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On the construction of graphs of nullity one

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Abstract

This paper studies singular graphs by considering minimal singular induced subgraphs of small order. These correspond to a number k of linearly dependent rows of the adjacency matrix determining what is termed as a core of the singular graph. For k at most 5, the distinct cores and corresponding minimal configurations (61 in number) are identified. This provides a method of constructing singular graphs from others of smaller order. Furthermore, it is shown that when a graph has a minimal configuration as an induced subgraph, then it is singular.

0. Introduction

If a graph G has n vertices, then the *order* n is denoted by $o(G)$. The *null graph* $\overline{K}_n$ is denoted by N_n and the *complete graph* by K_n. The *circuit* and *path* on n vertices are denoted by C_n and P_n, respectively. The *disjoint union* of two graphs H and K is denoted by $H \dot{+} K$.

The *adjacency matrix* $A(G)$ or A of a graph G having vertex set $\mathcal{V}(G) = \{v_1, v_2, \ldots, v_n\}$ is an $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. A is also represented by $(R_1, R_2, \ldots, R_n)^{\mathrm{T}}$, where R_i is the ith row vector of A corresponding to vertex v_i. The *rank* of a graph G is the rank of its adjacency matrix A.

All the graphs we consider are *simple,* i.e. without multiple edges or loops and the vertex set is labelled. A graph is said to be *singular* if its adjacency matrix A is a singular matrix; then at least one of the eigenvalues of A is zero. There corresponds a non-zero vector v_0 such that $Av_0 = 0$. The nullspace of A consists of the set of vectors v_0 together with the zero vector.

Since the adjacency matrix A is symmetric, the algebraic multiplicity is the same as its geometric multiplicity for each eigenvalue λ. This common value for $\lambda = 0$ is the *nullity* of G, and is therefore the number of zero eigenvalues of matrix A.

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Definition. The *nullity* of a singular graph G, denoted by $\eta(G)$, is the dimension of the nullspace of A, i.e., the multiplicity of the zero eigenvalue of A.

It follows that the rank of G, denoted by rank (G), is $o(G) - \eta(G)$.

This paper considers the problem of identifying singular graphs, which has been posed by Collatz and Sinogowitz [1] and was later discussed by various authors including Cvetković and Gutman [3] and others [2,13,14]. The results of a systematic search for graphs, of nullity one, the adjacency matrix of which has a linearly dependent set of t row vectors, where $2 \leqslant t \leqslant 5$, are presented. For a singular graph G, each linearly dependent set of row vectors of A corresponds to an eigenvector called a kernel eigenvector [1] that determines a subgraph called a core[1]. A particular core may be 'grown' into distinct non-isomorphic graphs of nullity one called minimal configurations[1]. It is shown that for $2 \leqslant t \leqslant 3$ the minimal configurations are P_3 and P_5. Those for $t = 4$ and $t = 5$ are drawn in Fig. 4 and Figs. 12(a) and (b), respectively. A minimal configuration can be extended[1] into larger graphs such that the eigenvector has the same non-zero components. A singular graph, the adjacency matrix of which has a set of t linearly dependent row vectors, for $2 \leqslant t \leqslant 5$, has at least one of the minimal configurations identified in this paper, as a subgraph.

In the last section singular graphs are constructed from smaller graphs, using two distinct methods. The first makes use of formulae relating characteristic polynomials of the adjacency matrix of graphs. The second uses the notions developed in the first two sections and it is shown that singular graphs can be obtained if the core is preserved.

As the adjacency matrix of a minimal configuration has a one-dimensional nullspace, the structure of the graph is not masked by overlapping cores. Using the lists of cores, kernel eigenvectors and minimal configurations, for $2 \leqslant t \leqslant 5$, given in this paper, properties common to singular graphs become apparent. The role played by the core of a singular graph of nullity one, as elaborated in this paper, leads to the development of related ideas which emphasise its importance, as follows. In [8], the vector space of cores of a singular graph induced by the nullspace of its adjacency matrix is defined and used to determine bounds on the rank of the graph. As graphs with cores for $t = 6$ contribute to those of rank 6 they are described in [8]. Graphs of rank 6 also include 'nut graphs', which are minimal configurations whose core has nullity one and which are discussed in [6,11]. In [9] it is shown that the coefficient of λ in the characteristic polynomial of a graph G of nullity one is closely related to the corresponding kernel eigenvector which in turn depends on the vertices of the core.

1. The core of a singular graph

Definition. Two vertices are said to be of *the same type* if they are not adjacent and have the same neighbours.

[1] Formal definitions of these terms will appear later.

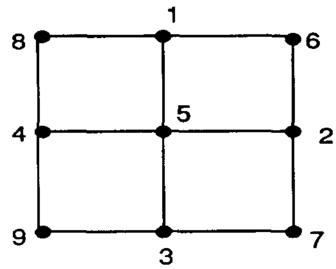

Fig. 1.

Thus, two vertices v_i, v_j of the same type have the same row vectors $R_i = R_j$ describing them. It is noted that the occurrence of s equal rows contributes $(s - 1)$ to the nullity.

Definition. A *kernel eigenvector* v_0 of a singular graph with adjacency matrix A, is an eigenvector in the nullspace of A.

A singular graph with $\eta > 1$ has more than one (linearly independent) kernel eigenvector. Thus, for the graph Γ_3 (see Fig.1)[2] of order 9 and rank 6, the eigenvectors $(1,-1,1,-1,0,0,0,0,0)^{\mathrm{T}}$, $(0,0,0,0,0,-1,1,1,-1)^{\mathrm{T}}$, $(0,0,0,0,1,0,-1,-1,0)^{\mathrm{T}}$, form a basis for the nullspace.

Definition. Let G be a singular graph having adjacency matrix $A = (R_1, R_2, \ldots, R_n)^{\mathrm{T}}$ and a kernel eigenvector $v_0 = (\alpha_1, \alpha_2, \ldots, \alpha_t, 0, \ldots, 0)^{\mathrm{T}}$, $\alpha_i \neq 0$, $\forall i$, $1 < t \leqslant n$. Then a *kernel relation* $\mathscr{R}$ of G (with respect to v_0) is the linear relation

$$\alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0. \tag{1}$$

The numbers $\alpha_i (i \in 1, 2, \ldots, t)$ are assumed to be non-zero integers with g.c.d. equal to 1.

If A has two row vectors R_1, R_2 which are linearly dependent then the corresponding vertices are of the same type. The smallest such graph which is connected is P_3.

Theorem 1. *Let G be a graph with adjacency matrix A having three linearly dependent row vectors (no two of which are linearly dependent). The three row vectors satisfy a unique relation $R_i + R_j = R_k$.*

This is proved by a routine case-by-case analysis which shows that there is a unique relation between the three linearly dependent row vectors of A. The smallest such graph which is connected is P_5.

