Commentary

Graphs and their Spectra

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From the contributions to conferences and journals, it is cvident that most of the rcsearch in mathematics is directed towards the development of the theoretical aspect of its various arcas. In this sense mathematics is an art fathomed and pondcred on for the sake of its own bcauty. It has determined the direction of most of the significant research in other fields. Being an incomparablc human achievement. mathematical creativity has fathered our understanding about the nature of man and his universe. Invariably, apparently futile results find inlniediatc applications in various fields.

Graph theory started as a musing brain teasers from the days of Euler, who showed, in the eighteenth century, that the seven Königsberg bridges cannot be crossed just once in a closed route, and of Guthrie and De Morgan who. in the nineteenth century. questioned the number of colours required to colour a map. Since then it has been taught under various guises including operational rcscarch in management studies, network theory in engineering and algorithms in computer science. It has become a valuablc forecasting tool in several applications in industry and commerce.

Since 1939. chemists investigating molecular orbitals noticed a relationship between the energy levels and the stability of a molecule. The Hückel molecular orbital theory gives an approximation of the π-molecular orbitals of a molecule by expressing them as a linear combination of the atomic pre-orbitals (Cotton. 1963; Coulson and Rushbrook. 1940; Zivkovic.1972). When Schrödinger's equation, that determines the molecular orbital energies. is simplified. the resulting equation is the characteristic equation Det(λI−A) = 0. where A is the adjacency matrix of the graph whose structure is the same as that of the molecule being considered (when hydrogens suppressed. as in the case of hydrocarbons. which is the case most commonly quoted in chemistry literature) (Spinlter. 1964). The spectrum of a graph is the solution of the characteristic equation of its adjacency matrix and the eigen values in the spectrum describe the energy of the orbitals of the molecule whose structure is the same as that of the graph.

The investigation of Graph Spectra is one of the foremost problems of current research in the theory of graphs. Several important researchers have addressed the problem and the theory is sufficiently advanced so that state-of-the-art books synthesizing results have already appeared. In spite of this, there is ample scope for further research. One of the best books that offers a survey of the work done in this area up to a few years ago. is Spectra of Graphs by Cvetkovic and co-workers. 1980. When Cvetkovic was about to present his Ph.D. thesis on the spectra of graphs, an established physical chemist, I. Gutman showed a keen interest in his results. He realised that for a class of molecules the eigenvalues in the spectrum of a graph were precisely the energy of the orbitals of the molecule whose structure is the same as that of the graph.

The zero of the energy scale is that for no interaction between the separate atomic orbitals within the molecule (Karplus and Porter, 1970). Thus the zero eigenvalues, $h=0$, determine the non-bonding molecular orbitals (NBMO) responsible for the instability of a molecule. The NBMO are described by the corresponding linearly independent kernel eigenvectors of A (Zivkovic, 1972). The solutions also shed light on the electron density distribution in a molecule (Cotton, 1963). So the results of graph spectra are of great interest in chemistry.

The mathematical analysis of an existing molecule in terms of its spectrum may be investigated if the bonds between the atoms are known. The data is represented as an adjacency list expressing the neighbouring atoms of each atom in the molecule or as a (0-1) adjacency matrix A in which an i-j entry is 1 if the corresponding atoms are bonded within the molecule and zero otherwise. The vanishing of the determinant of A is an indication of instability. Even the characteristic equation itself, Det(λI−A) = 0, where A is the adjacency matrix of the graph whose structure is the same as that of the molecule being considered gives a number of results about the structure of the molecule.

A graph whose adjacency matrix has the number zero in its spectrum is said to be singular. Although some results regarding bipartite graphs have already appeared in the literature, identification especially for arbitrary graphs is complex as with increasing order the number of basic structures responsible for the singularities increases enormously.

