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RELATION BETWEEN THE LAPLACIAN AND THE ORDINARY CHARACTERISTIC POLYNOMIAL[1]

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Abstract

Let G be a graph and $v_1, v_2, \ldots, v_n$ be its vertices. Let d_r be the degree of the vertex v_r. The Laplacian characteristic polynomial of G can be viewed as the ordinary characteristic polynomial of a weighted graph G^*, obtained by attaching to each vertex v_r of G a self-loop of weight $-d_r$. Based on this observation a general relation between the Laplacian and the ordinary characteristic polynomials can be deduced. Several consequences of this relation are pointed out. An expreession for the Wiener index W of trees is obtained, in which W is expressed in terms of numbers of selections of independent edges of the graph G and of its subgraphs.

INTRODUCTION

Graph spectra and characteristic polynomials belong among the standard tools of mathematical chemistry [1–3]. Laplacian spectra and the corresponding characteristic

[1] Part VIII of the series "*Chemical Applications of the Laplacian Spectrum*"; parts I–VII are the references [7–13].

polynomials are much less studied objects, but also for them a number of chemical applications were recently communicated [4-13].

Let G be a graph on n vertices. Its (ordinary) characteristic polynomial is defined in the usual manner as [1,2,14]

$$\phi(G) = \phi(G, \lambda) = \det[\lambda\, I_n - A(G)] \tag{1}$$

where $A(G)$ is the adjacency matrix of G and I_n the unit matrix of order n.

Let $v_1, v_2, \ldots, v_n$ be the vertices of G. The degree d_r of the vertex v_r is the number of the first neighbors of this vertex. The diagonal matrix of vertex degrees will be denoted by $D(G)$. Then $L(G) = D(G) - A(G)$ is the Laplacian matrix of G and

$$\psi(G) = \psi(G, \lambda) = \det[\lambda\, I_n - L(G)] \tag{2}$$

is the Laplacian characteristic polynomial of G. (More details on Laplacian matrices and their spectra are found in the book [14] and the reviews [15-18].)

Both $\phi(G)$ and $\psi(G)$ are monic polynomials of order n. In what follows we shall write them in the coefficient form as

$$\phi(G, \lambda) = \sum_j a_j(G)\, \lambda^{n-j} \quad ; \quad \psi(G, \lambda) = \sum_j (-1)^j\, c_j(G)\, \lambda^{n-j} \, . \tag{3}$$

Note that in this notation, $c_j(G) \geq 0$ for all G and for all j [15-18], whereas a_j may assume both positive, negative and zero values [14]. Note, in addition, that

$$(-1)^n\, \psi(G, -\lambda) = \sum_j c_j(G)\, \lambda^{n-j} \tag{4}$$

a relation that is an immediate consequence of (3).

In the following considerations we shall encounter subgraphs of the graph G, obtained by deleting from it certain vertices. In order to simplify our notation, if $v_{r_1}, v_{r_2}, \ldots, v_{r_k}$ are distinct vertices of G, then the subgraph obtained by deleting these vertices from G is denoted by $G_{r_1, r_2, \ldots, r_k}$. This subgraph has $n - k$ vertices. In particular, G_r stands for the $(n-1)$-vertex graph, obtained by deleting from G the vertex v_r; by $G_{r,s}$ is denoted the $(n-2)$-vertex graph, obtained by deleting from G the vertices v_r and v_s.

AN AUXILIARY FORMULA

Let as before G be an arbitrary graph and v_r, v_s its two distinct vertices. Let $G[h_r]$ be the graph obtained from G by attaching to the vertex v_r a self-loop of weight h_r. Analogously, $G[h_s]$ is obtained from G by attaching to v_s a self-loop of weight h_s. Further, $G[h_r, h_s]$ is obtained by attaching to both v_r and v_s self-loops of weight h_r and h_s, respectively. Finally, $G[h_1, h_2, \ldots, h_n]$ is the graph obtained by attaching a self-loop of weight h_r to vertex v_r, for each $r = 1, 2, \ldots, n$.

