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Some Spectral Properties of the Arc-Graph

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Abstract

The arc-graph of a digraph is a directed generalization of the line-graph of an undirected graph. Vertices of the arc-graph are arcs of a digraph; an ordered pair of arcs of a digraph is a pair of adjacent vertices in its arc-graph if and only if the head of the one arc coincides with the tail of the other, whether the remaining tail and head coincide or not. Self-loops, if any, of a digraph are considered as arcs whose head and tail coincide and participate in the above considerations as well.

The arc-graph of an undirected graph can also be constructed if one initially replaces each edge of the second with opposite darts and then reverts to the above pattern.

It is proven that the spectrum of a weighted (di-)graph admitting self-loops and the spectrum of its weighted arc-graph coincide with accuracy to the number of zero eigenvalues. Also, we give a partial result for the permanent of the adjacency matrix of the arc-graph and speculate upon chemical relevance of the present study.

1 Preliminaries

Let $D = D(V, L)$ be a digraph with the set V of vertices and set L of arcs (self-loops, if any, are considered as self-adjacent arcs whose head and tail coincide); $|V| = n$, $|L| = l$. The arc-graph $\Gamma(D) = \Gamma(L, M)$ of a digraph D is a derivative digraph whose vertex set L

is the set of arcs of D; each ordered pair pq and rv of arcs, of D, is a pair of adjacent vertices in Γ iff the head q of pq coincides with the tail r of rv ($q = r$), whether the remaining tail p and head v coincide or not.

The arc-graph $\Gamma(G)$ of an undirected graph $G = G(V, E)$ can also be constructed if we initially replace each edge ij with a pair of opposite darts ($1 \leq i, j \leq |V| = n; |E| = m$), which results in the so-called symmetric digraph $S = S(G) = S(V, L)$ ($|L| = 2|E| +$ the number of self-loops, if any), and then revert to the above pattern.

For any weighted digraph D (D may also be S) the corresponding weighted arc-graph $\Gamma(D)$ is defined unambiguously. Let $A = [a_{ij}]_{i,j=1}^{n}$ and $A(\Gamma(D)) = [w_{tu}]_{t,u=1}^{l}$ denote the weighted adjacency matrices of D and $\Gamma(D)$, respectively, wherein the entries are the weights of respective arcs (self-loops); in the special case that D is an unweighted digraph, the two matrices are reduced to matrices of zeros and ones. Under this, if $b = pq$ and $c = qr$ is an ordered pair of incident (adjacent) arcs in D, the weight w_{bc} of the derivative arc bc in $\Gamma(D)$ is just the weight a_{qr} of the second arc, qr, of D; however, $w_{uv} \equiv 0$ for every pair, u and v, of nonadjacent arcs of D, disregarding any weights of u and v, in D.

In the arc-vertex incidency matrix $B = [b_{rs}]_{r,s=1}^{l,n}$ of G, an entry $b_{rs} = 1$ if a vertex s is the head of an arc $r = pq$ ($s = q$) and $b_{rs} = 0$ if $s \neq p$; obviously, B has exactly one 1 in row. In its weighted vertex-arc analog $C = [c_{sr}]_{s,r=1}^{n,l}$, an entry $c_{sr} = a_{pq}$ (an entry of $A(G)$) if a vertex s is the tail of an arc $r = pq$ ($s = p$) and $c_{sr} = 0$ if $s \neq p$; apparently, C has just one nonzero entry in column.

2 The characteristic polynomial of the arc-graph

Our first statement is elementary but it will play an important role below.

Lemma 1. Let B and C be the two incidency matrices introduced above. Then

$$BC = A(\Gamma(G)), \tag{1}$$

$$CB = A(G). \tag{2}$$

Proof. Pick (1). The (i, j)-th entry of the product matrix BC is $\sum_{s=1}^{n} b_{is}c_{sj}$. Because B has only one 1 in row, the last sum contains at most one nonzero summand. Since i and j are fixed, the nonzero summand $b_{is}c_{sj}$ requires that s is the head of an arc $i = ps$ and the tail of an arc $j = sq$, in G or, alternatively, $S(G)$; in this case, $b_{is} = 1$ and $c_{sj} = a_{sq}$. Therefore, the (i, j)-th entry of BC is $b_{is}c_{sj} = a_{sq}$ for some s and q completely determined by arcs i and j. On the other hand, the quantity a_{sq} is also the (i, j)-th entry of $A(\Gamma(G))$, because, by definition, the latter entry is the weight of the second arc $j = sq$. Thus, indeed, $BC = A(\Gamma(G))$. The remaining case (2) can be treated in a similar vein and we so arrive at the overall proof. □

Throughout this paper, we shall denote by I the diagonal identity matrix.

