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On Kirchhoff Index and Resistance–Distance Energy of a Graph

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Abstract

We report lower bounds for the Kirchhoff index of a connected (molecular) graph in terms of its structural parameters such as the number of vertices (atoms), the number of edges (bonds), maximum vertex degree (valency), second maximum vertex degree and minimum vertex degree. Also we give the Nordhaus–Gaddum-type result for Kirchhoff index.

In this paper we define the resistance distance energy as the sum of the absolute values of the eigenvalues of the resistance distance matrix and also we obtain lower and upper bounds for this energy.

1 Introduction

It is well known that the resistance distance between two arbitrary vertices in an electrical network can be obtained in terms of the eigenvalues and eigenvectors of the combinatorial Laplacian matrix and normalized Laplacian matrix associated with the network. By studying Laplacian matrix, people have proved many properties of resistance distances [1,2]. The resistance distance is a novel distance function on a graph proposed by Klein and

Randić [3]. The term "resistance distance" was used because of the physical interpretation (see [4], for the details).

Throughout this paper G will denote a simple undirected graph and the vertices of it will be labeled by v_1, $v_2, \ldots,$ v_n. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by δ, the maximum by Δ and the second maximum by Δ_2. In [5], it has been depicted that the standard distance between two vertices v_i and v_j of a connected graph G, denoted by d_{ij}, is defined as the length (=number of edges) of a shortest path that connects v_i and v_j. Moreover in order to examine other distances in graphs (or more formally, molecular graphs), Klein and Randić [6] considered the resistance distance between vertices of a graph G, denoted by r_{ij}, as defined in [1]. In fact the resistance distance concept has been much studied in the chemical studies (see, for instance, [2, 6]). In [6, 7], it has been introduced the sum of resistance distances of all pairs of vertices of a molecular graph G,

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

that named as the "Kirchhoff index".

Let J denote the square matrix of order n such that all of whose elements are unity. Then for all connected graphs (with two or more vertices) the matrix $L + \frac{1}{n}J$ is non-singular, its inverse

$$X = \|x_{ij}\| = \left(L + \frac{1}{n}J\right)^{-1}$$

exists and, as depicted in [1], $r_{ij} = x_{ii} + x_{jj} - 2x_{ij}$. The matrix whose (i, j)-entry is r_{ij}, is called the *resistance distance matrix* and will be denoted by $RD = RD(G)$. This matrix is symmetric and has a zero diagonal.

The Laplacian matrix of a graph G is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees and $A(G)$ is the $(0, 1)$-adjacency matrix of graph G. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$ denote the eigenvalues of $L(G)$. They are usually called the Laplacian eigenvalues of G.

The Kirchhoff index $Kf(G)$ can also be written as

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

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$ are the eigenvalues of the Laplacian matrix $L(G)$. As usual, K_n, $K_{1,n-1}$ and $K_{p,q}$ denote respectively the complete graph, the star and complete bipartite graph. The union ($\cup$) of two graphs is the graph whose set of vertices is the union of the sets of vertices of the two graphs, and whose set of edges is the union of the sets of edges of the two graphs. The graph join ($\vee$) of two graphs is their graph union with all the edges that connect the vertices of the first graph with the vertices of the second graph.

Now we study the Kirchhoff index in more detail, especially its relationship with the the number of vertices (atoms), the number of edges (bonds), maximum vertex degree (valency), second maximum vertex degree and minimum vertex degree. The paper is organized as follows. In section 2, we present the lower bounds on the Kirchhoff index of graph, and, the Nordhaus–Gaddum-type result for the Kirchhoff index. In section 3, we obtain the various lower and upper bounds on the *resistance distance energy* (*resistance distance energy* is the sum of the absolute values of the eigenvalues of the resistance distance matrix).

2 Lower bounds on the Kirchhoff index

In this section we give an upper bound on the resistance-distance index.