As highly reactive molecules are difficult to prepare and to isolate, and very unstable, it would be useful to predict their possible structure. The characterisation of singular graphs is still an open question. In this respect the author has had some success in characterising minimal configurations (Sciriha, 1996). A systematic search for the minimal configurations in singular graphs that give rise to a singularity was carried out on the grounds that a linearly dependent set of t row vectors of A, the adjacency matrix of the graph, is present. The linear combination between the t row vectors is termed a kernel relation and is denoted R_t. It is noted that the coefficients of the kernel relation are the ordered entries of the corresponding kernel eigenvector in the nullspace of A. An algorithm was set up to identify the non-isomorphic singular graphs for successive values of t. This theory becomes more and more cumbersome when applied to large systems. One can practically not avoid the use of an appropriate software package, such as MATHEMATICA, used in programming mode, for values of t larger than or equal to 5.

The first stage was to determine the core, χ_t, which is the subgraphs induced by the vertices corresponding to these t row vectors of A. From the core χ_t, a minimal configuration (Γ_t, χ_t, R_t) is "grown" by adding a periphery, a set of vertices adjacent to those of the core, until the number of zero eigenvalues in the spectrum of the resulting graph G, called the nullity of the graph G, is reduced to one. In the case when the core has one zero eigenvalue in its spectrum then the minimal configuration, Γ_t is the core itself. Such a graph has been called a nut graph as the periphery is empty (Gutman and Sciriha, 1995). The core χ_t and kernel relation R_t of the minimal configurations Γ_t, thus obtained will be unique. There may be several peripheries for the same core and kernel relation so that there is a many-to-one correspondence between the structures of minimal configurations Γ_t and the pair (χ_t, R_t). Such minimal configurations are the subgraphs found in all singular graphs. The 61 minimal configurations for t less or equal to 5 have been characterized. Several properties for larger t have also been established.

The core may shed light on the charge density distribution in a molecule. The vertices of the core have been shown to correspond to atoms that are charge rich in some ions and molecules. These are the atoms that are likely to be involved in chemical reactions.

As different minimal configurations may be "grown" from the same core, a maximum configuration may be set up by including all the peripheral vertices used to build up the minimal configurations from a core χ_t satisfying the relation R_t. In this way the largest graph with the number zero in its spectrum satisfying a particular kernel relation R_t with all the vertices of the periphery joined to those of the core and themselves inducing a null graph, is obtained. This configuration may have more than one zero eigenvalue. Corresponding to each zero eigenvalue is a core and a particular kernel relation (Sciriha, 1995a).

The graph may be enlarged further by including edges between the vertices in the periphery and also by joining arbitrary graphs to the vertices in the periphery. In this way the order of the graph may be increased indefinitely without upsetting the core χ_t or the relation R_t. So will the rank of the graph which is equal to the order less the nullity.

In 1993 M. Ellingham published a paper showing that he has addressed the problem of singular graphs from a different point of view (Ellingham, 1993). He also built a singular graph G from "basic subgraphs". These he defined as non-singular graphs of order r where r is the rank of the adjacency matrix of G. It has also been interesting to investigate graphs of small rank. As the order of a graph is increased the rank is kept fixed or under control at small values by adding vertices which increase the nullity, that is the number of zero eigenvalues in the spectrum. Thus as new vertices are included more minimal configurations are discovered as subgraphs. For very small rank only complete k-partite graphs are admissible, allowing only vertices of the same type, that is vertices having the same set of neighbouring vertices. For rank greater than or equal to 4 more minimal configurations contribute to the nullity.

As the set of minimal configurations characterizing singular graphs is being collected and their properties studied, certain common properties are already apparent. In fact several conjectures have been made, the validity of which will be investigated. One such conjecture is on the common value L of the coefficient of λ of the characteristic polynomial $\mathrm{Det}(\lambda I - A)$ where A is the adjacency matrix of the graph, for minimal configurations grown from the same core for the same kernel relation. It is conjectured that L may be expressed in terms of the properties of the vertex-deleted subgraphs of the corresponding minimal configuration (Sciriha, 1995b).

J.J. Seidel who is one of the pioneers of the development of Graph Spectra stressed his belief that the eigensolution holds the secrets to the understanding of graphs and the systems they model. The aim of this work is to unravel some solutions of significant importance.

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