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A lower bound for the energy of symmetric matrices and graphs

Enide Andrade [a,*], María Robbiano [b], B. San Martín [b]

[a] *CIDMA-Center for Research and Development in Mathematics and Applications, Departamento de Matemática, Universidade de Aveiro, 3810-193, Aveiro, Portugal*
[b] *Departamento de Matemáticas, Universidad Católica del Norte, Av. Angamos 0610, Antofagasta, Chile*

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ABSTRACT

The energy of a symmetric matrix is the sum of the absolute values of its eigenvalues. We introduce a lower bound for the energy of a symmetric matrix partitioned into blocks. This bound is related to the spectrum of its quotient matrix. Furthermore, we study necessary conditions for the equality. Applications to the energy of the generalized composition of a family of arbitrary graphs are obtained. A lower bound for the energy of a graph with a bridge is given. Some computational experiments are presented in order to show that, in some cases, the obtained lower bound is incomparable with the well known lower bound $2\sqrt{m}$, where m is the number of edges of the graph.

1. Motivation and main goal

In this work we deal with an (n, m)-graph G which is an undirected simple graph with a vertex set $\mathcal{V}(G)$ of cardinality n and an edge set $\mathcal{E}(G)$ of cardinality m. The concept of

* Corresponding author.
E-mail address: enide@ua.pt (E. Andrade).

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energy of graphs appeared in Mathematical Chemistry and we review in this section its importance. In Chemistry *Molecular graphs* represent the structure of molecules. They are generated, in general, by the following rule: vertices stand for atoms and edges for bonds. A *matching* N in a graph G is a nonempty set of edges such that no two have a vertex in common. A *perfect matching* is a matching whose set of vertices (set of end vertices of the edges forming the matching) coincides with the set of vertices of G. There are two basic types of molecular graphs: those representing *saturated hydrocarbons* and those representing *conjugated π-electron systems*. In the second class, the molecular graph should have perfect matchings (called "Kekulé structure"). In the 1930s, Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called *conjugated hydrocarbons* (conjugated π-electron systems) which have a system of connected π-orbitals with *delocalized* π-electrons (electrons in a molecule that are not associated with a single atom or a covalent bond). Thus, the HMO (Hückel molecular orbital model) enables to describe approximately the behavior of the so-called π-electrons in a conjugated molecule, especially in conjugated hydrocarbons. For more details see [12] and the references therein. As usual we denote the adjacency matrix of G by $A(G)$. The eigenvalues of G are the eigenvalues of this matrix.

Following to HMO theory, the total π-electron energy, E_π, is a quantum-chemical characteristic of conjugated molecules that agrees with their thermodynamic properties. For conjugated hydrocarbons in their ground electronic states, E_π is calculated from the eigenvalues of the adjacency matrix of the molecular graph:

$$E_\pi = n\alpha + E\beta,$$

where n is the number of carbon atoms, α and β are the HMO carbon-atom coulomb and carbon–carbon resonance integrals, respectively. For the majority of conjugated π-electron systems

$$E = \sum_{i=1}^{n} |\lambda_i|\,, \tag{1}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the underlying molecular graph. For molecular structure researches, E is a very interesting quantity. In fact, it is traditional to consider E as the total π-electron energy expressed in β-units. The spectral invariant defined by (1) is called the *energy* of the graph G (see [9]). It is worth mentioning that in the contemporary literature, a plethora of upper bounds for this invariant has been reported. On the other hand, lower bounds for energy are much fewer in number, probably because these are much more difficult to deduce. For these (recently determined) lower bounds, the reader should be referred to [1,3,11,13,16].

Let $M = (M_{ij})$ be a partitioned matrix, we say that M has a symmetric partitioning if $M_{ij} = (M_{ji})^t$, for all $1 \leq i, j \leq k$. Note that a matrix with a symmetric partitioning is symmetric. The *energy of a symmetric matrix* is defined as the sum of the absolute values of its eigenvalues, see [14,15].