Lemma 2.1. *[8] Let G be a connected (molecular) graph on $n > 2$ vertices, m edges with maximum degree Δ. Then*

$$Kf(G) \geq \frac{n}{\Delta+1} + \frac{n(n-2)^2}{2m-\Delta-1} \tag{1}$$

with equality holding if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Lemma 2.2. *[9] Let G be a connected (molecular) graph of order n and maximum degree Δ with at least one edge. Then $\lambda_1 \geq \Delta+1$ with equality holding if and only if $\Delta = n-1$.*

Lemma 2.3. *[10] Let G be a connected (molecular) graph of order $n \geq 3$. Then*

$$\lambda_2 \geq \Delta_2$$

with equality holding if G is a complete bipartite graph $K_{r,s}$ or a tree with degree sequence $\pi(T) = \left(\frac{n}{2}, \frac{n}{2}, 1, 1, \ldots, 1\right)$, where $n \geq 4$ is even.

Lemma 2.4. *[11] Let G $(\neq K_n)$ be a connected (molecular) graph with minimum degree δ. Then $\lambda_{n-1} \leq \delta$.*

Lemma 2.5. *[12] Let G be a connected (molecular) graph on n vertices. Then $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$ if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$ or $G \cong K_{\Delta,\Delta}$.*

Now we are ready to give lower bound on Kirchhoff index and characterize extremal graphs.

Theorem 2.6. *Let G be a connected (molecular) graph on $n > 2$ vertices, m edges with maximum degree Δ, second maximum degree Δ_2 and minimum degree δ. Then*

$$Kf(G) \geq \frac{n}{\Delta+1} + \frac{n}{2m-\Delta-1}\Big((n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\delta}\Big) \tag{2}$$

with equality holding if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Proof: If $G = K_n$, then the equality holds in (2). Otherwise, $G \neq K_n$. By Lemma 2.3, $\lambda_2 \geq \Delta_2$ and by Lemma 2.4, $\lambda_{n-1} \leq \delta$. So, we have

$$\sqrt{\frac{\lambda_2}{\lambda_{n-1}}} - \sqrt{\frac{\lambda_{n-1}}{\lambda_2}} \geq \frac{\Delta_2-\delta}{\sqrt{\Delta_2\delta}}. \tag{3}$$

Now,

$$\begin{aligned}
\sum_{i=2}^{n-1}\lambda_i\sum_{i=2}^{n-1}\frac{1}{\lambda_i} &= n-2+\sum_{1<i<j<n}\Big(\frac{\lambda_i}{\lambda_j}+\frac{\lambda_j}{\lambda_i}\Big) \\
&= n-2+(n-2)(n-3)+\sum_{1<i<j<n}\frac{(\lambda_i-\lambda_j)^2}{\lambda_i\lambda_j} \\
&\geq (n-2)^2+\frac{(\Delta_2-\delta)^2}{\Delta_2\delta} \quad \text{as } \sqrt{\frac{\lambda_i}{\lambda_j}}-\sqrt{\frac{\lambda_j}{\lambda_i}} \geq 0 \text{ for } 1<i<j<n \qquad (4) \\
&\qquad\qquad \text{and by (3).}
\end{aligned}$$

Since $\sum_{i=1}^{n-1}\lambda_i = 2m$, from (4), we get

$$\sum_{i=1}^{n-1}\frac{1}{\lambda_i} \geq \frac{1}{\lambda_1} + \frac{1}{2m-\lambda_1}\Big((n-2)^2+\frac{(\Delta_2-\delta)^2}{\Delta_2\delta}\Big).$$

Note that

$$f(x) = \frac{1}{x} + \frac{1}{2m-x}\Big((n-2)^2+\frac{(\Delta_2-\delta)^2}{\Delta_2\delta}\Big)$$

is an increasing function for $[\Delta+1, n]$ as $(n-2)x \geq 2m - x$, that is, $(n-1)x \geq 2m = \sum_{i=1}^{n} d_i$. Since $\lambda_1 \geq \Delta + 1$, we get the required result (2).

