Energy of a graph is never an odd integer

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Abstract

It is shown that if the energy of a graph is rational then it must be an even integer.

We consider simple graphs, that is, graphs which do not contain loops or parallel edges. Let G be a graph with n vertices. Let A be the adjacency matrix of G. Recall that A is an $n \times n$ matrix with its rows and columns being indexed by the vertices of G. The (i, j)-entry of A is 1 if the i-th and the j-th vertices of G are adjacent and it is zero otherwise. Thus A is a symmetric $0-1$ matrix with zeros along the diagonal.

An interesting quantity in Hückel theory is the sum of the energies of all the electrons in a molecule, the so-called total π-electron energy E_π. For a molecule with $n = 2k$ atoms, the total π-electron energy can be shown to be $E_\pi = 2\sum_{i=1}^{k} \lambda_i$ where $\lambda_i, i = 1, 2, \ldots, k$, are the top k eigenvalues of the adjacency matrix of the graph of the molecule. For a bipartite graph, because of the symmetry of the spectrum, we can write $E_\pi = \sum_{i=1}^{n} |\lambda_i|$, and this has motivated the following definition. For any (not necessarily bipartite) graph G, the *energy* of the graph is defined as $\sum_{i=1}^{n} |\lambda_i|$ where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. For additional information and background on the energy of graphs we refer to ([1],[4],[5]) and the references contained therein.

Characterizing the set of positive numbers which can occur as energy of a graph has been a problem of interest. In this connection, Professor S. B. Rao has asked whether the energy of a graph can ever be an odd integer [6]. In this note we prove that the energy can never be an odd integer. In fact we show that if the energy is rational then it must be an even integer.

The proof is based on the concept of the *additive compound* introduced by Fiedler ([2],[3]).

Let B be an $n \times n$ matrix and let $1 \leq k \leq n$ be an integer. The k-th additive compound $\mathcal{A}_k(B)$ is a matrix of order $\binom{n}{k} \times \binom{n}{k}$ defined as follows. The rows and the columns of $\mathcal{A}_k(B)$ are indexed by the k-subsets of $\{1, 2, \ldots, n\}$, arranged in an arbitrary, but fixed, order. Let S and T be subsets of $\{1, 2, \ldots, n\}$. The (S, T)-entry of $\mathcal{A}_k(B)$ is the coefficient of x in the expansion of the determinant of the submatrix of $B + xI$ indexed by the rows in S and the columns in T.

As an example, let

$$B = \begin{bmatrix} 2 & 3 & 1 \\ -1 & 0 & 2 \\ 4 & 1 & 3 \end{bmatrix}.$$

Let the 2-subsets of $\{1, 2, 3\}$ be arranged as $\{1, 2\}, \{1, 3\}, \{2, 3\}$.

The submatrix of $B + xI$, indexed by the rows and the columns in $\{1, 2\}$ is given by $\begin{bmatrix} 2+x & 3 \\ -1 & x \end{bmatrix}$. The coefficient of x in the determinant of this matrix is 2 and hence the $(1, 1)$-entry of $\mathcal{A}_2(B)$ is 2. It can be checked that the second additive compound of B is given by

$$\mathcal{A}_2(B) = \begin{bmatrix} 2 & 2 & -1 \\ 1 & 5 & 3 \\ -4 & -1 & 3 \end{bmatrix}.$$

The main result of Fiedler on additive compounds is the following. If

$\mu_1, \ldots, \mu_n$ are the eigenvalues of B, then the eigenvalues of $\mathcal{A}_k(B)$ are given by $\mu_{i_1} + \cdots + \mu_{i_k}$, for all $1 \leq i_1 < \cdots < i_k \leq n$.

Now consider the graph G with the $n \times n$ adjacency matrix A. As before, let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A. We assume that $\lambda_1, \ldots, \lambda_k$ are positive and the rest are nonpositive. Since the trace of A is zero, the energy of G is $2\sum_{i=1}^k \lambda_i$. Note that the characteristic polynomial of $\mathcal{A}_k(A)$ is a monic polynomial with integer coefficients. Also, $\sum_{i=1}^k \lambda_i$ is an eigenvalue of $\mathcal{A}_k(A)$ by the result of Fiedler mentioned above. It follows that if $\sum_{i=1}^k \lambda_i$ is rational, then it must be an integer. Thus if the energy of G is rational, then it must be an even integer.

We conclude with some remarks. Clearly, the technique of the paper yields the more general result that if A is an $n \times n$ symmetric matrix with integer entries then the sum of the moduli of the eigenvalues of A cannot be an odd integer. This was also conjectured by Professor S. B. Rao in a personal communication. It may also be remarked that every positive even integer is the energy of a graph. In fact the energy of the complete bipartite graph K_{1,p^2} is $2p$.

References

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