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ON SECOND–STAGE SPECTRUM AND ENERGY OF A GRAPH

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Abstract. Let G be a simple graph. The *derived graph* of G, denoted by $G^\dagger$, is the graph having the same vertex set as G, in which two vertices are adjacent if and only if their distance in G is two. We establish several spectral properties of $G^\dagger$, including its energy.

1. Introduction

Let G be a graph with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$. The *distance* between the vertices v_i and v_j, $v_i, v_j \in \mathbf{V}(G)$, is equal to the length (= number of edges) of a shortest path starting at v_i and ending at v_j (or vice versa) [2].

In inorganic chemistry [12], there is a concept called second electron affinity. It is the energy supplied to an $X^-(g)$ ion to form an $X^{2-}(g)$ ion i. e., to form a second–stage ion from the original ion. This concept motivated us to define the second–stage matrix $\mathbf{A}_2(G)$ of a graph G, which is the symmetric $n \times n$ matrix whose (i,j)-entry is unity if the vertices v_i and v_j are at distance two, and zero otherwise. As $\mathbf{A}_2(G)$ is a symmetric $(0,1)$-matrix, with zero diagonal, it may be viewed as the adjacency matrix of some graph $G^\dagger$, that in [1] was named *derived graph* of G.

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Examples.

Let K_n, P_n, S_n, and C_n be, respectively, the n-vertex complete graph, path, star, and cycle, and let $K_{a,b}$ be the complete bipartite graph on $a+b$ vertices. Let $\overline{G}$ denote the complement of the graph G. Then $(K_n)^\dagger \cong \overline{K_n}$, $(P_n)^\dagger \cong P_{\lfloor n/2 \rfloor} \cup P_{\lceil n/2 \rceil}$, $(S_n)^\dagger \cong K_{n-1} \cup K_1$, $(K_{a,b})^\dagger \cong K_a \cup K_b$, and

$$(C_n)^\dagger \cong \begin{cases} \overline{K_3} & \text{if } n = 3, \\ K_2 \cup K_2 & \text{if } n = 4, \\ C_{n/2} \cup C_{n/2} & \text{if } n \text{ is even and } n \geq 6, \\ C_n & \text{if } n \text{ is odd and } n \geq 5. \end{cases}$$

Since $(G_1 \cup G_2)^\dagger \cong (G_1)^\dagger \cup (G_2)^\dagger$, the derived graph of a disconnected graph is necessarily disconnected. However, in numerous cases (e. g. for all bipartite graphs) the derived graph of a connected graph is also disconnected. In [1], classes of graphs were characterized whose derived graphs are connected. In [1] also upper bounds for the largest eigenvalue of $G^\dagger$ were established.

Denote the eigenvalues of the graph G by $\lambda_i = \lambda_i(G)$, $i = 1, 2, \ldots, n$, and order them so that

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n. \tag{1.1}$$

These eigenvalues form the spectrum of G, denoted by $Spec(G)$. Two graphs G and H are said to be cospectral if $Spec(G) = Spec(H)$. For more details on graph spectral theory see [3].

The eigenvalues of $G^\dagger$ are also real and will be ordered according to (1.1). As usual [7], [9], the energy of $G^\dagger$ is defined as

$$E(G^\dagger) = \sum_{i=1}^{n} |\lambda_i(G^\dagger)|. \tag{1.2}$$

Recall that the graph energy has long known chemical applications; for details see the surveys [6], [8]. Two graphs with the same energy are called equienergetic. Equienergetic graphs need not be cospectral. Cospectral graphs are equienergetic in a trivial manner. We are interested in those equienergetic graphs which are not cospectral.

All graphs considered in this paper are simple. In the subsequent considerations we need the following previously established results:

Lemma 1.1. [4] *Let*

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_0 & \mathbf{A}_1 \\ \mathbf{A}_1 & \mathbf{A}_0 \end{bmatrix}$$

be a 2×2 block symmetric matrix. Then the eigenvalues of $\mathbf{A}$ are those of $\mathbf{A}_0 + \mathbf{A}_1$ together with those of $\mathbf{A}_0 - \mathbf{A}_1$.

