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Coulson's integral formula for digraphs

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Abstract

We extend the concept of energy to directed graphs in such a way that Coulson's Integral Formula remains valid. As a consequence, it is shown that the energy is increasing over the set $\mathcal{D}_{n,h}$ of digraphs with n vertices and cycles of length h, with respect to a quasi-order relation. Applications to the problem of extremal values of the energy in various classes of digraphs are considered.

1 Introduction and terminology

A digraph (or directed graph) $G = (\mathcal{V}, \mathcal{D})$ is defined to be a finite set $\mathcal{V}$ and a set $\mathcal{D}$ of ordered pairs of elements of $\mathcal{V}$. The elements of $\mathcal{V}$ are called vertices and the elements of $\mathcal{D}$ are called directed edges or arcs. Sometimes we denote by $\mathcal{V}_G$ and $\mathcal{D}_G$ the set of vertices and arcs of G, respectively. We consider here simple digraphs.

Two vertices are called adjacent if they are connected by an arc. If there is an arc from vertex x to vertex y we indicate this by writing xy. A path of length $n-1$ ($n \geq 2$), denoted by P_n, is a graph with n vertices $\{v_1, \ldots, v_n\}$ and with $n-1$ arcs $v_i v_{i+1}$, where $i = 1, \ldots, n-1$. A cycle of length n, denoted by C_n, is the digraph with the vertex set $\{v_1, \ldots, v_n\}$ having arcs $v_i v_{i+1}$, $i = 1, \ldots, n-1$ and $v_n v_1$. A linear digraph is a digraph in which every vertex has indegree and outdegree equal to 1. Clearly, a linear digraph consists of cycles.

The adjacency matrix A of a digraph G whose vertex set is $\{v_1, \ldots, v_n\}$ is the $n \times n$ matrix whose entry a_{ij} is defined as

$$a_{ij} = \begin{cases} 1 & \text{if} \quad v_i v_j \in \mathcal{D} \\ 0 & \quad\text{otherwise} \end{cases}$$

The characteristic polynomial $|xI - A|$ of the adjacency matrix A of G is called the characteristic polynomial of G and it is denoted by Φ_G. The eigenvalues of A are called the eigenvalues of G.

The coefficients of the characteristic polynomial contain information on the structure of the digraph, as we can see in the Coefficient Theorem for Digraphs [1, Theorem 1.2]

Theorem 1.1 *Let G be a digraph with characteristic polynomial*

$$\Phi_G = x^n + b_1 x^{n-1} + \cdots + b_{n-1} x + b_n$$

Then

$$b_k = \sum_{L \in \mathcal{L}_k} (-1)^{comp(L)}$$

for every $k = 1, \ldots, n$, where $\mathcal{L}_k$ is the set of all linear subdigraphs L of G with exactly k vertices; $comp\,(L)$ denotes the number of components of L.

If G is an undirected graph then G can be viewed as a digraph $\overline{G}$ by identifying each edge of G with a cycle of length 2 in $\overline{G}$. Then Theorem 1.1 can be reformulated for undirected graphs as follows [1, Theorem 1.3]:

Theorem 1.2 *Let G be a graph with characteristic polynomial*

$$\Phi_G = x^n + b_1 x^{n-1} + \cdots + b_{n-1} x + b_n$$

Then

$$b_j = \sum_{L} (-1)^{comp(L)}\, 2^{cyc(L)}$$

where the sum is over all subgraphs L of G consisting of disjoint edges and cycles, having j vertices; $comp\,(L)$ is the number of components and $cyc\,(L)$ is the number of cycles in L.

It follows from Theorem 1.2 that if G is a bipartite graph then the characteristic polynomial of G can be expressed in the form

$$\Phi_G = x^n + \sum_{k \geq 1} (-1)^k\, b\,(G, 2k)\, x^{n-2k} \tag{1}$$

where $b\,(G, 2k) \geq 0$ for all $k \geq 1$. This expression for Φ_G induces in a natural way a quasi-order relation " $\preceq$ " (i.e. a reflexive and transitive relation) over the set of all bipartite graphs: if G_1 and G_2 are bipartite graphs whose characteristic polynomials are in the form (1)

$$G_1 \preceq G_2 \Longleftrightarrow b\,(G_1, 2k) \leq b\,(G_2, 2k) \text{ for all } k \geq 1 \tag{2}$$

If $G_1 \preceq G_2$ and there exists a k such that $b\,(G_1, 2k) < b\,(G_2, 2k)$ then we write $G_1 \prec G_2$.

