is the cosine of the angle between the corresponding eigenspace and the main vector j. Main eigenvalues are those with a nonzero main angle. Two graphs are called *comain* if they have the same main angles.

Vertices x and y of a graph G are *similar* if there is an automorphism of G which takes x to y. Equivalence classes of the similarity relation are called *orbits* of G. The automorphism group of G is denoted by G.

Given a square matrix $B = ||b_{ij}||_1^s$, let the vertex set X of a graph G be partitioned into (nonempty) subsets $X_1, X_2, ..., X_s$ so that for any $i, j = 1, 2, ..., s$ each vertex from X_i is adjacent to b_{ij} vertices of X_j. Then the multidigraph H with the adjacency matrix B is called a *divisor* of G.

Theorem 1.[5] *The spectrum of any divisor of a graph G contains all main eigenvalues of G.*

See ref 3, pp 118−124, for the next two theorems.

Theorem 2.[6] *For any graph G there is a divisor of G whose number of vertices equals the number of orbits of the automorphism group of G.*

Theorem 3.[6] *The characteristic polynomial of any divisor of a graph G is a divisor of the characteristic polynomial of G.*

The topic of interest in this paper is the following theorem:

Theorem 4. *The number of main eigenvalues of a graph G does not exceed the number of orbits into which the vertex set of G is partitioned by the automorphism group of G.*

This theorem is an immediate consequence of theorems 1−3. However, the proof of theorem 1, pp 39−40 of ref 5) is rather involved (cf. also ref 4). Therefore we present here an independent proof of theorem 4. This proof uses group theoretical concepts and, in particular, the theory of matrix representation of groups[7] (see also ref 3, pp 141−149).

In section 2 we give a proof of theorem 4. In section 3 we present several examples and comments on the general case, while in section 4 we treat bipartite graphs.

2. PROOF OF THEOREM 4

Given a graph G on n vertices, a vector of dimension n is called *totally symmetric* (with respect to G) if its coordinates corresponding to any two similar vertices are mutually equal.

The main vector has coefficients of 1 on every vertex; therefore, it is unchanged by any exchange of vertices or

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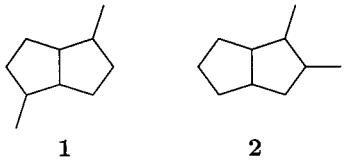

Figure 1. Two graphs that are both cospectral and comain.

any symmetry operation performed on the graph and so is a totally symmetric vector.

In the automorphism group of the graph, the main direction belongs to the totally symmetric representation Γ_0, which is nondegenerate and has character $\chi_0(R) = 1$ for all $R \in G$.

The full set of eigenvectors of G span the reducible representation $\Gamma_\sigma(v)$, the permutation representation of the vertices, which is defined by the fact that its character $\chi_\sigma(R)$ under any $R \in G$ is equal to the number of vertices left unshifted by R.

$\Gamma_\sigma(v)$ contains exactly n_0 copies of Γ_0, where n_0 is the number of orbits. The scalar product of any two vectors that belong to *different* irreducible representations of G is zero.

A main eigenvector has a nonzero scalar product with the main vector; therefore, it must contain a component that has the same, totally symmetric representation as that vector.

Therefore, only those eigenvalues λ whose eigenspaces contain a totally symmetric component can be main. n_0 is thus an upper bound on the number n_m of main eigenvalues of G: $n_m \leq n_0$.

This completes the proof.

Group theory takes us only as far as theorem 4, but some additional remarks can be made.

3. EXAMPLES AND COMMENTS

The notation $c_i^{(k)}$ ($i = 1, ..., n$) stands for the coefficients (coordinates) of the kth eigenvector; where no ambiguity is likely, the superscript (k) can be omitted.

1. The bound is an inequality; there are graphs G for which $n_m = n_0$ and others for which $n_m < n_0$. *All* graphs have $n_m \geq 1$, as the principal eigenvector (corresponding to the largest eigenvalue) has all coefficients of the same sign, is of symmetry Γ_0, and has therefore a nonzero main angle for any graph.

