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On Complementary Distance Signless Laplacian Spectral Radius and Energy of Graphs

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Abstract. Let D be the diameter and $d_G(v_i, v_j)$ be the distance between the vertices v_i and v_j of a connected graph G. The complementary distance matrix of a graph G is $CD(G) = [cd_{ij}]$ in which $cd_{ij} = 1 + D - d_G(v_i, v_j)$ if $i \neq j$ and $cd_{ij} = 0$ if $i = j$. The complementary transmission $CT_G(v)$ of a vertex v is defined as $CT_G(v) = \sum_{u \in V(G)} [1 + D - d_G(u, v)]$. Let $CT(G) = diag[CT_G(v_1), CT_G(v_2), \ldots, CT_G(v_n)]$. The complementary distance signless Laplacian matrix of G is $CDL^+(G) = CT(G) + CD(G)$. In this paper, we obtain the bounds for the largest eigenvalue of $CDL^+(G)$. Further we determine Nordhaus-Gaddum type results for the largest eigenvalue. We also establish some bounds for the complementary distance signless Laplacian energy.

Keywords: Complementary distance signless Laplacian matrix (energy); diameter; complementary transmission regular graph.

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1. Introduction

In this work we concern only simple graphs, that is graphs without loops, multiple and directed edges. Let G be such a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $A = A(G)$ be its $(0,1)$-adjacency matrix. Suppose N_i be the neighbor set of vertex $v_i \in V(G)$. Then $|N_i| = d_G(v_i)$, where $d_G(v_i)$ is the degree of a vertex v_i, for $i = 1, 2, \ldots, n$. The maximum and minimum vertex degrees are denoted by $\triangle$ and δ, respectively. The distance between two vertices u and v, which is the smallest length of any $u - v$ path in G, is denoted by $d_G(u, v)$. The greatest distance between any two vertices of a connected graph G is called the diameter of G and is denoted by $diam(G) = D$.

For developing structure property models in drug design, virtual synthesis, chemical database searching, similarity and diversity assessments, there is a significant interest in deriving additional structural descriptors for quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) models. So that Ivanciuc [26] introduced the complementary distance matrix for molecular graphs, and discussed by Balaban et al. [4] and Ivanciuc et al. [27], which has been successfully applied in the structure property modeling of the molar heat capacity, standard Gibbs energy of formation and vaporization enthalpy of 134 alkanes $C_6 - C_{10}$ [27].

The complementary distance matrix of a graph G is defined as $CD(G) = [cd_{ij}]$, where

$$cd_{ij} = \begin{cases} 1 + D - d_{ij} & \text{if} \quad i \neq j \\ 0 & \text{otherwise,} \end{cases}$$

where D is the diameter of G and d_{ij} is the distance between the vertices v_i and v_j in G. The complementary Wiener index of a graph G is defined as

$$CW(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}(1 + D - d_{ij}) = \sum_{1 \leq i < j \leq n}(1 + D - d_{ij}). \tag{1.1}$$

We define the complementary transmission $CT_G(v)$ of a vertex v as $CT_G(v) = \sum_{u \in V(G)}[1 + D - d_G(u, v)]$ and $CT(G)$ is the diagonal matrix

$$diag[CT_G(v_1), CT_G(v_2), \ldots, CT_G(v_n)].$$

For $1 \leq i \leq n$, one can easily see that $CT_G(v_i)$ is just the i-th row sum of $CD(G)$. Clearly $CW(G) = \frac{1}{2}\sum_{v \in V(G)} CT_G(v)$. A graph G is said to be complementary transmission regular if $CT_G(v)$ is a constant for each $v \in V(G)$.

Since A is a real and symmetric adjacency matrix of order n, its eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ are real numbers. These eigenvalues form the spectrum of G [9, 12]. The energy of a graph G is defined as the sum of absolute values of its eigenvalues [22], that is,

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

The mathematical properties of this spectrum-based graph invariant has been extensively studied, see the book [30], the recent articles [16, 17, 18, 19, 21, 23, 34, 33] and the references cited therein.

The complementary distance energy of a graph G, denoted by $E_{CD}(G)$ and is defined as,

$$E_{CD}(G) = \sum_{i=1}^{n} |\mu_i|, \tag{1.2}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the complementary distance matrix $CD(G)$ of G. B. Zhou, and N. Trinajstić [37], gave bounds for the largest eigenvalues of the complementary distance matrix. Recent results related to the complementary distance energy can be found in [31, 32, 35].

The eigenvalues of the complementary distance matrix of a graph G satisfies the relations

$$\sum_{i=1}^{n} \mu_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} \mu_i^2 = 2 \sum_{1 \le i < j \le n} (1 + D - d_{ij})^2. \tag{1.3}$$

Let $Deg(G) = diag[d_G(v_1), d_G(v_2), \ldots, d_G(v_n)]$ be the diagonal degree matrix of G. The Laplacian matrix of G is defined as $L(G) = Deg(G) - A(G)$ and signless Laplacian matrix of G is defined as $L^+(G) = Deg(G) + A(G)$. Let $\mu_1^-, \mu_2^-, \ldots \mu_n^-$ and $\mu_1^+, \mu_2^+, \ldots, \mu_n^+$ be the eigenvalues of the matrices $L(G)$ and $L^+(G)$, respectively. Then the Laplacian energy of G is defined in [24] as,

$$E_L(G) = \left| \mu_i^- - \frac{2m}{n} \right|$$

and, in analogy to $E_L(G)$, the signless Laplacian energy is defined as

$$E_L^+(G) = \left| \mu_i^+ - \frac{2m}{n} \right|.$$

For studies of the signless Laplacian spectrum and energy see [1, 3, 11, 13, 14, 15, 16, 17, 29, 36].