The properties of characteristic polynomials of weighted graphs were established long time ago [19–22]. The recursion relation (5) is a well known and often used result:

$$\phi(G[h_r]) = \phi(G) - h_r\,\phi(G_r)\ . \tag{5}$$

By repeated application of (5) for $G[h_r, h_s]$ one obtains:

$$\begin{aligned}\phi(G[h_r, h_s]) &= \phi(G[h_r]) - h_s\,\phi(G_s[h_r]) \\ &= \{\phi(G) - h_r\,\phi(G_r)\} - h_s\,\{\phi(G_s) - h_r\,\phi(G_{r,s})\}\end{aligned}$$

i. e.,

$$\phi(G[h_r, h_s]) = \phi(G) - h_r\,\phi(G_r) - h_s\,\phi(G_s) + h_r\,h_s\,\phi(G_{r,s})\ . \tag{6}$$

Formula (6) is also previously known, see, for instance [23]. Its immediate generalization is:

$$\begin{aligned}\phi(G[h_1, h_2, \ldots, h_n]) &= \phi(G) - \sum_{r=1}^{n} h_r\,\phi(G_r) + \sum_{1 \le r_1 < r_2 \le n} h_{r_1}\,h_{r_2}\,\phi(G_{r_1,r_2}) \\ &\quad - \sum_{1 \le r_1 < r_2 < r_3 \le n} h_{r_1}\,h_{r_2}\,h_{r_3}\,\phi(G_{r_1,r_2,r_3}) + \cdots\end{aligned}$$

i. e.,

$$\begin{aligned}\phi(G[h_1, h_2, \ldots, h_n]) &= \phi(G) - \sum_{r=1}^{n} h_r\,\phi(G_r) \\ &\quad + \sum_{k \ge 2}(-1)^k \sum_{1 \le r_1 < r_2 \cdots < r_k \le n} h_{r_1}\,h_{r_2}\cdots h_{r_k}\,\phi(G_{r_1,r_2,\ldots,r_k})\end{aligned}$$

which we shall write in a shorter manner as

$$\phi(G[h_1, h_2, \ldots, h_n]) = \phi(G) + \sum_{k \ge 1}(-1)^k \sum_{r_1 < \cdots < r_k} h_{r_1}\cdots h_{r_k}\,\phi(G_{r_1,\ldots,r_k})\ . \tag{7}$$

THE MAIN RESULT

Using the definitions (1) and (2) of the two characteristic polynomials we readily obtain:

$$\begin{aligned}(-1)^n\,\psi(G,-\lambda) &= (-1)^n\,\det[-\lambda\,I_n - D(G) + A(G)] \\ &= \det[\lambda\,I_n - A(G) + D(G)] \\ &= \det[\lambda\,I_n - A(G^*)] = \phi(G^*,\lambda)\end{aligned}$$

where $A(G^*) = A(G) - D(G)$ can be viewed as the adjacency matrix of some weighted graph G^*. Now, $A(G^*)$ and $A(G)$ differ only in the diagonal elements: whereas all diagonal elements in $A(G)$ are equal to zero, those in $A(G^*)$ are equal to $-d_1, -d_2, \ldots, -d_n$. Clearly, G^* is obtained from G by attaching to its vertices $v_1, v_2, \ldots, v_n$ self-loops of weights $-d_1, -d_2, \ldots, -d_n$, respectively.