2. All totally symmetric eigenvectors *except* those for which $\sum_{i=1}^{n} c_i = 0$ belong to a main eigenvalue. This zero-sum condition can occur systematically, leading to various classes of graphs for which the inequality is strict. It can conceivably occur as an accident, too. An example is the cospectral, comain pair of graphs **1** and **2** in Figure 1.

Considered as maps on the sphere, these graphs have different symmetry groups: in this setting, **1** has C_2 symmetry but **2** has only the trivial symmetry C_1. Both graphs have eigenvalues (and main angles): 2.4368(0.9485), 1.6582(0), 1.1651(0), 0.7495(0.2104), 0.4314(0.1192), −0.1576(0), −0.6426(0.1953), −1.5593(0), −1.9752(0.0605), and −2.1064(0). The number of main eigenvalues of **1** is consistent with its five orbits and five totally symmetric eigenvectors. However, **2** has ten orbits, and all ten eigenvectors are totally symmetric in C_1, so the vanishing of half of the coefficient sums appears, from the point of view of symmetry, as an accident. This pair has all main angles equal. In fact, there are examples of cospectral graphs with (a) the same main angles, (b) the same main eigenvalues but different main angles, (c) the same number of main eigenvalues but different main eigenvalues, and (d) different numbers of main eigenvalues.

An example for b is the smallest pair of connected cospectral graphs (they have six vertices and are graphs no. 79 and no. 80 in a published catalogue[8]).

3. If the automorphism group of the graph is trivial, then each vertex of G constitutes a distinct orbit and $n_0 = n$. A graph with n main eigenvalues has the trivial symmetry.

4. For a *regular* graph, the eigenvector for the largest eigenvalue is equal to j, and orthonormality of the full set of n eigenvectors of G therefore implies that all other vectors have $\sum_{i=1}^{n} c_i = 0$. Thus a regular graph has $n_m = 1$. Any graph whose vertices form a single orbit is regular.

5. A complete graph K_n has $n_m = 1$ but also $n_0 = 1$, so for K_n ($n > 0$), the bound is sharp. The bound is also sharp for cycles C_n ($n > 2$) as they are regular, of degree 2. The bound is also sharp for paths P_n ($n > 0$) ($n_0 = n/2$ for n even, $n_0 = (n + 1)/2$ for n odd): the proof is direct, given the analytical solution for the eigenvalues $\lambda_k = 2\cos(k\pi/(n + 1))$, ($k = 1, ..., n$) and corresponding eigenvectors $c_r^{(k)} = [2/(n + 1)]^{1/2} \sin(k\pi r/(n + 1))$, for vertices $r = 1, ..., n$ (cf., e.g., ref 1 or 3, p 214). The sum of coefficients is nonvanishing for all totally symmetric (odd k) vectors.

6. The subdivision graphs $S(K_n)$ of complete graphs K_n, $n > 1$, for $n \neq 3$ have $n_m = n_0 = 2$; $S(K_3)$ is C_6 and has $n_m = n_0 = 1$, as do all C_n.

Proof. $S(K_n)$ has "old" vertices of K_n and "new" vertices dividing edges of K_n. The local eigenvalue conditions are

$$-\lambda C_{\text{old}} + (n-1)C_{\text{new}} = 0$$
$$-\lambda C_{\text{new}} + 2C_{\text{old}} = 0$$

where every old vertex carries an equal coefficient C_{old} and every new vertex an equal coefficient C_{new}. Equality within sets follows from the fact that the old vertices form one orbit, the new vertices another. Therefore

$$\begin{vmatrix} -\lambda & n-1 \\ 2 & -\lambda \end{vmatrix} = 0 \Rightarrow \lambda = \pm[2(n-1)]^{1/2}$$

and normalization gives $C_{\text{old}} = 1/(2n)^{1/2}$ and $C_{\text{new}} = \pm 1/[n(n-1)]^{1/2}$.

The coefficients are finite as $n \neq 0$, $n \neq 1$ by simplicity of $S(K_n)$, and scalar products with j are

$$\frac{1}{[n+1]^{1/2}}\left(1 \pm \left[\frac{n-1}{2}\right]^{1/2}\right)$$

i.e. two distinct nonzero values except when $n = 3$ and $S(K_3) = C_6$.