Lemma 1.2. [3] *Let $L(G)$ denote the line graph of the graph G. If G is r-regular and connected, $r \geq 3$, with $Spec(G) = \{r, \lambda_2, \dots, \lambda_n\}$, then*

$$Spec(L(G)) = \begin{pmatrix} 2r-2 & \lambda_2 + r - 2 & \cdots & \lambda_n + r - 2 & -2 \\ \\ 1 & 1 & \cdots & 1 & \frac{1}{2}n(r-2) \end{pmatrix}.$$

Lemma 1.3. [13]. *Let G be same as in Lemma 1.2, and let $L^2(G) = L(L(G))$. Then*

$$Spec(L^2(G)) = \begin{pmatrix} 4r-6 & \lambda_2 + 3r - 6 & \dots & \lambda_n + 3r - 6 & 2r-2 & -2 \\ \\ 1 & 1 & \dots & 1 & \frac{1}{2}n(r-2) & \frac{1}{2}nr(r-2) \end{pmatrix}.$$

Lemma 1.4. [3] *Let G be a connected r-regular graph with spectrum $\{r, \lambda_2, \dots, \lambda_n\}$. Then $Spec(\overline{G}) = \{n - r - 1, -(\lambda_2 + 1), \dots, -(\lambda_n + 1)\}$.*

Lemma 1.5. [3] *For every $p \geq 3$, there exists a pair of non-cospectral cubic graphs on $2p$ vertices.*

Lemma 1.6. [10] *For every $n \geq 8$, there exists a pair of 4-regular non-cospectral graphs on n vertices.*

This paper is organized as follows. First, we determine the spectrum of some derived graphs $G^\dagger$, in the case when the graph G has diameter 2. Then we state a few bounds for the energy of $G^\dagger$. Finally, we describe a few cases of equienergetic derived graphs.

2. Graphs of diameter two

The diameter of a graph is the maximum distance between its vertices. If the diameter of the graph G is two, then any pair of non-adjacent vertices is at distance two, and is thus connected in $G^\dagger$. Consequently,

$$G^\dagger \cong \overline{G}.$$

In other words, if G is an (n,m)-graph, then $G^\dagger$ is an $\left(n, \binom{n}{2} - m\right)$-graph. Consequently, all previously known spectral results, depending only on the number of vertices and edges of a graph G, can now be re-stated for $G^\dagger$. For instance, by Lemma 1.4 we have

Theorem 2.1. *Let G be an r-regular graph of diameter 2 and let its spectrum be $\{r, \lambda_2, \ldots, \lambda_n\}$. Then $Spec(G^\dagger) = \{n-r-1, -(\lambda_2+1), \ldots, -(\lambda_n+1)\}$.*

As special cases of Theorem 2.1 we have:

$$Spec((K_{n,n})^\dagger) = \begin{pmatrix} n-1 & -1 \\ 2 & 2n-2 \end{pmatrix}; \qquad Spec((CP(n))^\dagger) = \begin{pmatrix} 1 & -1 \\ n & n \end{pmatrix}$$

where $CP(n)$ denotes the "cocktail party graph", namely the $(2n)$-vertex regular graph of degree $2n-2$ (obtained by deleting n independent edges from the complete graph K_{2n}).

Let $G_1 \times G_2$ denote the Cartesian product of the graphs G_1 and G_2 [3].

Theorem 2.2. *Let G be an r-regular graph of diameter 2 and spectrum $\{r, \lambda_2, \ldots, \lambda_n\}$. Then*

$$Spec((G \times K_2)^\dagger) = \begin{pmatrix} 3n-2(r+2) & -2(\lambda_i+1) & -n & 0 \\ 1 & 1 & 1 & n-1 \end{pmatrix}, \qquad i = 2, \ldots, n.$$

Proof. Since G is of diameter 2, its second–stage matrix is $\mathbf{A}(\overline{G})$. The product $H \cong G \times K_2$ is $(r+1)$-regular and of diameter 3. Its second–stage matrix is of the form

$$\begin{pmatrix} \mathbf{A}(\overline{G}) & \mathbf{A}(\overline{G}) + \mathbf{J} \\ \mathbf{A}(\overline{G}) + \mathbf{J} & \mathbf{A}(\overline{G}) \end{pmatrix}$$

where $\mathbf{J}$ is the all-one square matrix of order n. Theorem 2.2 follows by Lemmas 1.1 and 1.4. $\square$

If G is of diameter 2 having m edges, then $G^\dagger$ has $m^\dagger = \binom{n}{2} - m$ edges. If, in addition, G is regular of degree r, then $G^\dagger$ is regular of degree $n-r-1$. Bearing these facts in mind, we may use known results from the theory of graph energy [7, 9] to state:

Theorem 2.3. *Let G be an (n,m)-graph of diameter 2. Then*

$$\begin{aligned}\sqrt{2m^\dagger + n(n-1)\Delta^{2/n}} &\leq E(G^\dagger) \leq \sqrt{2nm^\dagger}\\ 2\sqrt{m^\dagger} &\leq E(G^\dagger) \leq 2m^\dagger\\ E(G^\dagger) &\leq \frac{2m^\dagger}{n} + \sqrt{(n-1)\left[2m^\dagger - \left(\frac{2m^\dagger}{n}\right)^2\right]}\end{aligned}$$

where $\Delta = |\det \mathbf{A}_2(G)|$.