Employing the notation specified in the preceding section, we have $G^* \equiv G[-d_1, -d_1, -d_2, \ldots, -d_n]$, and consequently,

$$\phi(G[-d_1, -d_1, -d_2, \ldots, -d_n], \lambda) = (-1)^n\,\psi(G,-\lambda)\ . \qquad (8)$$

Combining Eqs. (7) and (8) we arrive at our main result:

$$(-1)^n\,\psi(G,-\lambda) = \phi(G,\lambda) + \sum_{k\geq 1}(-1)^k \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\,\phi(G_{r_1,\ldots,r_k},\lambda)\ . \qquad (9)$$

Formula (9) shows that the Laplacian characteristic polynomial of a graph G can be expressed in terms of the ordinary characteristic polynomials of G and of all vertex-deleted subgraphs of G. Its derivation (as shown above) is elementary and is based on a straightforward application of the familiar identity (5). A result analogous to Eq. (9) was communicated some time ago [24], but was obtained using a different, much less transparent, approach.

Bearing in mind (3) the right-hand side of Eq. (9) can be transformed into

$$\sum_j \left[a_j(G) + \sum_{k\geq 1} \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\,a_{j-k}(G_{r_1,\ldots,r_k}) \right] \lambda^{n-j}$$

which, in view of relation (4) gives

$$c_j(G) = a_j(G) + \sum_{k\geq 1} \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\,a_{j-k}(G_{r_1,\ldots,r_k})\ . \qquad (10)$$

Needless to say that (10) is just another form of the identity (9) and is fully equivalent to it.

SIMPLE AND LESS SIMPLE APPLICATIONS

Denote by m the number of edges of the graph G, and recall that $a_0(G) = 1$, $a_1(G) = 0$, $a_2(G) = -m$, and that the sum of the vertex degrees of G is equal to $2m$. For $j = 0, 1$, and 2, Eq. (10) yields:

$$\begin{aligned}
c_0(G) &= a_0(G) = 1 \\
c_1(G) &= a_1(G) + \sum_r d_r\, a_0(G_r) = 0 + \sum_r d_r = 2m \\
c_2(G) &= a_2(G) + \sum_r d_r\, a_1(G_r) + \sum_{r<s} d_r\, d_s\, a_0(G_{r,s}) = -m + 0 + \sum_{r<s} d_r\, d_s \\
&= \frac{1}{2}\left(\sum_r \sum_s d_r\, d_s - \sum_r (d_r)^2\right) - m = \frac{1}{2}(2m)^2 - \frac{1}{2}\sum_r (d_r)^2 - m \\
&= 2m^2 - m - \frac{1}{2}\sum_r (d_r)^2 .
\end{aligned}$$

These are known results [15-18].

All graphs possess a zero Laplacian eigenvalue [6,7,15-18] and therefore it is always $c_n(G) = 0$. Therefrom we arrive at the curious and generally valid identity:

$$a_n(G) + \sum_{k \geq 1} \sum_{r_1 < \cdots < r_k} d_{r_1} \cdots d_{r_k}\, a_{n-k}(G_{r_1,\ldots,r_k}) = 0 . \tag{11}$$

Another relation of the same kind is obtained from the equality [15-18] $c_{n-1}(G) = n\, t(G)$, where $t(G)$ is the number of spanning trees of the graph G:

$$a_{n-1}(G) + \sum_{k \geq 1} \sum_{r_1 < \cdots < r_k} d_{r_1} \cdots d_{r_k}\, a_{n-k-1}(G_{r_1,\ldots,r_k}) = n\, t(G) . \tag{12}$$

Note that (11) and (12) are identities in which only the coefficients of the ordinary characteristic polynomials (of G and of its subgraphs) occur. Hence, these are generally valid formulas from (ordinary) graph spectral theory [14]. It seems that these have not been reported previously.

