Iranian Journal of Mathematical Chemistry, Vol. 6, No. 2, October 2015, pp. 185 – 187 **IJMC**

Open problems for equienergetic graphs

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Received 31 May 2015; Accepted 15 June 2015

ACADEMIC EDITOR: ALI REZA ASHRAFI

ABSTRACT The energy of a graph is equal to the sum of the absolute values of its eigenvalues. Two graphs of the same order are said to be equienergetic if their energies are equal. We point out the following two open problems for equienergetic graphs. **(1)** Although it is known that there are numerous pairs of equienergetic, non-cospectral trees, it is not known how to systematically construct any such pair. **(2)** If by numerical calculation one finds that two non-cospectral graphs seem to be equienergetic, in the general case no method is known for proving that this indeed is the case.

KEYWORDS graph energy • equienergetic graphs • spectrum (of graph).

Let G be a (molecular) graph of order n, and let its eigenvalues be $\lambda_1, \lambda_2, \ldots, \lambda_n$, forming the spectrum of G. The energy of the graph G is defined as

$$E = E(G) = \sum_{i=1}^{n} | \lambda_i | .$$

This quantity has applications in chemistry [1]. Its mathematical theory is nowadays well elaborated [2], but some open problems still exist. In what follows we point out two of these.

Two graphs G_a and G_b of the same order are said to be *equienergetic* if $E(G_a) = E(G_b)$. Evidently, two cospectral graphs are equienergetic, but there also exist non-cospectral equienergetic graphs. In fact, there are very many such graphs, the simplest being C_4 (with spectrum $\{2,0,0,-2\}$), $K_2 \cup K_2$ (with spectrum $\{1,1,-1,-1\}$), and $K_3 \cup K_1$ (with spectrum $\{2,0,-1,-1\}$), all three having $n=4$ and $E=4$. An example of non-cospectral equienergetic trees is the pair T_1, T_2, the molecular graphs of 3-methyloctane and 3,3-diethylpentane (both with $n=9$) [3].

Several systematic constructions of families of non-cospectral equienergetic cycle-containing graphs have been described [2]. Computer-aided studies reveal that also among trees there are numerous non-cospectral equienergetic species [3,4]. Thus, it is easy to **find** pairs of non-cospectral equienergetic trees. On the other hand, no progress has been achieved in solving the apparently similar task:

(1) ***Construct*** *at a pair of non-cospectral equienergetic trees.*

If by numerical calculation one finds that two non-cospectral graphs G_a, G_b seem to be equienergetic (i.e., that their energies agree on, say, 20 decimal places), it still remains to demonstrate that the equality $E(G_a) = E(G_b)$ holds in a mathematically exact manner.

In the case of the trees T_1, T_2 this demonstration can be done as follows [3]. By standard and mathematically exact calculation, one finds that the characteristic polynomials of T_1 and T_2 are $\lambda^9 - 8\lambda^7 + 20\lambda^5 - 17\lambda^3 + 4\lambda$ and $\lambda^9 - 8\lambda^7 + 18\lambda^5 - 16\lambda^3 + 5\lambda$, respectively. Since $\lambda^9 - 8\lambda^7 + 20\lambda^5 - 17\lambda^3 + 4\lambda = \lambda(\lambda^2-1)(\lambda^2-4)(\lambda^4-3\lambda^2+1)$ and $\lambda^9 - 8\lambda^7 + 18\lambda^5 - 16\lambda^3 + 5\lambda = \lambda(\lambda^2-1)^3(\lambda^2-5)$, explicit algebraic expressions exists for all eigenvalues of T_1 and T_2. Then by a straightforward calculation one verifies that both $E(T_1)$ and $E(T_2)$ are equal to $6+2\sqrt{5}$.

Such a verification of equienergeticity cannot be employed in the general case, because the roots of the vast majority of characteristic polynomials cannot be explicitly expressed in radicals. However, until now no other method has been proposed. Therefore, another open problem in the theory of graph energy is:

(2) *Design a general method for proving that two graphs are equienergetic.*

In the present author's opinion, the solutions of the open problems **(1)** & **(2)** may require developments of new proof techniques in spectral graph theory.

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