Gutman [3] introduced this quasi-order relation in order to compare the energies of different graphs. The energy of a graph G, denoted by $E\,(G)$, is defined to be the sum of the absolute values of the eigenvalues of A. For a survey of the mathematical properties of the energy we refer to [5]. Other recent results can be found in ([10],[11],[12],[13]).

It is well known that if G is a bipartite graph, then the energy of G can be expressed by means of the Coulson integral formula ([4] and [5])

$$E(G) = \frac{2}{\pi} \int_0^\infty x^{-2} \ln \left[1 + \sum_{k=0}^{\left[\frac{p}{2}\right]} b(G,k)\, x^{2k} \right] dx \tag{3}$$

which implies

$$\begin{aligned} G_1 &\preceq G_2 \Rightarrow E(G_1) \leq E(G_2) \\ G_1 &\prec G_2 \Rightarrow E(G_1) < E(G_2) \end{aligned} \tag{4}$$

This increasing property of E have been successfully applied in the study of the extremal values of the energy over a significant class of graphs ([6]-[9],[14]-[18]).

In this paper we extend the concept of energy to directed graphs in such a way that Coulson's Integral Formula remains valid. As a consequence, it is shown that the energy is increasing over the set $\mathcal{D}_{n,h}$ of digraphs with n vertices and cycles of length h, with respect to a quasi-order relation. Applications to the problem of extremal values of the energy in various classes of digraphs are considered.

2 Energy of digraphs

In this section we generalize the concept of energy to digraphs. Note that in the case of digraphs, the adjacency matrix is not necessarily symmetric and so the eigenvalues can be complex numbers.

Definition 2.1 *Let G be a digraph with n vertices and eigenvalues $z_1, \ldots, z_n$. The energy of G is defined as*

$$E(G) = \sum_{i=1}^{n} |Re(z_i)|$$

where $Re(z_i)$ denotes the real part of z_i.

Example 2.2 *Let G be the digraph shown in Figure 1. By Theorem 1.1, the characteristic polynomial of G is*

$$\Phi_G = x^{10} - x^7 - 2x^6 + 2x^3 = x^3\left(x^4 - 2\right)\left(x^3 - 1\right)$$

The eigenvalues of G are $0, 0, 0, \pm\sqrt[4]{2}, \pm\sqrt[4]{2}i, 1$ and $-\frac{1}{2} \pm \frac{\sqrt{3}}{2}i$. Consequently,

$$E(G) = 2\sqrt[4]{2} + 2$$

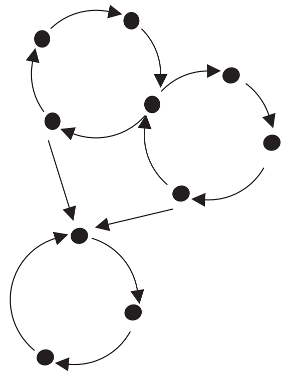

Figure 1

Of course, there are different ways to generalize the energy to digraphs. However, as we shall see later, this generalization is consistent with some of the fundamental results in the theory.

Example 2.3 *If G is a (undirected) graph we define a directed graph $\overline{G}$ with the same adjacency matrix of G: $\mathcal{V}_G = \mathcal{V}_{\overline{G}}$ and every edge of G is replaced by a directed cycle of length 2. Clearly $A_G = A_{\overline{G}}$ and so $E(G) = E(\overline{G})$. In this way, Definition 2.1 generalizes the concept of energy of (undirected) graphs.*

In the following examples we use Theorem 1.1 to calculate the characteristic polynomial of the digraphs.