Now we suppose that the equality holds in (2). Then all inequalities in the above argument must be equalities. Since $\lambda_1 = \Delta + 1$, we have $\Delta = n - 1$, by Lemma 2.2. From equality in (4), we get $\lambda_2 = \lambda_3 = \cdots = \lambda_{n-1}$. By Lemma 2.5, we conclude that $G \cong K_{1,n-1}$. For $G = K_{1,n-1}$, both $\lambda_2 = \Delta_2$ and $\lambda_{n-1} = \delta$ holds. Hence $G \cong K_{1,n-1}$ or $G \cong K_n$.

Conversely, one can easily see that the equality holds in (2) for star $K_{1,n-1}$ or complete graph K_n. □

Remark 2.7. *One can easily see that our lower bound (2) is better than the previous lower bound (1).*

A kite $Ki_{n,\omega}$ is the graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an end point from the path. We now give another lower bound for Kirchhoff index and characterize extremal graphs.

Theorem 2.8. *Let G ($\neq K_n$) be a connected (molecular) graph on $n > 2$ vertices, m edges with maximum degree Δ and minimum degree δ. Then*

$$Kf(G) \geq 1 + \frac{n}{\delta} + \frac{n(n-3)^2}{2m - \Delta - \delta - 1} \tag{5}$$

with equality holding if and only if $G \cong K_{1,n-1}$ or $G \cong Ki_{n,n-1}$ or $G \cong K_n - e$, where $K_n - e$ is the graph of order n, obtained from K_n by deleting an edge.

Proof: We have

$$\begin{aligned} Kf(G) &= \frac{n}{\lambda_1} + \frac{n}{\lambda_{n-1}} + \sum_{i=2}^{n-2} \frac{n}{\lambda_i} \\ &\geq 1 + \frac{n}{\lambda_{n-1}} + \frac{n(n-3)^2}{2m - \lambda_1 - \lambda_{n-1}} \qquad (6) \\ &\quad \text{by } \lambda_1 \leq n \text{ and by arithmetic–harmonic mean inequality} \\ &\geq 1 + \frac{n}{\lambda_{n-1}} + \frac{n(n-3)^2}{2m - \Delta - \lambda_{n-1} - 1} \quad \text{by Lemma 2.2.} \qquad (7) \end{aligned}$$

Note that

$$f(x)=\frac{1}{x}+\frac{(n-3)^2}{2m-\Delta-x-1}, \quad x\leq\delta$$

is a decreasing function if and only if $(n-2)x \leq 2m-\delta-1$, that is, $(n-2)x \leq \sum_{i=2}^{n} d_i - 1$, which is true for $x \leq \delta$ and G is connected. Thus we have

$$f(x)\geq\frac{1}{\delta}+\frac{(n-3)^2}{2m-\Delta-\delta-1} \ .$$

From above we get the required result (5).

Now we suppose that the equality holds in (5). Then all inequalities in the above argument must be equalities. From equality in (7), we get

$$\lambda_1=\Delta+1$$

that is, $\Delta=n-1$, by Lemma 2.2. From equality in (6), we get

$$\lambda_1=n \quad \text{and} \quad \lambda_2=\lambda_3=\cdots=\lambda_{n-2} \ .$$

Thus we conclude that $\overline{G}$ is disconnected with at least one isolated vertex and

$$S(\overline{G})=(n-\lambda_{n-1},\underbrace{n-\lambda_2,\,n-\lambda_2,\ldots,n-\lambda_2}_{n-3},0,0).$$

If $\overline{G}$ has exactly two connected components, then $\overline{G}\cong K_1\cup K_{1,n-2}$ or $\overline{G}\cong K_1\cup K_{n-1}$ or $\overline{G}\cong K_1\cup K_{\frac{n-1}{2},\frac{n-1}{2}}$, n is odd, by Lemma 2.5. Since $\lambda_2=\lambda_3=\cdots=\lambda_{n-2}$, we must have $G\cong Ki_{n,n-1}$ or $G\cong K_{1,n-1}$. Otherwise, $\overline{G}$ contains at least $n-2$ isolated vertices. Since $G\neq K_n$, we must have $\overline{G}\cong(n-2)K_1\cup K_2$, that is, $G\cong K_n-e$.

