

Research Article

Some Bounds for the Kirchhoff Index of Graphs

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The resistance distance between two vertices of a connected graph G is defined as the effective resistance between them in the corresponding electrical network constructed from G by replacing each edge of G with a unit resistor. The Kirchhoff index of G is the sum of resistance distances between all pairs of vertices. In this paper, general bounds for the Kirchhoff index are given via the independence number and the clique number, respectively. Moreover, lower and upper bounds for the Kirchhoff index of planar graphs and fullerene graphs are investigated.

1. Introduction

Let G be a connected graph with vertices labeled as $1, 2, \dots, n$. It is natural to view G as an electrical network by imagining each edge of G to be a (unit) resistor. In this guise, it is reasonable to consider the effective resistance between any two vertices of G , and the novel concept of *resistance distance* [1] $r_{ij}(G)$ between any two vertices i and j of G is thus defined as the effective resistance between them. Compared to the (shortest-path) distance $d_{ij}(G)$ between i and j in G , it is well known that $r_{ij}(G) \leq d_{ij}(G)$ with equality if and only if i and j are connected by unique path [1].

There are many distance-based molecular structure descriptors, as reviewed in [2], which have played important roles in QSAR and QSPR. Among these structure descriptors, the most famous one is the Wiener index $W(G)$ [3], which is known as the sum of distances between all pairs of vertices. Analogous to the Wiener index, the Kirchhoff index of G [1, 4], denoted by $Kf(G)$, is defined as the sum of resistance distances between all pairs of vertices; that is,

$$Kf(G) = \sum_{i < j} r_{ij}(G). \quad (1)$$

As summarized in [2], much work has been done by many researchers to investigate bounds for the Kirchhoff index. There are not only general bounds that are given in terms of various graph structural parameters like the number of vertices, the number of edges, the matching number,

the chromatic number, the maximum degree, and the number of spanning trees [5–20], but also bounds for some special interesting classes of graphs, such as circulant graphs, unicyclic graphs, and bicyclic graphs [21–27]. Along this line, we consider the relation between the Kirchhoff index and the independence number as well as the clique number, and bounds are obtained for the Kirchhoff index of graphs via the two graph invariants. In addition, lower and upper bounds for the Kirchhoff index of planar graphs and fullerene graphs are investigated. For more information on the Kirchhoff index of graphs, the readers are referred to the most recent papers [28–36] and references therein.

2. General Bounds

2.1. A Lower Bound via the Independence Number. We first introduce some notations. Denote the vertex set and edge set of G , respectively, by $V(G)$ and $E(G)$. A subset X of $V(G)$ is called independent if its vertices are mutually nonadjacent. The independence number $\alpha(G)$ is the largest cardinality among all independent sets of G . The clique number $\omega(G)$ of G is the largest set of mutually adjacent vertices in G . The degree of vertex i , denoted by $d_i(G)$, is the number of neighbors of i . The adjacency matrix $A(G)$ of G is an $n \times n$ matrix with the (i, j) -entry equal to 1 if vertices i and j are adjacent and 0 otherwise. Let $D(G) = \text{diag}(d_1(G), d_2(G), \dots, d_n(G))$ be the diagonal matrix of vertex degrees. Then the Laplacian matrix of G is $L(G) = D(G) - A(G)$. Let $\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{n-1}$

be the eigenvalues of $L(G)$, called the Laplacian eigenvalues of G . Since G is connected, $\lambda_0 = 0$ and $\lambda_k > 0$ for $k = 1, 2, \dots, n-1$ [37]. The spectrum of $L(G)$, also known as the Laplacian spectrum of G , is

$$S(G) = (\lambda_0, \lambda_1, \dots, \lambda_{n-1}). \quad (2)$$

Zhu et al. [38] and Gutman and Mohar [39] established a classical result for computing the Kirchhoff index via the Laplacian spectrum of G .