The second statement is out of known fundamental results of the spectral theory of matrices (see 2.15.15 in [1]), viz.:

Lemma 2. Let Q be an arbitrary $l \times n$ matrix and R be an arbitrary $n \times l$ matrix $(l \geq n)$ over the field of complex numbers. Let further $P(U; x) = \det(U - xI)$ be the characteristic polynomial of a square matrix U. Then

$$P(QR; x) = x^{l-n} P(RQ; x). \tag{3}$$

Evidently, Lemma 2 must also hold true for the case $n > l$ because the roles of matrices R and Q are completely symmetrical therein.

Here, we recall that the characteristic polynomial $P(H; x)$ of any graph H is the characteristic polynomial $P(A(H); x)$ of its adjacency matrix $A(H)$ [2].

¿From the last crucial result, it immediately follows

Theorem 3. Let $P(G; x)$ and $P(\Gamma(G); x)$ be the characteristic polynomial of an arbitrary weighted (di-)graph G and that of its arc-graph $\Gamma(G)$, respectively. Then

$$P(\Gamma(G); x) = x^{l-n} P(G; x), \tag{4}$$

where l and n are the numbers of vertices in $\Gamma(G)$ and G, respectively.

In other words, the spectra of $\Gamma(G)$ and G may differ only in the number of zero eigenvalues and this difference in the multiplicities is $|l - n|$.

We would like to propose an elementary application. Let the adjacency matrix $A(G)$, of a weighted molecular graph G, be the matrix of the Hückel Hamiltonian $\mathcal{H}$ of some quantum-chemical system. Since there always exists the above derivative matrix $A(\Gamma(G))$, one may also raise a question about a derivative (non-Hermitian) Hamiltonian $\mathcal{H}^*$ corresponding to $A(\Gamma)$. Theoretically, $\mathcal{H}^*$ must possess the same spectrum of eigenvalues that

$\mathcal{H}$ does and, moreover, contain extra zero eigenvalues. The latter eigenvalues, unforeseen in the usual Hückel method, may be conjectured to play a key role in gaining a more complete understanding of electronic and photonic properties of some materials. In author's opinion, an instance of materials that may be retreated in such a way are nanoporous ionic conductors exhibiting mesoscopic features. Here, it is especially valuable that Theorem 3 affords us a way for deriving the complete spectrum of $\mathcal{H}^*$ from that of $\mathcal{H}$, without any special computation.

3 The permanental polynomial of the arc-graph

Here we indicate some partial results, without going into very much detail in the derivation of these results.

By definition (see p. 34 in [2]), the permanental polynomial $P^+(H;x)$ of a weighted graph H is the permanental polynomial $P^+(A(H);x)$ of its adjacency matrix $A(H)$; herein, $P^+(A(H);x) = \mathrm{per}[A(H) + xI]$.

An digraph D is called Eulerian if there exists a closed spanning walk W traversing every arc, in D, exactly once and consistently with its orientation; under this, the number of arcs entering any vertex of D equals the number of arcs emanating from it. The mentioned closed walk W, in D, is called the Eulerian trail. The cyclical order of arcs in an Eulerian trail is of value because one and the same Eulerian digraph D admits more than one Eulerian trail whenever the order of cyclically touring its arcs may be varied. The last circumstance plays a crucial role when Eulerian trails formalize the cyclical motion of particles in the respective models of statistical physics, where every possible closed walk of a particle must necessarily be taken into account. All the said can readily be adapted to undirected graphs if one reconsiders every edge as opposite darts, as it was already done while introducing the notion of the symmetric digraph $S(G)$. In the last sense, any connected undirected graph G admits at least one Eulerian trail passing every its edge strictly twice and just in opposite directions.