Example 2.4 *Let G be an acyclic digraph (i.e., G has no cycles). Then $E(G) = 0$. In fact, the characteristic polynomial of G is $\Phi_G = x^n$, where n is the number of vertices of G. Consequently, 0 is the unique eigenvalue of G (of multiplicity n) and so $E(G) = 0$.*

Example 2.5 *Let C_n be the cycle of n vertices. Then the characteristic polynomial of C_n is $\Phi_C = x^n - 1$. Therefore,*

$$E(C_n) = \sum_{k=0}^{n-1} \left| cos\left(\frac{2k\pi}{n}\right) \right|$$

Example 2.6 *Let G be a digraph with n vertices and unique cycle C_r of length r, where $2 \le r \le n$. Then*

$$\Phi_G = x^n - x^{n-r} = x^{n-r}(x^r - 1)$$

Hence, the eigenvalues of G are the r-th roots of unity, each with multiplicity 1, and 0 with multiplicity $n - r$. It follows that

$$E(G) = E(C_r) = \sum_{k=0}^{r-1} \left| cos\left(\frac{2k\pi}{r}\right) \right|$$

In [7] and [9] the authors considered the problem of finding the maximal and minimal energy among unicyclic graphs with a fixed number of vertices. It is natural to consider the same problem for unicyclic digraphs.

Theorem 2.7 *Among all unicyclic digraphs with n vertices, the minimal energy is attained in digraphs which contain a cycle of length $2, 3$ or 4. The maximal energy is attained in the cycle C_n of length n.*

Proof. Let G be a digraph with n vertices and unique cycle C_r of length $r \geq 2$. It follows from Example 2.6 that

$$E\left(G\right) = E\left(C_r\right) = \sum_{k=0}^{r-1} \left| cos\left(\frac{2k\pi}{r}\right) \right|$$

If $r = 2, 3$ or 4 then $E\left(C_r\right) = 2$. Assume that $r \geq 5$. We will show that

$$E\left(C_r\right) > 2$$

Recall that for every positive integer p

$$\sum_{k=0}^{p-1} cos\left(\frac{2k\pi}{p}\right) = 0$$

which implies that

$$\sum_{k=0}^{\left[\frac{p}{4}\right]} cos\left(\frac{2k\pi}{p}\right) = -\sum_{k=\left[\frac{p}{4}\right]+1}^{\left[\frac{p}{2}\right]} cos\left(\frac{2k\pi}{p}\right) \tag{5}$$

Since $r \geq 5$ then

$$cos\left(\frac{2\pi}{r}\right) > 0$$

Hence

$$1 < 1 + cos\left(\frac{2\pi}{r}\right) \leq \sum_{k=2}^{r-1} \left| cos\left(\frac{2k\pi}{r}\right) \right|$$

Then

$$\begin{aligned} E\left(C_r\right) &= \sum_{k=0}^{r-1} \left| cos\left(\frac{2k\pi}{r}\right) \right| \\ &= 1 + cos\left(\frac{2\pi}{r}\right) + \sum_{k=2}^{r-1} \left| cos\left(\frac{2k\pi}{r}\right) \right| \\ &\geq 2\left(1 + cos\left(\frac{2\pi}{r}\right)\right) > 2 \end{aligned}$$

Now we show that if $n > r \geq 5$ then

$$E(C_r) < E(C_n)$$

If $n > r \geq 5$ and $k = 1, \ldots, \left[\frac{r}{4}\right]$ then $\frac{2k\pi}{n} < \frac{2k\pi}{r}$ which implies $cos\left(\frac{2k\pi}{r}\right) < cos\left(\frac{2k\pi}{n}\right)$ since $\frac{2k\pi}{n}, \frac{2k\pi}{r} \in (0, \frac{\pi}{2}]$. Hence

$$\sum_{k=0}^{\left[\frac{r}{4}\right]} cos\left(\frac{2k\pi}{r}\right) < \sum_{k=0}^{\left[\frac{r}{4}\right]} cos\left(\frac{2k\pi}{n}\right) \leq \sum_{k=0}^{\left[\frac{n}{4}\right]} cos\left(\frac{2k\pi}{n}\right) \tag{6}$$