Theorem 1.

$$Kf(G) = n \sum_{k=1}^{n-1} \frac{1}{\lambda_k}. \quad (3)$$

The join of G_1 and G_2 , denoted by $G_1 + G_2$, is the graph obtained from $G_1 \cup G_2$ by adding all edges between vertices of G_1 and that of G_2 , where \cup denote the disjoint union. The Laplacian eigenvalues of $G_1 + G_2$ are characterized in the following result.

Lemma 2 (see [37]). *Let G_1 and G_2 be graphs such that $|V(G_1)| = n$ and $|V(G_2)| = m$. Suppose that $0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-1}$ and $0 = \mu_0 \leq \mu_1 \leq \mu_2 \leq \dots \leq \mu_{m-1}$ are Laplacian eigenvalues of G_1 and G_2 . Then the Laplacian eigenvalues of $G_1 + G_2$ are $0, m+n, m+\lambda_i, n+\mu_j, i = 1, 2, \dots, n-1, j = 1, 2, \dots, m-1$.*

The nonincreasing property of the Kirchhoff index, as stated below, plays an important role in estimating bounds for the Kirchhoff index.

Lemma 3 (see [12]). *Let G be a noncomplete graph. If G' is obtained from G by adding an edge, then $Kf(G') < Kf(G)$.*

For simplicity, if there is no confusion, we always abbreviate $r_{ij}(G), d_{ij}(G), d_v(G), \alpha(G)$, and $\omega(G)$ to $r_{ij}, d_{ij}, d_v, \alpha$, and ω , respectively. Throughout the paper, we use K_n, P_n to denote the complete and path graph of order n , respectively. We use \overline{G} to denote the complement of G . Then the main result of this subsection is given as follows.

Theorem 4. *Let G be a connected graph with n vertices and independence number α . Then*

$$Kf(G) \geq n - \alpha + \frac{n(\alpha - 1)}{n - \alpha}, \quad (4)$$

with equality if and only if $G \cong \overline{K_\alpha} + K_{n-\alpha}$.

Proof. Let G_0 be a graph having the minimum Kirchhoff index among all connected graphs with n vertices and independence number α . Then by the nonincreasing property of the Kirchhoff index as given in Lemma 3, it is easily seen that $G_0 \cong \overline{K_\alpha} + K_{n-\alpha}$. Now we compute the Kirchhoff index of G_0 . Since it is well known that $S(\overline{K_\alpha}) = (0, 0, \dots, 0)$ and $S(K_{n-\alpha}) = (n - \alpha, n - \alpha, \dots, n - \alpha)$, by Lemma 2, we get

$$S(G_0) = \left(0, \underbrace{n - \alpha, \dots, n - \alpha}_{\alpha - 1}, \underbrace{n, \dots, n}_{n - \alpha} \right). \quad (5)$$

Then according to Theorem 1, it follows that

$$Kf(G_0) = n \left(\frac{\alpha - 1}{n - \alpha} + \frac{n - \alpha}{n} \right) = n - \alpha + \frac{n(\alpha - 1)}{n - \alpha}. \quad (6)$$

□

2.2. An Upper Bound via the Clique Number. Let \mathcal{G}_ω be the set of graphs with n vertices and clique number ω . Let G_p denote the graph obtained by identifying one end vertex of path $P_{n-\omega+1}$ with any vertex of K_ω . In the following, we have shown that, among all the graphs in \mathcal{G}_ω , G_p has the maximum Kirchhoff index. To this end, we need the following two lemmas.

Lemma 5 (see [40]). *Let G be a graph with a cut edge $e = xy$ and G_1 and G_2 the components of $G - e$ containing x and y , respectively. Then*

$$Kf(G) = Kf(G_1) + Kf(G_2) + |V(G_2)| Kf_x(G_1) + |V(G_1)| Kf_y(G_2) + |V(G_1)| |V(G_2)|, \quad (7)$$

where $Kf_x(G)$ denote the sum of resistance distances between x and all the other vertices of G .

