Rectifying a misbelief: Frank Harary's role in the discovery of the coefficient-theorem in chemical graph theory

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It is shown that the formula relating the coefficients of the characteristic polynomial of a graph G to certain structural features of G (which in mathematical chemistry is traditionally referred to as the Sachs theorem) is a straightforward and relatively easily inferable corollary of an earlier result by Frank Harary.

1. Introduction

Let G be a graph on n vertices and A its adjacency matrix. Then the characteristic polynomial of G is defined as

$$\phi(G,x) = \det(xI - A)\,, \tag{1}$$

where I is the identity matrix of order n. Hence $\phi(G,x)$ is a polynomial of degree n in the variable x, and can be written in the form

$$\phi(G,x) = \sum_{h=0}^{n} a_h x^{n-h}\,. \tag{2}$$

The knowledge of the dependence of the coefficients a_h of the characteristic polynomial on the structure of G is of paramount importance in chemical graph theory. The precise form of this dependence is known. The most frequently repeated version of this result is that which follows Sachs [1].

By K_2 we denote the graph consisting of two vertices connected by an edge. A *cycle* is a connected graph whose all vertices are of degree 2. A graph whose all components are cycles and/or K_2-graphs is called a *basic figure*. The numbers of components and circuits in a basic figure B are denoted by $k(B)$ and $c(B)$, respectively. Then the famous coefficient-theorem can be formulated as follows:

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THEOREM 1

For $h = 0, a_h = 1$. For $h \geqslant 1$,

$$a_h = \sum_B (-1)^{k(B)} 2^{c(B)}$$

with the summation ranging over all basic figures that possess exactly h vertices, and that are as subgraphs contained in the graph G.

2. Some historical remarks

Among mathematical chemists the result states above as theorem 1 is commonly known under the name "Sachs Theorem". Indeed, this is just the "Koeffizientsatz" reported by Sachs in 1963 [1]. The chemical community was unaware of it until 1972, when the members of the Zagreb group published a "chemist-friendly" version of it [2], followed by numerous chemical applications; for an early review see [3]. The Zagreb group learned about the coefficient-theorem from Dragoš Cvetković, a mathematician from Belgrade, and, in particular, from this Ph.D. thesis [4]. (In the 1970s such a cooperation was still feasible.)

The name "Sachs Theorem" is found for the first time in ref. [2]. Together with the name "Sachs graph" for what Sachs called a basic figure (Grundfigur), this terminology became a part of the traditional folklore of mathematical chemistry. Of the many reviews and monographs in which the Sachs theorem is outlined and its chemical usages discussed, we mention just a few [3,5–11].

One year before Sachs' article [1] appeared, Harary published a paper on the determinant of the adjacency matrix of a graph [12], in which he elaborated certain ideas from an earlier work [13]. This "determinant-theorem" was eventually included in Harary's seminal textbook [14] as well as in a later monograph [15] and is thus widely known. Using the notation and terminology from the previous section, the determinant-theorem reads as follows:

THEOREM 2

$$\det A = \sum_B (-1)^{e(B)} 2^{c(B)},$$

where $e(B)$ is the number of components of B having even number of vertices, and where the summation goes over all basic figures with n vertices that are as subgraphs contained in the graph G.

In 1963, Sachs knew of Harary's paper [12]. He quoted it in [1], immediately after stating the "Koeffizientsatz", but without indicating that this paper may be of any particular relevance for the "Koeffizientsatz".

In practically all mathematico-chemical writings dealing with the "Sachs Theorem", Harary's result on the determinant is either completely ignored (e.g. in [8]) or mentioned only superficially (e.g. in [7]).

The aim of this paper is to demonstrate that theorem 1 can be relatively easily deduced from theorem 2.

3. Theorem 1 follows from theorem 2

The main reason why the statement given in the title of this section was not immediately recognized seems to lie in the fact that Harary preferred to consider graphs without loops (or, in his terminology [12]: "ordinary graphs which correspond to an irreflexive symmetric relation"). He, however, continues with the remark that "the extension to arbitrary relations, which are not necessarily irreflexive, is straightforward". In other words, Harary hints that his theorem 2 can be straightforwardly extended to embrace graphs with (weighted) loops.

This can be done as follows.

Let B be a graph whose components are cycles and/or K_2-graphs and/or isolated vertices possessing loops. Then instead of theorem 2 we have

THEOREM 2a

$$\det A = \sum_B (-1)^{e(B)} 2^{c(B)} w(B)\,,$$

where $w(B)$ is the product of the loop-weights of B.

If we rewrite eq. (1) as

$$\phi(G,x) = (-1)^n \det(A - xI)\,,$$

then the matrix $A - xI$ can be understood as the adjacency matrix of a graph where every vertex has a loop of weight $-x$. Applying theorem 2a we then readily arrive at

$$\phi(G,x) = (-1)^n \sum_B (-1)^{e(B)} 2^{c(B)} (-x)^{l(B)}\,, \tag{3}$$

where $l(B)$ stands for the number of loops in the basic figure B.

