Journal of Mathematical Extension
Journal Pre-proof
ISSN: 1735-8299
URL: http://www.ijmex.com
Original Research Paper

Harary Energy, Complementary Distance Energy and Equienergetic Graphs

B. Parvathalu*
Karnatak University's Karnatak Arts/Science College

K. G. Mirajkar
Karnatak University's Karnatak Arts College

R. S. Naikar
Karnatak University's Karnatak Arts College

Abstract. The energy of a graph G is defined as the absolute sum of its eigenvalues. Numerous studies have focused on similar aspects of graph energy, including Harary energy, distance energy, complementary distance energy, and Laplacian energy. However, relatively few investigations have addressed the class of graphs of the same order that exhibit equienergetic properties with respect to more than two associated matrices. In this paper, we characterize a class of graphs that share equienergetic attributes with respect to adjacency, Harary, and complementary distance matrices. Additionally, we present a large class of graphs demonstrating equienergetic attributes concerning four matrices associated with graphs of the same order.

AMS Subject Classification: 05C50; 05C76
Keywords and Phrases: Harary energy, Graph energy, Complementary distance energy, Equienergetic graphs

Received: July 2024; Accepted: November 2024
*Corresponding Author

1 Introduction

Let G be a simple and connected graph of order n and size m. The degree of a vertex v is the number of edges incident to it. A graph G is said to be r-regular if every vertex of G has degree r. The length of the shortest path connecting any two vertices v_j and v_k is the distance between them, denoted by d_{jk}. The diameter of G, denoted as $diam(G)$, is the maximum distance between any two vertices of a graph G.

Let $A(G) = [a_{jk}]$ denote the *adjacency matrix* of a graph G, where $a_{jk} = 1$ if v_j is adjacent to v_k and 0 otherwise. The Harary matrix was defined in honor of Professor Frank Harary. The *Harary matrix* [10] of a graph G, denoted by $H(G)$, is also called the reciprocal distance matrix [12] and is expressed as $H(G) = [h_{jk}]$, where $h_{jk} = 1/d_{jk}$ if $j \neq k$ and 0 otherwise. The *complementary distance matrix* [11] of a graph G, denoted by $CD(G)$, is expressed as $CD(G) = [cd_{jk}]$, where $cd_{jk} = 1 + diam(G) - d_{jk}$ if $j \neq k$ and 0 otherwise. The eigenvalues associated with the adjacency, Harary, and complementary distance matrices are known as the adjacency (A), Harary (H), and complementary distance (CD) eigenvalues of a graph G respectively. The *energy or A-energy* of graph G, introduced by I. Gutman in 1978 [6], is defined as the absolute sum of the eigenvalues of the adjacency matrix of a graph G and is denoted by $\mathcal{E}_A(G)$. In chemistry, the energy of a molecular graph is significant because it corresponds to the total π-electron energy of the molecule it represents. If $\mathcal{E}_A(G_1) - \mathcal{E}_A(G_2) = 0$, then the two graphs G_1 and G_2 of the same order are called *equienergetic graphs* or *A-equienergetic graphs*. The *Harary energy or H-energy* [5] is defined as the absolute sum of the Harary eigenvalues of a graph G and is denoted by $\mathcal{E}_H(G)$. If $\mathcal{E}_H(G_1) - \mathcal{E}_H(G_2) = 0$, then the two graphs G_1 and G_2 of the same order are called *Harary equienergetic graphs* or *H-equienergetic graphs*. The *complementary distance energy or CD-energy* [21] is defined as the absolute sum of the complementary distance eigenvalues of a graph G and is denoted by $\mathcal{E}_{CD}(G)$. If $\mathcal{E}_{CD}(G_1) - \mathcal{E}_{CD}(G_2) = 0$, then the two graphs G_1 and G_2 of the same order are called *complementary distance equienergetic graphs* or *CD-equienergetic graphs*. There are other matrices associated with graphs in which the graph's energy invariants are studied; here, we mention a few [2, 13, 14, 18]. Some studies on H-energy and CD-energy can be found in [3, 5, 17, 19, 20, 21, 23, 24, 25].