[2] For justification of this notation, refer to Fig. 4.

Definition. Let v_0 be a kernel eigenvector of a singular graph G, of order $n \geqslant 3$. A subgraph of G induced by the vertices corresponding to the non-zero components of v_0 is said to be a *core* $\chi_t (= \chi)$ (w.r.t v_0), where t is the number of vertices of the core called the *core size*.

Lemma. *A core χ of a singular graph G (with respect to a kernel eigenvector v_0 of G) is a vertex-induced subgraph of G which is itself singular and has a vector in its nullspace each of whose components is non-zero.*

Proof. Let v_0 be a kernel eigenvector of G with t non-zero components. Let G be relabelled such that the first t vertices correspond to the non-zero components of v_0. If $v_0 = (\alpha_1, \alpha_2, \ldots, \alpha_t, 0, \ldots, 0)^{\mathrm{T}}, \alpha_i \neq 0, \forall i,\ 1 < t \leqslant n$ and A is the adjacency matrix of G, then $\chi (= \chi_t) = \langle v_1, v_2, \ldots, v_t \rangle$. The principal $t \times t$ submatrix of A is the adjacency matrix of the subgraph χ and has a kernel eigenvector $v_0' = (\alpha_1, \alpha_2, \ldots, \alpha_t)^{\mathrm{T}}$. Hence χ is singular. Also each component α_i of v_0' is not zero. □

Definition. For a graph of nullity *one* the number of non-zero components of the kernel eigenvector is called the *core number* of the singular graph.

Thus in a graph G of nullity one the core number is the core size of the unique core in G. For a graph with $\eta > 1$, a core χ is determined by the eigenvector being considered.

It is noted that χ_t may well be disconnected. It can be shown that the core number of P_7, the path of order 7, is 4, $v_0 = (1, -1, 1, -1, 0, 0, 0)^{\mathrm{T}}$ and that the core is N_4, whose vertices are the alternate vertices of the path starting from a terminal vertex.

The Hűckel molecular orbital theory (HMO) gives an approximation of the π-molecular orbitals of a molecule by expressing them as a linear combination of the atomic pπ-orbitals [2, 14]. When Schrődinger's equation, which determines the molecular orbital energies, is simplified, the resulting equation is the characteristic equation $\mathrm{Det}(\lambda I - A) = 0$, where A is the adjacency matrix of the graph whose structure is the same as that of the molecule (when hydrogen-suppressed, as in the case of hydrocarbons, which is the case most commonly quoted in chemistry literature) [12]. The zero of the energy scale is that for no interaction between the separate atomic orbitals within the molecule. Thus, $\lambda = 0$ determines the non-bonding molecular orbitals (NBMO) described by the corresponding linearly independent kernel eigenvectors of A [14]. The solutions also shed light on the electron density distribution in a molecule [2].

The graph ${}^1C_6$,which is C_6 with one pendant edge (shown later in Fig. 4) represents the structure of the benzyl ion (C_6H_5–CH_2) when hydrogen-suppressed. The graph has core number 4 and one kernel eigenvector $(2, 1, -1, -1, 0, 0, 0)^{\mathrm{T}}$ that describes its NBMO. In this case, the vertices of the core represent atoms that have large charge densities. Thus, reactions tend to involve the electron orbitals of these atoms.

A molecule having the shape of Γ_3 mentioned above and bonds represented by the edges of the graph would have 3 NBMOs described by the 3 linearly independent eigenvectors in the nullspace of $A(\Gamma_3)$.

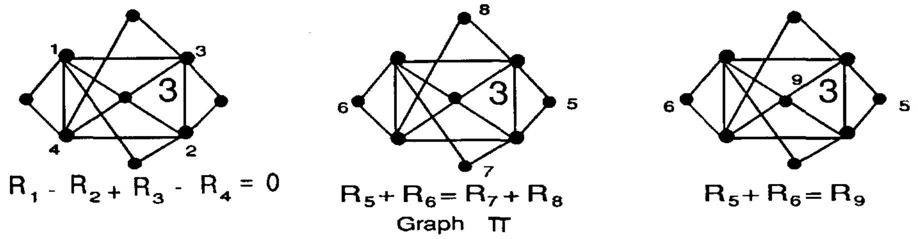

Fig. 2.

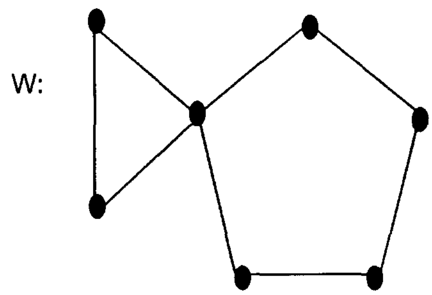

Fig. 3.

A graph may satisfy a number of different relations corresponding to different (labelled) cores. Thus, the graph Π satisfies $R_1 - R_2 + R_3 - R_4 = 0$ which corresponds to core C_4. It also satisfies $R_5 + R_6 = R_7 + R_8$ which corresponds to another core N_4 and $R_9 = R_5 + R_6$ which corresponds to yet another core N_3. This graph is not planar and hence, HMO theory is not applicable [4]. (The numbers, in large type, in Fig. 2 and later in Fig. 4, denote the nullity of the graph depicted.)

Definition. The *Periphery* $\mathscr{P}$ of a singular graph G (with respect to a kernel eigenvector v_0 of G) is the vertex set $\mathscr{V}(G) - \mathscr{V}(\chi)$, where χ is the core corresponding to v_0.

Let G_1 be a connected graph of order n with one zero eigenvalue. If its core χ has nullity 1 and $G_1 = \chi$, then $\mathscr{P} = \phi$ and the kernel eigenvector has $t (= n)$ non-zero components, given by (1). Such a graph, called a nut graph, is W of order 7 (given in Fig. 3) [5]. If χ has nullity $\eta(\chi) > 1$, then in G_1, $\mathscr{P} \neq \phi$. To form G_1, from the same core χ, different sets of edges joining the vertices of the periphery $\mathscr{P}$ to two or more vertices of the core may be found.

2. Minimal configurations

Definition. A connected graph $\mathscr{T}$ is an *Extension* of a graph G if G is an induced subgraph of $\mathscr{T}$ such that

1. $\mathrm{o}(G) < \mathrm{o}(\mathscr{T})$,

2. $\langle \mathscr{V}(T) - \mathscr{V}(G) \rangle$ is null.
$\mathscr{T}$ is also said to be *extended* from G.