The complementary distance Laplacian matrix of a connected graph G is defined as

$$CDL^-(G) = CT(G) - CD(G).$$

The complementary distance Laplacian energy of a graph G is denoted by $E_{CDL^-}(G)$ and is defined as

$$E_{CDL^-}(G) = \sum_{i=1}^{n} \left| \delta_i - \frac{1}{n}\sum_{j=1}^{n} CT_G(v_j) \right|, \tag{1.4}$$

where $\delta_1, \delta_2, \ldots, \delta_n$ are the eigenvalues of the complementary distance Laplacian matrix of G.

The complementary distance signless Laplacian matrix of a connected graph G is an $n \times n$ matrix $CDL^+(G) = [c_{ij}]$, where

$$c_{ij} = \begin{cases} 1 + D - d_{ij} & \text{if} \quad i \neq j \\ \sum_{j=1, j\neq i}^{n}(1 + D - d_{ij}) & \text{if} \quad i = j, \end{cases}$$

where d_{ij} is the distance between the vertices v_i and v_j.

In other words, complementary distance signless Laplacian matrix is

$$CDL^+(G) = CT(G) + CD(G). \tag{1.5}$$

The investigation of matrices related to various graphical structures is a very large and growing area of research. The matrix $CDL^+(G)$ is irreducible, non-negative, symmetric and positive semidefinite. Let $\rho_i = \rho_i(G)$, $i = 1, 2, \ldots, n$ be the eigenvalues of the complementary distance signless Laplacain matrix $CDL^+(G)$ and they can be labeled in the non-increasing order as $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The largest eigenvalue ρ_1 of $CDL^+(G)$ is called the complementary distance signless Laplacian spectral radius of G. By the Perron-Frobenius theorem, there is a unique normalized positive eigenvector of $CDL^+(G)$ corresponding to $\rho_1(G)$, which is called the (complementary distance signless Laplacian) principal eigenvector of G.

A column vector $x = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex v_i to x_i, that is, $x(v_i) = x_i$ for $i = 1, 2, \ldots, n$. Then,

$$x^T CDL^+(G)x = \sum_{\{u,v\}\subseteq V(G)} (1 + D - d_{uv})(x(u) + x(v))^2,$$

and ρ is an eigenvalue of $CDL^+(G)$ corresponding to the eigenvector x if and only if $x \neq 0$ and for each $v \in V(G)$,

$$\rho x(v) = \sum_{u\in V(G)} (1 + D - d_{uv})(x(u) + x(v)).$$

These equations are called the (ρ, x)-eigenequations of G. For a normalized column vector $x \in \mathbb{R}^n$ with at least one non-negative component, by the

Rayleigh's principle, we have

$$\rho(G) \geq x^T CDL^+(G)x,$$

with equality if and only if x is the principal eigenvector of G (see [10]). For other undefined notations and terminology from graph theory, one can refer the books [5, 7, 8].

The paper is organized as follows. In Sections 2 and 3 we determine the bounds and Nordhaus-Gaddum type results for $\rho_1(G)$. In Section 4, we determine the upper bounds for $\rho_1(G)$ of bipartite graphs. In Section 5, we get the eigenvalues of the complementary distance signless Laplacian matrix of graphs obtained by some graph operations. Finally, in the Section 6, we obtain the bounds for the complementary distance signless Laplacian energy of graphs. The results of this paper are analogous to the results obtained in [2].

2. Bounds for $\rho_1(G)$

In this section, we get upper and lower bounds for the maximum eigenvalue of the complementary distance signless Laplacian matrix of a graph G. We start with the following lemma.

Lemma 2.1. *Let G be a connected graph on n vertices. Then*

$$\rho_1(G) \geq \frac{4CW(G)}{n},$$

with equality if and only if G is complementary transmission regular.

Proof. Since $\mathbf{1} = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T \in \mathbb{R}^n$ is normalized, we have

$$\begin{aligned} \rho_1(G) &\geq \mathbf{1}^T CDL^+(G)\mathbf{1} \\ &= \sum_{1\leq i<j\leq n} (1 + D - d_{ij}) \left(\frac{1}{\sqrt{n}} + \frac{1}{\sqrt{n}}\right)^2 \\ &= \frac{4CW(G)}{n}. \end{aligned}$$

Equality holds if and only if the graph G has the principal eigenvector $\mathbf{1}$, that is, $CT_G(v)$ is a constant for each vertex $v \in V(G)$, i.e., G is complementary transmission regular.

□

Corollary 2.2. *Let G be a connected graph with $n \geq 2$ vertices, m edges and $D = diam(G)$. Then*

$$\rho_1(G) \geq \frac{4m}{n}(D - 1) + 2(n - 1). \tag{2.1}$$

Equality holds if and only if G is a regular graph of diameter $D \leq 2$.

Proof. Suppose $G = K_n$ or G is a regular graph of diameter $D = 2$, then it is easy to see that (2.1) is an equality. Conversely, since there are m pairs of vertices at distance 1 and $\left[\binom{n}{2} - m\right]$ pairs of vertices at distance at most D, we have,

$$CW(G) \geq Dm + \left[\binom{n}{2} - m\right] = (D-1)m + \frac{n(n-1)}{2}.$$

Therefore by Lemma 2.1, we get the required result. □

Corollary 2.3. *Let G be a triangle and quadrangle free connected graph with $n \geq 2$ vertices, m edges and diameter D. Then*

$$\rho_1(G) \geq 2\left[n - 1 + \frac{1}{n}\left[(D-2)M_1(G) + 2m\right]\right],$$

where $M_1(G) = \sum_{u \in V(G)} [d_G(u)]^2$.
Equality holds if and only if G is a complementary transmission regular and $D \leq 3$.