Let n_G^+, n_G^-, and n_G^0 represent the number of positive, negative, and zero A-eigenvalues of a graph G, respectively. The graphs $\overline{G}$, K_n, $K_{m,n}$, and $L(G)$ represent the complement of a graph G, the complete graph of order n, the complete bipartite graph of order $m+n$, and the line graph of G, respectively. The k^{th} iterated line graph of G, for $k = 0, 1, 2, \ldots$, is defined as $L^k(G) = L(L^{k-1}(G))$, where $L^0(G) = G$ and $L^1(G) = L(G)$.

The Harary matrix and complementary distance matrix play crucial roles in developing quantitative structure-property relationship (QSPR) models in chemistry [11, 12, 16]. Indulal [8, 9] introduced an open problem which focused on characterizing or constructing families of graphs exhibiting equienergetic properties with respect to both the adjacency and distance matrices. In the paper [22] Ramane et al. subsequently offered solutions by introducing certain families of graphs that demonstrate equienergetic characteristics with respect to both adjacency and distance matrices. Also in [7], Ilić et al. presented the results concerning adjacency, Laplacian and distance equienergetic graphs. Moreover, for many large classes of graphs, the precise relationships among A-energy, H-energy, and CD-energy are not known. This naturally leads us to explore the precise relationships among A-energy, H-energy, and CD-energy and to construct the graphs which exhibit equienergetic properties with respect to three or more than three matrices associated with graphs of same order. For undefined terminology and notation we follow [4].

Theorem 1.1. [3] *Let G be an r-regular graph of order n with $diam(G) \leq 2$. If $r = \lambda_1, \lambda_2, \ldots, \lambda_n$ are the A-eigenvalues of G, then the H-eigenvalues of G are $\frac{1}{2}(n + r - 1)$ and $\frac{1}{2}(\lambda_i - 1)$; $i = 2, 3, \ldots, n$.*

Proposition 1.2. [15] *If G is an r-regular graph of order n, then $diam(G) \leq 2$ or $diam(\overline{G}) \leq 2$.*

Theorem 1.3. [15] *If G is an r-regular graph of order $n(\geq 8)$, then $diam(\overline{L^k(G)}) = 2$ for all $k \geq 1$.*

Let n_k, m_k, and r_k represent the order, size, and regularity of $L^k(G)$ for $k = 0, 1, 2, \ldots$.

Remark 1.4. [22] Let G be an $r_0(\geq 4)$-regular graph of order n_0 and size m_0. Then for all $k \geq 2$, the graphs $\overline{L^k(G)}$ have the following A-eigenvalues: $n_k - r_k - 1$, 1 with multiplicity $m_{k-1} - n_{k-1}$, and $n_k - m_{k-1} + n_{k-1} - 1$ negative A-eigenvalues all of which are less than or equal to -3.

Let $\square$ denote the Cartesian product of graphs.

Theorem 1.5. [26] *For all $n \geq 4$, the regular graphs $\overline{L^k(K_{n,n} \square K_{n-1})}$ and $\overline{L^k(K_{n-1,n-1} \square K_n)}$ have the same regularity and same order. These graphs exhibit integral A-eigenvalues and are A-equienergetic.*

Theorem 1.6. [21] *Let G be an r-regular graph of order n with diam(G) ≤ 2. If $r = \lambda_1, \lambda_2, \ldots, \lambda_n$ are the A-eigenvalues of G, then the CD-eigenvalues of G are $n + r - 1$ and $\lambda_i - 1$; $i = 2, 3, \ldots, n$.*

2 Main Results

Proposition 1.2 assures us that most regular graphs have a diameter of at most 2. This motivates us to investigate the various energy invariants of such regular graphs. In the following discussion, we elucidate a direct relationship between the A-energy, H-energy, and CD-energy of regular graphs with a diameter of at most 2.