Definition. A singular graph Γ of order $n \geqslant 3$, having a core χ_t and periphery $\mathscr{P} := \mathscr{V}(\Gamma) - \mathscr{V}(\chi_t)$ is a *minimal configuration*, of core number t, if the following conditions are satisfied:
(i) $\eta(\Gamma) = 1$,
(ii) $\mathscr{P} = \phi$ or $\mathscr{P}$ induces a null graph,
(iii) and in the case when $\mathscr{P} \neq \phi$, the deletion of $v \in \mathscr{P}$ increases the nullity of Γ.

As the one-dimensional nullspace of $A(\Gamma)$ determines both the core $\chi_t = \langle v_1, v_2, \ldots, v_t \rangle$ and the kernel relation $\mathscr{R}_t : \alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0$, where α_i are non-zero integers, it is convenient to refer to the minimal configuration Γ as $(\Gamma, \mathscr{R}_t, \chi_t)$.

Theorem 2. *A minimal configuration $(\Gamma, \mathscr{R}_t, \chi_t)$ is an extension of the core, χ_t, so that it is connected. The valency of a vertex in the periphery is at least* 2.

Proof. Suppose that Γ is not connected. Then it has a component K containing some of or all the vertices of the core χ_t. The adjacency matrix of Γ may be partitioned as follows:

$$A(\Gamma) = \begin{pmatrix} A(K) & \vdots & 0 \\ \cdots & & \cdots \\ 0 & \vdots & A(H) \end{pmatrix}.$$

Let v_0 be a kernel eigenvector. If the core is a subgraph of K, then the vertices of H are in the periphery and so H is a null graph. Thus, the nullity of Γ is more than one; a contradiction. If, on the other hand, the core has vertices both in K and H, let $v_0 = (\alpha_1, \alpha_2, \ldots, \alpha_r, 0, 0, \ldots, 0, \beta_1, \beta_2, \ldots, \beta_s, 0, \ldots, 0)^{\mathrm{T}}$ where the αs are the non-zero components of v_0 corresponding to the vertices of K and the βs are those corresponding to the vertices of H. Then each of the vectors $(\alpha_1, \alpha_2, \ldots, \alpha_r, 0, 0, \ldots, 0)^{\mathrm{T}}$ and $(0, 0, \ldots, 0, \beta_1, \beta_2, \ldots, \beta_s, 0, \ldots, 0)^{\mathrm{T}}$ are kernel eigenvectors of Γ; again a contradiction. Hence, Γ is connected. Furthermore, the vertices in $\mathscr{P}$ (if not empty) have no edges between them and so are adjacent to those of the core, by definition of minimal configuration. So Γ is an extension of the core.

Suppose, now, that $v \in \mathscr{P}$ and v is a terminal vertex adjacent to vertex v_j of the core. Then if α_j is the component of a kernel eigenvector v_0 of Γ corresponding to vertex v_j then $A(\Gamma)(v_0) = 0 \Longrightarrow \alpha_j = 0$; a contradiction as α_j is also a component of a kernel eigenvector of the core. Hence, the valency of a vertex in the periphery is at least 2. $\square$

2.1. Illustration: construction of the minimal configurations of core number 4

An algorithm to construct the *minimal configurations*, $(\Gamma, \mathscr{R}_4, \chi_4)$ of core-number 4, is now presented. A graph Γ, with adjacency matrix $A = (R_1, R_2, \ldots)^{\mathrm{T}}$, for which a relation $\mathscr{R}_4$:

$$\alpha_1 R_1 + \alpha_2 R_2 + \alpha_3 R_3 + \alpha_4 R_4 = 0 \tag{2}$$

(where α_i are non-zero integers and g.c.d.(α_i)=1) holds, is required.
The corresponding core is $\chi_4 = \langle v_1, v_2, v_3, v_4 \rangle$ and the kernel eigenvector v_0 is $(\alpha_1, \alpha_2, \alpha_3, \alpha_4, 0, \ldots, 0)^{\mathrm{T}}$, with exactly 4 non-zero components.

For $\chi_4 - v_4 = \langle v_1, v_2, v_3 \rangle$, all graphs on 3 vertices, namely K_3, $K_{1,2}$, $K_2 \dot{+} N_1$ and N_3 are considered. To determine the core, all possible one-vertex extensions of each, satisfying $\mathscr{R}_4$, are considered in turn. Let the additional vertex be v_4. There are $2^3 = 8$ possibilities for v_4. Taking each in turn and solving the resulting equations, only two cores are found to satisfy (2). These are C_4 which has nullity 2 and N_4 which has nullity 4.

At this stage (2) is not determined having 1 and 3 unknowns, respectively, relative to α_1. To form a minimal configuration from C_4, with (2) completely determined, another vertex, adjacent to two or more vertices of the core, is required to reduce the nullity to 1. A unique extension Λ (up to isomorphism) is obtained with nullspace $\{v_0\} = \{(1, -1, 1, -1, 0)^{\mathrm{T}}\}$. To form a minimal configuration from N_4 another three vertices, each of which is adjacent to two or more vertices of the core, are required to reduce the nullity to 1. Four distinct one-dimensional nullspaces are obtained, viz.,

$$\{(1, -1, 1, -1, 0, 0, 0)^{\mathrm{T}}\}, \quad \{(1, 1, -1, 1, 0, 0, 0)^{\mathrm{T}}\}, \quad \{(1, 1, -2, 1, 0, 0, 0)^{\mathrm{T}}\},$$
$$\{(2, 1, -1, -1, 0, 0, 0)^{\mathrm{T}}\}.$$

Each eigenvector gives at least one minimal configuration. With reference to Fig. 4, $v_0 = (1, -1, 1, -1, 0, 0, 0)^{\mathrm{T}}$ gives two minimal configurations P_7 and Γ_1; $v_0 = (1, 1, -1, 1, 0, 0, 0)^{\mathrm{T}}$ gives $S(K_{1,3})$; $v_0 = (1, 1, -2, 1, 0, 0, 0)^{\mathrm{T}}$ gives $H(K_4)$; $v_0 = (2, 1, -1, -1, 0, 0, 0)^{\mathrm{T}}$ gives ${}^1C_6$. This completes the construction.

There may be different minimal configurations for the same relation $\mathscr{R}_t$: $\alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0$, and core $\chi = \langle v_1, v_2, \ldots, v_t \rangle$. These have different sets of edges joining the vertices of the periphery whose vertices correspond to different submatrices $(R_{t+1}, R_{t+2}, \ldots, R_n)^{\mathrm{T}}$ of A. Thus, P_7 and Γ_1 are two minimal configurations for the same core N_4 and the same eigenvector

$$v_0 = (1, -1, 1, -1, 0, 0, 0)^{\mathrm{T}}. \tag{3}$$

The graph Γ_1 has P_7 as a subgraph but both Γ_1 and P_7 are minimal configurations as each has nullity one, $\langle \mathscr{P} \rangle = N_3$, and the deletion of a vertex from the periphery increases the nullity in the resulting graph in each case.