Proof. Here m pairs of vertices are at distance 1, $\left[\frac{1}{2}M_1(G) - m\right]$ pairs of vertices are at distance 2 and $\left[\binom{n}{2} - \frac{1}{2}M_1(G)\right]$ pairs of vertices are at distance at most $D \geq 3$, then from Lemma 2.1 we have the following

$$\begin{aligned} \rho_1(G) &\geq \frac{4}{n}\left[Dm + (D-1)\left[\frac{1}{2}M_1(G) - m\right] + \frac{n(n-1)}{2} - \frac{1}{2}M_1(G)\right] \\ &= 2\left[n - 1 + \frac{1}{n}\left[(D-2)M_1(G) + 2m\right]\right]. \end{aligned}$$

□

Lemma 2.4. [6] *Let B be a non-negative irreducible matrix with row sums $B_1, B_2, \ldots, B_n$. If $\rho_1(B)$ is the largest eigenvalue of B, then $min_{1 \leq i \leq n} B_i \leq \rho_1(B) \leq max_{1 \leq i \leq n} B_i$, with either equality if and only if $B_1 = B_2 = \cdots = B_n$.*

Lemma 2.5. *Let G be a connected graph with $n \geq 2$ vertices and diameter D. Let Δ and δ be the maximum and minimum vertex degrees of G respectively. Then*

$$2[n - 1 + (D-1)\delta] \leq \rho_1(G) \leq 2[(n-1)(D-1) + \Delta],$$

with equality on both sides if and only if G is a regular graph of diameter $D \leq 2$.

Proof. We can easily see that the sum of the elements of i-th row in a matrix $CDL^{+}(G)$ is

$$\begin{aligned} CDL_i^{+} &= \sum_{j=1}^{n} c_{ij} \\ &= 2\sum_{j=1,\ j\neq i}^{n}(1+D-d_{ij}) \\ &\leq 2[(1+D-1)d_G(v_i)+(1+D-2)(n-1-d_G(v_i))] \\ &= 2[(n-1)(D-1)+d_G(v_i)] \end{aligned}$$

and

$$\begin{aligned} CDL_i^{+} &= \sum_{j=1}^{n} c_{ij} \\ &= 2\sum_{j=1,\ j\neq i}^{n}(1+D-d_{ij}) \\ &\geq 2[(1+D-1)d_G(v_i)+(1+D-D)(n-1-d_G(v_i))] \\ &= 2[n-1+(D-1)d_G(v_i)]. \end{aligned}$$

Equality holds in both cases if and only if $D \leq 2$ for all i. Clearly $CDL_1^{+} = CDL_2^{+} = \cdots = CDL_n^{+}$ if and only if $d_G(v_1) = d_G(v_2) = \cdots = d_G(v_n)$ and $D \leq 2$. By Lemma 2.4, the maximum eigenvalue of an irreducible non-negative matrix is at most the maximum row sum of the matrix and is at least the minimum row sum of the matrix, which is attained if and only if all the row sums are equal. Further $\delta \leq d_G(v_i) \leq \Delta$ for all $i = 1, 2, \ldots, n$. Hence the result follows from Lemma 2.4.

□

We obtain another upper bound for $\rho_1(G)$ in terms of order, size and maximum vertex degree, which is as follows.

Theorem 2.6. *Let G be a connected graph with $n \geq 2$ vertices, m edges and $\triangle$ is the maximum vertex degree. Then*

$$\rho_1(G) \leq \sqrt{[n-1][4(n-1)(D-1)^2] + 2[2D-1][2m+(n-2)\triangle]}, \qquad (2.2)$$

with equality if and only if $G = K_n$.

Proof. Let $X = (x_1, x_2, \ldots, x_n)^T$ be an unit eigenvector corresponding to $\rho_1(G)$ of $CDL^{+}(G)$. We have

$$CDL^{+}(G)X = \rho_1(G)X.$$

From the i^{th} equation of the above expression and applying the Cauchy-Schwarz inequality, we have

$$\begin{aligned}\rho_1(G)x_i &= \sum_{k:k\neq i}(1+D-d_{ik})(x_k+x_i)\\ &\leq \sqrt{\sum_{k:k\neq i}(1+D-d_{ik})^2\sum_{k:k\neq i}(x_k+x_i)^2}. \qquad (2.3)\end{aligned}$$

Let $CT_i^* = \sum_{k:k\neq i}(1+D-d_{ik})^2$, for $i = 1, 2, \ldots, n$ and $CT_p^* = max_{i\in V} CT_i^*$. Squaring both sides in (2.3) and taking sum for $i = 1$ to n, we get

$$\begin{aligned}\rho_1^2(G) &\leq \sum_{i=1}^{n} CT_i^*\left(1-x_i^2+(n-1)x_i^2+1-x_i^2+(n-1)x_i^2\right) \qquad (2.4)\\ &= \sum_{i=1}^{n} CT_i^*\left(2+(2n-4)x_i^2\right)\\ &\leq 2\sum_{i=1}^{n} CT_i^* + (2n-4)CT_p^* \qquad \text{as} \quad \sum_{i=1}^{n} x_i^2 = 1. \qquad (2.5)\end{aligned}$$

Since,

$$\begin{aligned}CT_i^* &= \sum_{k:k\neq i}(1+D-d_{ik})^2\\ &\leq (n-1)(D-1)^2 + (2D-1)d_G(v_i)\end{aligned}$$

and also, $CT_p^* = (D-1)^2(n-1) + (2D-1)\triangle$, that is, $\sum_{i=1}^{n} CT_i^* = n(n-1)(D-1)^2 + 2m(2D-1)$. Therefore we get

$$\rho_1^2(G) \leq [n-1][4(n-1)(D-1)^2] + 2[2D-1][2m+(n-2)\triangle]. \qquad (2.6)$$

For the equality, suppose that equality holds in (2.2). Then all inequalities in the above argument must be equalities. From equality in (2.6), G has $D \leq 2$ and $CT_i^* = (D-1)^2(n-1) + (2D-1)d_G(v_i)$, for $i = 1, 2, \ldots, n$. From equality in (2.4), G is a regular graph because we get $CT_1^* = CT_2^* = \cdots = CT_n^*$. Then $d_G(v_1) = d_G(v_2) = \cdots = d_G(v_n)$. If $D = 1$, then $G \cong K_n$. Otherwise $D = 2$ and hence we have $d_{ij} = 1$ or $d_{ij} = 2$, for all i, j. Without loss of generality we can assume that the shortest distance between vertex v_1 and v_n is 2. From equality in (2.3) and (2.4), we get $d_{i,1}x_1 = d_{i,2}x_2 = \cdots = d_{i,i-1}x_{i-1} = d_{i,i+1}x_{i+1} = \cdots = d_{i,n}x_n$, $i = 1, 2, \ldots, n$ and for $i = 1$ we get $x_k = 2x_n$, $k \in N(1)$ and $x_k = x_1$, $k \notin N(1)$, $k \neq 1$. Similarly, for $i = n$ we get $x_k = 2x_1$, $k \in N(n)$ and $x_k = x_1$,$k \notin N(n)$, $k \neq n$. Thus we have $x_1 = x_n$ and two type of eigencomponents x_1 and $2x_1$ in eigenvector X, which is a contradiction as G is regular graph of diameter 2. Hence G is complete graph K_n. Conversely, one can easily see that the equality holds in (2.2) for complete graph K_n. Hence the proof.