On the other hand

$$\begin{aligned} \frac{1}{2}E(C_r) &= \sum_{k=0}^{\left[\frac{r}{2}\right]} \left| cos\left(\frac{2k\pi}{r}\right)\right| = \\ &= \sum_{k=0}^{\left[\frac{r}{4}\right]} \left| cos\left(\frac{2k\pi}{r}\right)\right| + \sum_{k=\left[\frac{r}{4}\right]+1}^{\left[\frac{r}{2}\right]} \left| cos\left(\frac{2k\pi}{r}\right)\right| \end{aligned}$$

so the result follows applying (5) and (6). ■

Example 2.6 shows that the energy of a unicyclic digraph is equal to the energy of its unique cycle. This situation can be generalized.

Definition 2.8 *Let G be a digraph. We define the cyclic part of G, denoted by G_c, as the subdigraph of G induced by the set of arcs which belong to a cycle of G.*

Example 2.9 *Figure 2 shows the cyclic part G_c of the digraph G in Figure 1.*

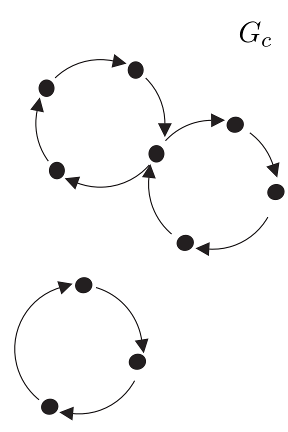

Figure 2

Theorem 2.10 *Let G be a digraph. Then $E(G) = E(G_c)$.*

Proof. By Theorem 1.1, if $a \in \mathcal{D}_G$ does not belong to a cycle of G then $\Phi_G = \Phi_{G-a}$. More generally, let $W = \{a \in \mathcal{D}_G : a \text{ does not belong to a cycle of } G\}$. Then it is clear that $G_c = G - W$ and $\Phi_G = \Phi_{G-W} = \Phi_{G_c}$. It follows that $E(G) = E(G_c)$. ■

It is clear now that Example 2.6 is a particular case of Theorem 2.10.

Definition 2.11 *A digraph G es pure-cyclic (abbreviated as pc) if G is weakly connected and $G_c = G$.*

In other words, a weakly connected digraph G is *pc* if every arc belongs to a cycle of G.

Recall that the direct sum $G_1 \dot{+} G_2$ of the digraphs $G_1 = (\mathcal{V}_1, \mathcal{D}_1)$ y $G_2 = (\mathcal{V}_2, \mathcal{D}_2)$, where $\mathcal{V}_1$ and $\mathcal{V}_2$ are disjoint, is the digraph $(\mathcal{V}, \mathcal{D})$ such that $\mathcal{V} = \mathcal{V}_1 \cup \mathcal{V}_2$ and $\mathcal{D} = \mathcal{D}_1 \cup \mathcal{D}_2$.

Proposition 2.12 *Let $G = G_1 \dot{+} G_2$. Then $E(G) = E(G_1) + E(G_2)$.*

Proof. The adjacency matrix of G has the form

$$\begin{pmatrix} A(G_1) & 0 \\ 0 & A(G_2) \end{pmatrix}$$

where $A(G_1)$ and $A(G_2)$ are the adjacency matrices of G_1 and G_2, respectively. It follows immediately that $\Phi_{G_1 \dot{+} G_2} = \Phi_{G_1}\Phi_{G_2}$ and so $E(G) = E(G_1) + E(G_2)$. ■

Theorem 2.13 *Let G be a digraph. Then G_c is a direct sum of (unique) pc subdigraphs of G. In particular, if $G_c = P_1 \dot{+} P_2 \dot{+} \cdots \dot{+} P_s$, where each P_k is pc, then $E(G) = \sum_{k=1}^{s} E(P_k)$.*