The questions considered now are whether larger extensions of the core exist for the *same* relation between the vertices of the core, and whether the nullity in the

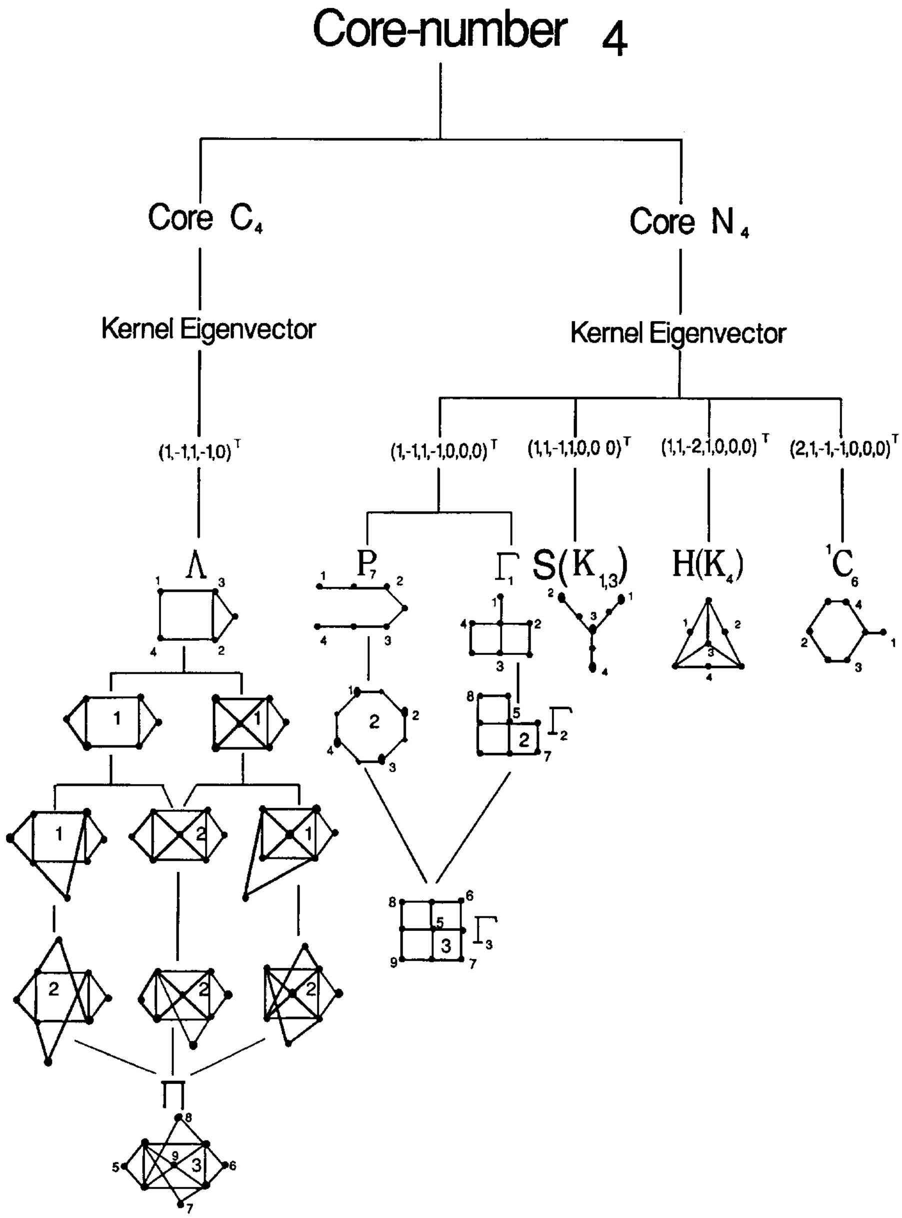

Fig. 4.

resulting extension is preserved. Adding another vertex adjacent to the core of Γ_1 so that the resulting graph Γ_2 has the eigenvector $v_0 = (1,-1,1,-1,0,0,0,0)^{\mathrm{T}}$ increases the nullity to 2 as besides the kernel relation of Γ_1

$$R_1 - R_2 + R_3 - R_4 = 0, \tag{4}$$

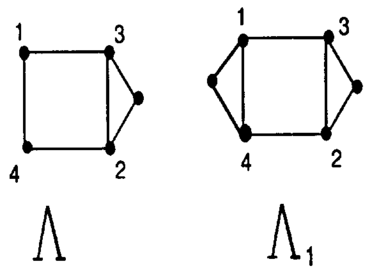

Fig. 5.

the graph Γ_2 also satisfies $R_7 + R_8 = R_5$. This graph is called an intermediate configuration[3] as another vertex may be added to it adjacent to the vertices of the core to obtain Γ_3. Relation (4) is still satisfied by Γ_3 but the nullity increases to 3 as

$$R_1 - R_2 + R_3 - R_4 = 0, \qquad R_7 + R_8 = R_5 \qquad \text{and} \quad R_6 + R_9 = R_5.$$

Thus, Γ_2 has the two linearly independent kernel eigenvectors $(1,-1,1,-1,0,0,0,0)^{\mathrm{T}}$ and $(0,0,0,0,-1,0,1,1)^{\mathrm{T}}$, respectively. Similarly, Γ_3 has 3 linearly independent kernel eigenvectors. Thus, molecules having structures Γ_1, Γ_2 and Γ_3 have 1, 2 and 3 NBMOs, respectively.

Since no more vertices adjacent to the core (other than those of the same type) may be added to Γ_3 without altering the kernel relation (4) then Γ_3 is called a maximum configuration[3] for core N_4 and relation(4). It is noted that Γ_3 may also be 'grown' from P_7 which has the same eigenvector $v_0 = (1,-1,1,-1,0,0,0)^{\mathrm{T}}$ as Γ_1. An intermediate configuration is then C_8 with nullity 2 and the maximum configuration is Γ_3 with nullity 3. Besides being an intermediate configuration, corresponding to minimal configuration P_7, the graph C_8 is a core for a minimal configuration of core number 8 as $(1,-1,1,-1,1,-1,1,-1)^{\mathrm{T}}$ is a kernel eigenvector.

This algorithm is illustrated in Fig. 4.

In the above construction, the nullity of the extensions of the graphs P_7 and Γ_1 has increased. An example of a minimal configuration of core number 4 whose nullity remained unchanged on extension is Λ shown in Fig. 5.