□

3. Nordhaus-Gaddum Type Results for $\rho_1(G)$

Theorem 3.1. *Let G be a connected graph on $n \geq 4$ vertices with a connected complement graph $\bar{G}$. Let D and $\bar{D}$ be the diameters of graphs G and $\bar{G}$, respectively. Then*

$$2(n-1)(k+1) \leq \rho_1(G) + \rho_1(\bar{G}) \leq 2[(2k'-1)(n-1) + (\Delta - \delta)], \tag{3.1}$$

where $k = min\{D, \bar{D}\}$ and $k' = max\{D, \bar{D}\}$. The equality holds if and only if both G and $\bar{G}$ are regular graphs of diameter 2.

Proof. Let m and $\bar{m}$ be the number of edges of G and $\bar{G}$. Therefore $m + \bar{m} = \binom{n}{2}$.

Lower bound: From the Corollary 2.2, we have

$$\begin{aligned}
\rho_1(G) + \rho_1(\bar{G}) &\geq \frac{4m}{n}(D-1) + 2(n-1) + \frac{4\bar{m}}{n}(\bar{D}-1) + 2(n-1) \\
&= \frac{4}{n}[mD + \bar{m}\bar{D} - (m+\bar{m})] + 4(n-1) \\
&\geq \frac{4}{n}[k(m+\bar{m}) - (m+\bar{m})] + 4(n-1) \\
&= \frac{4}{n}\left[k\frac{n(n-1)}{2} - \frac{n(n-1)}{2}\right] + 4(n-1) \\
&= 2(n-1)(k+1).
\end{aligned} \tag{3.2}$$

Now suppose that equality holds in the left hand side of Eq. (3.1). Then the equality holds in Eq. (3.2) if $k = D = \bar{D} = 2$. Therefore by Corollary 2.2 we get both G and $\bar{G}$ are regular graph of diameter 2.

Conversely, let both G and $\bar{G}$ be regular graph of diameter 2, that is $D = \bar{D} = k = 2$. Then by Corollary 2.2, $\rho_1(G) = \frac{4m}{n}(k-1) + 2(n-1)$ and $\rho_1(\bar{G}) = \frac{4\bar{m}}{n}(k-1) + 2(n-1)$. Hence

$$\rho_1(G) + \rho_1(\bar{G}) = 2(k+1)(n-1).$$

Upper bound: From the Lemma 2.5, we have

$$\begin{aligned}
\rho_1(G) + \rho_1(\bar{G}) &\leq 2[(n-1)(D-1) + \Delta] + 2[(n-1)(\bar{D}-1) + n - 1 - \delta] \\
&= 2[(n-1)(D+\bar{D}) - (n-1) + (\Delta - \delta)] \\
&\leq 2[(2k'-1)(n-1) + (\Delta - \delta)].
\end{aligned} \tag{3.3}$$

Now suppose that equality holds in the right hand side of Eq. (3.1). Then the equality holds in Eq. (3.3) if $k' = D = \bar{D} = 2$. Therefore by Lemma 2.5 we get both G and $\bar{G}$ are regular graphs of diameter 2.

Conversely, let both G and $\bar{G}$ be regular graph of diameter 2, that is $D = \bar{D} = k' = 2$. Then by Lemma 2.5, $\rho_1(G) = 2[n-1-\Delta]$ and $\rho_1(\bar{G}) = 2[n-1-\delta]$.

Hence

$$\rho_1(G) + \rho_1(\bar{G}) = 2[3(n-1) + \Delta - \delta].$$

□

The following theorem gives an upper bound for $\rho_1(G) + \rho_1(\bar{G})$ in terms of graph parameters like order n, maximum degree $\triangle$ and minimum degree δ.

Theorem 3.2. *Let G be a connected graph on $n \geq 4$ vertices with a connected $\bar{G}$. Then*

$$\begin{aligned} &\rho_1(G) + \rho_1(\bar{G}) \\ \leq\ & \sqrt{\frac{\begin{array}{rl} & 8(n-1)^2(D-1)^2(2\bar{D}-1)(2D-1)(D+\bar{D}-1) \\ + & 2(2D-1)\left[2(n-1)^2[\bar{D}^2(2D-1)^2 - (D-1)^2(2\bar{D}-1)^2]\right. \\ + & \left.(n-2)(2D-1)^2(2\bar{D}-1)(\triangle-\delta)\right] \end{array}}{2(2D-1)(2\bar{D}-1)(D+\bar{D}-1)}} \\ +\ & \sqrt{\frac{\begin{array}{rl} & 8(n-1)^2\bar{D}^2(2\bar{D}-1)(2D-1)(D+\bar{D}-1) \\ - & 2(2\bar{D}-1)\left\{2(n-1)^2[\bar{D}^2(2D-1)^2 - (D-1)^2(2\bar{D}-1)^2]\right. \\ + & \left.(n-2)(2D-1)(2\bar{D}-1)^2(\delta-\triangle)\right\} \end{array}}{2(2D-1)(2\bar{D}-1)(D+\bar{D}-1)}}. \end{aligned}$$

