What is the meaning of the graph energy after all?

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Abstract

For a simple graph \( G = (V, E) \) with eigenvalues of the adjacency matrix \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \), the energy of the graph is defined by \( E(G) = \sum_{j=1}^{n} |\lambda_j| \). Myriads of papers have been published in the mathematical and chemistry literature about properties of this graph invariant due to its connection with the energy of (bipartite) conjugated molecules. However, a structural interpretation of this concept in terms of the contributions of even and odd walks, and consequently on the contribution of subgraphs, is not yet known. Here, we find such interpretation and prove that the (adjacency) energy of any graph (bipartite or not) is a weighted sum of the traces of even powers of the adjacency matrix. We then use such result to find bounds for the energy in terms of subgraphs contributing to it. The new bounds are studied for some specific simple graphs, such as cycles and fullerenes. We observe that including contributions from subgraphs of sizes not bigger than 6 improves some of the best known bounds for the energy, and more importantly gives insights about the contributions of specific subgraphs to the energy of these graphs.

Keywords: graph energy, graph spectra, matrix functions, conjugated molecules.

1. Introduction

The concept of graph energy arose in the context of the study of conjugated hydrocarbons using a tight-binding method known in chemistry as the Hückel molecular orbital (HMO) method (see for instance [1,2]). In this context, the total energy of a conjugated molecule \( M \) is defined by

\[
E(M) = 2 \sum_{j: \lambda_j > 0} \lambda_j = \sum_{j=1}^{n} |\lambda_j|,
\]

where the last equality is a consequence of the fact that such conjugated molecules can be represented by bipartite graphs, thus the spectra of their adjacency matrices are symmetric. Here, \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) are the eigenvalues of
the adjacency matrix of the (molecular) graph—typically a simple, connected, undirected graph. It should be remarked that such energy is given in units of a parameter known as $\beta$ which has a negative value.

This concept was then generalized to any graph—not necessarily bipartite—by Ivan Gutman, who named it the graph energy $[4]$. Then, for a simple, undirected graph $G = (V,E)$, the energy is defined as

$$E(G) = \sum_{j=1}^{n} |\lambda_j|.$$  

(2)

A myriad of papers and a couple of monographs have been written about the graph energy $[5, 6, 8]$. The monograph $[8]$ is an excellent compilation of results, historical background and methodological approaches that may serve as a guide to the reader who wants to get deeper into this field. The concept has been generalized to other matrices apart from the adjacency one $[10]$ (see also the corresponding Chapters of the monographs $[4, 8]$), and many bounds and extremal properties have been reported for these graph/matrix energies. Many researchers claim in their papers that they are studying the graph energy because of the chemical implications of that quantity. As soon as this concept is extended to non-bipartite graphs, however, it completely loses all its chemical and physical meaning. Nevertheless, as a graph invariant, the graph energy can bring important structural information about the graph. But, the problem is to know what exactly the graph energy means in terms of the structure of a graph. Thus, after nearly 40 years of research on graph energy, what is it after all?

Here we provide a structural interpretation of the graph energy using the concept of matrix function (see next Section for formal definitions). In particular, we prove that the graph energy is given by the sum of the traces of the even powers of the adjacency matrix weighted in a specific way. Using this new representation we find new bounds for the energy as sums of contributions of subgraphs. Consequently, armed with this structural interpretation the graph energy can now be used in the general context of structural graph theory or even to study some real-world graphs.

2. Preliminaries

We consider here simple, undirected, connected graphs $G = (V,E)$, without multiple edges or self-loops. The adjacency matrix $A$ of $G$ is then a square, symmetric matrix with spectral decomposition $A = V \Lambda V^T$, where

$$V = \begin{bmatrix} \vec{\psi}_1 & \ldots & \vec{\psi}_n \end{bmatrix}$$

is the matrix of orthonormalized eigenvectors $\vec{\psi}_j$ associated with the eigenvalues $\lambda_j$, and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$. If $f$ is a scalar function defined on the spectrum of $A$ we can define a function of the matrix $A$, $f(A)$, by means of

$$f(A) = V f(\Lambda) V^T.$$  

(3)
where \( f(\Lambda) = \text{diag}(f(\lambda_1), \ldots, f(\lambda_n)) \). For example, for any symmetric positive semidefinite matrix \( A \) we can define its (positive semidefinite) square root by means of \( S = \sqrt{A} = V\sqrt{\Lambda}V^T \). This is the only symmetric positive semidefinite matrix with the property that \( S^2 = A \).

We observe that if \( f \) is defined by a power series expansion of the form

\[
f(x) = \sum_{k=0}^{\infty} a_k x^k
\]

such that the series converges on an open disk containing the \( \lambda_j \), then the above definition is equivalent to

\[
f(A) = \sum_{k=0}^{\infty} a_k A^k.
\]

(4)

For further information on matrix functions, the reader is referred to [7].

