Topological Resonance Energy is Real

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It is proved that the zeros of the matching polynomial of a graph are real. Hence, topological resonance energy is also a real quantity.

In two recent papers Aihara [1] and independently Gutman et al. [2] discovered an algebraic approach to the Dewar resonance energy, based on purely topological considerations. The new "topological resonance energy" TRE was defined as [1, 2]

$$\mathrm{TRE} = \sum_{i=1}^{n} g_i (e_i - x_i) ,$$

where e_i is a zero of the characteristic polynomial of the molecular graph, x_i is a zero of the matching polynomial and g_i is the occupation number of the i-th molecular orbital.

TRE was successively used for predicting the stability and reactivity of conjugated molecules in both ground [3] and excited state [4]. Attempts to apply TRE to boron compounds were also reported [5].

The crucial concept in the new theory is the matching polynomial $\alpha(G)$ defined as

$$\alpha(G) = \alpha(G, x) = \sum_{k=0}^{[n/2]} (-1)^k p(G, k) x^{n-2k}, \quad (1)$$

where n is the number of vertices of the molecular graph G and $p(G, k)$ is the number of selections of k independent edges in G. In [1] $\alpha(G)$ was called the "reference polynomial" while in [2] the name "acyclic polynomial" was proposed. The name "matching polynomial" is, however, more appropriate since in standard graph theoretical terminology $p(G, k)$ is just the number of matchings of $2k$ vertices in the graph G [6, 7].

The numbers e_i are real because they are eigenvalues of the adjacency matrix of the molecular graph (which is a symmetric real matrix). The numbers g_i are, of course, real since $g_i = 0$ or 1 or 2. However, the theory developed in [1–5] gave no guarantee that the x_i's will also be real numbers. The matching polynomial is defined by means of purely combinatorial terms and there is no *a priori* reason to expect that its zeros will be real.

On the other hand it is clear that the question of the reality of the zeros of $\alpha(G)$ is of utmost importance for the theory of TRE. If in certain cases TRE would be a complex number, then its interpretation would be obscure and the whole theory would lose its significance for chemistry.

In the present work we resolve this difficulty by proving the following result. Let G be an arbitrary graph and v its arbitrary vertex. Then $G - v$ is the subgraph obtained by deletion of v from G.

Theorem

The zeros of $\alpha(G)$ are real. Moreover, the zeros of $\alpha(G-v)$ interlace the zeros of $\alpha(G)$, i.e. between any two zeros of $\alpha(G)$ there is a zero of $\alpha(G-v)$.

This theorem immediately implies that TRE is real.

Proof will be given by total induction on the number n of vertices. It can be easily checked that our theorem holds for all graphs with $n = 1, 2, 3$ and 4 vertices.

In the following we shall assume that the theorem is true for all graphs with less than n vertices and show that then it holds also for graphs with n vertices.

Let the vertex v of G be adjacent to the vertices $w_1, w_2, \ldots, w_d$. Then among the $p(G, k)$ selections of k independent edges in G there are $p(G - v - w_j, k - 1)$ selections which contain the edge incident to v and w_j, and $p(G - v, k)$ selections which do not contain any edge incident to v. Hence

$$p(G, k) = p(G - v, k) + \sum_{j=1}^{d} p(G - v - w_j, k - 1).$$

Substitution of this identity back into (1) yields

$$\alpha(G) = x\,\alpha(G - v) - \sum_{j=1}^{d} \alpha(G - v - w_j) . \quad (2)$$

$G - v$ is a graph with $n - 1$ vertices while the subgraphs $G - v - w_j$ possess $n - 2$ vertices. Then according to our hypothesis, the zeros of $\alpha(G - v - w_j)$ interlace the zeros of $\alpha(G - v)$ for all $j = 1, 2, \ldots, d$.

It is evident from Eq. (2) that if y is a zero of both $\alpha(G - v)$ and $\alpha(G - v - w_j)$ $(j = 1, 2, \ldots, d)$,

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then it is also a zero of $\alpha(G)$. Let the polynomial $D(x)$ of degree $n-h$ be the greatest common divisor of $\alpha(G)$, $\alpha(G-v)$ and $\alpha(G-v-w_j)$ ($j = 1, 2, \ldots, d$). Let further

$$\alpha(G) = D(x)\,\beta(G)\,,$$
$$\alpha(G-v) = D(x)\,\beta(G-v) \quad \text{and}$$
$$\alpha(G-v-w_j) = D(x)\,\beta(G-v-w_j)\,.$$

According to our hypothesis the zeros of $D(x)$ are real. Therefore it remains to be proved that the h zeros of $\beta(G)$ are also real. We shall verify this by showing that the values of $\beta(G)$ change sign h times in the interval $(-\infty, +\infty)$.

Dividing Eq. (2) by $D(x)$ we obtain

$$\beta(G) = x\,\beta(G-v) - \sum_{j=1}^{d} \beta(G-v-w_j)\,. \tag{3}$$

The zeros of $\beta(G-v-w_j)$ interlace the zeros of $\beta(G-v)$. Therefore $\beta(G-v)$ must possess only distinct zeros. Let the zeros of $\beta(G-v)$ be

$$y_1 < y_2 < \cdots < y_{h-1}\,.$$

Two cases have to be distinguished, namely h is either even or odd. We shall consider here only the case when h is even. If the opposite is true, then the proof is analogous, but has to be changed accordingly.

For even h, $\beta(G, x) > 0$ and $\beta(G-v-w_j, x) > 0$ if $x \to \pm\infty$. Since the zeros of $\beta(G-v-w_j)$ lie between the zeros of $\beta(G-v)$, we deduce that for all $j = 1, 2, \ldots, d$,

$$\beta(G-v-w_j, y_1) \geqq 0\,,$$
$$\beta(G-v-w_j, y_2) \leqq 0, \ldots, \beta(G-v-w_j, y_{h-1}) \geqq 0\,.$$

Consequently,

$$\sum_{j=1}^{d} \beta(G-v-w_j, y_i) > 0 \quad \text{for} \quad i = 1, 3, \ldots, h-1$$

and

$$\sum_{j=1}^{d} \beta(G-v-w_j, y_i) < 0 \quad \text{for} \quad i = 2, 4, \ldots, h-2\,.$$

(The above sums must be different from zero since in the opposite case y_i would be a zero of all $\beta(G-v-w_j)$'s and therefore also a zero of $\beta(G)$.)

Finally, from (3) we conclude that

$$\beta(G, -\infty) > 0\,, \quad \beta(G, y_1) < 0\,,$$
$$\beta(G, y_2) > 0, \ldots, \beta(G, y_{h-1}) < 0\,,$$
$$\beta(G, +\infty) > 0$$

i.e. $\beta(G, x)$ changes sign h times in the interval $(-\infty, +\infty)$.

Hence $\beta(G)$ has h real zeros and $\alpha(G)$ has n real zeros. The zeros of $\beta(G-v)$ lie between the zeros of $\beta(G)$. This completes the proof of the theorem.

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