Conversely, one can easily see that the equality holds in (5) for star $K_{1,n-1}$ or for kite $Ki_{n,n-1}$ or for K_n-e. This completes the proof. □

Remark 2.9. *The lower bound in (5) is sharp for $K_{1,n-1}$, $Ki_{n,n-1}$ or K_n-e. But (1) and (2) are sharp only for $K_{1,n-1}$ or K_n.*

Lemma 2.10. *[12] Let G be a graph of order n with at least one edge. Then $\lambda_1=\lambda_2=\cdots=\lambda_{n-1}$ if and only if $G\cong K_n$.*

Lemma 2.11. *[9] Let G be a connected (molecular) graph with diameter d. Suppose $L(G)$ has exactly k distinct eigenvalues. Then $d+1\leq k$.*

Zhou and Trinajstić [8] obtained the following Nordhaus–Gaddum-type result for the Kirchhoff index:

Lemma 2.12. *Let G be a connected (molecular) graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then*

$$Kf(G) + Kf(\overline{G}) \geq 4n - 2 \,.$$

Another structure–descriptor introduced long time ago [13] is the so-called first Zagreb index (M_1) equal to the sum of the squares of the degrees of all vertices of G. Some basic properties of M_1 can be found in [14, 15]. Denote by H^*, a graph of diameter 2 such that $\lambda_1(H^*) = \cdots = \lambda_k(H^*) \neq \lambda_{k+1}(H^*) = \cdots = \lambda_{n-1}(H^*)$, $\lambda_k(H^*) + \lambda_{n-1}(H^*) = n$ for some value of k, $1 \leq k < n-1$. For example, cycle of length 5, C_5 is H^*-type graph as $S(C_5) = (3.618, 3.618, 1.382, 1.382, 0)$ and diameter of C_5 is 2. We now give lower bound for $Kf(G) + Kf(\overline{G})$:

Theorem 2.13. *Let G be a connected (molecular) graph of order n (≥ 5) and m edges with connected $\overline{G}$. Then*

$$Kf(G) + Kf(\overline{G}) \geq \frac{n^2(n-1)^2}{2m(n-1) - M_1(G)} \tag{8}$$

where $M_1(G)$ is the first Zagreb index of G. Moreover, the equality holds in (8) if and only if $G \cong H^*$.

Proof: We have

$$\begin{aligned} Kf(G) + Kf(\overline{G}) &= n \sum_{i=1}^{n-1} \Big(\frac{1}{\lambda_i} + \frac{1}{n-\lambda_i} \Big) \\ &= n^2 \sum_{i=1}^{n-1} \frac{1}{\lambda_i(n-\lambda_i)} \\ &\geq \frac{n^2(n-1)^2}{2mn - \sum_{i=1}^{n-1} \lambda_i^2} \quad \text{by arithmetic–harmonic mean inequality.} \end{aligned} \tag{9}$$

Since $2m = \sum_{i=1}^{n} d_i$, we have $\sum_{i=1}^{n-1} \lambda_i^2 = \sum_{i=1}^{n} d_i(d_i+1) = M_1(G) + 2m$, we get (8) from (9).

Now suppose that the equality holds in (8). Then the equality holds in (9). From equality in (9), we get

$$\lambda_i(n-\lambda_i) = \lambda_j(n-\lambda_j) \quad \text{for all } v_i, v_j \in V,$$

that is,

$$(\lambda_i - \lambda_j)(n - \lambda_i - \lambda_j) = 0 \text{ for all } v_i, v_j \in V,$$