Proof. Keeping the notation in the proof of Theorem 2.10, it is clear that

$$G_c = G - W = P_1 \dot{+} P_2 \dot{+} \cdots \dot{+} P_s,$$

where each P_k is *pc*. Therefore, by Theorem 2.10 and Proposition 2.12, we conclude that

$$E(G) = E(G_c) = \sum_{k=1}^{s} E(P_k)$$

■

3 Coulson's integral formula for the energy of a digraph

Let G be a digraph with n vertices and eigenvalues $z_1, \ldots, z_n$. If A is the adjacency matrix of G then

$$Tr(A) = \sum_{k=1}^{n} z_k = 0$$

which implies

$$\sum_{k=1}^{n} Re(z_k) = 0 = \sum_{k=1}^{n} Im(z_k)$$

and consequently,

$$E(G) = 2 \sum_{+} Re(z_k) \tag{7}$$

where $\sum\limits_{+}$ indicates the summation over all eigenvalues with positive real part.

Theorem 3.1 *(Coulson's integral formula for digraphs) Let G be a digraph with n vertices. Then*

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{ix\Phi'_G(ix)}{\Phi_G(ix)} \right] dx \tag{8}$$

In the above formula, $\int\limits_{-\infty}^{+\infty} F(x)\, dx$ stands for the principal value of the respective integral, i.e.,

$$\lim_{t \to \infty} \int_{-t}^{t} F(x)\, dx$$

Proof. The proof is similar to the graph version with some modifications. If

$$\Phi_G(z) = \prod_{j=1}^{p} (z - w_j)^{\mu_j}$$

is the characteristic polynomial of the digraph G then the eigenvalues $w_1, \ldots, w_p$ are in general complex numbers. Since the coefficients of $\Phi_G(z)$ are real numbers (integers) we know that if w_k is an eigenvalue then $\overline{w_k}$ is also an eigenvalue. Furthermore, these can appear on the imaginary axis. Bearing in mind that it is not possible to integrate along a curve passing through a singularity, the contour Γ is changed to the one shown in Figure 3

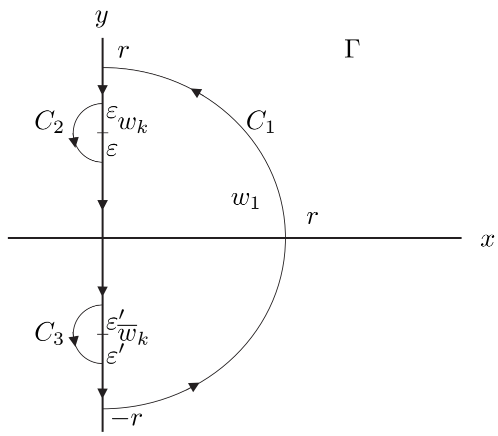

Figure 3

In this contour we choose $r > \|w_1\|$, where w_1 has maximal module among all w_k, $k = 1, \ldots, p$. As we can see, Γ consists of the counterclockwise oriented semicircles C_1, C_2 and C_3, with radius r, ε and ε', respectively, and three line segments.

As a consequence of the Cauchy integral formula [2] applied to the function

$$f(z) := z\frac{\Phi_G'(z)}{\Phi_G(z)} = z\sum_{j=1}^{p}\frac{\mu_j}{z - w_j}$$

we deduce

$$\frac{1}{2\pi i}\oint_{\Gamma} f(z)\,dz = \sum_{+}\mu_j w_j = \sum_{+} z_j = \sum_{+} Re(z_j) = \frac{1}{2}E(G) \tag{9}$$

On the other hand, evaluating the above integral along each of the curves which conform Γ, and letting $r \to \infty$, $\varepsilon \to 0$ and $\varepsilon' \to 0$ then

$$\begin{aligned}\frac{1}{2\pi i}\oint_{\Gamma} f(z)\,dz &= \frac{1}{2\pi i}\oint_{\Gamma}[f(z) - n]\,dz \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}[n - f(iy)]\,dy \end{aligned} \tag{10}$$

since $\int_{C_1}[f(z) - n]\,dz = 0$ if $r \to +\infty$ and $\int_{C_2}[f(z) - n]\,dz + \int_{C_3}[f(z) - n]\,dz = 0$ if $\varepsilon \to 0$ and $\varepsilon' \to 0$. The result follows from (9) and (10). In case there are more eigenvalues on the imaginary axis we proceed similarly. ■

