Research Article

Some Chemistry Indices of Clique-Inserted Graph of a Strongly Regular Graph

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In this paper, we give the relation between the spectrum of strongly regular graph and its clique-inserted graph. The Laplacian spectrum and the signless Laplacian spectrum of clique-inserted graph of strongly regular graph are calculated. We also give formulae expressing the energy, Kirchoff index, and the number of spanning trees of clique-inserted graph of a strongly regular graph. And, clique-inserted graph of the triangular graph $T(t)$, which is a strongly regular graph, is enumerated.

1. Introduction

Gutman in [1] officially gave the definition of graph energy, which has a widespread application in chemistry and physics [1–3]. Koolen and Moulton in [4] proved that the graph with maximal energy is a strongly regular graph. Furthermore, Haemers in [5] show that the maximal energy of strongly regular graphs is corresponding to a type of Hadmada matrix. Zhang in [6] suggested that the iterative operation of clique-insertion can be considered as a way to extend complex networks. It is meaningful to calculate some indices of clique-inserted graph of a strongly regular graph.

Algebraic graph theory, as a part of graph theory, mainly investigates the relationship between parameters and structure of a graph by matrix theory. The research on the spectrum of graph enriches graph theory. Collatz and Sinogowitz [7] firstly used adjacency matrix to study the spectrum and structure of graphs. However, many scholars gradually find that the adjacency spectrum has limitations, especially in solving the chemical problem of distinguishing isomers (i.e., homographs). Compared with adjacency matrix, Laplacian matrix can reflect the properties of graphs more accurately, see [8]. The Laplacian spectrum of a graph contributes to many invariants of a graph, such as Kirchhoff index and connectivity. These indices can further reflect some of the chemical properties of a graph. A tree of diameter 4 with minimum Laplacian spectral radius is determined in [9]. The properties of the Laplacian matrix and the application of the topological indices were studied in [10]. Cvetkovic’ et al. in [8] defined the signless Laplacian spectrum of finite graphs and their properties. With the further research on the internal characteristics of networks, some scholars have found that many actual networks are composed of several groups or clusters. These groups or clusters have relatively close connections among nodes, but relatively few connections between each cluster, which is called “community structure.” Revealing its community structure is very important for the analysis of network structure, and the community division method based on the graph spectrum effectively solves this problem.

The research on topological indices of graphs is a hot topic in graph theory. Many topological indices have applied in the field of chemistry and physics [11]. For an electrical network, the Kirchhoff index is proportional to the electrical energy consumed by the network per unit time [6]. Richard defines the Bruhat graph and gives the topological indices for it in [12]. From the perspective of complex networks, topological indices can reflect the overall characteristics [13], effectively evaluate the overall characteristics of complex networks [14], protect useful networks, and block viral network [15]. The geometric arithmetic indices are proposed by Vukičević and...
Furtula in [16], which have a nice predictive ability to entropy, centrifugal factor, and other physical properties.

The paper is arranged as follows. We give some preliminaries and calculate spectrum of clique-inserted graph of a strongly regular graph in Section 2. In Section 3, we introduce some energies and typical topological indices. An example is given with respect to indices in Section 4.

2. Spectra of Clique-Inserted Graph of a Strongly Regular Graph

All graphs in this paper are simple and connected. A simple graph requires that there be neither a cycle nor a pair of vertices connected by two edges. Let $G$ be a graph whose vertices are $1, 2, \ldots, n$. The adjacency matrix of $G$ is a square matrix of order $n$, represented by $A(G)$. If vertices $i$ and $j$ are adjacent, then $(i, j) = 1$ and $0$, otherwise. The eigenvalues of a graph $G$ are the eigenvalues of the adjacency matrix $A(G)$, denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Let $D(G)$ be a diagonal matrix, and the diagonal elements are the degrees of the corresponding vertices of $G$. The Laplacian matrix and the signless Laplacian matrix of $G$ are $L(G) = D(G) - A(G)$ and $L^+(G) = D(G) + A(G)$, respectively. We denote the eigenvalues of $L(G)$ by $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_n$, and the eigenvalues of $L^+(G)$ by $\mu_1^+ \geq \mu_2^+ \geq \cdots \geq \mu_n^+$.