Λ and its extension Λ_1 have core C_4, eigenvectors $(1,-1,1,-1,0)^{\mathrm{T}}$ and $(1,-1,1,-1,0,0)^{\mathrm{T}}$, respectively, and $\eta = 1$.

Definition. A *maximum configuration*, $(\Gamma'', \mathscr{R}_t, \chi_t)$, is an extension of the core χ_t of a minimal configuration $(\Gamma, \mathscr{R}_t, \chi_t)$ if Γ'' is a singular graph with adjacency matrix A such that

1. Γ is a subgraph of Γ'',
2. $\langle \mathscr{P} \rangle$ is a null graph and

[3] The formal definition will appear later.

3. Γ'' has the maximum number of vertices $v_{t+1}, v_{t+2}, \ldots, v_n$, in $\mathscr{P}$, adjacent to vertices of the core, corresponding to rows $R_{t+1}, R_{t+2}, \ldots, R_n$ of A (no two of which are equal) such that relation $\mathscr{R}_t$ is still satisfied.

It follows that the maximum configuration is a connected graph.

Lemma. *Let χ_t be a graph of nullity* more than one *having a kernel eigenvector with no zero components and a kernel relation $\mathscr{R}_t$. An extension of χ_t of the least order such that $\eta(\Gamma) = 1$ is a minimal configuration $(\Gamma, \mathscr{R}_t, \chi_t)$. The largest extension of χ_t (excluding vertices of the same type) such that the kernel relation still holds is the maximum configuration $(\Gamma'', \mathscr{R}_t, \chi_t)$.*

Thus, the maximum configuration has core χ_t and periphery which includes the union of the peripheries, of all the minimal configurations having the same core and relation, as described by the row vectors in their respective adjacency matrices.

Lemma. *Every minimal configuration of core number t, satisfying the same relation $\alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0$, and having the same core $\chi_t = \langle v_1, v_2, \ldots, v_t \rangle$, is a subgraph of the same maximum configuration.*

Extensions leading to a maximum configuration may be constructed when, for the same core and relation, there are more than one minimal configuration or isomorphic minimal configurations (with different labellings).

Definition. An *intermediate configuration* $(\Gamma', \Gamma, \mathscr{R}_t, \chi_t)$ corresponding to the minimal configuration $(\Gamma, \mathscr{R}_t, \chi_t)$ is a connected singular graph Γ' such that
1. Γ' has Γ as a subgraph
2. Γ' has more vertices than Γ but only a proper subset of the peripheral vertices of the corresponding maximum configuration Γ'' and
3. the relation $\mathscr{R}_t$ is still satisfied.

2.2. *Algorithm to construct a minimal configuration*

The algorithm constructs $(\Gamma, \mathscr{R}_t, \chi_t)$, a minimal configuration of core number t satisfying the relation $\mathscr{R}_t$: $\alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0$, $\alpha_i \neq 0, \forall i$.
Let $A = (R_1, R_2, \ldots, R_t, R_{t+1}, \ldots, R_n)^{\mathrm{T}}$ and H_{t-1} be an arbitrary graph of order $(t-1)$.
To determine the core χ_t and the corresponding relation $\mathscr{R}_t$, all possible one-vertex extensions of H_{t-1} that satisfy $\mathscr{R}_t$ are considered systematically. Let the additional vertex be v_t. There are 2^{t-1} possibilities to consider. For each possible core χ_t, the nullity μ is determined. Since N_t is a possible core and $v_0 = (\alpha_1, \alpha_2, \ldots, \alpha_t, 0, \ldots, 0)^{\mathrm{T}}$, $\alpha_i \neq 0, \forall i$, is in the eigenspace of $\lambda = 0$ (i.e., in the nullspace of A) then $\mu \geqslant 1$. Once the core χ_t is determined, v_0 has $(\mu - 1)$ 'unknowns' relative to α_1. To determine these unknowns, groups of $(\mu - 1)$ vertices are considered in turn from the set of t-tuples

(having entries 0 or 1), which are row vectors describing vertices adjacent to χ_t. Each group $\mathscr{B}$ of $(\mu - 1)$ vertices that determine v_0 uniquely provides an extension of χ_t of order $(t+\mu-1)$. This extension of χ_t by $\mathscr{B}$ is a minimal configuration $(\Gamma, \mathscr{R}_t, \chi_t)$. The procedure is repeated for all other possible graphs H_{t-1}. Since straightforward proofs show that a core can neither have a terminal vertex, nor does it have an odd circuit or a complete graph as a disjoint component, nor is it an extension of K_{t-1}, the algorithm can be shortened considerably.

This algorithm determines the kernel eigenvectors v_0 for $2 \leqslant t \leqslant 5$. The minimal configurations for $t \leqslant 4$ were calculated manually but for $t = 5$ the use of an appropriate software could not practically be avoided. The next two theorems present the unique minimal configurations (up to isomorphism) obtained for $2 \leqslant t \leqslant 5$.

Theorem 3. *The minimal configurations* $(\Gamma, \mathscr{R}_t, \chi_t)$ *for* $t \leqslant 4$ *are*

- $t = 2$ $\mathscr{R}_t$: $R_1 = R_2$, $\chi_2 = N_2$, $\Gamma = P_3$ of rank 2.
- $t = 3$ $\mathscr{R}_t$: $R_1 + R_2 = R_3$, $\chi_3 = N_3$, $\Gamma = P_5$ of rank 4.
- $t = 4$ $\mathscr{R}_t$: $R_1 - R_2 + R_3 - R_4 = 0$, $\chi_4 = C_4$, $\Gamma = \Lambda$ of rank 4,
  $\mathscr{R}_t$: $R_1 - R_2 + R_3 - R_4 = 0$, $\chi_4 = N_4$, $\Gamma = P_7$ *or* Γ_1 both of rank 6,
  $\mathscr{R}_t$: $R_1 + R_2 - R_3 + R_4 = 0$, $\chi_4 = N_4$, $\Gamma = S(K_{1,3})$ of rank 6,
  $\mathscr{R}_t$: $R_1 + R_2 - 2R_3 + R_4 = 0$, $\chi_4 = N_4$, $\Gamma = H(K_4)$ of rank 6,
  $\mathscr{R}_t$: $2R_1 + R_2 - R_3 - R_4 = 0$, $\chi_4 = N_4$, $\Gamma = {}^1C_6$ of rank 6.

The minimal configurations for $t = 4$ are given in Fig. 4.

Theorem 4. *There are* 53 *distinct minimal configurations* $(\Gamma, \mathscr{R}_5, \chi_5)$, *of core number* 5, *represented in Figs.* 12(a) *and* (b).