Proof. By the inequality (2.2) from Theorem 2.6, we get

$$\begin{aligned} \rho_1(G) + \rho_1(\bar{G}) \ \leq\ & \sqrt{(n-1)\,[4(n-1)(D-1)^2] + 2(2D-1)\,[2m + (n-2)\triangle]} \\ +\ & \sqrt{(n-1)[4(n-1)(\bar{D}-1)^2] + 2(2\bar{D}-1)[2\bar{m} + (n-2)\bar{\triangle}]}. \end{aligned}$$

Then we get

$$\begin{aligned} &\rho_1(G) + \rho_1(\bar{G}) \\ \leq\ & \sqrt{(n-1)\,[4(n-1)(D-1)^2] + 2(2D-1)\,[2m + (n-2)\triangle]} \\ +\ & \sqrt{(n-1)[4(n-1)(\bar{D}-1)^2] + 2(2\bar{D}-1)[2(n-1)^2 - 2m - (n-2)\delta]}, \end{aligned} \tag{3.4}$$

as $\bar{m} = \binom{n}{2} - m$, and $\bar{\triangle} = n - 1 - \delta$, where $\bar{m}$, $\bar{D}$ are the number of edges and diameter of $\bar{G}$. Consider the function

$$\begin{aligned} &f(m) \\ =\ & \sqrt{(n-1)\,[4(n-1)(D-1)^2] + 2(2D-1)\,[2m + (n-2)\triangle]} \\ +\ & \sqrt{(n-1)[4(n-1)(\bar{D}-1)^2] + 2(2\bar{D}-1)[2(n-1)^2 - 2m - (n-2)\delta]}. \end{aligned} \tag{3.5}$$

One can easily get that

$$f(m) \ \leq\ f\left(\frac{\begin{array}{c}(n-1)^2\left[\bar{D}^2(2D-1)^2 - (D-1)^2(2\bar{D}-1)^2\right] \\ -(n-2)(2D-1)(2\bar{D}-1)\left[(2\bar{D}-1)\triangle + (2D-1)\delta\right]\end{array}}{(2D-1)(2\bar{D}-1)4(D+\bar{D}-1)}\right).$$

Now, from the equations (3.4) and (3.5), we get the required result. □

Corollary 3.3. *Let G be a connected graph on $n \geq 4$ vertices and $\bar{G}$ be its complement graph. If $D = \bar{D}$, then*

$$\rho_1(G) + \rho_1(\bar{G}) \leq 2\sqrt{4(n-1)^2(D-1)^2 + (2D-1)(n-2)[2(n-1) + (\triangle - \delta)]},$$

where D and $\bar{D}$ are the diameters of G and $\bar{G}$, respectively.

4. On $\rho_1(G)$ of Bipartite Graphs

In this section we present upper bounds for the complementary distance signless Laplacian spectral radius of bipartite graphs in terms of diameter and number of vertices and characterize the extremal graphs.

Theorem 4.1. *Let G be a connected bipartite graph on n vertices with bipartition of vertices as $V(G) = V_1 \cup V_2$ where $|V_1| = p$, $|V_2| = q$. Then*

$$\begin{aligned} \rho_1(G) \leq\ & \frac{1}{2}(D(3n-4) - 2(n-2)) \qquad (4.1)\\ +\ & \frac{1}{2}\sqrt{\begin{matrix}[D(3n-4)-2(n-2)]^2 \\ -4\left[2D(Dn^2 - 3Dn + 2D - n^2 + 5n - 2pq - 4) + 4(pq - n + 1)\right]\end{matrix}}, \end{aligned}$$

with equality if and only if G is $K_{p,q}$.

Proof. Let $V_1 = \{v_1, v_2, \ldots, v_p\}$ and $V_2 = \{v_{p+1}, v_{p+2}, \ldots, v_{p+q}\}$, where $p+q = n$. Let $X = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector of $CDL^+(G)$ corresponding to the spectral radius $\rho_1(G)$ of a graph G. Let us assume that $x_i = max_{v_k \in V_1} x_k$ and $x_j = max_{v_k \in V_2} x_k$.

For $v_i \in V_1$,

$$\begin{aligned} \rho_1(G)x_i &= \sum_{k=1, k\neq i}^{p} (1 + D - d_{ik})(x_k + x_i) + \sum_{k=p+1}^{p+q} (1 + D - d_{ik})(x_k + x_i) \\ &\leq [D(2p + q - 2) - 2(p-1)]\, x_i + Dqx_j. \qquad (4.2) \end{aligned}$$

For $v_i \in V_2$,

$$\begin{aligned} \rho_1(G)x_j &= \sum_{k=1}^{p} (1 + D - d_{ik})(x_k + x_j) + \sum_{k=p+1, k\neq j}^{p+q} (1 + D - d_{ik})(x_k + x_j) \\ &\leq Dpx_i + [D(2q + p - 2) - 2(q-1)]\, x_j. \qquad (4.3) \end{aligned}$$

Since G is connected, hence $x_k > 0$, for all $v_k \in V(G)$. From (4.2) and (4.3), we get

$$[\rho_1(G) - (D(2p + q - 2) - 2(p-1))]\, [\rho_1(G) - (D(2q + p - 2) - 2(q-1))] \leq D^2pq,$$

as $x_i, x_j > 0$.

That is,

$$\rho_1^2(G) - \rho_1(G)\left[D(2(n-1)+(n-2)) - 2(n-2)\right] + D^2(2n^2-6n+4) \\ -2D(n^2-5n+2pq+4) + 4(p-1)(q-1) \leq 0.$$

From the above inequality we get the required result (4.1).

Now suppose that equality holds in (4.1), then all inequalities in the above argument must be equal.
From the equality in (4.2), we get

$$x_k = x_j, \text{ and } v_i v_k \in E(G), \ \forall v_k \in V_2.$$

From the equality in (4.3), we get

$$x_k = x_i \text{ and } v_j v_k \in E(G), \forall v_k \in V_1.$$

Thus each vertex in each set is adjacent to all the vertices on the other set and vice versa. Hence G is complete bipartite graph $K_{p,q}$.