The partition function, or statistical sum, Z of the Ising problem may be written as the product $Z = Z_1Z_2$, where Z_1 stands for unary and binary interactions and Z_2 does for multiparticle interactions (of three particles and more) in a simulated physico-chemical system Ω [3–7]. In 1958, Frank Harary obtained an exact graph-theoretical estimation of Z_2 as the generating function $Z_2(z)$ of even subgraphs (having all vertex degrees even and all components Eulerian) of a weighted graph $G(\Omega)$ of Ω, where a special physical quantity is substituted for a formal variable z (see [3–7] for details and below).

We can simultaneously propose the following two refinements of his solution ([3–5]):
1) To consider all types of unary and binary interactions, in Ω, given by the adjacency matrix $A(G)$ with (many) distinct diagonal and nondiagonal entries, respectively;
2) To enumerate all vertex covers of $G(\Omega)$ by Eulerian trails traversed in its strongly connected subgraphs instead of enumerating "less informative" covers by even subgraphs [3–7], which is necessary for description of moving particles (in contrast to [3–5], where particles were fixed in the knots of crystalline lattice).

Among our modifications to the original Harary's approach (see [3–5]), it should specially be noted that the above-mentioned physical quantity (substituted for z in [3–7]) herein renders a dynamic parameter adapted to many sorts of interactions. A variable x in $P^+(H;x)$ will be employed without any physical sense while all physical information in Z_2 will be introduced via the entries a_{ij} of $A(G)$ (res. $A(\Gamma)$). Specifically, an entry of $A(G)$ is this (cf [3–5])

$$a_{ij} = \tanh\left(\frac{\varepsilon_{ij}}{kT}\right) \qquad (1 \le i, j \le n)\,, \tag{5}$$

where $\tanh(\cdots)$ is the hyperbolic tangent, ε_{ij} is the energy of interaction between the i-th and j-th particles, k is the Boltzman constant, and T is an absolute temperature.

Now return to purely mathematical matters. The Greek character "Γ" in "$\Gamma(G)$" may be considered as an operator Γ transferring a graph G into another one $\Gamma(G)$. This operator has some remarkable properties. In particular, it can give for any loopless Eulerian digraph G with all out-degrees $d_i = d > 1$ $(l > n)$ an infinite series of such digraphs: $\Gamma^0(G) := G, \Gamma^1(G) = \Gamma(G), \Gamma^2(G) = \Gamma(\Gamma^1(G)), \ldots, \Gamma^{s+1}(G) = \Gamma(\Gamma^s(G))$ $(s \ge 0)$, whose spectra differ only in the number of zero eigenvalues. But, out of all properties of the operator Γ, the most important for us is that Γ "unties" every Eulerian trail θ of a graph $\Gamma^s(G)$, transferring it into an oriented cycle $\Gamma(\theta)$ of Γ^{s+1} $(s \ge 0)$ with the same weight $w(\Gamma(\theta)) = w(\theta)$. Here, we recall that the weight $w(\sigma)$ of any cycle σ, in an arbitrary digraph D, is the product of the weights of arcs comprising σ. Moreover, Γ assures one-to-one correspondence between the set of all Eulerian trails on G and the set of all oriented cycles of $\Gamma(G)$.

As a substitute to the cofactor Z_2, in the partition function Z [3–5], that already takes into account the two refinements above, we shall propose the quantity ζ. By definition, ζ is the sum of the weights of all vertex covers of G by Eulerian trails of its subgraphs. Due to the mentioned property of the operator Γ, the numerical value of ζ can also be obtained if one, instead of that, computes the sum of the weights of all vertex covers of $\Gamma(G)$ by its oriented cycles. This latter value for $\Gamma(G)$ is, by definition, the sum of all coefficients of the permanental polynomial $P^+(\Gamma(G);x)$ of $\Gamma(G)$; see [2] for details. Thus, we arrive at the following