Remark 3.2 *It is easy to see that Coulson's formula for the energy of digraphs is also valid for multidigraphs in general.*

Corollary 3.3 *If G be a digraph with n vertices then*

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} log\left[x^n \Phi_G\left(\frac{i}{x}\right)\right]$$

Proof. By Theorem 3.1,

$$\begin{aligned} E(G) &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{ix\Phi'_G(ix)}{\Phi_G(ix)}\right] dx \\ &= \frac{1}{\pi} \int_{-\infty}^{0} \left[n - \frac{ix\Phi'_G(ix)}{\Phi_G(ix)}\right] dx + \frac{1}{\pi} \int_{0}^{+\infty} \left[n - \frac{ix\Phi'_G(ix)}{\Phi_G(ix)}\right] dx \end{aligned}$$

Setting $x = \frac{1}{t}$ it follows that

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{i\frac{1}{t}\Phi'_G\left(i\frac{1}{t}\right)}{\Phi_G\left(i\frac{1}{t}\right)}\right] \frac{dt}{t^2}$$

Integrating by parts and considering

$$u = \frac{1}{t} \text{ and } dv = \left[\frac{n}{t} - \frac{i\frac{1}{t^2}\Phi'_G\left(i\frac{1}{t}\right)}{\Phi_G\left(i\frac{1}{t}\right)}\right] dt$$

we deduce that

$$du = -\frac{1}{t^2} dt \text{ y } v = log\left[t^n \Phi_G\left(\frac{i}{t}\right)\right]$$

and so

$$\begin{aligned} E(G) &= \frac{1}{\pi}\left(\frac{1}{t} log\left[t^n \Phi_G\left(\frac{i}{t}\right)\right]\right)_{-\infty}^{+\infty} \\ &\quad + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{t^2} log\left[t^n \Phi_G\left(\frac{i}{t}\right)\right] dt \\ &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{t^2} log\left[t^n \Phi_G\left(\frac{i}{t}\right)\right] \end{aligned}$$

■

4 Increasing property of the energy of digraphs

Consider the set $\mathcal{D}_{n,h}$ consisting of digraphs with n vertices and every cycle has length h.

Theorem 4.1 *If $G \in \mathcal{D}_{n,h}$ then the characteristic polynomial of G has the form*

$$\Phi_G = x^n + \sum_{k\geq 1} (-1)^k \, b\,(G, kh)\, x^{n-kh} \tag{11}$$

where $b\,(G, kh) \geq 0$ for every $k \geq 1$.

Proof. By Theorem 1.1, the companion coefficient of x^{n-kh} is given by

$$b_{kh} = \sum_{L\in\mathcal{L}_{kh}} (-1)^{comp(L)}$$

Since every cycle of G has length h, it follows that

$$L \in \mathcal{L}_{kh} \Leftrightarrow L \text{ is a direct sum of } k \text{ cycles of length } h \text{ of } G$$

Hence $b_{kh} = (-1)^k \, b\,(G, kh)$, where $b\,(G, kh) \geq 0$ is the number of linear subdigraphs of G consisting of k cycles of length h. Furthermore, it is clear that $b_j = 0$ if j is not a multiple of h, because in this case $\mathcal{L}_j = \emptyset$. ■

Now we define a quasi-order relation over $\mathcal{D}_{n,h}$.

Definition 4.2 *Let G_1 and G_2 elements of $\mathcal{D}_{n,h}$. Then we define $G_1 \preceq G_2$ if the following condition holds:*

$$b\,(G_1, kh) \leq b\,(G_2, kh) \text{ for every } k \geq 1.$$

If $G_1 \preceq G_2$ and there exists k such that $b\,(G_1, kh) < b\,(G_2, kh)$ then $G_1 \prec G_2$.

Clearly, this is a reflexive and transitive relation over $\mathcal{D}_{n,h}$.