Conversely, it is easy to see that (4.1) holds for complete bipartite graph $K_{p,q}$. □

Theorem 4.2. *Let G be a connected bipartite graph of order n and size m with bipartition of the vertex set as $V(G) = V_1 \cup V_2$, where $|V_1| = p$ and $|V_2| = q$, $p + q = n$. Then*

$$\rho_1(G) \leq \frac{1}{2}\left[A^* + \sqrt{\begin{array}{l} A^{*2} - 4\{2(D-1)\left[2(pq-n+1+(p-1)\triangle_2+(q-1)\triangle_1)\right. \\ \left. + (D-2)(n(n-1)-2pq)\right]\} \end{array}}\right], \tag{4.4}$$

where $A^* = 2(D-1)(n-2) + n(D-2) + 2(\triangle_1 + \triangle_2)$, $\triangle_1$ and $\triangle_2$ are the maximum degree among vertices from V_1 and V_2, respectively.

Proof. Let $V_1 = \{v_1, v_2, \ldots, v_p\}$ and $V_2 = \{v_{p+1}, v_{p+2}, \ldots, v_{p+q}\}$. Let $X = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $CDL^+(G)$ corresponding to the maximum eigenvalue $\rho_1(G)$ such that $x_i = max_{v_k \in V_1} x_k$ and $x_j = max_{v_k \in V_2} x_k$. Then we have, for $v_i \in V_1$,

$$\begin{aligned} \rho_1(G)x_i &= \sum_{k=1, k\neq i}^{p} (1+D-d_{ik})(x_k+x_i) + \sum_{k=p+1}^{p+q} (1+D-d_{ik})(x_k+x_i) \\ &\leq \left[2(D-1)(p-1) + q(D-2) + 2\triangle_1\right] x_i + \left[q(D-2)+2\triangle_1\right] x_j. \quad (4.5) \end{aligned}$$

For $v_i \in V_2$,

$$\begin{aligned} \rho_1(G)x_j &= \sum_{k=1}^{p} (1+D-d_{jk})(x_k+x_j) + \sum_{k=p+1, k\neq j}^{p+q} (1+D-d_{jk})(x_k+x_j) \\ &\leq \left[p(D-2)+2\triangle_2\right] x_i + \left[2(D-1)(q-1) + p(D-2) + 2\triangle_2\right] x_j. \quad (4.6) \end{aligned}$$

Combining the inequalities (4.5) and (4.6), we arrive at

$$\begin{gathered}[\rho_1(G) - (2(D-1)(p-1) + q(D-2) + 2\triangle_1)] \\ \times [\rho_1(G) - (2(D-1)(q-1) + p(D-2) + 2\triangle_2)].\end{gathered}$$

Since $x_k > 0$ for $1 \leq k \leq p+q$,

$$\begin{aligned}&\rho_1^2(G) - \rho_1(G)\,[2(D-1)(n-2) + n(D-2) + 2(\triangle_1 + \triangle_2)] + 2(D-1) \\ &\times \left[2(pq - n + 1 + (p-1)\triangle_2 + (q-1)\triangle_1) + (D-2)(p^2+q^2-1)\right] \leq 0. \quad (4.7)\end{aligned}$$

From the inequality (4.7) we get the desired result.

For the equality, we have $x_i = x_k$ for $k = 1, 2, \ldots, p$ and $x_j = x_k$ for $k = p+1, p+2, \ldots, p+q$. This means that the eigenvector x has at most two different coordinates, the degrees of vertices in V_1 and V_2 are equal to $\triangle_1$ and $\triangle_2$, respectively, implying that G is a semi-regular graph. If G is not a complete bipartite graph, it follows from $p\triangle_1 = q\triangle_2$ that $\triangle_1 < q$ and $\triangle_2 < p$ and the eccentricity of every vertex must be equal to 3. □

Corollary 4.3. *Let G be a connected bipartite graph of order n and size m with bipartition of the vertex set as $V(G) = V_1 \cup V_2$, where $|V_1| = p$ and $|V_2| = q$, $p+q = n$. Let $\triangle_1$ and $\triangle_2$ be the maximum degree among vertices from V_1 and V_2, respectively. If $\triangle_1 = \triangle_2 = \triangle$, then*

$$\rho_1(G) \leq \frac{1}{2}\left[\hat{A} + \sqrt{\begin{array}{l}\hat{A}^2 - 4\{2(D-1)\,[2(pq-n+1+\triangle(n-2) \\ +(D-2)(n(n-1)-2pq)]\}\end{array}}\right], \quad (4.8)$$

where $\hat{A} = 2(D-1)(n-2) + n(D-2) + 4\triangle$.

5. Eigenvalues of $CDL^+(G)$ of Graphs Obtained by Some Graph Operations

In this section we compute eigenvalues of the complementary distance signless Laplacian matrix with respect to some graph operations. The following lemma will be helpful in the sequel.

Lemma 5.1. [20] *Let $A = \begin{bmatrix} A_0 & A_1 \\ A_1 & A_0 \end{bmatrix}$ be a symmetric 2×2 block matrix. Then the spectrum of A is the union of the spectra of $A_0 + A_1$ and $A_0 - A_1$.*

The graph $G \bigtriangledown G$ is obtained by joining every vertex of G to every vertex of another copy of G.

