OPEN PROBLEMS IN MATHEMATICAL CHEMISTRY

A PROPERTY OF THE CIRCUIT CHARACTERISTIC POLYNOMIAL

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Denote by G a (molecular) graph and by C a circuit contained in G. Then $G-C$ is the subgraph obtained by deleting the vertices of C from G. The matching polynomial (also called reference or acyclic polynomial) of G is defined as [1]:

$$\alpha(G)=\sum_k(-1)^k m(G,k)x^{n-2k}, \tag{1}$$

where n stands for the number of vertices of G and $m(G,k)$ is the number of k-matchings of G. (Recall that a k-matching is a collection of k mutually non-touching edges [1].)

It was established some time ago [1] that all the zeros of the matching polynomial of any graph are real-valued numbers. In 1977, Aihara [2] introduced a local resonance energy associated with the circuit C of the molecular graph G as

$$CE=\sum_{i=1}^{n} g_i(y_i-x_i), \tag{2}$$

where x_i, $i=1,2,\ldots,n$ are the zeros of the matching polynomial $\alpha(G)$, whereas y_i, $i=1,2,\ldots n$ are the zeros of the so-called circuit characteristic polynomial $\beta(G,C)$,

$$\beta(G,C)=\alpha(G)\pm 2\alpha(G-C). \tag{3}$$

The minus sign in eq. (3) is used in the case of a Hückel-type circuit and the plus sign for a Möbius-type circuit [3]. In formula (2), g_i denotes the occupation number of the ith π-molecular orbital of the respective conjugated system.

Note: Solutions to this and other problems published in this series should be addressed to Professor P.G. Mezey. It is anticipated that valid solutions to problems appearing in our series will be published in future issues of the Journal of Mathematical Chemistry.

For the success of Aihara's circuit resonance energy defined via eq. (2), it is essential that the zeros of the polynomial $\beta(G, C)$ are real-valued numbers. Already at this time, Aihara [2] mentioned that the numbers y_i were real, but gave no argument to support his claim. In the meantime, we examined a large number (several hundreds) of molecular graphs and found not one single case in which $\beta(G, C)$ would have a complex-valued zero. Therefore, we wish to formulate the following conjecture.

CONJECTURE

For any circuit C contained in any graph G, all the zeros of the circuit characteristic polynomial $\beta(G, C)$, eq. (3), are real-valued numbers.

At present, we are unable to prove the above statement, but we know a few partial results:

(1) If no edge of G belongs to more than one circuit, then all the zeros of $\beta(G, C)$ are real [4]. This case, of course, includes monocyclic graphs.

(2) If G is a bicyclic graph, then for all C the zeros of $\beta(G, C)$ are real [4].

(3) If G is a cyclic graph in which the size of the maximum matching is 2 (see fig. 1), then for all C the zeros of $\beta(G, C)$ are real

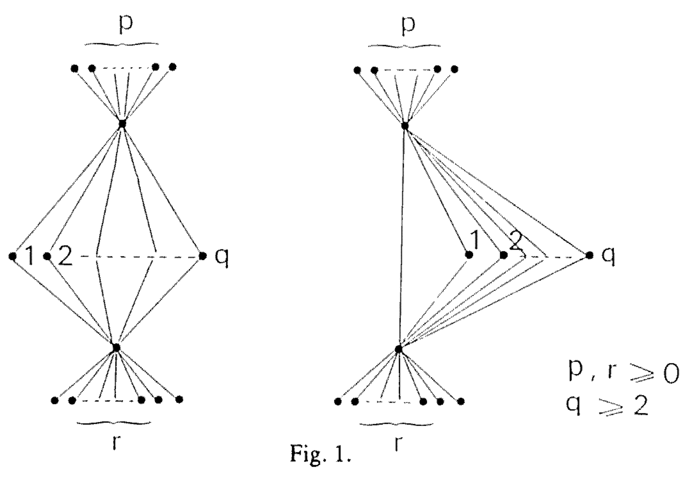

Fig. 1.

The person who first proves (or disproves) our conjecture is invited to a dinner. He or she can claim this prize from I.G. in Yugoslavia.

References

[1] For details of the theory of matching polynomials and an exhaustive bibliography, see: D. Cvetković, M. Doob, I. Gutman and A. Torgašev, *Recent Results in the Theory of Graph Spectra* (North-Holland, Amsterdam, 1988).

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[3] N. Mizoguchi, J. Phys. Chem. 92(1988)2754.

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