Lemma 6 (see [41]). *Let T be an n vertex tree different from P_n and S_n . Then*

$$W(S_n) < W(T) < W(P_n). \quad (8)$$

Theorem 7. *Let $G \in \mathcal{G}_\omega$ be different from G_p . Then*

$$Kf(G) < Kf(G_p). \quad (9)$$

Proof. If $\omega = 2$, then G_p is a path. Noticing that the Kirchhoff index is equal to the Wiener index for trees, by Lemmas 3 and 6, the assertion holds. In the following, we assume that $\omega \geq 3$.

Let G_0 be the graph with the maximum Kirchhoff index and let H be the subgraph of G_0 such that $H \cong K_\omega$.

Claim 1 (every component of $G_0 - H$ is connected to H by only one edge). Suppose to the contrary that there exists a component of $G_0 - H$ such that it is connected to H with edges e_1, e_2, \dots, e_k ($k > 1$). Let G_1 be the graph obtained from G_0 by the deletion of e_2, e_3, \dots, e_k . Then it is easily seen that $G_1 \in \mathcal{G}_\omega$ and G_1 is a proper spanning subgraph of G_0 . Thus by Lemma 3, we have $Kf(G_1) > Kf(G_0)$, contradicting the property that G_0 has the maximum Kirchhoff index.

Claim 2 (every component of $G_0 - H$ is a tree). Suppose to the contrary that there exists a component C of $G_0 - H$ such that C is not a tree. Let T be a spanning tree of C . Remove from G_0 all the edges in C but not in T to obtain G_1 . Then $G_1 \in \mathcal{G}_\omega$ and G_1 is a proper subgraph of G_0 . Again by Lemma 3, we have $Kf(G_1) > Kf(G_0)$, a contradiction.

Claim 3 (every component of $G_0 - H$ is a path, which connects to H via an end vertex). Let C be any component of $G_0 - H$. By Claims 1 and 2, we know that C is a tree and C is connected to H by a single edge $e = xy$ ($y \in C$). Clearly $G - e$ has two

components, one is C , and denote the other one by G_1 . Then by Lemma 5,

$$Kf(G_0) = Kf(G_1) + Kf(C) + |V(C)|Kf_x(G_1) + |V(G_1)|Kf_y(C) + |V(G_1)||V(C)|. \quad (10)$$

Since $Kf(G_0)$ has the maximum Kirchhoff index and by Lemma 6 and the fact that the Kirchhoff index is equal to the Wiener index for trees, we know that $Kf(G_0)$ is maximized if and only if C is a path and y is an end vertex of C ; the claim holds.

Claim 4 (every vertex of H has degree at most ω in G_0). Suppose to the contrary that there exists $x \in H$ such that the degree of x in G_0 is larger than ω . Then by Claim 1, x is connected to at least two components of $G_0 - H$. Let C_1 and C_2 be two such components connecting to x by edges xy_1 and xy_2 , respectively. By Claim 3, both C_1 and C_2 are paths with y_1 and y_2 being end vertices of them. Without loss of generality, suppose that the length of C_1 is less than or equal to the length of C_2 . Let z_1 (resp., z_2) be the end vertex of C_1 (resp., C_2) different from y_1 (resp., y_2), and let u be the unique neighbor of z_1 . Now construct a new graph G_1 from G_0 by first deleting the edge z_1u and then adding a new edge z_1z_2 . Clearly $G_1 \in \mathcal{E}_\omega$. We show $Kf(G_0) < Kf(G_1)$ so that Claim 4 is proved by contradiction. It is easily seen that, for any two vertices u, v distinct from z_1 ,

$$r_{uv}(G_0) = r_{uv}(G_1). \quad (11)$$

Thus to show $Kf(G_0) < Kf(G_1)$, we need only to show that $Kf_{z_1}(G_0) < Kf_{z_1}(G_1)$. On one hand, it is easily verified that

$$\sum_{a \in (V(C_1) \cup V(C_2) \cup \{x\})} r_{z_1a}(G_0) = \sum_{a \in (V(C_1) \cup V(C_2) \cup \{x\})} r_{z_1a}(G_1). \quad (12)$$

On the other hand, for any vertex b that is not contained in $(V(C_1) \cup V(C_2) \cup \{x\})$, we have

$$\begin{aligned} r_{z_1b}(G_0) &= r_{z_1x}(G_0) + r_{xb}(G_0) < r_{z_1x}(G_1) + r_{xb}(G_0) \\ &= r_{z_1x}(G_1) + r_{xb}(G_1) = r_{z_1b}(G_1). \end{aligned} \quad (13)$$

Hence it follows that $Kf_{z_1}(G_0) < Kf_{z_1}(G_1)$, as required.