Theorem 5.2. *Let G be a connected r-regular graph on n-vertices with diameter $D \leq 2$. If $r, \lambda_2, \lambda_3, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G, then the eigenvalues of the complementary distance signless Laplacian matrix of $G \bigtriangledown G$ are*

$$4Dn-2D-2n+2+2r,$$

$$2Dn-2D-2n+2+2r \qquad \textit{and}$$

$$2Dn-2D-n+2+r+\lambda_i, \qquad 2 \textit{ times}, \quad i=2,3,\ldots,n.$$

Proof. As G is an r-regular graph of diameter $D \le 2$, the complementary distance signless Laplacian matrix of $G \bigtriangledown G$ can be written as

$$\begin{bmatrix} \begin{array}{c}(2Dn-D-n+r+1)\,I\\ +DA+(D-1)\bar{A}\end{array} & DJ \\ \\ DJ & \begin{array}{c}(2Dn-D-n+r+1)\,I\\ +DA+(D-1)\bar{A}\end{array} \end{bmatrix},$$

where A is the adjacency matrix of G, $\bar{A}$ is the adjacency matrix of $\bar{G}$, J is a matrix of order $n \times n$ whose all entries are equal to 1 and I is an identity matrix of order n. Since $\bar{A} = J - I - A$, then by applying Lemma 5.1, we get the result. □

Definition 5.3. [25] Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Take another copy of G with the vertices labeled by $\{u_1, u_2, \ldots, u_n\}$ where u_i corresponds to v_i for each i. Make u_i adjacent to all the vertices in $N(v_i)$ in G, for each i. The resulting graph, denoted by D_2G is called the double graph of G.

Theorem 5.4. *Let G be a connected r-regular graph on n vertices with diameter 2 and let $r, \lambda_2, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of G. Then the eigenvalues of the complementary distance signless Laplacian matrix of D_2G are*

$$2r(D-1)+2n+D(n+r-1),$$

$$D(n+r-1), \qquad n \textit{ times}, \quad \textit{and}$$

$$2\lambda_i(D-1)+D(n+r-1), \qquad i=2,3,\ldots,n.$$

Proof. By definition of D_2G, the complementary distance signless Laplacian matrix of D_2G is of the form

$$\begin{bmatrix} DA+\bar{A}+(D(n+r)-(D-1))\,I & DA+\bar{A}+I \\ DA+\bar{A}+I & DA+\bar{A}+(D(n+r)-(D-1))\,I \end{bmatrix},$$

where D is the diameter of graph G, A is the adjacency matrix of G, $\bar{A}$ is the adjacency matrix of $\bar{G}$ and I is an identity matrix. Since $\bar{A} = J - I - A$, then by applying Lemma 5.1, the result follows. □

6. Bounds for the Complementary Distance Signless Laplacian Energy

In this section we obtain some bounds for the complementary distance signless Laplacian energy of a graph. To preserve the main features of the complementary distance energy and complementary distance Laplacian energy and bearing in mind the Eq. (1.3), we define here

$$\xi_i = \rho_i - \frac{1}{n}\sum_{j=1}^{n} CT_G(v_j), \qquad i = 1, 2, \ldots, n, \tag{6.1}$$

where ρ_i, $i = 1, 2, \ldots n$ are the eigenvalues of $CDL^+(G)$.

Definition: Let G be a connected graph of order n. Then the complementary distance signless Laplacian energy of G, denoted by $E_{CDL^+}(G)$ is defined as

$$E_{CDL^+}(G) = \sum_{i=1}^{n} |\xi_i| = \sum_{i=1}^{n} \left| \rho_i - \frac{1}{n}\sum_{j=1}^{n} CT_G(v_j) \right|. \tag{6.2}$$

Lemma 6.1. *Let G be a connected graph of order n. Then*

$$\sum_{i=1}^{n} \xi_i = 0 \text{ and } \sum_{i=1}^{n} \xi_i^2 = 2S,$$

where

$$S = s + \frac{1}{2}\sum_{i=1}^{n}\left[CT_G(v_i) - \frac{1}{n}\sum_{j=1}^{n} CT_G(v_j)\right]^2 \text{ and } s = \sum_{1\le i<j\le n} (1 + D - d_{ij})^2.$$

Proof.

$$\begin{aligned}
\sum_{i=1}^{n} \rho_i &= \text{trace}[CDL^{+}(G)] = \sum_{i=1}^{n} CT_G(v_i) \quad \text{and} \\
\sum_{i=1}^{n} \rho_i^2 &= \text{trace}[CDL^{+}(G)]^2 \\
&= 2 \sum_{1 \le i < j \le n} (1 + D - d_{ij})^2 + \sum_{i=1}^{n} (CT_G(v_i))^2 \\
&= 2s + \sum_{i=1}^{n} (CT_G(v_i))^2
\end{aligned}$$

Now,

$$\begin{aligned}
\sum_{i=1}^{n} \xi_i &= \sum_{i=1}^{n} \left(\rho_i - \frac{1}{n} \sum_{j=1}^{n} CT_G(v_j) \right) \\
&= \sum_{i=1}^{n} \rho_i - \sum_{j=1}^{n} CT_G(v_j) = 0,
\end{aligned}$$

and

$$\begin{aligned}
\sum_{i=1}^{n} \xi_i^2 &= \sum_{i=1}^{n} \left(\rho_i - \frac{1}{n} \sum_{j=1}^{n} CT_G(v_j) \right)^2 \\
&= \sum_{i=1}^{n} \rho_i^2 - \frac{2}{n} \sum_{j=1}^{n} CT_G(v_j) \sum_{i=1}^{n} \rho_i + \frac{1}{n} \left[\sum_{j=1}^{n} CT_G(v_j) \right]^2 \\
&= 2 \sum_{1 \le i < j \le n} (1 + D - d_{ij})^2 + \sum_{j=1}^{n} (CT_G(v_j))^2 \\
&- \frac{2}{n} \sum_{j=1}^{n} CT_G(v_j) \sum_{i=1}^{n} CT_G(v_i) + \frac{1}{n} \left[\sum_{j=1}^{n} CT_G(v_j) \right]^2 \\
&= 2s + \sum_{i=1}^{n} \left[CT_G(v_i) - \frac{1}{n} \sum_{j=1}^{n} CT_G(v_j) \right]^2 \\
&= 2S.
\end{aligned}$$

□

Corollary 6.2. *Let G be a connected graph of order n and size m with diameter $D \le 2$. Then*

$$\sum_{i=1}^{n} \xi_i^2 = 6m + n(n-1) + M_1(G) - \frac{4m^2}{n},$$

where $M_1(G) = \sum\limits_{i=1}^{n} (d_G(v_i))^2$.