that is, either $\lambda_i = \lambda_j$ or $\lambda_i + \lambda_j = n$ for all $v_i, v_j \in V$. Thus $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$ or $\lambda_1 = \cdots = \lambda_k \neq \lambda_{k+1} = \cdots = \lambda_{n-1}$, $\lambda_k + \lambda_{n-1} = n$ for some value of k, $1 \leq k < n-1$. If $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$, then by Lemma 2.10, $G \cong K_n$, a contradiction as $\overline{G}$ is connected. Otherwise, $\lambda_1 = \cdots = \lambda_k \neq \lambda_{k+1} = \cdots = \lambda_{n-1}$, $\lambda_k + \lambda_{n-1} = n$ for some value of k, $1 \leq k < n-1$. By Lemma 2.11, $d = 2$ as $G \neq K_n$. Hence $G \cong H^*$.

Conversely, let G be isomorphic to some H^*. Then

$$\begin{aligned} Kf(G) + Kf(\overline{G}) &= \frac{nk}{\lambda_1} + \frac{n(n-k-1)}{n-\lambda_1} + \frac{n(n-k-1)}{\lambda_1} + \frac{kn}{n-\lambda_1} \\ &= \frac{n^2(n-1)}{\lambda_1(n-\lambda_1)} \\ &= \frac{n^2(n-1)^2}{2m(n-1) - M_1(H^*)} \quad \text{as } \textstyle\sum_{i=1}^n \lambda_i^2 = \sum_{i=1}^n d_i(d_i+1)\,. \end{aligned}$$

Hence the theorem. □

3 Bounds for resistance-distance energy

Graph spectral theory, based on eigenvalues of the adjacency matrix, has well and long known applications in chemistry [16,17]. One of the chemically (and also mathematically) most interesting graph-spectrum that based quantities in the graph energy is defined as follows:

Let G be a simple graph on n vertices and let A be its adjacency matrix. Let $\mu_1, \mu_2, \cdots, \mu_n$ be the eigenvalues of A. These are said to be the eigenvalues of the graph G and to form of its spectrum [18]. The energy $E(G)$ of the graph G is defined as the sum of the absolute values of its eigenvalues

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

For more details on graph energy one can see, for instance, the reference [19].

In view of evident success of the concept of graph energy, and because of the rapid decrease of open mathematical problems in its theory, energies based on the eigenvalues of other graph matrices have, one-by-one, been introduced. Of these, the Laplacian energy $LE(G)$, pertaining to the Laplacian matrix, sees to be the first [20]. Followed the distance energy [21] based on the distance matrix, and variety of energy - like graph invariants - introduced by Consonni and Todeschini [22]. After that Nikiforov extended the definition of energy to arbitrary matrices [23], making thus possible to conceive the incidence energy [24], based on the incidence matrix, etc.

Along these above lines of reasoning, we could think of the resistance-distance energy as the sum of absolute values of the eigenvalues of the resistance-distance matrix. More formally, let $\rho_1, \rho_2, \cdots, \rho_n$ be the eigenvalues of the resistance-distance matrix RD. Knowing that these eigenvalues are necessarily real numbers, the resistance-distance energy can be defined as

$$RDE = RDE(G) = \sum_{i=1}^{n} |\rho_i| \ . \tag{10}$$

It is easy to see that this definition can be applicable to all graphs in the literature. Yet, the actual route to resistance-distance energy is somewhat less straightforward.

In this section, by considering the definition in (10), we first present some fundamental results for convenience.

Lemma 3.1. *[1] Let G has $n \geq 2$ vertices. Assume that λ_1 and λ_{n-1} are the largest and smallest positive Laplacian eigenvalues of G, respectively. Then, for $1 \leq s \leq n$, each eigenvalue ρ_s of the resistance-distance matrix RD satisfy the inequality*

$$\begin{array}{rcl} \nu_1(B) + \min\Big(\dfrac{-2}{\lambda_{n-1}}, -2\Big) \leq & \rho_1 & \leq \nu_1(B) - \dfrac{2}{\lambda_1} \\ \min\Big(\dfrac{-2}{\lambda_{n-1}}, -2\Big) \leq & \rho_k & \leq \dfrac{-2}{\lambda_1}; \quad 2 \leq k \leq n-1 \\ \nu_n(B) + \min\Big(\dfrac{-2}{\lambda_{n-1}}, -2\Big) \leq & \rho_n & \leq \nu_n(B) - \dfrac{2}{\lambda_1} \end{array} \tag{11}$$