Claim 5 ($G - H$ has only one component). Suppose to the contrary that $G - H$ has at least two components C_1 and C_2 . Then by Claim 4, C_1 and C_2 must be connected with H via different vertices of H , say x and y . Let $e_1 = xu$ and $e_2 = yv$ be the two edges connecting H with C_1 and C_2 , respectively. Then both C_1 and C_2 are paths with u and v being their end vertices. Suppose that the lengths of C_1 and C_2 are l_1 and l_2 , respectively. Without loss of generality, we may assume that $l_1 \leq l_2$. Let z_1 (resp., z_2) be the other end vertex of C_1 (resp., C_2) different from u (resp., v), and let z be the unique neighbor of z_1 . Construct a new graph G_1 from G_0 by first deleting the edge zz_1 and then adding a new edge between z_1 and z_2 . Now we show $Kf(G_0) < Kf(G_1)$, which thus gives

the desired contradiction. For any two vertices p, q distinct from z_1 , it is easily seen that

$$r_{pq}(G_0) = r_{pq}(G_1). \quad (14)$$

Thus it suffices to show that $Kf_{z_1}(G_0) < Kf_{z_1}(G_1)$. On one hand,

$$\begin{aligned} \sum_{a \in V(C_1) \cup V(C_2) \cup \{x, y\}} r_{z_1a}(G_0) &= 1 + 2 + \cdots + l_1 + \left(l_1 + \frac{2}{\omega}\right) \\ &\quad + \left(l_1 + 1 + \frac{2}{\omega}\right) + \left(l_1 + 2 + \frac{2}{\omega}\right) + \cdots + \left(l_1 + l_2 + \frac{2}{\omega}\right), \end{aligned} \quad (15)$$

while

$$\begin{aligned} \sum_{a \in V(C_1) \cup V(C_2) \cup \{x, y\}} r_{z_1a}(G_1) &= 1 + 2 + \cdots + l_2 + (l_2 + 1) + \left(l_2 + 1 + \frac{2}{\omega}\right) \\ &\quad + \left(l_2 + 2 + \frac{2}{\omega}\right) + \cdots + \left(l_2 + l_1 + \frac{2}{\omega}\right), \end{aligned} \quad (16)$$

which implies that

$$\sum_{a \in V(C_1) \cup V(C_2) \cup \{x, y\}} r_{z_1a}(G_0) < \sum_{a \in V(C_1) \cup V(C_2) \cup \{x, y\}} r_{z_1a}(G_1). \quad (17)$$

On the other hand, for any vertex b that is not contained in $(V(C_1) \cup V(C_2) \cup \{x, y\})$, we have

$$\begin{aligned} r_{z_1b}(G_0) &= r_{z_1x}(G_0) + r_{xb}(G_0) < r_{z_1y}(G_1) + r_{xb}(G_0) \\ &= r_{z_1x}(G_1) + r_{yb}(G_1) = r_{z_1b}(G_1). \end{aligned} \quad (18)$$

Hence it follows that $Kf_{z_1}(G_0) < Kf_{z_1}(G_1)$ as required.

From Claims 1–5, we deduce that $G_0 \cong G_p$, as desired. \square

By Lemma 5, simple calculation leads to

$$\begin{aligned} Kf(G_p) &= \frac{(n-\omega)^3 - (n-\omega)}{6} + \frac{\omega(n-\omega)(n-\omega-1)}{2} \\ &\quad + \frac{2(\omega-1)(n-\omega)}{\omega} + \omega - 1 + \omega(n-\omega) \\ &= (n-\omega) \left(\frac{n^2 + n\omega - 2\omega^2 + 3\omega + 11}{6} - \frac{2}{\omega} \right) + \omega - 1. \end{aligned} \quad (19)$$

Consequently, the upper bound on the Kirchhoff index is given in terms of the clique number.