Proof. If G is having diameter less than or equal to two, then G has m pairs of vertices at distance 1 and $\binom{n}{2} - m$ pairs of vertices at distance 2.

Therefore

$$\sum_{1 \le i < j \le n} (1 + D - d_{ij})^2 = \frac{6m + n(n-1)}{2},$$

and

$$CT(v_i) = \sum_{i=1}^{n} (1 + D - d_{ij}) = (n - 1 + d_G(v_i)).$$

Therefore,

$$\begin{aligned} \sum_{i=1}^{n} \xi_i^2 &= 2 \sum_{1 \le i < j \le n} (1 + D - d_{ij})^2 + \sum_{i=1}^{n} \left[CT(v_i) - \frac{1}{n} \sum_{j=1}^{n} (CT(v_j)) \right]^2 \\ &= 6m + n(n-1) + \sum_{i=1}^{n} \left[d_G(v_i) - \frac{2m}{n} \right]^2 \\ &= 6m + n(n-1) + M_1(G) - \frac{4m^2}{n}. \end{aligned}$$

□

Theorem 6.3. *Let G be a connected graph of order n. Then*

$$2\sqrt{S} \le E_{CDL^+}(G) \le \sqrt{2nS}.$$

Proof. By direct computation, we get

$$\begin{aligned} T &= \sum_{i=1}^{n} \sum_{j=1}^{n} (|\xi_i| - |\xi_j|)^2 \\ &= 2n \sum_{i=1}^{n} |\xi_i|^2 - 2 \left(\sum_{i=1}^{n} |\xi_i| \right) \left(\sum_{j=1}^{n} |\xi_j| \right) \\ &= 4nS - 2(E_{CDL^+}(G))^2. \end{aligned}$$

Since $T \ge 0$, hence $E_{CDL^+}(G) \le \sqrt{2nS}$.

Now, $\left(\sum\limits_{i=1}^{n} \xi_i \right)^2 = 0$. This implies $\sum\limits_{i=1}^{n} \xi_i^2 + 2 \sum\limits_{1 \le i < j \le n} (\xi_i)(\xi_j) = 0$.

Therefore,

$$\begin{aligned}
2S &= -2\sum_{1\le i<j\le n}(\xi_i\xi_j)\\
&\le 2\left|\sum_{1\le i<j\le n}(\xi_i\xi_j)\right|\\
&\le 2\sum_{1\le i<j\le n}|\xi_i||\xi_j|.
\end{aligned}$$

Thus,

$$\begin{aligned}
(E_{CDL^+}(G))^2 &= \left(\sum_{i=1}^{n}|\xi_i|\right)^2\\
&= \sum_{i=1}^{n}|\xi_i|^2+2\sum_{1\le i<j\le n}|\xi_i||\xi_j|\\
&\ge 2S+2S\\
&= 4S.
\end{aligned}$$

Hence we get the desired. □

Corollary 6.4. *If G is a connected graph on n vertices, then*

$$E_{CDL^+}(G)\ge\sqrt{2n(n-1)}.$$

Proof. Since $d_{ij}\le D$, for $i,j=1,2,\dots,n$, hence by Theorem 6.3 we have

$$\begin{aligned}
E_{CDL^+}(G) &\ge 2\sqrt{\sum_{1\le i<j\le n}(1+D-d_{ij})^2+\frac{1}{2}\sum_{i=1}^{n}\left[CT_G(v_i)-\frac{1}{n}\sum_{j=1}^{n}CT_G(v_j)\right]^2}\\
&\ge 2\sqrt{\sum_{1\le i<j\le n}(1+D-d_{ij})^2}\\
&\ge 2\sqrt{\sum_{1\le i<j\le n}1}\\
&= 2\sqrt{\frac{n(n-1)}{2}}\\
&= \sqrt{2n(n-1)}.
\end{aligned}$$

□

By Corollary 6.2 and Theorem 6.3, we get the following immediate corollary.

Corollary 6.5. *Let G be a connected graph with n vertices, m edges and $D\le 2$. Then*

$$\begin{aligned} E_{CDL^+}(G) &\geq \sqrt{12m + 2n(n-1) + 2M_1(G) - \frac{8m^2}{n}} \text{ and} \\ E_{CDL^+}(G) &\leq \sqrt{6mn + n^2(n-1) + nM_1(G) - 4m^2}, \end{aligned}$$

where $M_1(G) = \sum_{i=1}^{n} (d_G(v_i))^2$.

Lemma 6.6. [28] *Let* $a_1, a_2, \ldots, a_n$ *be non-negative numbers. Then*

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

Lemma 6.7. *Let* G *be a connected graph with* n *vertices,* I *is the unit matrix of order* n *and* $\Gamma = \left|det\left(CDL^+(G) - \frac{1}{n}\sum_{i=1}^{n} CT(v_i)I\right)\right|$. *Then*

$$\sqrt{2S + n(n-1)\Gamma^{(2/n)}} \leq E_{CDL^+}(G) \leq \sqrt{2(n-1)S + n\Gamma^{(2/n)}}.$$

Proof. Let $a_i = |\xi_i|^2$, $i = 1, 2, \ldots, n$ and

$$\begin{aligned} K &= n\left[\frac{1}{n}\sum_{i=1}^{n}|\xi_i|^2 - \left(\prod_{i=1}^{n}|\xi_i|^2\right)^{1/n}\right] \\ &= n\left[\frac{2S}{n} - \left(\prod_{i=1}^{n}|\xi_i|\right)^{2/n}\right] \\ &= 2S - n\Gamma^{2/n}. \end{aligned}$$

By Lemma 6.6, we get

$$K \leq n\sum_{i=1}^{n}|\xi_i|^2 - \left(\sum_{i=1}^{n}|\xi_i|^2\right)^2 \leq (n-1)K.$$

That is,

$$2S - n\Gamma^{2/n} \leq 2nS - (E_{CDL^+}(G))^2 \leq (n-1)[2S - n\Gamma^{2/n}].$$

By simplification of above inequality we get the required result. $\square$

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