where the matrix B whose (i,j)-entry is equal to $x_{ii} + x_{jj}$ (for $X = \|x_{ij}\| = (L + \frac{1}{n}J)^{-1}$, J denote the square matrix of order n such that all of whose elements are unity) and each $\nu_s(B)$ $(1 \leq s \leq n)$ is an s-th largest eigenvalue of the matrix B.

Lemma 3.2. *[1] Let G has $n \geq 2$ vertices (possessing $t(G) > 0$ spanning trees) and let $\lambda_1, \lambda_2, \cdots, \lambda_{n-1}, \lambda_n = 0$ be its Laplacian eigenvalues. Then the determinant of its resistance-distance matrix RD is equal to*

$$(-1)^{n-1} \frac{2^{n-1}}{nt(G)} \Big(S + 2\sum_{k=1}^{n-1} \frac{1}{\lambda_k}\Big)$$

where

$$S = \frac{n}{2}(x_{11}, x_{22}, \cdots, x_{nn})L(x_{11}, x_{22}, \cdots, x_{nn})^T \ .$$

Now we are ready to give some bounds on the resistance-distance energy:

Theorem 3.3. *Let G has $n \geq 2$ vertices and let $\lambda_1, \lambda_2, \cdots, \lambda_{n-1}, \lambda_n = 0$ be its Laplacian eigenvalues. Then*

$$RDE = RDE(G) \leq M + \sqrt{(n-1)(D - M^2)} \tag{12}$$

where D is the sum of the squares of entries of the resistance-distance matrix, B is given as in Lemma 3.1 and, by (11),

$$M = \nu_1(B) + \min\left(\frac{-2}{\lambda_{n-1}}, -2\right). \tag{13}$$

Proof. Let $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ be the eigenvalues of the resistance-distance matrix RD. We know that

$$RDE = \sum_{i=1}^{n} |\rho_i| \quad and \quad \sum_{i=1}^{n} \rho_i^2 = D = \sum_{i=1}^{n}\sum_{j=1}^{n}(r_{ij})^2.$$

By the Cauchy–Schwarz inequality, we get

$$\sum_{i=2}^{n} |\rho_i| \leq \sqrt{(n-1)\sum_{i=2}^{n}(\rho_i)^2} = \sqrt{(n-1)(D - \rho_1^2)}.$$

Therefore

$$RDE \leq \rho_1 + \sqrt{(n-1)(D - \rho_1^2)}.$$

By Lemma 3.1, since

$$\rho_1 \geq \nu_1(B) + min\left(\frac{-2}{\lambda_{n-1}}, -2\right)$$

we obtain the required result. □

Theorem 3.4. *Let G be a graph with $n \geq 2$ vertices. Then*

$$RDE = RDE(G) \leq \sqrt{nD} \tag{14}$$

where D is the sum of the squares of entries of the resistance-distance matrix.

Proof: We have that

$$RDE = \sum_{i=1}^{n} |\rho_i| \quad and \quad \sum_{i=1}^{n} \rho_i^2 = D = \sum_{i=1}^{n}\sum_{j=1}^{n}(r_{ij})^2.$$

By the Cauchy–Schwarz inequality, we get

$$RDE \leq |\rho_1| + |\rho_n| + \sqrt{(n-2)\sum_{i=2}^{n-1}\rho_i^2} = |\rho_1| + |\rho_n| + \sqrt{(n-2)(D-\rho_1^2-\rho_n^2)}\,.$$