Theorem 8. Let G be a connected graph with n vertices and clique number ω . Then

$$Kf(G) \leq (n - \omega) \left(\frac{n^2 + n\omega - 2\omega^2 + 3\omega + 11}{6} - \frac{2}{\omega} \right) + \omega - 1 \quad (20)$$

with equality holds if and only if $G \cong G_p$.

3. Planar Graphs

A planar graph is a graph which can be drawn in the plane without edges crossing. In this section, we investigate bounds for Kirchhoff index of planar graphs. The following lemma is used.

Lemma 9 (see [17]). $\lambda_1 = \lambda_2 = \dots = \lambda_{n-1}$ if and only if $G \cong K_n$.

Theorem 10. For an n vertex planar graph G ($n \geq 3$),

$$\frac{n(n-1)^2}{6(n-2)} \leq Kf(G) \leq \frac{n^3 - n}{6}. \quad (21)$$

The first equality holds if and only if $G \cong K_3, K_4$, and the second does if and only if G is a path.

Proof. The upper bound is well known and we suffice to show the lower bound. Bearing in mind that, for a planar graph G , $|E(G)| \leq 3n-6$, together with the fact that $\sum_{i=1}^n \lambda_i = \sum_{i=1}^{n-1} \lambda_i = \sum_{i=1}^n d_i = 2|E(G)|$, by Cauchy-Schwarz inequality, we have

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i} \geq \frac{(n-1)^2}{2|E(G)|} \geq \frac{(n-1)^2}{2(3n-6)} = \frac{(n-1)^2}{6(n-2)}. \quad (22)$$

The equality holds if and only if $1/\lambda_1 = 1/\lambda_2 = \dots = 1/\lambda_{n-1}$, that is, $\lambda_1 = \lambda_2 = \dots = \lambda_{n-1}$, which implies by Lemma 9 that G is a complete graph. Then the proof is completed by noticing that only K_3 and K_4 are planar complete graphs for $n \geq 3$. \square

Though the lower bound is not sharp for $n \geq 5$, it can be shown that, up to a scale factor, the bound is asymptotically attainable. One example is the star graph S_n , which has Kirchhoff index $(n-1)^2$. This indicates that the lower bound can be asymptotically attained up to a scale factor of at least $1/6$. In fact, the scale factor could be improved to at least $\sqrt{3}/6$. For example, consider the planar graph $G = K_2 + P_{n-2}$. Since the Laplacian eigenvalues of P_n are [42]

$$4\sin^2 \frac{k\pi}{2n}, \quad k = 0, 1, \dots, n-1, \quad (23)$$

by Lemma 2, we readily obtain that the Laplacian eigenvalues of G are

$$0, n, n, 2 + 4\sin^2 \frac{k\pi}{2(n-2)}, \quad k = 1, 2, \dots, n-3. \quad (24)$$

Therefore, by Theorem 1, we have

$$\begin{aligned} Kf(G) &= 2 + \frac{n}{2} \sum_{k=1}^{n-3} \frac{1}{1 + 2\sin^2(k\pi/2(n-2))} \\ &= 2 + \frac{n}{2} \sum_{k=1}^{n-3} \frac{1}{2 - \cos(k\pi/(n-2))}. \end{aligned} \quad (25)$$

Now we consider the asymptotic behavior of $Kf(G)$ as $n \rightarrow \infty$:

