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Minimizing Kirchhoff index among graphs with a given vertex bipartiteness

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ABSTRACT

The resistance distance between any two vertices of a graph G is defined as the effective resistance between them if each edge of G is replaced by a unit resistor. The Kirchhoff index $Kf(G)$ is the sum of the resistance distances between all the pairs of vertices in G. The vertex bipartiteness υ_b of a graph G is the minimum number of vertices whose deletion from G results in a bipartite graph. In this paper, we characterize the graph having the minimum $Kf(G)$ values among graphs with a fixed number n of vertices and fixed vertex bipartiteness, $1 \le \upsilon_b \le n-3$.

1. Introduction

We only consider finite and simple graphs here. Let $G = (V(G), E(G))$ denote a graph with vertex-set $V(G)$ and edge-set $E(G)$. If $e \in E(G)$ has end vertices u and v, then we say that u and v are adjacent and this edge is denoted by uv. The cardinality of $V(G)$ is called the order of G. The subgraph induced by a vertex subset $S \subseteq V(G)$, denoted by $\langle S\rangle$, is a graph with vertex set S and edge set $E(\langle S\rangle) = \{uv : u, v \in S, uv \in E(G)\}$. The complement of the graph G, denoted by $\overline{G}$, is the graph for which $V(\overline{G}) = V(G)$ and $E(\overline{G}) = \{uv : uv \notin E(G)\}$. Let $\mathscr{G}_{n,m}$ be the graphs with n vertices and $\upsilon_b(G) \le m$. i.e.,

$$\mathscr{G}_{n,m} = \Big\{G = (V(G), E(G)) : |V(G)| = n, \upsilon_b(G) \le m.\Big\},$$

where m is a natural number such that $m \le n-3$. For other undefined terminology and notation, the reader is referred to [1].

The adjacency matrix of G, denoted by $A(G) = (a_{ij})_{n\times n}$, is an $n \times n$ symmetric matrix such that $a_{ij} = 1$ if vertices v_i and v_j are adjacent and 0 otherwise. The number of neighbors of a vertex v_i is its degree. Let $d_G(v_i)$ be the degree of vertex v_i of G and $D(G) = diag\Big(d_G(v_1), d_G(v_2), \ldots, d_G(v_n)\Big)$ be the diagonal matrix of vertex degrees of G. Then the Laplacian matrix of G is $L(G) = D(G) - A(G)$ [18,19]. The spectrum of Laplacian matrix $L(G)$ is denoted by $\sigma(L(G)) = \{\mu_1, \ldots, \mu_n\}$, where this sequence of Laplacian eigenvalues is given in non-increasing order [9,20].

The basic model for a chemical molecule is that the vertices represent the atoms and the edges represent the chemical bonds. Among the descriptors used in Mathematical Chemistry to study these models, one that has received numerous

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attention [2,10–12,28,30,33,34,36–39] since its introduction by Klein and Randić in [17] is the Kirchhoff index, defined as

$$Kf(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} r_{ij}(G),$$

where r_{ij} is the effective resistance between vertices v_i and v_j computed with Ohm's law when the edges of the graph are supposed to have unit resistances. For more work on $Kf(G)$, the readers are referred to [6,7,21–23,26,31,32] and recent papers [3,8,16,24,25,27,29,35].

Motivated by the above results, in this paper we further investigate the graph having the minimum Kirchhoff index among graphs with a fixed number n of vertices and fixed vertex bipartiteness, $1 \le v_b \le n-3$.

The rest of the paper is organized as follows. An introduction to a generalized join graph operation is provided in Section 2. Some lemmas and the proof of main result are presented in Sections 3 and 4, respectively.

2. A generalized join graph operation

Usually, considering two vertex disjoint graphs G_1 and G_2, the join $G_1 \vee G_2$ is the graph such that

$$V(G_1 \vee G_2) = V(G_1) \cup V(G_2)$$

and

$$E(G_1 \vee G_2) = E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1), v \in V(G_2)\}.$$

A generalization of the join operation was introduced in [4] as follows:

Let $\mathscr{F} = \{G_1, \ldots, G_k\}$ be a family of vertex disjoint graphs, where G_i has order n_i, for $1 \le i \le k$. Let H is an arbitrary graph with vertex-set $V(H) = \{1, \ldots, k\}$. Each vertex $i \in V(H)$ is assigned to the graph $G_i \in \mathscr{F}$. The H-join of $G_1, \ldots, G_k$ is the graph $G = H[G_1, \ldots, G_k]$ such that

$$V(G) = \bigcup_{i=1}^{k} V(G_i)$$

and

$$E(G) = \left(\bigcup_{i=1}^{k} E(G_i)\right) \bigcup \left(\bigcup_{rs\in H} \Big\{uv \mid u \in V(G_r), v \in V(G_s)\Big\}\right).$$

Remark 1. If $H = K_2$, the H-join is the usual join graph operation. The same generalization of the join operations was considered in [4], under the designation of generalized composition of the graphs $G_1, \ldots, G_k$ along the graph H and denoted by $H[G_1, \ldots, G_k]$.

3. Lemmas

In this section, we give some lemmas that will be used in the proofs of main results.

Lemma 3.1. *[30] The Kirchhoff index is strictly monotonic in the number of edges: if G' is the graph which results from adding a new edge to a graph G. Then*

$$Kf(G') < Kf(G).$$

There is a famous relationship between $Kf(G)$ and the Laplacian eigenvalues of G as below.

Lemma 3.2. *[15, 40] Let G be a connected graph of order n. Then*

$$Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i},$$

where $\mu_1 \ge \mu_2 \cdots \ge \mu_n = 0$ are the Laplacian eigenvalues of G.

Next, we specify some notation. For $1 \le i \le k$. Define

$$N_i = \sum_{ij\in E(H)} n_j.$$

By applying the results to the Laplacian matrix of $H[G_1, \ldots, G_k]$ where $G_1, \ldots, G_k$ are arbitrary graphs (see [4], Theorem 8), Cardoso et al. have the following lemma.