Theorem 2.1. *Let G be an r-regular graph of order n with diam$(G) \leq$ 2. If $r = \lambda_1, \lambda_2, \ldots, \lambda_n$ are the A-eigenvalues of G, then*

$$\mathcal{E}_H(G) = n - n_G^+ - \sum_{\lambda_i \in (0,1)} (\lambda_i - 1) + \frac{1}{2}\mathcal{E}_A(G) = \frac{1}{2}\mathcal{E}_{CD}(G).$$

Proof. Let $\mu_1, \mu_2, \ldots, \mu_n$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the H and A-eigenvalues of G, respectively. Then by Theorem 1.1, the H-eigenvalues of G are $\frac{1}{2}(n + r - 1)$ and $\frac{1}{2}(\lambda_i - 1)$; $i = 2, 3, \cdots, n$. Therefore, the

H-energy of G is

$$\begin{aligned}
\mathcal{E}_H(G) &= \sum_{i=1}^{n}|\mu_i| = \frac{1}{2}\left(n + r - 1 + \sum_{i=2}^{n}|\lambda_i - 1|\right) \\
&= \frac{1}{2}\left(n + \sum_{i=1}^{n}|\lambda_i - 1|\right) \\
&= \frac{1}{2}\left(n + \sum_{\lambda_i \leq 1}(-\lambda_i + 1) + \sum_{\lambda_i > 1}(\lambda_i - 1)\right) \\
&= \frac{1}{2}\left(n + \sum_{\lambda_i \leq 1} -\lambda_i + n_\lambda[\lambda_n, 1] + \sum_{\lambda_i > 1}\lambda_i - n_\lambda(1, \lambda_1]\right),
\end{aligned}$$

where $n_\lambda(I)$ shows the number of A-eigenvalues λ of G that are contained in I, here I represents any interval.

$$\begin{aligned}
&= \frac{1}{2}\Bigg(n + n_\lambda[\lambda_n, 1] - n_\lambda(1, \lambda_1] + \sum_{\lambda_i \leqslant 0}|\lambda_i| + \sum_{\lambda_i \in (0,1]} -\lambda_i \\
&\qquad + \sum_{\lambda_i > 1}\lambda_i\Bigg). \qquad (1)
\end{aligned}$$

The $\mathcal{E}_A(G)$ can be expressed as,

$$\mathcal{E}_A(G) = \sum_{\lambda_i \leq 0} |\lambda_i| + \sum_{\lambda_i \in (0,1]} \lambda_i + \sum_{\lambda_i > 1} \lambda_i. \qquad (2)$$

The order n of a graph G can be expressed as,

$$n = n_\lambda[\lambda_n, 1] + n_\lambda(1, \lambda_1] = n_\lambda(0, 1] + n_\lambda(1, \lambda_1] + n^0 + n^-. \qquad (3)$$

Using the equalities (2) and (3) in (1) we obtain,

$$\begin{aligned}\mathcal{E}_H(G) &= \frac{1}{2}\left(n + n + \mathcal{E}_A(G) - 2n_\lambda(1, \lambda_1] - 2\sum_{\lambda_i \in (0,1]} \lambda_i\right)\\ &= \frac{1}{2}\left(2n + \mathcal{E}_A(G) - 2n_G^+ + 2n_\lambda(0,1] - 2\sum_{\lambda_i \in (0,1]} \lambda_i\right)\\ &= \frac{1}{2}\Big(2n + \mathcal{E}_A(G) - 2n_G^+ + 2n_\lambda(0,1] - 2\sum_{\lambda_i \in (0,1]} (\lambda_i - 1)\\ &\qquad - 2n_\lambda(0,1]\Big)\\ &= \frac{1}{2}\left(2n + \mathcal{E}_A(G) - 2n_G^+ - 2\sum_{\lambda_i \in (0,1)} (\lambda_i - 1)\right)\\ \mathcal{E}_H(G) &= n - n_G^+ - \sum_{\lambda_i \in (0,1)} (\lambda_i - 1) + \frac{1}{2}\mathcal{E}_A(G),\end{aligned}$$

The equality $2\mathcal{E}_H(G) = \mathcal{E}_{CD}(G)$ follows directly from the interrelations between H-eigenvalues and CD-eigenvalues from Theorems 1.1 and 1.6 which concludes the proof. □

The following observations are immediate from Theorem 2.1,

1. If there is no A-eigenvalues in the interval $(0, 1)$, then $\sum_{\lambda_i \in (0,1)} (\lambda_i - 1) = 0$ and vice-versa.
2. For each A-eigenvalue $\lambda_i \in (0, 1)$, we have $\sum_{\lambda_i \in (0,1)} (\lambda_i - 1) < 0$ and also $n_G^+ + \sum_{\lambda_i \in (0,1)} (\lambda_i - 1) > 0$.