$$\begin{aligned} &\lim_{n \rightarrow \infty} \frac{1}{n^2} Kf(T_n) \\ &= \lim_{n \rightarrow \infty} \left(2 + \frac{n}{2} \sum_{k=1}^{n-3} \frac{1}{2 - \cos(k\pi/(n-2))} \right) \\ &= \lim_{n \rightarrow \infty} \frac{2}{n^2} + \lim_{n \rightarrow \infty} \frac{1}{2n} \sum_{k=1}^{n-3} \frac{1}{2 - \cos(k\pi/(n-2))} \\ &= \lim_{n \rightarrow \infty} \frac{n-3}{2n} \sum_{k=1}^{n-3} \frac{1}{2 - \cos(k\pi/(n-2))} \frac{1}{n-3} \\ &= \frac{1}{2} \lim_{n \rightarrow \infty} \sum_{k=1}^{n-3} \frac{1}{2 - \cos(k\pi/(n-2))} \frac{1}{n-3} \\ &= \frac{1}{2} \int_0^1 \frac{1}{2 - \cos x\pi} dx \\ &= \frac{1}{2} \frac{\sqrt{3}}{3} = \frac{\sqrt{3}}{6}. \end{aligned} \quad (26)$$

Hence $Kf(T_n)$ grows as $(\sqrt{3}/6)n^2$ as $n \rightarrow \infty$, and the scale factor is improved to at least $\sqrt{3}/6$.

4. Fullerene Graphs

A fullerene graph G is a cubic 3-connected planar graph with exactly 12 pentagons and other hexagons. Fullerene graphs are well studied in both mathematical and chemical literatures. To give bounds for fullerene graphs, we need some preparations.

The famous Foster first formula, given by Foster [43], states that

$$\sum_{i \sim j} r_{ij} = n - 1, \quad (27)$$

where $i \sim j$ means i and j are adjacent. Foster's second formula [44], also given by Foster, perhaps less well known, states that

$$\sum_v \frac{r_{ij}}{d_v} = n - 2, \quad (28)$$

where r_{ij} is measured across the end vertices of two adjacent edges iv and vj and the sum is taken over all adjacent edges. Palacios [14] extended Foster's first and second formulae and obtained the so-called Foster third formula, which states that

$$\sum_{v,w} \sum_{i < j} \frac{r_{ij}}{d_v d_w} = n - 3 + \sum_j \frac{1}{d_j} \sum_{k \sim j} \frac{1}{d_k}, \quad (29)$$

where the sum is taken over all pairs of vertices i and j such that $ivwj$ is a 3-walk. In particular, if G is k regular, then the above equation can be simply written as

$$\sum_{3\text{-walks}} r_{ij} \kappa_{ij} = (n-3)k^2 + nk, \quad (30)$$

where κ_{ij} is the number of 3-walks from i to j .

Now we give lower bounds for resistance distance between any two nonadjacent vertices in G in terms of the distance between them.

Lemma 11. *Let G be a fullerene graph and let $i, j \in V(G)$. Suppose that $d_{ij} = d \geq 2$. Then*

$$r_{ij} \geq \begin{cases} \frac{2}{3} (2 - 2^{1-(d/2)}), & \text{if } d \text{ is even,} \\ \frac{2}{3} (2 - 2^{(3-d)/2} + 2^{(-1-d)/2}), & \text{otherwise.} \end{cases} \quad (31)$$

Proof. If $d = 2$, by the inequality $r_{ij} \geq 1/d_i + 1/d_j$ [45], we know that $r_{ij} \geq 1/3 + 1/3 = 2/3$, as desired. Now suppose that $d \geq 3$. We distinguish the following two cases.

Case 1 (d is even). We partition vertices in $V(G) \setminus \{i, j\}$ into the following parts. For $k = 1, 2, \dots, (d/2) - 1$, let

$$\begin{aligned} I_k &= \{x \mid x \in V(G) \setminus \{i, j\}, d_{ix} = k\}, \\ J_k &= \{x \mid x \in V(G) \setminus \{i, j\}, d_{jx} = k\}, \end{aligned} \quad (32)$$

and let $I_{d/2}$ be the set of the remaining vertices. For $k = 1, 2, \dots, d/2$, contract I_k into a single vertex i_k . For $k = 1, 2, \dots, (d/2) - 1$, contract J_k into a single vertex j_k . Then we obtain a path P of length d with multiple edges;

$$P : (i =) i_0, i_1, \dots, i_{(d/2)-1}, i_{d/2}, j_{(d/2)-1}, \dots, j_1, j_0 (= j). \quad (33)$$