Corollary 2.1. *Let G be an r-regular graph of diameter 2. Then,*

$$E(G^\dagger) \leq (n-r-1) + \sqrt{(n-1)(n-r-1)(r+1)}.$$

Let the graphs G_1 and G_2 have disjoint vertex sets. Their *join*, $G_1 \nabla G_2$, is the graph obtained by joining every vertex of G_1 with every vertex of G_2. If $G_1 \cong K_a$ and $G_b \cong K_b$, then $G_1 \nabla G_2 \cong K_{a+b}$, having diameter equal to one. In all other cases, the join $G_1 \nabla G_2$ has diameter two. Therefore, the derived graph of $G_1 \nabla G_2$ satisfies:

$$(G_1 \nabla G_2)^\dagger \cong \overline{G}_1 \cup \overline{G}_2 \ . \tag{2.1}$$

From (2.1) and Lemma 1.4 we obtain:

Theorem 2.4. *For $i = 1, 2$, let G_i be an r_i-regular graph with n_i vertices and spectrum $\{r_i, \lambda_{i,2}, \ldots, \lambda_{i,n_i}\}$. Then Spec$((G_1 \nabla G_2)^\dagger)$ consists of eigenvalues $-\lambda_{i,j} - 1$ for $i = 1, 2$ and $j = 2, 3, \ldots, n_i$, and two more eigenvalues $n_1 - r_1 - 1$ and $n_2 - r_2 - 1$.*

Corollary 2.2. *Let G be a connected r-regular graph on n vertices. Then*

$$Spec((G \nabla G)^\dagger) = \begin{pmatrix} n-r-1 & -(\lambda_i(G)+1) \\ 2 & 2 \end{pmatrix}, \quad i = 2, 3, \ldots, n.$$

3. Equienergetic derived graphs

Theorem 3.1. *For every $n \equiv 0$ $(mod\ 6) \geq 18$, there exists a pair of equienergetic n-vertex derived graphs.*

Proof. Let $n = 6p$, $p \geq 3$. Let G_1 and G_2 be non-cospectral cubic graphs on $2p$ vertices, cf. Lemma 1.5. Then their line graphs, $L(G_1)$ and $L(G_2)$, are 4-regular on $3p$ vertices. By Lemma 1.2 and Corollary 2.2, the only positive eigenvalues of $(G_1 \nabla G_1)^\dagger$ are $3p-5$ and $3p-5$. The same is true for $(G_2 \nabla G_2)^\dagger$. Thus,

$$E((G_1 \nabla G_1)^\dagger) = E((G_2 \nabla G_2)^\dagger) = 2 \cdot 2 \cdot (3p-5) = 12p - 20.$$

The theorem follows now from the fact that both $(G_1 \nabla G_1)^\dagger$ and $(G_2 \nabla G_2)^\dagger$ have $6p$ vertices. □

In [11] a result similar to Theorem 3.1 can be found, pertaining to distance-equienergetic graphs.

We now find the spectrum of some derived self–complementary graphs, in terms of the spectra of the parent graphs. These results are then used to show that there exist equienergetic derived self–complementary graphs.

A graph G is said to be self–complementary if $G \cong \overline{G}$. The following construction [5] yields self–complementary graphs.

Construction [5, 10]. Let G be an n-vertex graph. Replace the end vertices of P_4 by a copy of G and the internal vertices of P_4 by a copy of $\overline{G}$. Join the vertices of these graphs by all possible edges whenever the corresponding vertices of P_4 are adjacent. The $4n$-vertex graph thus constructed will be denoted by H. The graph H is self–complementary.

Theorem 3.2. *Let G be a connected r-regular graph on n vertices, with spectrum $\{r, \lambda_2, \lambda_3 \ldots, \lambda_n\}$. Let H be the graph constructed from G in the above described manner. Then the spectrum of $H^\dagger$ consists of λ_i , $-(\lambda_i + 1)$ $i = 2, 3, \ldots, n$, each with multiplicity 2, together with the numbers $\frac{1}{2}\left[1 \pm \sqrt{5n^2 + 4r(r+1-n) - 2n + 1}\right]$, each with multiplicity 2.*

Proof. The second–stage matrix of H is of the form

$$\begin{pmatrix} \mathbf{A}(\overline{G}) & \mathbf{0} & \mathbf{J} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}(G) & \mathbf{0} & \mathbf{J} \\ \mathbf{J} & \mathbf{0} & \mathbf{A}(G) & \mathbf{0} \\ \mathbf{0} & \mathbf{J} & \mathbf{0} & \mathbf{A}(\overline{G}) \end{pmatrix}.$$

Being regular, the graph G has the all-one vector $\mathbf{j}$ as an eigenvector, corresponding to eigenvalue r. All other eigenvectors of G are orthogonal to $\mathbf{j}$. The complement $\overline{G}$ has an eigenvalue $-\lambda - 1$ corresponding to eigenvalue $\lambda \neq r$ of G, such that both eigenvalues have the same multiplicities and eigenvectors.