A graph with $n$ vertices is said to be $k$-regular if each of its vertices has degree $k$. Furthermore, if any two adjacent vertices have a common neighbour and any pair of distinct nonadjacent vertices have $c$ common neighbours, then the graph is called a strongly regular graph with parameters $(n, k, a, c)$. The strongly regular graph has exactly three eigenvalues: $k, \theta$, and $\tau$ (because $\theta \tau < 0$, we usually assume that $\tau < 0$) with $\theta = (a - c + \sqrt{E})/2$ and $\tau = (a - c - \sqrt{E})/2$, where $E = (a - c)^2 + 4(k - c)$. The multiplicities $m_\theta$ and $m_\tau$ corresponding to $\theta$ and $\tau$ are given, respectively, by

$$m_\theta = \frac{(n - 1)\tau + k}{\theta - \tau},$$

$$m_\tau = \frac{(n - 1)\theta + k}{\theta - \tau}.\quad (1)$$

By the property of the adjacency matrix, we have

$$m_\theta + m_\tau = n - 1,$$

$$m_\theta \theta + m_\tau \tau = -k.\quad (2)$$

The graph obtained by replacing every vertex of a graph $G$ by a clique (i.e., a complete graph) with $s$ vertices is called an $s$-clique-inserted graph of $G$ [17, 18]. Let $u$ be a vertex in $G$ whose degree is greater than 0. If we obtain $G$ by replacing the vertex $u$ with a 3-clique (as illustrated in Figure 1), then $G$ is said to be an $s$-clique-inserted graph at $u$.

Next, we will calculate the spectrum of clique-inserted graph of a strongly regular graph. We firstly introduce a lemma before this.

**Lemma 1** (see [19]). Let $\tilde{G}$ be an $s$-clique-inserted graph of a graph $G$. If the adjacency spectrum of $G$ is

$$\{\lambda_1^n, \lambda_2^n, \ldots, \lambda_n^n\},$$

then the adjacency spectrum of $\tilde{G}$ is

$$\left\{ (s(\lambda_0 + 1) - 1)^n, (s(\lambda_1 + 1) - 1)^n, \ldots, (s(\lambda_n + 1) - 1)^n, (-1)^{s(n-1)}(n_1+n_2+\cdots+n_s) \right\}.\quad (4)$$

Let $G$ be a strongly regular graph; its parameters and spectrum are $\{n, k, a, c\}$ and $\{k^1, \theta^{m_\theta}, \tau^{m_\tau}\}$. And, $\tilde{G}$ is a clique-inserted graph of $G$. We can see that $\tilde{G}$ is a regular graph with degree $k = s(k + 1) - 1$. By Lemma 1, we conclude that the adjacency spectrum of $\tilde{G}$ is

$$\{ (s(k + 1) - 1)^1, (s(\theta + 1) - 1)^{m_\theta}, (s(\tau + 1) - 1)^{m_\tau},$$

$$(-1)^{(s-1)(1+m_\theta+m_\tau)} \}$$. The eigenvalues of $\tilde{G}$, denoted by $\lambda_i (1 \leq i \leq 4)$, are $s(k + 1) - 1, s(\theta + 1) - 1, s(\tau + 1) - 1, -1$.

For the regular graph $\tilde{G}$, we have $\mu_i = \bar{k} - \lambda_i$. Then, we obtain that the Laplacian eigenvalues of $\tilde{G}$ are $0, s(k - \theta), s(k - \tau),$ and $s(k + 1)$. So, the Laplacian spectrum of $\tilde{G}$ is

$$\{ (s(k + 1) - 1)^1, (s(\theta + 1) - 1)^{m_\theta}, (s(\tau + 1) - 1)^{m_\tau}, (-1)^{(s-1)(1+m_\theta+m_\tau)} \}$$.\quad (5)
3. Applications of Spectra

In Section 2, we obtain the spectrum of $\bar{G}$. Now, we use the spectrum of $\bar{G}$ to explore the corresponding other quantities. There are a lot of literature studies about the applications of spectrum of matrix, see [3, 9, 20, 21]. Some definitions will be given at first in each part.

3.1. Energy, Laplacian Energy, and Signless Laplacian Energy of $\bar{G}$. The energy of a graph is defined as the spectrum of adjacency matrix of graph which is put forward firstly by Gutman in [1]. The study of graph energy is one of the earliest and the most extensively studied in graph theory. The chemist Huckel obtained the graph model of the corresponding molecules through the approximate treatment of unsaturated hydrocarbons when he studied organic molecular energy. And, he used the eigenvalues of the corresponding matrix to represent the energy levels of specific electrons [8]. Graph energy has a strong application background in chemistry, such as establishing mathematical models for organic molecules and analysing energy levels and stability.