— Core : $C_4 \dot{+} N_1$: There are 3 linearly independent kernel eigenvectors to which correspond 10 minimal configurations of rank 6.
— Core : $K_{2,3}$: There is 1 kernel eigenvector to which correspond 3 minimal configurations of rank 6.
— Core : N_5: There are 17 linearly independent kernel eigenvectors to which correspond 40 minimal configurations of rank 8.

The above configurations were obtained using the software package 'Mathematica' in programming mode. Two main programs were processed. The first produced the one-dimensional nullspace $\{v_0\}$ of each of the possible minimal configurations with one of the three cores in turn. The output of the second consisted of the sets $\mathscr{B}$, each of which describes a minimal configuration for a particular core and a particular nullspace $\{v_0\}$.

To ensure that $\alpha_i \neq 0$ $\forall i, 1 \leqslant i \leqslant 5$, the sets $\mathscr{B}$ of vertices were found such that $A(v_0) = 0$ and $A(G - v_i)(v_0) \neq 0$, where v_i is each of the vertices of the core in turn and $G - v_i$ is the corresponding vertex-deleted subgraph of G. Care was taken to select only non-isomorphic minimal configurations from the output. For instance, for core

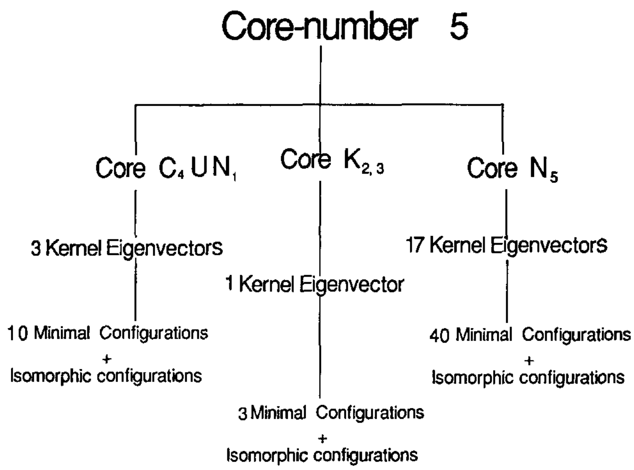

Fig. 6.

N_5, the kernel eigenvectors whose non-zero components were the same but ordered differently, produce isomorphic minimal configurations.

3. Construction of larger singular graphs

3.1. Use of the characteristic polynomial

A well-known relation for the characteristic polynomial $\phi(G)$ of a graph G is given in the following theorem [7, 10]:

Theorem 5. *If $G-v$ is the subgraph obtained from G by deleting vertex v, and $N(v)$ denotes the set of neighbouring vertices of v, then the characteristic polynomial $\phi(G)$ of G is*

$$\phi(G) = \lambda\phi(G-v) - \sum_{w \in N(v)} \phi(G-v-w), \tag{5}$$

provided no subgraph of G is a circuit passing through v.

Corollary 1. *If $\forall w \in N(v)$, $G-v-w$ is singular then so is G.*

Definition. Let G be a graph and $v \in \mathscr{V}(G)$.
(i) v is *critical* in G if G is non-singular and $G-v$ is singular.
(ii) G is a *critically non-singular* graph if $\forall v \in \mathscr{V}(G)$, v is critical in G.

An infinite family of critically nonsingular graphs consists of the bipartite nonsingular graphs of even order such as C_{4t+2} and P_{2t}.

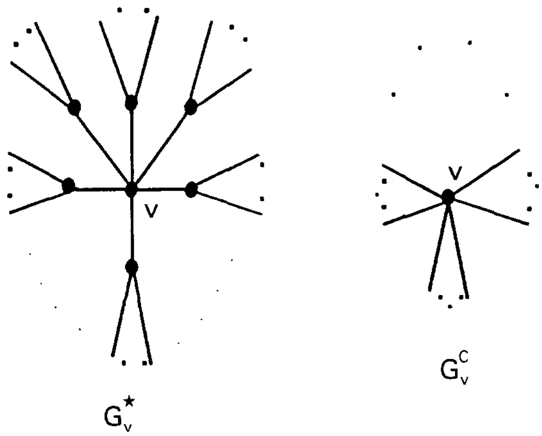

Fig. 7.

Definition. The graph G_v^* is constructed by joining an isolated vertex v to one vertex v_j of each of r disjoint connected graphs $G_j, j = 1, 2, \ldots, r$.

Corollary 2. *The characteristic polynomial of G_v^* is given by*

$$\phi(G_v^*) = \lambda \prod_j \phi(G_j) - \sum_j \Big(\phi(G_j - v_j) \prod_{i \neq j} \phi(G_i) \Big).$$

Proof. Since $G_v^* - v$ is the disjoint union of $G_1, G_2, \ldots, G_r$, then $\phi(G_v^* - v)$ is the product of $\phi(G_1), \phi(G_2), \ldots, \phi(G_r)$. If a component G_j of $G_v^* - v$ has v_j connected to v then $G_v^* - v - v_j$ is the disjoint union of $G_j - v_j$ and G_i, $i \neq j$. The result follows from (5). □

Theorem 6. *Let the connected components of the graph $G_v^* - v$ be $G_1, G_2, \ldots, G_r$. If two or more of the graphs $G_1, G_2, \ldots, G_r$, are singular or if v_i is critical in G_i, $\forall i = 1, 2, \ldots, r$, then G_v^* is singular.*

A similar result may be obtained using Schwenk's formula for the characteristic polynomial of the coalescence $K.H$ of two rooted graphs (K, u), (H, w) obtained by identifying the vertices u, and w so that this vertex $v = u = w$ becomes a cut-vertex [7]:

$$\phi(K.H) = \phi(K)\phi(H - w) + \phi(K - u)\phi(H) - \lambda\phi(K - u)\phi(H - w).$$

Definition. The graph G_v^C is constructed by identifying one vertex v_j of each of r disjoint graphs $G_j, j = 1, 2, \ldots, r$.

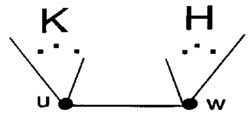

Fig. 8.

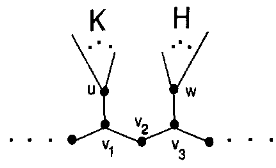

Fig. 9.

Lemma. *The characteristic polynomial of* G_v^C *is given by*

$$\phi(G_v^C) = \sum_j \Big(\phi(G_j)\prod_{i \neq j}\phi(G_i - v_i)\Big) - (r-1)\lambda\prod_j(\phi(G_j - v_j).$$

The proof follows by induction on r.

Definition. Let K, H be two labelled graphs such that graph $G = K \cup H$ and graph $P = K \cap H$. Then K, H are said to be the *parts* of G.