Proposition 4. Let ζ be the refined cofactor Z_2 in the partition function Z of a physico-chemical system Ω modeled with a graph G. Then

$$\zeta = P^+(\Gamma(G);1) = \mathrm{per}[A(\Gamma) + I]. \tag{6}$$

Proof. Evidently, $P^+(\Gamma(G);1)$ is just the sum of coefficients of $P^+(\Gamma(G);x)$ and, thus, the desired result for ζ. □

Corollary 4.1. Let ζ be the above cofactor of the partition function Z. Then

$$\zeta = \sum_{0}^{2^l} \mathrm{per} A_\mu = \sum_{0}^{2^l} \zeta_\mu , \tag{7}$$

where the first sum runs over all principal minors A_μ of $A(\Gamma)$ while the second does over all the partition functions ζ_μ of subsystems Ω_μ, of Ω, given by the respective minors A_μ.

Since we modified the cofactor Z_2 in Z, the expression for Z renders into $Z = Z_1\zeta$, wherein Z_1 is estimated as in [3–5] and ζ was rigorously evaluated above. Taking the said on trust, as a working conjecture, we shall propose the following resulting solution for Z, viz.:

Proposition 5. Let $Z = Z_1\zeta$ be the generalized partition function of a system Ω modeled with a graph G. Then

$$Z = 2^l \left[\prod_{i,j=1}^{n,n} \cosh\left(\frac{\varepsilon_{ij}}{kT}\right) \right] \mathrm{per}[A(\Gamma(G)) + I], \tag{8}$$

where $\cosh(\frac{\varepsilon_{ij}}{kT})$ is the hyperbolic cosine and the product embraces only all nonzero values of it (while i and j run over all values within the indicated limits).

The above raises a question about an efficient method for calculating the permanental polynomial $P^+(\Gamma(G);x)$ or, what is sufficient in our applied context, the value of $P^+(\Gamma(G);1)$. In general, it stays unsolved. Nevertheless, herein we give an affirmative answer to our previous question [7] about analytically solving the above problem for ζ through the permanent of whatever matrix relevant to it.

In conclusion, we shall present a partial result for the tail coefficient of the permanental polynomial $P^+(\Gamma(H);x)$ of the arc-graph $\Gamma(H)$ of an Eulerian digraph H. In particular, H may be the above symmetric digraph $S(G)$ and, consequently, the arc-graph $\Gamma(G)$ of an undirected graph G may also be considered below in place of $\Gamma(H)$.

Proposition 6. Let $A(H)$ be the adjacency matrix of a weighted Eulerian digraph H (res. undirected graph H) admitting self-loops and $A(\Gamma(H))$ be the adjacency matrix of the arc-graph $(\Gamma(H))$. Then

$$\mathrm{per}\,[A(\Gamma(H))] = \left(\prod_{i,j=1}^{n,n} a_{ij}\right)\prod_{i=1}^{n} d_i!\,, \tag{9}$$

where the first product is taken over all nonzero entries of $A(H)$, d_i stands for the out-degree (res. degree) of a vertex i in H and the second product is taken over all factorials of vertex out-degrees (res. degrees) in H.

Proof. Sketch it. The permanent of any matrix is independent of permuting its rows and/or columns. In particular, nonsimultaneously (!) permuting rows and columns of $A(\Gamma(H))$ can give a block-diagonal matrix B whose every diagonal block B_i $(1 \le i \le n)$ is a $d_i \times d_i$ submatrix with fixed-value columns and the entries in every row, of B_i, are exactly all nonzero entries of the i-th row of $A(H)$. Obviously, $\mathrm{per}B_i = \left(\prod_{j=1}^{n} a_{ij}\right) d_i!$, where the product involves all nonzero entries of the i-th row of $A(H)$. Since the permanent of B is $\prod_{i=1}^{n} B_i$, we immediately obtain that $\mathrm{per}\Gamma(H) = \mathrm{per}B = \prod_{i=1}^{n}\left(\left(\prod_{j=1}^{n} a_{ij}\right) d_i!\right) = \left(\prod_{j=1}^{n} a_{ij}\right)\prod_{i=1}^{n} d_i!$, where, on the last side, the first product embraces all nonzero entries of $A(H)$ while the second symmetrically does factorials of all vertex out-degrees (res. degrees) of H. The proof is over. □

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