7. Any two-orbit graph is either (a) regular and has $n_m = 1$ or (b) not regular and has $n_m = 2$.

Proof. We have $n_0 = 2$. In a totally symmetric vector all vertices of orbit i carry the same coefficient c_i. Solutions for the two possible values of λ and their corresponding coefficient sets obey

$$-\lambda c_1 + d_{11}c_1 + d_{12}c_2 = 0, \quad -\lambda c_2 + d_{22}c_2 + d_{21}c_1 = 0 \tag{1}$$

with normalization

$$n_1 c_1^{\,2} + n_2 c_2^{\,2} = 1$$

where each member of orbit i has d_{ik} neighbors in orbit k and $n_1 d_{12} = n_2 d_{21}$. The question to be solved is, under what conditions are solutions of (1) compatible with

$$n_1 c_1 + n_2 c_2 = 0 \qquad (1)$$

i.e. when is a λ value obeying (1) nonmain?

From (2), a normalized, nonmain, totally symmetric eigenvector has $c_1 = [n_2/n_1(n_1 + n_2)]^{1/2}$ and $c_2 = -[n_1/n_2(n_1 + n_2)]^{1/2}$.

The λ equations for this set of c_i are

$$-\lambda + d_{11} - \frac{n_1 d_{12}}{n_2} = 0, \quad \lambda\frac{n_1}{n_2} - \frac{n_1}{n_2} d_{22} + d_{21} = 0$$

and hence $\lambda = d_{11} - d_{21} = d_{22} - d_{12}$, which implies $d_{11} + d_{12} = d_{22} + d_{21}$. Hence, the degrees of vertices are equal in both orbits, and G is regular. Therefore, if one λ value of the two totally symmetric eigenvectors is nonmain, G is regular. From remark 3, if G is regular, we have $n_m = 1$.

8. Γ_0 is a nondegenerate representation. It follows that any degenerate main eigenvalue of G is *accidentally degenerate*—its degeneracy is not forced by the symmetry of the graph. Indeed, there are no examples of graphs with main degenerate eigenvalues in the table of eigenvalues, angles, and main angles of connected graphs up to five vertices.[4] However, the largest eigenvalue is always main, and in disconnected graphs it can be degenerate. The smallest such example is $2K_1$. In the table of connected graphs on six vertices[8] we can find graphs (both bipartite and non-bipartite) having zero as a degenerate main eigenvalue (e.g. graphs no. 111 and 63). Connected graphs with a main degenerate eigenvalue different from zero can be found in the table of connected graphs on seven vertices.[9] For example, the graph 8-95 has 1 as a main 2-fold eigenvalue. In spite of the accidental character of the degeneracy in main eigenvalues, we can come across classes of graphs with this phenomenon; one result[10] characterizes the so-called *generalized line graphs* in which the (least) eigenvalue -2 is main. Examples of accidental degeneracy in chemically relevant graphs include the 9-fold (nonmain) eigenvalue 1 of the truncated icosahedron which is $G_g + H_g$ when analyzed in I_h symmetry.

9. In the case of three orbits the number of main eigenvalues is 1, 2, or 3. An example for the second alternative is provided by the subdivision $S(K_{1,3})$ of the star $K_{1,3}$. This graph has seven vertices and the spectrum 2, 1^2, 0, -1^2, -2, where the exponent denotes the multiplicity. Main eigenvalues are 2 and 0. This graph appears[11] as a counterexample to a conjecture[12] that the spectrum of a divisor with the smallest number of vertices is just the main part of the spectrum. The conjecture had been previously disproven[5] by a counterexample on 21 vertices. If the conjecture were true, we would have in theorem 4 an equality instead of the present inequality.

10. The problem of characterizing graphs with exactly k main eigenvalues, posed in ref 5 (cf. ref 4, p 40), remains open. A theorem from ref 11 identifying the main part of the spectrum with the spectrum of a companion matrix is an algebraic reformulation of the definition rather than a real structural characterization.

4. REMARKS ON BIPARTITE GRAPHS

1. In a bipartite graph the vertices fall into two sets, called the partite sets, such that each vertex of any one set is adjacent only to members of the other. The adjacency matrix of a bipartite graph has the following property: if $+\lambda$ is an eigenvalue of the graph, then so is $-\lambda$, and the eigenvectors that form a basis for eigenvalue $+\lambda$ are transformed into a basis for eigenvalue $-\lambda$ by reversing the sign on the coefficients of one partite set.

