Research Article

Discussion on reciprocal graph from graph theoretical point of view

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Abstract

Over the few years graph theory has been one of the most rapidly growing areas of mathematics. Very basic ideas of graph theory with its introduction as well as its few applications in the field of Chemistry are discussed here. In the field of graph theory reciprocal graphs are very important because of their distinct characteristics. Eigenspectral properties of such graphs are mainly focused here.

Key Words: Graph theory; Reciprocal graphs; Eigenspectral properties.

Introduction

Graph theoretical ideas were first introduced in the year of 1736 when Leonhard Euler presented his solution of Königsberg bridge problem\(^1^\)\(^\text{-}^6\). In the year of 1857 Aurther Cayley used graphical concept of tree while he was trying to enumerate the number of isomers of alkanes, \(C_nH_{2n+2}\)\(^1\)\(^\text{-}^7\). Four colours problem first presented by A. F. Möbius became well known after Cayley published it in the first volume of the Proceedings of the Royal Geographical Society in 1879\(^1^\)\(^\text{-}^5\),\(^8\). Till date, the four colours conjecture so far is a famous unsolved problem in graph theory, although an enormous amount of research has been done in this field. The first mention of a graph was not before 1878. J.J. Sylvester first introduced the terminology ‘graph’ in the year of 1878\(^9\). From the time of terminology ‘graph’ was used in mathematics and also in the field of chemistry to represent the molecular structural formulas. The essence and beauty of graph theory attracted mathematicians thus a great deal of research has been done and is being done in this area. By now graph theory exists as a separate field in Mathematics. Huge numbers of books on mathematical graph theory have been appeared. Oystein Ore, Robin J.Wilson and Frank Harary have a great contribution to this field\(^2\),\(^10\),\(^11\). Although graph theory is a discipline of pure mathematics, it is applied in theoretical chemistry along with its
considerable applications\textsuperscript{12-16}. A great deal of research has been done and is being done in this area. Graph theoretical ideas are applied in quantum mechanical molecular orbital theory. Determination of eigenspectral properties\textsuperscript{17-20} and correlations with some important physico-chemical properties are interesting research area to the theoretical chemists. Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies are the active areas of chemical research\textsuperscript{21-25}. Topological indices are the graph invariants and are enormously used in these studies particularly for searching molecular databases, selecting compounds for drug screening, drug designing, predicting molecular properties and modeling drug receptor sites. New molecular descriptors are introduced to explore the structure-dependent properties of molecules with important physico-chemical properties.

**Finite Graphs and Infinite Graphs:**

A graph $G = (v, E)$ consists of a set of objects $v = (v_1, v_2, v_3, ...)$ called vertices and another set $E = (e_1, e_2, e_3, ...)$ whose elements are called edges. A graph is represented by a diagram, in which each vertex is represented by dot and each edge is represented by segment of line joining its end vertices.

A finite graph and infinite graph are shown in Figure 1a and Figure 1b respectively. In Figure-1(a) $v_1, v_2, v_3$ and $v_4$ are the vertices and $e_1, e_2, e_3, e_4, e_5, e_6$ and $e_7$ are the edges of the graph. Here $e_6$ is called loop because its initial and final vertices are the same i.e. $v_4$. An infinite graph consists of infinite number of edges and vertices as in Figure 1b. Crystal lattice is an example of infinite graph.

![Figure 1](image_url)

**Figure 1:** (a) A finite graph (b) An infinite graph
Reciprocal graphs and its some properties:

Different types of graphs are considered depending on the number of vertices or edges, mode of connection among the vertices or edges or the value of their eigenspectra etc. Reciprocal graphs are very special type of graphs. Reciprocal graphs²⁶-²⁹ are those whose eigenvalues occur in the form of reciprocal pair ($\lambda, 1/\lambda$) with palendromic characteristic polynomials. Four-vertex reciprocal graphs of linear chain, cycle and star are shown in Figure 2.

![Figure 2: 4-vertex reciprocal graphs of linear chain, cyclic and star graphs](image)

**Characteristic polynomial of reciprocal graphs**

Characteristic polynomial of any graph can be written as follows.

$$a_0x^n + a_1x^{n-1} + a_2x^{n-2} + \ldots + a_{n-2}x^2 + a_{n-1}x + a_n = 0$$  \hspace{1cm} (1)

Here $a_i, i = 0, 1, 2, \ldots, (n-1), n$, are called characteristic polynomial coefficients and $x$ represents the eigenvalue of the graph. If $x$ be the eigenvalue for a reciprocal graph according to the definition $1/x$ will be another eigenvalue so equation can also be written in the form given below

$$a_0(1/x)^n + a_1(1/x)^{n-1} + a_2(1/x)^{n-2} + \ldots + a_{n-2}(1/x)^2 + a_{n-1}(1/x) + a_n = 0$$  \hspace{1cm} (2)

Multiplying equation (2) by $x^n$ we get

$$a_0 + a_1x + a_2x^2 + \ldots + a_{n-2}x^{n-2} + a_{n-1}x^{n-1} + a_nx^n = 0$$  \hspace{1cm} (3)

Comparing equation (1) and equation (3) we can write

$$a_0 = a_n, a_1 = a_{n-1}, a_2 = a_{n-2}, \ldots$$ so on.
Characteristics polynomials of reciprocal graphs with such special relation among its coefficients are called palendromic type of characteristics polynomial.

A method\textsuperscript{28} for construction of characteristics polynomial (CP) coefficients of three classes of reciprocal graphs (linear, cyclic and star graphs) has been developed. In this method working formula was expressed in matrix product form.

**Cardinalities of reciprocal graphs:**

Two vertices are said to be ‘independent’ if they are not connected by an edge. The number of sets of such independent is called “cardinality”. Mandal and et.al.\textsuperscript{30} studied on the cardinalities of three classes of reciprocal graphs (linear, cyclic and star graphs). Recurrence as well as analytical formula was derived. These relations were applied to calculate the bond orders of some conjugated molecules.

**Topological indices of reciprocal graphs:**

Topological indices are graph invariants are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. Two important topological indices namely Hosoya indices and Wiener indices of three classes of reciprocal graphs (linear, cyclic and star graphs) are extensively studied\textsuperscript{31}. Mandal et.al.\textsuperscript{32} farther studied to express these two topological indices for reciprocal graphs in terms of number of pendant vertices.

**Conclusion**

Reciprocal graphs are not all hypothetical; some represents real molecules which are fairly synthesized. Reciprocal graph of the type cyclic graph with six base vertices attached with six pendant vertices represents hexamethylene cyclohexane molecule was already synthesized. When pendant vertices of reciprocal graphs are replaced by hetero atoms particularly sulphur, oxygen or nitrogen it has been conjectured that their electrical conductivity should be very high. These reciprocal graphs are very important to theoretical chemists because of their reciprocal and also self-complementary eigenvalues.

**References**

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