Evidently, if B possesses l loops then its remaining $n - l$ vertices belong either to cycles or to K_2-graphs. It is also clear that l may assume any value between 0 and n. Collecting those basic figures that contain a fixed number of loops, say $n - h$, we can write the right-hand side of (3) as

$$\phi(G,x) = (-1)^n \sum_{h=0}^{n} \left[\sum_B (-1)^{e(B)} 2^{c(B)} \right] (-1)^{n-h} x^{n-h}\,, \tag{4}$$

where the second summation embraces only those basic figures that have n vertices and exactly $n - h$ loops. Because the loops do not influence the values of the parameters $e(B)$ and $c(B)$, the second summation in (4) can also be conceived as going over the basic figures that possess h vertices and no loops.

Comparing eqs. (2) and (4) we see that

$$a_h = (-1)^h \sum_B (-1)^{e(B)} 2^{c(B)}$$

and that theorem 1 will result provided the terms $h + e(B)$ and $k(B)$ have equal parities for all basic figures B. To see this denote by n_j the number of components of B having j vertices. Then

$$h = \sum_j j n_j = \sum_j 2j n_{2j} + \sum_j (2j+1) n_{2j+1} ,$$

$$k(B) = \sum_j n_j = \sum_j n_{2j} + \sum_j n_{2j+1} ,$$

$$e(B) = \sum_j n_{2j} .$$

Consequently,

$$h + e(B) - k(B) = 2\sum_j j n_{2j} + 2\sum_j j n_{2j+1} ,$$

i.e. the difference between $h + e(B)$ and $k(B)$ is always an even number. Consequently,

$$(-1)^{h+e(B)} = (-1)^{k(B)} ,$$

implying the validity of theorem 1.

4. Discussion

As shown in the previous section it is a not-too-difficult task to deduce the "Sachs Theorem" from Harary's determinant-formula. The reasons why so few have realized this and why so little credit has been given to the actual inventor of the result, are not easy to fully understand. Those who knew were not motivated enough to publicize this "straightforward", yet for chemical graph theory so important a connection. Those who knew less did not read carefully enough either [1] or [12]. The majority has just overtaken from [2] and the later publications both the coefficient-theorem and its putative name.

Although much delayed, but hopefully not too late, this scientific injustice should be corrected. Because Harary did not, whereas Sachs did formulate an explicit and ready-to-use coefficient-theorem, one could, maybe, call it the "Harary–Sachs Theorem".

5. Bibliographic notes

(a) The seeds of the determinant-theorem are found in [13]: F. Harary, *A graph theoretic method for the complete reduction of a matrix with a view toward finding its eigenvalues*, J. Math. Phys. 38 (1959) 104–111. [Note that J. Math. Phys. is the "Journal of Mathematics and Physics" and not the "Journal of Mathematical Physics".]

(b) The determinant-theorem is stated and proved in [12]: F. Harary, *The determinant of the adjacency matrix of a graph*, SIAM Rev. 4 (1962) 202–210. As a curiosity it should be mentioned that in this paper the author conjectures that 16 is the smallest number of vertices for which two graphs can be isospectral. He also says that "by exhaustive methods it has been verified" that there are not isospectral graphs with up to 6 vertices. In reality, the smallest isospectral graphs are $C_4 \cup K_1$ and $K_{1,4}$, having 5 vertices each.

(c) The coefficient-theorem is stated, proved and discussed in detail in [1]: H. Sachs, *Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem charakterischen Polynom*, Publ. Math (Debrecen) 11 (1963) 119–134. Harary's previous work is mentioned only in a footnote that says nothing more than that "the determinant of the adjacency matrix was investigated by Harary".

(d) The terms "Sachs Theorem" and "Sachs graph" were put forward in [2]: A. Graovac, I. Gutman, N. Trinajstić and T. Živković, *Graph theory and molecular orbitals. Application of the Sachs theorem*, Theor. Chim. Acta 26 (1972) 67–78. Harary's paper was not quoted. Sachs' paper was quoted with an unintentional printing error. The same misquotation was then repeated by numerous other authors who referred to the Sachs theorem.

(e) Since 1962/63 the coefficient-theorem was rediscovered many times. A detailed account of this issue and bibliographic details can be found in [16].

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[14] F. Harary, *Graph Theory* (Addison-Wesley, Reading, 1969) theorems 13.2 and 13.2a.
[15] F. Buckley and F. Harary, *Distance in Graphs* (Addison-Wesley, Reading, 1990) theorem 6.2.
[16] D. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs – Theory and Application* (Academic Press, New York, 1980) p. 36.