In symmetry terms, the representations of eigenspaces for $+\lambda$ and $-\lambda$ are related as

$$\Gamma(\lambda) = \Gamma_\star \times \Gamma(-\lambda) \qquad (3)$$

where $\Gamma_\star$ is the nondegenerate irreducible representation of the *alternating vector* which has coefficients $+1$ on all members of one partite set and -1 on all members of the other.

Γ_0 is the symmetry of the ground eigenvector, the vector corresponding to the greatest eigenvalue $+\lambda_{max}$, and $\Gamma_\star$ is the symmetry of the nondegenerate eigenvector corresponding to the least eigenvalue $-\lambda_{max}$.

2. Bipartite graphs are of two types. *Either* (a) some orbit is broken across the two partite sets, in which case $\Gamma_\star \neq \Gamma_0$, *or* (b) each partite set consists of whole orbits of G, in which case $\Gamma_\star = \Gamma_0$ and $\Gamma(\lambda) = \Gamma(-\lambda)$ for all $+\lambda$.

3. (a) In case a, in the absence of accidental degeneracy at λ, at most one of $+\lambda$ and $-\lambda$ may be main, and if $+\lambda$ is main, then $\Gamma(\lambda)$ contains Γ_0 and $\Gamma(-\lambda)$ contains $\Gamma_\star$. In case a, although $\Gamma_\star$ is *not* Γ_0, $\Gamma(\lambda)$ and $\Gamma(-\lambda)$ may still be equal but only if $+\lambda$ is degenerate. A corollary is that $+\lambda = 0$, if present in the spectrum of a case a graph, must be a degenerate eigenvalue.

3. (b) All graphs of trivial symmetry C_1; where each vertex forms a distinct orbit of size 1, necessarily belong to case b. In case b, eigenspaces for $+\lambda$ and $-\lambda$ contain equal numbers of totally symmetric eigenvectors, but this does not imply that the eigenvalues have the same main/nonmain status. In fact, the pair $\{+\lambda, -\lambda\}$ of a case b graph may contain 0, 1, or 2 main eigenvalues, depending on λ and G. Clearly, if $\Gamma(\lambda)$ does not contain Γ_0, neither $+\lambda$ nor $-\lambda$ are main.

The possibilities when $\Gamma(\lambda)$ *does* contain Γ_0 are distinguished by partitioning the graph into black and white partite sets and separating the contributions B_λ, W_λ to the summation in the computation of the main angle for eigenvalue $+\lambda$. The main angle is then $|B_\lambda + W_\lambda|$ for $+\lambda$ and $|B_\lambda - W_\lambda|$ for $-\lambda$.

The three cases are then (for nondegenerate $+\lambda$): (i) Neither of $\pm\lambda$ is main $\leftrightarrow B_\lambda = W_\lambda = 0$; (ii) Exactly one of $\pm\lambda$ is main $\leftrightarrow |B_\lambda| = |W_\lambda| \neq 0$; (iii) Both $\pm\lambda$ are main $\leftrightarrow |B_\lambda| \neq |W_\lambda|$.

5. CONCLUSION

This paper deals with some properties of graph eigenvalues and eigenvectors, exploring the connection between the symmetry ideas familiar to chemists and the mathematical property of "mainness". Chemical graph theory tends to concentrate first and foremost on eigen*values*, as these differentiate between radical and closed-shell, stable and

unstable, aromatic and antiaromatic systems, but eigen*vectors* also carry chemically significant information, particularly in the symmetry properties of HOMO and LUMO, and the number of distinct nonbonding vectors. They also specify the π charges and bond orders, the former requiring only the graph angles.[4] The present work highlights one aspect of the eigenvalue/eigenvector problem: the number of main eigenvalues. Although nonzero main angles may not at first sight appear to be chemically significant, theorem 4 shows that they are signs of the presence of a totally symmetric component of the eigenspace, and thus of a π molecular orbital that survives unchanged under all group operations. Further connections between graph angles and chemical properties can be expected in future work.

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