According to the structure of G , it is easily seen that, for $k = 1, 2, \dots, (d/2) - 1$, $|I_k| \leq 3 \times 2^{k-1}$, $|J_k| \leq 3 \times 2^{k-1}$. For $k = 1, 2, \dots, (d/2) - 1$, since every vertex in I_k has at least one neighbor in I_{k-1} , the number of edges connecting i_k and i_{k+1} is no more than $2|I_k| \leq 3 \times 2^k$. Similarly, for $k = 1, 2, \dots, (d/2) - 2$, the number of edges connecting j_k and j_{k+1} is no more than 3×2^k , and the number of edges connecting $j_{(d/2)-1}$ and $i_{d/2}$ is no more than $3 \times 2^{d-1}$. Hence, according to the series and parallel connection rules of resistors, we know that

$$\begin{aligned} r_{ij}(P) &= r_{i_0, i_1}(P) + r_{i_1, i_2}(P) + \dots + r_{i_{(d/2)-1}, i_{d/2}}(P) \\ &\quad + r_{j_{(d/2)-1}, i_{d/2}}(P) + r_{j_{(d/2)-2}, j_{(d/2)-1}}(P) \\ &\quad + \dots + r_{j_1, j_2}(P) + r_{j_0, j_1}(P) \\ &\geq \frac{1}{3} + \frac{1}{3 \times 2} + \dots + \frac{1}{3 \times 2^{(d/2)-1}} + \frac{1}{3 \times 2^{(d/2)-1}} \\ &\quad + \frac{1}{3 \times 2^{(d/2)-2}} + \dots + \frac{1}{3 \times 2} + \frac{1}{3} \\ &= \frac{2}{3} (2 - 2^{1-(d/2)}). \end{aligned} \quad (34)$$

Then by Rayleigh's short-cut principle [46], which states that shorting certain vertices together can only decrease the resistance distances between two given vertices, whereas cutting certain edges can only increase the resistance distance between two given vertices, it follows that

$$r_{ij}(G) \geq r_{ij}(P) \geq \frac{2}{3} (2 - 2^{1-(d/2)}). \quad (35)$$

Case 2 (d is odd). First partition vertices in $V(G) \setminus \{i, j\}$ in the following way. For $k = 1, 2, \dots, (d-1)/2 - 1$, let

$$I_k = \{x \mid x \in V(G) \setminus \{i, j\}, d_{ix} = k\}, \quad (36)$$

for $k = 1, 2, \dots, (d-1)/2$, let

$$J_k = \{x \mid x \in V(G) \setminus \{i, j\}, d_{jx} = k\}, \quad (37)$$

and let $I_{(d-1)/2}$ be the set of remaining vertices. Contract I_k to a single vertex i_k and contract J_k to a single vertex j_k , $k = 1, 2, \dots, (d-1)/2$. Using the same argument as the proof of Case 1, we could obtain that $r_{ij} \geq (2/3)(2 - 2^{(3-d)/2} + 2^{(-1-d)/2})$. \square

The following result is useful.

Lemma 12 (see [47]). *There are exactly $(9n/2 - 30)$ pairs of vertices at distance 3 in G .*

Next we introduce a classical result in graph theory—Menger's Theorem.

Theorem 13 (see [48], Menger's Theorem). *Let G be an undirected graph, and let u and v be nonadjacent vertices in G . Then, the maximum number of pairwise internally disjoint (u, v) paths in G equals the minimum number of vertices from $V(G) - \{u, v\}$ whose deletion separates u and v .*

Now we are ready for our main result.