With these observations, we have the following result

Corollary 2.2. *Let G be an r-regular graph of order n with diam$(G) \leq 2$. Then*

$$n - n_G^+ + \frac{1}{2}\mathcal{E}_A(G) \leq \mathcal{E}_H(G) < n + \frac{1}{2}\mathcal{E}_A(G).$$

Equality holds in the left side if and only if G has no A-eigenvalues in the interval $(0,1)$.

The following result provides a procedure for generating the H-equienergetic graphs. Furthermore, it offers a method to produce a class of graphs that exhibit both A-equienergetic and H-equienergetic properties.

Let G_i; $i=1,2$, be r_i-regular graphs. The A-eigenvalues of G_1 are $\lambda'_1, \lambda'_2, \ldots, \lambda'_n$, and the A-eigenvalues of G_2 are $\lambda''_1, \lambda''_2, \ldots, \lambda''_n$. The number of positive A-eigenvalues for G_1 is $n^+_{G_1}$, and for G_2 it is $n^+_{G_2}$.

Corollary 2.3. *Let G_i; $i=1,2$ be r_i-regular graphs, both of same order n with $diam(G_i) \leq 2$. If G_i; $i=1,2$ are A-equienergetic graphs, then G_i; $i=1,2$ are H-equienergetic if and only if*

$$n^+_{G_1} + \sum_{\lambda'_i \in (0,1)} (\lambda'_i - 1) = n^+_{G_2} + \sum_{\lambda''_i \in (0,1)} (\lambda''_i - 1).$$

Specifically, when G_i; $i=1,2$ have no A-eigenvalues in the interval $(0,1)$*, these graphs are H-equienergetic if and only if the number of positive A-eigenvalues are equal, i.e., $n^+_{G_1} = n^+_{G_2}$.*

Example 2.4. Let us consider the graphs $G_1 = \overline{L^k(K_{n,n} \Box K_{n-1})}$ and $G_2 = \overline{L^k(K_{n-1,n-1} \Box K_n)}$ as stated in Theorem 1.5. According to Remark 1.4 and Theorem 1.5, the graphs G_i; $i=1,2$ are A-equienergetic and have the same number of positive integral A-eigenvalues. Additionally, for all $k \geq 1$ and $n \geq 6$, these graphs have a diameter of 2, as established by Theorem 1.3. Therefore, by Corollary 2.3, these graphs are H-equienergetic. Hence, the graphs G_i; $i=1,2$ are A-equienergetic as well as H-equienergetic for all $k \geq 1$ and $n \geq 6$.

Motivated by orderenergetic graphs [1], we define Harary orderenergetic graph or H-orderenergetic graph as a graph whose Harary energy is equal to its order. In the following, we characterize H-orderenergetic graphs.

Corollary 2.5. *Let G be an r-regular graph of order n with $diam(G) \leq$ 2. Then G is H-orderenergetic if and only if $G \equiv K_2$.*

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the A-eigenvalues of G. By definition of H-orderenergetic graph and Theorem 2.1, G is H-orderenergetic graph if and only if

$$\mathcal{E}_A(G) = 2\left(n_G^+ + \sum_{\lambda_i \in (0,1)} (\lambda_i - 1)\right).$$

Also, an equivalent expression for A-energy of graph G is

$$\mathcal{E}_A(G) = 2\sum_{\lambda_i > 0} \lambda_i.$$

When combined, these two expressions provide the following

$$n_G^+ + \sum_{\lambda_i \in (0,1)} (\lambda_i - 1) = \sum_{\lambda_i > 0} \lambda_i \text{ or}$$

$$n_G^+ + \sum_{\lambda_i \in (0,1)} \lambda_i - n_\lambda(0,1) = \sum_{\lambda_i \in (0,1)} \lambda_i + \sum_{\lambda_i \geq 1} \lambda_i \text{ or}$$

$$n_\lambda[1, \lambda_1] = \sum_{\lambda_i \geqslant 1} \lambda_i,$$

which is possible only when G is K_2 as G is a regular graph. □

Remark 2.6. Let G be a regular graph. Then, the line graph of G is also a regular graph. In [20] and [17], the authors investigated the H-energy of line graphs and the complements of line graphs, respectively, where the graphs have a diameter of at most 2. It is worth noting that the results presented here are more general than those reported in [20] and [17].