Theorem 7. *Let the parts of the graph* G_v^C *be* $G_1, G_2, \ldots, G_r$, *and their intersection be* $\langle v\rangle$. *If* G_i *is singular,* $\forall i = 1, 2, \ldots, r$, *or* v_i *is critical in* G_i, *for* 2 (*or more*) *distinct* $i \in 1, 2, \ldots, r$, *then* G_v^C *is singular.*

If (K, u) and (H, w) are two rooted graphs, then the characteristic polynomial of the graph $KH + uw$, given in Fig. 8, obtained by joining vertices u, w [7] is

$$\phi(KH + uw) = \phi(K)\phi(H) - \phi(K - u)\phi(H - w). \tag{6}$$

Theorem 8. *Let the components of the graph obtained by deleting edge* uw *from* $KH + uw$ *be* (K, u) *and* (H, w). *If one of the following conditions is satisfied then* $KH + uw$ *is singular.*

1. *One component and its root-deleted subgraph are singular.*
2. *One component and the root-deleted subgraph of the other component are singular.*

Theorem 9. *Let path* P_{2t-1}, $t \geqslant 2$ *be labelled so that* v_1, v_2, v_3 *are* 3 *consecutive vertices and* v_2 *is a vertex of the core of the path. Let* (K, u) *and* (H, w) *be two rooted*

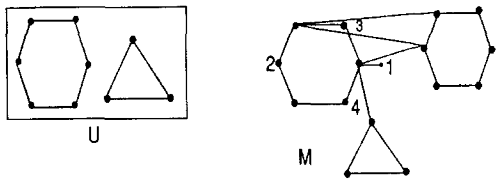

Fig. 10.

non-singular graphs and $KH + P_{2t-1}$, drawn in Fig. 9, be constructed such that v_1 is joined to u and v_3 is joined to w. Then $KH + P_{2t-1}$ has nullity one.

The proof follows from (6).

This result agrees with that obtained by using a well-known theorem that states that the nullity is preserved when a terminal vertex and its neighbour are deleted [3,13]. A more general construction is presented in the next theorem.

3.2. Extension of $\langle P \rangle$

The importance of the distinction between the vertices of the core and of the periphery is apparent from the following theorem.

Theorem 10. *Let G be a singular graph satisfying a relation $\mathscr{R}_t$, $t < o(G)$. If such a graph G has a core χ_t and periphery $\mathscr{P}$, and graph G^N is produced by joining one or more vertices in $\mathscr{P}$ to vertices of a graph N, then the kernel relation $\mathscr{R}_t$ will still be satisfied.*

Proof. There exists a labelling of G for which a relation between the row vectors of $A(G)$ is

$$\mathscr{R}_t: \quad \alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0, \; \alpha_i \neq 0, \tag{7}$$

$t \leqslant o(G)$. The corresponding kernel eigenvector is $(\alpha_1, \alpha_2, \ldots \alpha_t, 0, 0, \ldots, 0)^{\mathrm{T}}$. The graph G^N has an eigenvector with the same non-zero components corresponding to the vertices of the core, all other components being zero. □

In Fig.10 graph U is $C_6 \dot{+} K_3$. Graph M is produced by joining vertices of the periphery of the minimal configuration ${}^1C_6$ to vertices of U. From the above theorem it follows that U and ${}^1C_6$ satisfy the same relation $2R_1 + R_2 - R_3 - R_4 = 0$.

Lemma. *Let G be a graph of order n. Let each vertex of G be joined to a terminal vertex to form a graph G^L of order $2n$ having n more edges than G and at least n terminal vertices. Then G^L is a non-singular graph.*

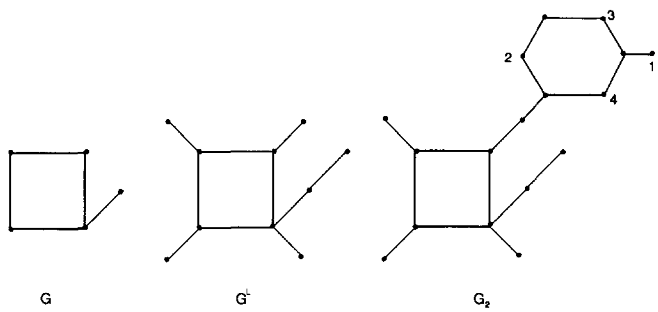

Fig. 11.

Proof. Let $v_1, v_2, \ldots, v_n$ be a labelling for G and let G^L be an extension of G so that v_{n+i} is the terminal vertex adjacent to v_i, $1 \leqslant i \leqslant n$. The adjacency matrix of G^L may be partitioned into 4 submatrices of order $n \times n$. Thus,

$$A(G^L) = \begin{pmatrix} A(G) & \vdots & I_n \\ \cdots & & \cdots \\ I_n & \vdots & 0 \end{pmatrix},$$

where the principal submatrix is $A(G)$, I_n is the identity matrix and 0 is the zero matrix. Since I_n is non-singular, the rank of G^L is $2n$ and $\eta(G^L) = 0$. $\square$

Theorem 11. *Let G_1 be a graph of nullity one satisfying the kernel relation $\mathscr{R}_t$: $\alpha_1 R_1 + \alpha_2 R_2 + \cdots + \alpha_t R_t = 0$, $\alpha_i \neq 0$, for $1 \leqslant i \leqslant t$ and $t < \mathrm{o}(G_1)$. Then a graph G_2, constructed by joining one vertex of the periphery of G_1 to one vertex of a non-singular graph of the form G^L, is also of nullity one, satisfying $\mathscr{R}_t$.*

Proof. When a terminal vertex and its neighbour are deleted from the graph G_2, the nullity is preserved. Thus, G_1 and G_2 have the same nullity, that is one. Furthermore, by Theorem 10, G_2 satisfies the kernel relation $\mathscr{R}_t$. Hence, the coefficients of $\mathscr{R}_t$ are the non-zero components of the kernel eigenvector of G_2, which is unique (up to scalar multiples). $\square$

In Fig. 11, G is a graph of order 5 and G^L is a non-singular graph of order 10. If G_1 is ${}^1C_6$, which has nullity one, then G_2 is also of nullity one.

It may be concluded that a sufficient condition for a graph to be singular is that it has one of the following induced subgraphs:

(i) a minimal configuration;

(ii) a minimal configuration having edges between the vertices in the periphery.