Let λ be an eigenvalue of G with eigenvector $\mathbf{x}$, such that $\mathbf{j}^T\mathbf{x} = 0$. Then $(\mathbf{x},\mathbf{0},\mathbf{0},\mathbf{0})^T$ and $(\mathbf{0},\mathbf{0},\mathbf{0},\mathbf{x})^T$ are the eigenvectors of $\mathbf{A}_2(H)$, corresponding to eigenvalue $-\lambda-1$. Similarly, $(\mathbf{0},\mathbf{x},\mathbf{0},\mathbf{0})^T$ and $(\mathbf{0},\mathbf{0},\mathbf{x},\mathbf{0})^T$ are the eigenvectors of $\mathbf{A}_2(H)$, corresponding to eigenvalue λ.

In this way, by means of $(\mathbf{x},\mathbf{0},\mathbf{0},\mathbf{0})^T$, $(\mathbf{0},\mathbf{x},\mathbf{0},\mathbf{0})^T$, $(\mathbf{0},\mathbf{0},\mathbf{x},\mathbf{0})^T$, and $(\mathbf{0},\mathbf{0},\mathbf{0},\mathbf{x})^T$ we constructed a total of $4(n-1)$ eigenvectors of $\mathbf{A}_2(H)$, all orthogonal to $(\mathbf{j},\mathbf{0},\mathbf{0},\mathbf{0})^T$, $(\mathbf{0},\mathbf{j},\mathbf{0},\mathbf{0})^T$, $(\mathbf{0},\mathbf{0},\mathbf{j},\mathbf{0})^T$, and $(\mathbf{0},\mathbf{0},\mathbf{0},\mathbf{j})^T$.

The four remaining eigenvectors of $H^\dagger$ are of the form $\mathbf{\Psi} = (\alpha\mathbf{j},\beta\mathbf{j},\gamma\mathbf{j},\delta\mathbf{j})^T$ for some $(\alpha,\beta,\gamma,\delta) \neq (0,0,0,0)$. Now, suppose that ν is an eigenvalue of $\mathbf{A}_2(H)$ with eigenvector $\mathbf{\Psi}$. Then from $\mathbf{A}_2(H)\,\mathbf{\Psi} = \nu\mathbf{\Psi}$ we get:

$$(n-r-1)\alpha + 0\,\beta + n\,\gamma + 0\,\delta = \nu\,\alpha \tag{3.1}$$

$$0\,\alpha + r\,\beta + 0\,\gamma + n\,\delta = \nu\,\beta \tag{3.2}$$

$$n\,\alpha + 0\,\beta + r\,\gamma + 0\,\delta = \nu\,\gamma \tag{3.3}$$

$$0\,\alpha + n\,\beta + 0\,\gamma + (n-r-1)\delta = \nu\,\delta \tag{3.4}$$

By solving Eqs. (3.1)–(3.4), we obtain the remaining four eigenvalues. □

Theorem 3.3. *Let B be a connected 4-regular graph on n vertices, with spectrum $\{4,\lambda_2,\ldots,\lambda_n\}$. Let $G = L^2(B)$ and let H be the self-complementary graph obtained from G according to the above described construction. Then*

$$E(H^\dagger) = 3\left(10n - 7 + 2\sqrt{20n^2 - 28n + 49}\right).$$

Proof. In [13] it was shown that the energy of the second line graph of an n-vertex regular graph of degree r depends only on n and r. Theorem 9 is obtained using an analogous argument: Apply Theorem 3.2 and Lemma 1.3 and observe that both $\lambda_i + 3r - 5$ and $\lambda_i + 3r - 6$ are positive when $r = 4$. □

Theorem 3.4. *For every $n = 48t$ and $n = 24(2t+1)$, for $t \geq 4$, there exists a pair of equienergetic derived graphs of self–complementary graphs.*

Proof. Case 1: $n = 48t$.
Let B_1 and B_2 be two non-cospectral 4-regular graphs on $2t$ vertices, as given by Lemma 1.6. Then both $L^2(B_1)$ and $L^2(B_2)$ are 10-regular and possess $12t$ vertices. Let H_1 and H_2 be the respective self–complementary graphs on $48t$ vertices, constructed by the above described method. Then by Theorem 3.3, the derived graphs of H_1 and H_2 are equienergetic.

Case 2: $n = 24(2t + 1)$.
This case is treated analogously, by considering pairs of non-cospectral 4-regular graphs on $2t + 1$ vertices, whose existence is guaranteed by Lemma 1.6. □

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