Theorem 4.3 *Let h be an integer of the form $h = 4l - 2$, where $l \geq 1$. Then the energy increases with respect to the quasi-order relation defined over $\mathcal{D}_{n,h}$. In other words, if $G_1, G_2 \in \mathcal{D}_{n,h}$ then*

$$G_1 \preceq G_2 \Rightarrow E\,(G_1) \leq E\,(G_2)$$

and

$$G_1 \prec G_2 \Rightarrow E\,(G_1) < E\,(G_2)$$

Proof. Let $B \in \mathcal{D}_{n,h}$. Then by Theorem 4.1

$$\Phi_B = x^n + \sum_{k\geq 1} (-1)^k \, b(B, kh) \, x^{n-kh}$$

Then

$$\begin{aligned}
\Phi_B \left(\frac{i}{x} \right) &= \frac{i^n}{x^n} + \sum_{k\geq 1} (-1)^k \, b(B, kh) \, \frac{i^{n-kh}}{x^{n-kh}} \\
&= \frac{i^n}{x^n} \left[1 + \sum_{k\geq 1} (-1)^k \, b(B, kh) \, x^{kh} i^{-k(4l-2)} \right] \\
&= \frac{i^n}{x^n} \left[1 + \sum_{k\geq 1} (-1)^k \, b(B, kh) \, x^{kh} \, (-1)^{-k} \right] \\
&= \frac{i^n}{x^n} \left[1 + \sum_{k\geq 1} b(B, kh) \, x^{kh} \right]
\end{aligned}$$

By Corollary 3.3

$$\begin{aligned}
E(B) &= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} log \left[x^n \frac{i^n}{x^n} \left[1 + \sum_{k\geq 1} b(B, kh) \, x^{kh} \right] \right] \\
&= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} log \left[i^n \left[1 + \sum_{k\geq 1} b(B, kh) \, x^{kh} \right] \right]
\end{aligned}$$

Since

$$\frac{1}{\pi} p.v. \int_{-\infty}^{+\infty} log \left[i^n \right] \frac{dx}{x^2} = 0$$

where $p.v.$ is the principal value of Cauchy's integral, it follows that

$$E(B) = \frac{1}{\pi} \int_{-\infty}^{+\infty} log \left[1 + \sum_{k\geq 1} b(B, kh) \, x^{kh} \right] \frac{dx}{x^2}$$

This clearly implies that the energy increases with respect to the quasi-order relation defined over $\mathcal{D}_{n,h}$. ■

We next use Theorem 4.3 to study the problem of extremal values of the energy for various classes of digraphs. As we mentioned before, a graph G can be considered as a digraph $\overline{G}$, where each edge of G corresponds to a cycle of length 2 in $\overline{G}$. We can extend this idea: let $h \geq 2$ an integer and G a graph. We construct a family of digraphs from G as follows: to each edge uv of G corresponds a directed path of length r from u to v and a directed path of length s form v to u, in such a way that $r+s=h$. This family of digraphs associated to G is denoted by $\mathcal{D}_h(G)$. It is clear that if $h=2$ then $\mathcal{D}_2(G)=\{\overline{G}\}$.

Example 4.4 *Figure 4 shows some elements of $\mathcal{D}_5(G)$ for the given graph G.*