SPECIAL CASES AND A CHEMICAL CONNECTION

If the graph G is bipartite, then its characteristic polynomial assumes the form:

$$\phi(G,\lambda) = \sum_j (-1)^j \, b_j(G) \, \lambda^{n-2j}$$

and $b_j(G) \geq 0$ for all G and for all j. Then Eq. (10) results in two different identities, one for even and another for odd coefficients of the Laplacian characteristic polynomial:

$$c_{2j}(G) = (-1)^j \left[b_j(G) + \sum_{k \geq 1} (-1)^k \sum_{r_1 < \cdots < r_{2k}} d_{r_1} \cdots d_{r_{2k}} \, b_{j-k}(G_{r_1,\ldots,r_{2k}}) \right] \quad (13)$$

$$c_{2j+1}(G) = (-1)^j \left[\sum_{k \geq 0} (-1)^k \sum_{r_1 < \cdots < r_{2k+1}} d_{r_1} \cdots d_{r_{2k+1}} \, b_{j-k}(G_{r_1,\ldots,r_{2k+1}}) \right] . \quad (14)$$

* * * * * *

Consider now trees (= connected acyclic graphs). Because trees are bipartite graphs, the above relations hold also for them. However, if T is a tree, then $b_j(T)$ is equal to $m(T,j)$, the number of selections of j mutually independent edges [2,14].

For an n-vertex tree T the identities (11) and (12) are additionally simplified. If n is even ($n = 2p$), then

$$m(T,p) + \sum_{k \geq 1} (-1)^k \sum_{r_1 < \cdots < r_{2k}} d_{r_1} \cdots d_{r_{2k}} \, m(T_{r_1,\ldots,r_{2k}}, p-k) = 0$$

$$\sum_{k \geq 0} (-1)^k \sum_{r_1 < \cdots < r_{2k+1}} d_{r_1} \cdots d_{r_{2k+1}} \, m(T_{r_1,\ldots,r_{2k+1}}, p-k-1) = (-1)^{p+1} n .$$

If n is odd ($n = 2p+1$), then

$$\sum_{k \geq 0} (-1)^k \sum_{r_1 < \cdots < r_{2k+1}} d_{r_1} \cdots d_{r_{2k+1}} \, m(T_{r_1,\ldots,r_{2k+1}}, p-k) = 0$$

$$m(T,p) + \sum_{k \geq 1} (-1)^k \sum_{r_1 < \cdots < r_{2k}} d_{r_1} \cdots d_{r_{2k}} \, m(T_{r_1,\ldots,r_{2k}}, p-k) = (-1)^p n .$$

Here we used the fact that for trees, $t(T) = 1$.

* * * * * *

Any tree T has the noteworthy property that its Laplacian coefficient $c_{n-2}(T)$ is equal to the Wiener topological index $W(T)$ [5-7,25]. (Recall that $W(T)$ is equal to the sum of distances between all pairs of vertices of T [2] and thus, at the first glance, has nothing in common with graph spectra and characteristic polynomials.) Bearing in mind the property $W(T) = c_{n-2}(T)$, we obtain, as special cases of the formulas (13) and (14), the following expression for the Wiener index.

For a tree T with an even number of vertices ($n = 2p$),

$$W(T) = (-1)^{p+1} \left[m(T, p-1) + \sum_{k \geq 1} (-1)^k \sum_{r_1 < \cdots < r_{2k}} d_{r_1} \cdots d_{r_{2k}} \, m(T_{r_1, \ldots, r_{2k}}, p-k-1) \right] \tag{15}$$

whereas if the number of vertices is odd ($n = 2p+1$),

$$W(T) = (-1)^{p+1} \left[\sum_{k \geq 0} (-1)^k \sum_{r_1 < \cdots < r_{2k+1}} d_{r_1} \cdots d_{r_{2k+1}} \, m(T_{r_1, \ldots, r_{2k+1}}, p-k-1) \right] . \tag{16}$$

Formulas (15) and (16), although inappropriate for actual calculation of the Wiener index, reveal some novel concealed algebraic properties of this structure-descriptor: By means of (15) and (16), the distance-based topological index W is expressed in terms of numbers of selections of independent edges of the tree T and its subgraphs. Thus we encounter another unexpected algebraic connection [26,27] between the Wiener index and other – formally unrelated – topological indices, in particular between Wiener index and Hosoya-index-type structure-descriptors.

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