Consider the function

$$f(x,y) = x + y + \sqrt{(n-2)(D-x^2-y^2)} \quad x>0,\; y>0.$$

Now our aim is to find the maximum value of $f(x,y)$. For this, we calculate

$$f_x = 1 - \frac{x\sqrt{n-2}}{\sqrt{D-x^2-y^2}},\; f_y = 1 - \frac{y\sqrt{n-2}}{\sqrt{D-x^2-y^2}},\; f_{xx} = -\frac{(D-y^2)\sqrt{n-2}}{(D-x^2-y^2)^{3/2}}$$

$$f_{xy} = f_{yx} = -\frac{xy\sqrt{n-2}}{(D-x^2-y^2)^{3/2}} \text{ and } f_{yy} = -\frac{(D-x^2)\sqrt{n-2}}{(D-x^2-y^2)^{3/2}}\,.$$

Now,

$$f_x = f_y = 0 \Rightarrow x = y = \sqrt{\frac{D}{n}}\,.$$

For $x = y = \sqrt{\frac{D}{n}}$,

$$f_{xx} < 0,\; f_{xx}f_{yy} - f_{xy}^2 = \frac{(n-2)(D-x^2-y^2)}{(D-x^2-y^2)^3} > 0\,.$$

From above we conclude that $f(x,y)$ has a maximum value at $x = y = \sqrt{\frac{D}{n}}$ and maximum value is $2\sqrt{\frac{D}{n}} + \sqrt{(n-2)\Big(D - 2\frac{D}{n}\Big)} = \sqrt{nD}$. Hence the theorem. □

Lemma 3.5. *[1] The resistance matrix of any connected (molecular) graph on n vertices, $n \geq 2$, has exactly one positive eigenvalue and exactly $n-1$ negative eigenvalues.*

Lemma 3.6. *[4] Let G be a graph of order n, m edges with diameter d. For all $v_i, v_j \in V$ $(i \neq j)$, the (i,j)-th element of the resistance distance matrix $RD(G)$ is*

$$\frac{1}{2}\Big(\frac{1}{d_i} + \frac{1}{d_j}\Big) \leq r_{ij} \leq 2md\Big(\frac{1}{d_i} + \frac{1}{d_j}\Big) \tag{15}$$

where d_i is the degree of vertex v_i in G.

Lemma 3.7. *[25] Let $B = ||b_{ij}||$ be an $n \times n$ irreducible non-negative matrix with spectral radius $\lambda_1(B)$, and let $R_i(B)$ be the i-th row sum of B, i. e., $R_i(B) = \sum_{j=1}^{n} b_{ij}$. Then*

$$\min\{R_i(B):\; 1 \leq i \leq n\} \leq \lambda_1(B) \leq \max\{R_i(B):\; 1 \leq i \leq n\}\,. \tag{16}$$

Moreover, if the row sums of B are not all equal, then both inequalities in (16) are strict.

Now we are ready to give another bound on the resistance-distance energy.

Theorem 3.8. *Let G be a graph of order $n \geq 2$ with m edges and diameter d. Then*

$$\min_i \left(\frac{n-2}{d_i} + \sum_{j=1}^{n} \frac{1}{d_j}\right) \leq RDE(G) \leq 4md\ \max_i \left(\frac{n-2}{d_i} + \sum_{j=1}^{n} \frac{1}{d_j}\right)$$

where d_i is the degree of the vertex v_i in G.

Proof: By Lemma 3.5, we have

$$RDE = RDE(G) = 2\rho_1 \ .$$

By Lemma 3.6 and Lemma 3.7, we have

$$\begin{aligned}\min_i \left(\frac{n-2}{d_i} + \sum_{j=1}^{n} \frac{1}{d_j}\right) \leq 2\min_i \sum_{j=1, j\neq i}^{n} r_{ij} \leq RDE(G) \leq 2\max_i \sum_{j=1, j\neq i}^{n} r_{ij} \\ \leq 4md\ \max_i \left(\frac{n-2}{d_i} + \sum_{j=1}^{n} \frac{1}{d_j}\right).\end{aligned}$$

Hence the theorem. □

The following lemma can be helped to show different bounds for resistance-distance energy.