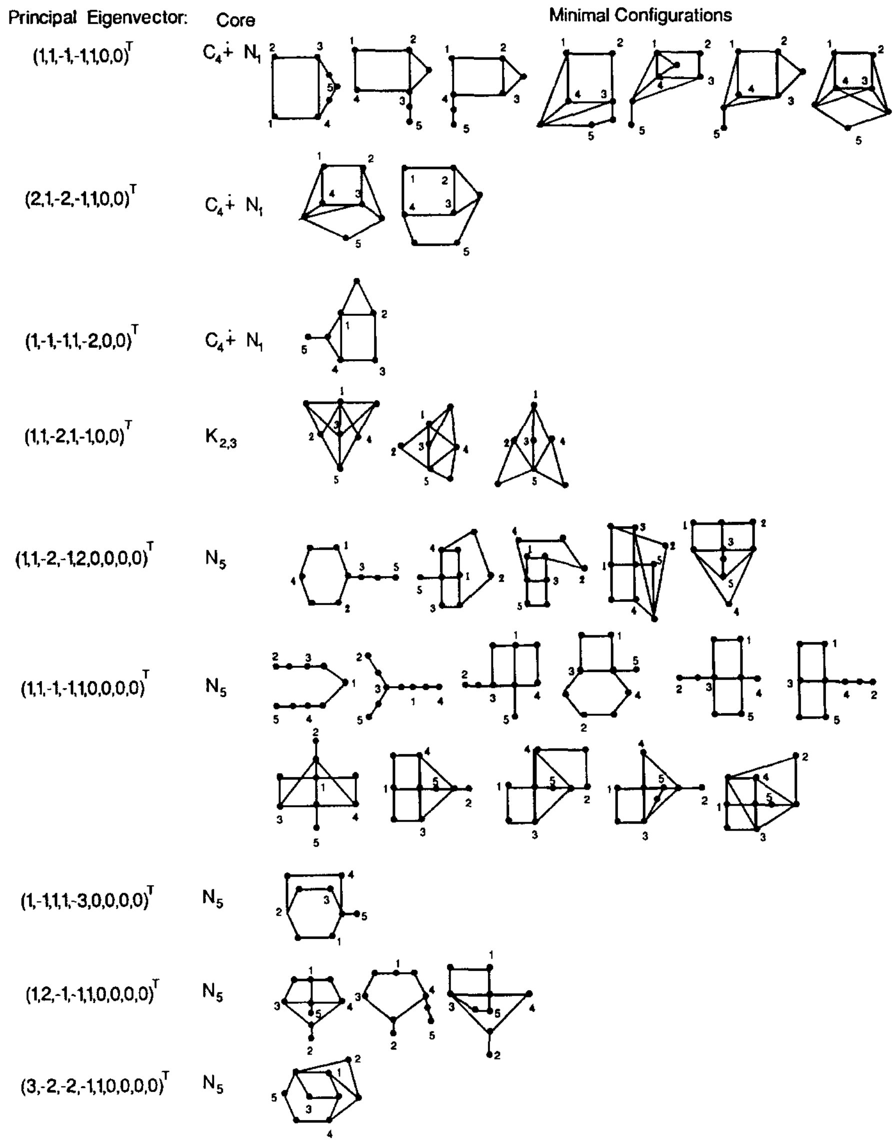

Fig. 12. a

The lists of kernel eigenvectors and their corresponding minimal configurations are useful to point out properties common to singular graphs. It is observed that the cores of order at most 5 (considered here) have nullity greater than one. It turns out from related work [6,11] that nullity one can be achieved for cores of all orders at least 7.

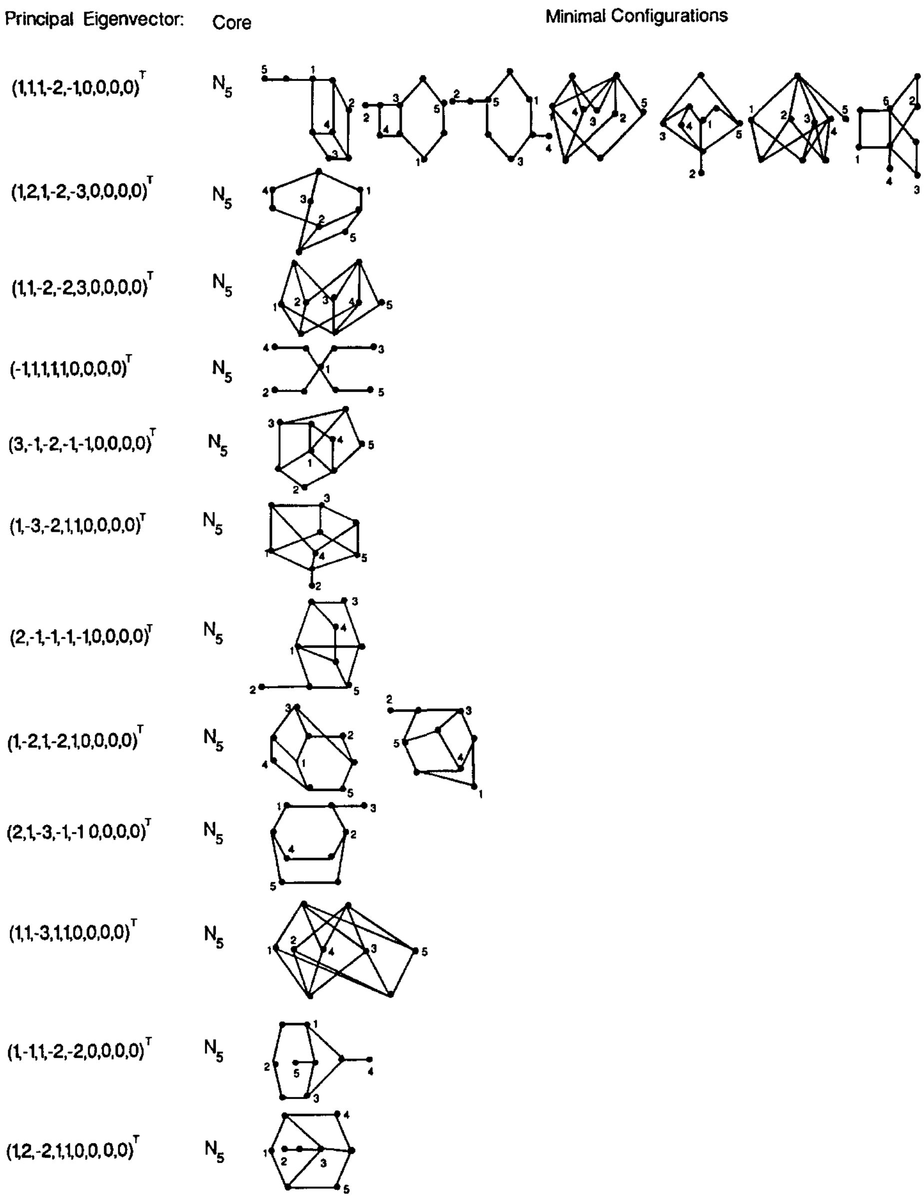

Fig. 12. b

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