Let $G$ be a connected simple graph with $n$ vertices. Then the energy of $G$ is

$$E(G) = \sum_{i=1}^{n} |\lambda_i(G)|.$$  

Now we calculate the energy of $\bar{G}$. For $\tau \leq - \tau/2$, by Theorem 1, we have

$$E(\bar{G}) = \sum_{i=1}^{m} |\lambda_i(\bar{G})| = 1 (s(k + 1) - 1) + m_\theta (s(\theta + 1) - 1) + m_\tau (1 - s(\tau + 1))$$

$$+ (s - 1)(1 + m_\theta + m_\tau) = s(k + 1 + m_\theta(\theta + 1) - m_\tau(\tau + 1) + (1 + m_\theta + m_\tau))$$

$$- 1 - m_\theta + m_\tau - (1 + m_\theta + m_\tau) = s(k + m_\theta\theta - m_\tau\tau) + 2(1 + m_\theta)(s - 1).$$

By (2),

$$E(\bar{G}) = s(-2m_\tau\tau) + 2(1 + m_\theta)(s - 1).$$

Substitute the values $m_\theta$ and $m_\tau$ in (1) into (10), we get

$$E(\bar{G}) = -2s (n-1)\theta + k \theta - \tau$$

$$+ 2 \left( 1 - \frac{(n-1)\tau + k}{\theta - \tau} \right) (s - 1).$$

For $-(1/2) \leq \tau < 0$, substitute the eigenvalue of $\bar{G}$ into equation (8):

$$E(\bar{G}) = \sum_{i=1}^{m} |\lambda_i(\bar{G})| = 1 (s(k + 1) - 1) + m_\theta (s(\theta + 1) - 1)$$

$$+ m_\tau (s(\tau + 1) - 1)$$

$$+ (s - 1)(1 + m_\theta + m_\tau) = 2n(s - 1).$$

The energy of the graph is calculated from the spectrum of the adjacency matrix, and in algebraic graph theory, the Laplacian spectrum of graphs and the applications have also received extensive attention. Although the adjacency spectrum can reflect some properties of the graph, there are
limitations, especially in the problem of the same spectrum. In [22], the Laplacian energy is used to propagate viruses in intuitionistic fuzzy networks. Cvetković et al. in [23] defined the signless Laplacian spectrum of finite graphs and their properties. Some scholars studied the maximization problem of the signless Laplacian spectrum of some special graphs [24, 25].

The Laplacian matrix adds degree matrix, a parameter closely related to graph structure, on the basis of adjacency matrix. The Laplacian spectrum has some properties of the adjacency spectrum. Let \( \mu_1, \mu_2, \ldots, \mu_n \) be the Laplacian eigenvalues of \( G \). And, the Laplacian energy is defined as

\[
LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.
\]  

(13)

Let \( \mu_1^+, \mu_2^+, \ldots, \mu_n^+ \) be the signless Laplacian eigenvalues of \( G \). The signless Laplacian energy is defined as

\[
LE^+(G) = \sum_{i=1}^{n} \left| \mu_i^+ - \frac{2m}{n} \right|.
\]  

(14)

If \( G \) is a regular graph with \( n \) vertices and \( m \) edges and degree \( k \), we have \( 2m = nk \). Then, \( LE(G) = \sum_{i=1}^{n} |\mu_i - k| = \sum_{i=1}^{n} \lambda_i = E(G) \) and \( LE^+(G) = \sum_{i=1}^{n} |\mu_i^+ - k| = \sum_{i=1}^{n} \lambda_i = E(G) \). So, for the clique-inserted graph \( \tilde{G} \), we have

\[
LE^+(\tilde{G}) = LE(\tilde{G}) = E(\tilde{G}) = \left\{ \begin{array}{ll}
-2\tau s \frac{(n-1)\theta + k}{\theta - \tau} + 2 \left( 1 - \frac{(n-1)\tau + k}{\theta - \tau} \right) (s-1), & \tau \leq \frac{1}{2} \\
2n(s-1), & \frac{1}{2} < \tau < 0.
\end{array} \right.
\]  

(15)

3.2. Kirchhoff Index of \( \tilde{G} \). In the early research on the topological index of graphs, many scholars focused their attention on the ordinary graph distance. Until the rise of electrical network theory, D. J. Klein and M. Randi built forward the concept of the resistance distance of graphs in [26], which is a topology index defined by the resistance distance. This new distance function has been favoured by chemists since it was proposed. In the field of physics and engineering, the calculation of resistance between two points is the core problem of circuit theory research. In mathematics, various formulae for calculating resistance distance are produced one after another. For an electrical network, it is a direct proportion to the electrical energy consumed by the network per unit time [10]. The Kirchhoff index can be used to describe the structural characteristics of molecules and define the topological radius of polymers in chemistry [26]. Small value of Kirchhoff index means strong network robustness in network science [27, 28].