Lemma 3.9. *[26] Let $a_1, a_2, \cdots, a_n$ be non-negative numbers. Then*

$$\begin{aligned} n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right] &\leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2 \\ &\leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right].\end{aligned}$$

Theorem 3.10. *Let G has $n \geq 2$ vertices (possessing $t(G) > 0$ spanning trees). Then*

$$\sqrt{n(n-1)[det(RD)]^{2/n} + D} \leq RDE(G) \leq \sqrt{(n-1)D + n[det(RD)]^{2/n}},$$

where

$$D = \sum_{i=1}^{n}\sum_{j=1}^{n} (r_{ij})^2.$$

Remark 3.11. *We note that, by considering the references [1,4], the bounds of RDE, that obtained in the left hand and right hand side of the inequality in the above theorem, can also be written in terms of the eigenvalues and eigenvectors of the combinatorial Laplacian and normalized Laplacian matrices.*

Proof. Note that

$$D = \sum_{i=1}^{n} \rho_i^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} (r_{ij})^2 \quad and \quad RDE = \sum_{i=1}^{n} |\rho_i| \ .$$

For $1 \leq i \leq n$, by taking $a_i = \rho_i^2$ in Lemma 3.9, we obtain

$$K \leq n \sum_{i=1}^{n} \rho_i^2 - (\sum_{i=1}^{n} |\rho_i|)^2 \leq (n-1)K$$

that is,

$$K \leq nD - [RDE]^2 \leq (n-1)K$$

where

$$K = n \left[\frac{1}{n} \sum_{i=1}^{n} \rho_i^2 - \left(\prod_{i=1}^{n} \rho_i^2 \right)^{1/n} \right] = n \left[\frac{1}{n} D - \left(\prod_{i=1}^{n} |\rho_i| \right)^{2/n} \right] = D - n \left[det(RD) \right]^{2/n} \ .$$

Hence the result. $\square$

In [5, 27], for any n-vertex tree T,

$$det(A(T)) = det(RD(T)) = (-1)^{n-1}(n-1)2^{n-2} \tag{17}$$

where $A(T)$ is the adjacency matrix of tree T.

Now using (17) in Theorem 3.10, we give the following result.

Corollary 3.12. *For any n-vertex tree T,*

$$\sqrt{D + n[(n-1)^{n+2} 4^{n-2}]^{1/n}} \leq RDE(T) \leq \sqrt{(n-1)D + n[(n-1)^2 4^{n-2}]^{1/n}}$$

where D is defined as in Theorem 3.10.

In [28], Bapat obtained the following two results:

(i) For unicyclic graph G of order n with unique cycle C_k of length k (≥ 3), then

$$det(RD(G)) = (-1)^{n-1} 2^{n-2} \cdot \frac{3kn - 2k^2 - 1}{3k^2} \ .$$

(ii) For cycle C_n of order n (≥ 3), then

$$det(RD(C_n)) = (-1)^{n-1} 2^{n-2} \cdot \frac{n^2 - 1}{3n^2} \ .$$

Using above results, we give the following corollary.

Corollary 3.13. *(i) For unicyclic graph G of order n with unique cycle C_k of length k (≥ 3), then*

$$\sqrt{D+n(n-1)\Big[2^{n-2}\cdot\frac{3kn-2k^2-1}{3k^2}\Big]^{2/n}} \leq RDE(T) \leq \sqrt{(n-1)D+n\Big[2^{n-2}\cdot\frac{3kn-2k^2-1}{3k^2}\Big]^{2/n}}$$

where D is defined as in Theorem 3.10.

(ii) For cycle C_n of order n (≥ 3), then

$$\sqrt{D+n(n-1)\Big[2^{n-2}\cdot\frac{n^2-1}{3n^2}\Big]^{2/n}} \leq RDE(T) \leq \sqrt{(n-1)D+n\Big[2^{n-2}\cdot\frac{n^2-1}{3n^2}\Big]^{2/n}}$$

where D is defined as in Theorem 3.10.

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