The equality $\mathcal{E}_{CD}(G) = 2\mathcal{E}_H(G)$ in Theorem 2.1 demonstrates that if any two graphs are CD-equienergetic, they are also H-equienergetic, and vice versa. Based on this observation, we derive the following result.

Corollary 2.7. *Let G_i; $i = 1, 2$ be r_i-regular graphs, both of same order n with diam$(G_i) \leq 2$. Then graphs G_i; $i = 1, 2$ are CD-equienergetic graphs if and only if they are H-equienergetic.*

Similar to the Corollary 2.2 and Corollary 2.3, we have the following results.

Corollary 2.8. *Let G be an r-regular graph of order n with diam$(G) \leq 2$. Then*

$$2n - 2n_G^+ + \mathcal{E}_A(G) \leq \mathcal{E}_{CD}(G) < 2n + \mathcal{E}_A(G).$$

Equality holds in the left side if and only if G has no A-eigenvalues in the interval $(0, 1)$.

Corollary 2.9. *Let G_i; $i = 1, 2$ be r_i-regular graphs, both of same order n with diam$(G_i) \leq 2$. If G_i; $i = 1, 2$ are A-equienergetic graphs, then G_i; $i = 1, 2$ are CD-equienergetic if and only if*

$$n_{G_1}^+ + \sum_{\lambda_i^{'} \in (0,1)} (\lambda_i^{'} - 1) = n_{G_2}^+ + \sum_{\lambda_i^{''} \in (0,1)} (\lambda_i^{''} - 1).$$

Specifically, if G_i; $i = 1, 2$ have no A-eigenvalues in the open interval $(0, 1)$, then G_i; $i = 1, 2$ are CD-equienergetic if and only if $n_{G_1}^+ = n_{G_2}^+$.

Remark 2.10. In [21] and [23], the authors investigated the CD-energy of line graphs and the complements of line graphs, respectively, where the graphs have a diameter of at most 2. It is noteworthy that the results presented here are more general than those reported in [21] and [23].

Remark 2.11. It is noted that the graphs G_i; $i = 1, 2$ in the Example 2.4 are A, H and CD-equienergetic graphs. Moreover, these graphs exhibit the equienergetic property with respect to the distance matrix, as demonstrated in Example 3.4 of [22].

3 Conclusion

In this paper, we present findings regarding the H and CD-energy of graphs along with some bounds on them. Additionally, we establish precise relationships among the A, H and CD-energies of graphs. The results of this paper and that of [22, 7] naturally motivates to raise the following question:

- Find the characterizations to determine the graphs of same order which share equienergetic characteristics with respect to more than four matrices associated with graphs.

Acknowledgments
The authors would like to thank the anonymous referee for their helpful comments. R. S. Naikar is thankful to the Karnataka Science and Technology Promotion Society, Bengalore, India for providing fellowship, No. DST/KSTePS/Ph.D.Fellowship/MAT-01:2022-23/1017.

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Bolle Parvathalu
Department of Mathematics
Assistant Professor of Mathematics
Karnatak University's Karnatak Arts/Science College
Dharwad, Karnataka, India
E-mail: bparvathalu@gmail.com

Keerthi Ganapath Rao Mirajkar
Department of Mathematics
Professor of Mathematics
Karnatak University's Karnatak Arts College
Dharwad, Karnataka, India
E-mail: keerthi.mirajkar@gmail.com

Roopa Subhas Naikar
Department of Mathematics
PhD Student in Mathematics
Karnatak University's Karnatak Arts College
Dharwad, Karnataka, India
E-mail: sroopa303@gmail.com