Theorem 14. *For an n vertex fullerene graph G , one has*

$$\frac{n^2}{2} - \frac{7n}{4} - 2 \leq Kf(G) < \frac{n^3}{18} - n^2 + \frac{329n}{18} - \frac{92}{3}. \quad (38)$$

Proof. We first prove the lower bound. By Foster's first formula,

$$\sum_{\substack{i < j \\ d_{ij}=1}} r_{ij} = n - 1. \quad (39)$$

Since G is triangle free, it is obvious that the end vertices of any two adjacent edges in G are at distance 2. Hence by Foster's second formula,

$$\sum_{\substack{i < j \\ d_{ij}=2}} r_{ij} = 3(n - 2). \quad (40)$$

Since there are exactly $6n - 60$ pairs of vertices at distance 3 and by Lemma 11 we know that $r_{ij} \geq 5/6$ for $d_{ij} = 3$, hence

$$\sum_{\substack{i < j \\ d_{ij}=3}} r_{ij} \geq \frac{5}{6} \left(\frac{9n}{2} - 30 \right) = \frac{15n}{4} - 25. \quad (41)$$

Since for $d_{ij} \geq 4$, by Lemma 11, $r_{ij} \geq 1$, we have

$$\sum_{\substack{i < j \\ d_{ij} \geq 4}} r_{ij} \geq \left[\binom{n}{2} - \frac{3n}{2} - 3n - \left(\frac{9n}{2} - 30 \right) \right] \times 1 = \frac{n^2 - 19n}{2} + 30. \quad (42)$$

Hence

$$\begin{aligned} Kf(G) &= \sum_{i < j} r_{ij} = \sum_{\substack{i < j \\ d_{ij}=1}} r_{ij} + \sum_{\substack{i < j \\ d_{ij}=2}} r_{ij} \\ &\quad + \sum_{\substack{i < j \\ d_{ij}=3}} r_{ij} + \sum_{\substack{i < j \\ d_{ij} \geq 4}} r_{ij} \\ &\geq n - 1 + 3n - 2 + \frac{15n}{4} - 25 + \frac{n^2 - 19n}{2} + 30 \\ &= \frac{n^2}{2} - \frac{7n}{4} - 2. \end{aligned} \quad (43)$$

For the upper bound, we consider any two nonadjacent vertices i and j . Since G is 3-connected, by Menger's Theorem, i and j are connected by at least three pairwise internally disjoint paths. Suppose that P_1 , P_2 , and P_3 are three pairwise internally disjoint paths connecting i and j . We consider the graph G^* induced by P_1 , P_2 , and P_3 . By Rayleigh's short-cut principle, $r_{ij}(G) \leq r_{ij}(G^*)$. Suppose that the lengths of P_1 , P_2 , and P_3 are l_1 , l_2 , and l_3 , respectively. Then by the series and parallel connection rules of resistors,

$$r_{ij}(G^*) = \frac{1}{(1/l_1) + (1/l_2) + (1/l_3)}. \quad (44)$$

Since it is obvious that $l_1 + l_2 + l_3 \leq n + 1$, it follows that

$$\frac{1}{l_1} + \frac{1}{l_2} + \frac{1}{l_3} \geq \frac{3}{n+1} + \frac{3}{n+1} + \frac{3}{n+1} = \frac{9}{n+1}. \quad (45)$$

Thus $r_{ij}(G) \leq r_{ij}(G^*) \leq (n+1)/9$.

By Foster's third formula (30) and noticing that there exist 3-walks which are not 3-path in G , we conclude that

$$\sum_{\substack{i < j \\ d_{ij}=3}} r_{ij} < \sum_{\text{3-walks}} r_{ij} \kappa_{ij} = (n-3)3^2 + 3n = 12n - 27. \quad (46)$$

Hence

$$\begin{aligned} Kf(G) &= \sum_{i < j} r_{ij} \\ &= \sum_{\substack{i < j \\ d_{ij}=1}} r_{ij} + \sum_{\substack{i < j \\ d_{ij}=2}} r_{ij} + \sum_{\substack{i < j \\ d_{ij}=3}} r_{ij} + \sum_{\substack{i < j \\ d_{ij} \geq 4}} r_{ij} \end{aligned}$$

$$\begin{aligned} &< n - 1 + 3(n - 2) + 12n - 27 \\ &\quad + \left(\frac{n^2 - 19n}{2} + 30 \right) \times \frac{n+1}{9} \\ &= \frac{n^3}{18} - n^2 + \frac{329n}{18} - \frac{92}{3}. \end{aligned} \quad (47)$$

□

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this article.

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