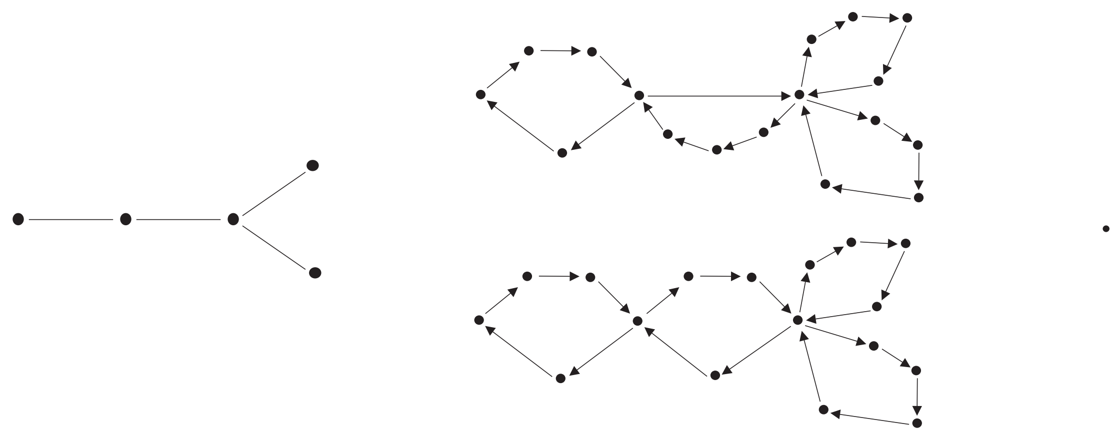

Figure 4

When T is a tree then $\mathcal{D}_h(T)$ has interesting properties.

Proposition 4.5 *Let $h\geq 2$ an integer and T a tree with n vertices. Then*

1. $\mathcal{D}_h(T)\subseteq\mathcal{D}_{p,h}$*, where* $p=(n-1)(h-2)+n$*;*

2. *If*

$$\Phi_T=x^n+\sum_{k\geq 1}(-1)^k b(T,2k)\,x^{n-2k}$$

then for every $X\in\mathcal{D}_h(T)$

$$\Phi_X=x^p+\sum_{k\geq 1}(-1)^k b(T,2k)\,x^{n-hk}$$

In particular, all digraphs in $\mathcal{D}_h(T)$ are cospectral.

Proof. 1. By definition, it is clear that the unique cycles in $X\in\mathcal{D}_h(T)$ correspond to the edges in T, and these have length h. Moreover, for each edge there are $h-2$ new vertices, together with the vertices in T gives $p=(n-1)(h-2)+n$ vertices in X.

2. By Theorem 1.1, the companion coefficient of x^{n-hk} in Φ_X is $\sum_{L\in\mathcal{L}_{hk}}(-1)^{comp(L)}$. Since $X\in\mathcal{D}_{p,h}$, every cycle of X has length h and consequently, $L\in\mathcal{L}_{hk}$ if and only if L is a direct

sum of k disjoint cycles of length h. From the definition of X, this number is equal to the number of k independent edges in T, which is exactly $b(T, 2k)$. ■

Theorem 4.6 *Let h be an integer and $\mathcal{T}$ a family of trees with n vertices. Assume that L is a minimal element and M is a maximal element of $\mathcal{T}$ with respect to the quasi-order defined in (2). Then every $X \in \mathcal{D}_h(L)$ and $Y \in \mathcal{D}_h(M)$ are, respectively, minimal and maximal elements of*

$$\mathcal{D}_h(\mathcal{T}) = \{\mathcal{D}_h(T) : T \in \mathcal{T}\}$$

Proof. Let $Z \in \mathcal{D}_h(T)$ for some $T \in \mathcal{T}$. Since $L \preceq T \preceq M$, it follows from the second part of Proposition 4.5 that $X \preceq Z \preceq Y$. ■

Corollary 4.7 *Let h be an integer of the form $h = 4k - 2$, where $k \geq 1$ and $\mathcal{T}$ a family of trees with n vertices. If L is a minimal element and M is a maximal element of $\mathcal{T}$ with respect to the quasi-order relation, then the minimal energy in $\mathcal{D}_h(\mathcal{T})$ is attained in $\mathcal{D}_h(L)$ and the maximal energy is attained in $\mathcal{D}_h(M)$.*

The previous Corollary states that if the extremal values (with respect to the quasi-order) of a family of trees $\mathcal{T}$ are known then the extremal values of the energy in $\mathcal{D}_h(\mathcal{T})$ can be determined.

Example 4.8 *Let $\mathcal{T}$ be the family of all trees with n vertices. It is well known that the star S_n and the path P_n are minimal and maximal elements, respectively [3]. It follows that the digraphs in $\mathcal{D}_h(S_n)$ and $\mathcal{D}_h(P_n)$ have minimal and maximal energy, respectively, in $\mathcal{D}_h(\mathcal{T})$.*

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