The Kirchhoff index and \( \mu_1, \mu_2, \ldots, \mu_n \) have the following relationship:

\[
Kf(G) = n \sum_{i=2}^{n} \frac{1}{\mu_i}
\]  

(16)

According to Theorem 1, substituting the Laplacian spectrum of \( \tilde{G} \) into equation (16), we get the Kirchhoff index of \( \tilde{G} \):

\[
Kf(\tilde{G}) = sn \sum_{i=2}^{n} \frac{1}{\mu_i} = sn \left( m_\theta \cdot \frac{1}{s(k-\theta)} + m_s \cdot \frac{1}{s(k-\tau)} + (s-1)n \cdot \frac{1}{s(k+1)} \right)
\]  

(17)

3.3. The Number of Spanning Trees of \( \tilde{G} \). The number of spanning trees is a minimum connected subgraph that containing all vertices of the connected graph. It is also a measure of the structure of a graph. The spanning trees are used in network reliability analysis, circuit design in physics, self-organized criticality [29], and so on. In computer network, it is an important index to evaluate network security [30, 31]. In the router system, the whole router network can be regarded as a graph \( G \), all routers as vertex \( i \) of graph \( G \), and the connection relationship between routers as edge \( e \) of graph \( G \). When a vertex and its adjacent edges are removed from a graph \( G \), the less the number of spanning trees of the new graph, the more important the point is.
The number of spanning trees of a graph $G$ with order $n$ is defined as
\[
\tau(G) = \frac{1}{n} \prod_{i=2}^{n} \mu_i. \tag{18}
\]

We can determine the connectivity of the graph $G$ from the number of spanning trees $\tau(G)$. The larger the number is, the more connected the graph is, see [8]. There are two graphs in Figure 2. The left graph of Figure 2 is Petersen graph with Laplacian spectrum $\{0, 2^5, 5^4\}$. The Laplacian spectrum of the right graph is $\{0, 1.4384, 3^3, 5.5616\}$. According to formula (16), we get $\tau(G)$ of the left graph is 2000 and the right graph is 43. The connectivity in left graph is stronger than that in the right graph.

According to Theorem 1, substitute the Laplacian spectrum of $G$ into formula (18), we obtain the number of spanning trees of $\tilde{G}$ is
\[
\tau(\tilde{G}) = \frac{1}{sn} \prod_{i=2}^{sn} \mu_i = \frac{1}{sn} (s(k-\theta)^{m_s} (s(k-\tau)^{m_s} (s(k+1))^{(s-1)n})
\]
\[
= \frac{1}{n} (s(k-\theta)^{m_s} (s(k-\tau)^{m_s} (s(k+1))^{(s-1)n}). \tag{19}
\]

4. An Example

In this section, we will give an example of calculations, that is, the clique-inserted graph of the triangular graph $T(t)$. The Johnson graph $J(t, 2)$ is also called the triangular graph $T(t)$ (see Figure 3, for example, $T(4)$).

In [20], we know $T(t)$ is a strongly regular graph with parameters $\left(\begin{array}{c} t \\ 2 \end{array}\right), 2t - 4, t - 2, 4$ and spectrum
\[
\{ (2t - 4)^1, (t - 4)^{t-1}, (t - 4)^{4t-4}, (2t - 4)^{(t^2 - 4t + 6)/2}\}. \hspace{1cm}
\]

Let $\tilde{T}$ be the clique-inserted graph of $T(t)$. Because $\tau = -2 < - (1/2)$, according to (10), the energy of $\tilde{T}$ is
\[
E(\tilde{T}) = 2s(t^2 - 3t) + 2t(s - 1) = 2t(s(t - 2) - 1). \hspace{1cm} \tag{20}
\]

By (17), the Kirchhoff index of $\tilde{T}$ is
\[
Kf(\tilde{T}) = \frac{t^2 (t - 1)^2}{4(2t - 3)} (s(t - 2) + \frac{(t - 1)^2}{2} + \frac{t^2(t - 3)}{8}). \hspace{1cm} \tag{21}
\]

By (19), the number of spanning trees of $\tilde{T}$ is
\[
\tau(\tilde{T}) = 4 \cdot s^{(s(t - 1)/2 - 2)} \cdot t^{t - 2} \cdot (2t - 2)^{(t(t - 3)/2 - 1)} \cdot (2t - 3)^{(s - 1)(t - 1)/2}. \hspace{1cm} \tag{22}
\]

5. Conclusions

In this paper, we get the graph $\tilde{G}$ by applying the operation of clique insertion to a strongly regular graph $G$ and obtain the relationships between the adjacency spectrum of graph $G$ and $\tilde{G}$. Furthermore, the Laplacian spectrum and signless Laplacian spectrum of $\tilde{G}$ are calculated. Based on the above conclusions, we give formulae expressing the energy, Kirchhoff index and the number of spanning trees of $\tilde{G}$.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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