3. Main result

The main result of this work is the finding that the (adjacency) graph energy of any graph can be obtained as a weighted sum of even powers of the adjacency matrix. First, we observe that

\[
E(G) = \text{tr} |A|,
\]

(5)

where \( |A| = V |A| V^T \) stands for the absolute value matrix function of \( A \). Then, we have the following result.

**Theorem 1.** The energy of a graph is given by

\[
E(G) = \lambda_1 \text{tr} \sum_{k=0}^{\infty} \left( \frac{1}{k!} \right) \sum_{\ell=0}^{k} (-1)^\ell \left( \frac{k}{\ell} \right) \left( \frac{A}{\lambda_1} \right)^{2\ell}.
\]

(6)

**Proof.** We start by recalling that every symmetric positive semidefinite matrix has a unique positive semidefinite square root. Then, we have that

\[
|A| = \sqrt{A^2}.
\]

(7)

We now expand the square root in a power series in \( A^2 \). Let \( \lambda_1 > 0 \) be the largest eigenvalue of \( A \). We note in passing that since \( G \) is connected, \( \lambda_1 \) is simple. Then, \( \frac{A}{\lambda_1} \) has spectral radius 1, and the matrix \( B = (\lambda_1^{-1}A)^2 - I \) has all its eigenvalues in the interval \([-1, 0]\). Hence, \( B \) is positive semidefinite and has spectral radius 1. Let us write

\[
|A| = \sqrt{A^2} = \lambda_1 \sqrt{\left( \frac{A}{\lambda_1} \right)^2} = \lambda_1 \sqrt{I + \left( \frac{A}{\lambda_1} \right)^2 - I} = \lambda_1 (I + B)^{1/2}.
\]

(8)

Recall now the following special case of the binomial theorem:
\[
\sqrt{1+x} = (1+x)^{\frac{1}{2}} = \sum_{k=0}^{\infty} \left(\frac{1}{2}\right)^{\frac{k}{2}} x^k,
\]
where the series converges for all \(x \in [-1, 1]\), and
\[
\binom{\alpha}{k} := \frac{\alpha (\alpha - 1) \cdots (\alpha - k + 1)}{k!}
\]
for any real \(\alpha\) (here \(\alpha = \frac{1}{2}\)). Therefore we can write
\[
|A| = \lambda_1 \sum_{k=0}^{\infty} \left(\frac{1}{2}\right)^{\frac{k}{2}} B^k = \lambda_1 \sum_{k=0}^{\infty} \left(\frac{1}{2}\right)^{\frac{k}{2}} \left(\left(\frac{A}{\lambda_1}\right)^2 - I\right)^k,
\]
which readily gives the desired result.

If we consider the first few terms of the expansion for \(E\) we have
\[
E = \text{tr} |A| = \lambda_1 \text{tr} \left[ I + \frac{1}{2} \left(\frac{A^2}{\lambda_1^2} - I\right) - \frac{1}{2 \cdot 4} \left(\frac{A^2}{\lambda_1^2} - I\right)^2 + \frac{1 \cdot 3}{2 \cdot 4 \cdot 6} \left(\frac{A^2}{\lambda_1^2} - I\right)^3 - \cdots \right],
\]
which clearly indicates that the energy of a graph only depends on even powers of the adjacency matrix of the corresponding graph. That is,
\[
E = \text{tr} |A| = \lambda_1 \sum_{k=0}^{\infty} \frac{2k}{2^{2k} (2k-1)} \text{tr} \left(\frac{A^2}{\lambda_1^2} - I\right)^k.
\]

4. Further developments

Here we use the main result in the previous section to obtain some upper bounds for the energy of a graph. Our goal is not to give very sharp bounds but to derive some that allow us to interpret the structural meaning of the graph energy, with special emphasis on the molecular energy in the HMO method. Recall that we have set
\[
B = \left(\frac{A^2}{\lambda_1^2} - I\right),
\]
and that \(B\) is a negative semidefinite matrix (with spectrum in \([-1, 0]\)). Furthermore,
\[
B_{ii} = \left(\frac{A^2}{\lambda_1^2} - I\right)_{ii} = \frac{k_i}{\lambda_1^2} - 1,
\]
where \(k_i\) is the degree of the corresponding vertex. Clearly, these diagonal terms are all negative. We now prove the following result.

**Theorem 2.** Let \(G\) be a graph with \(n\) nodes and \(m\) edges. Then,
\[ E(G) \leq \left( \frac{\lambda_1}{2} \right) n + \left( \frac{1}{\lambda_1} \right) m. \] 

Proof. It is easy to see that
\[ E(G) \leq \lambda_1 \text{tr} I = \lambda_1 n, \]
and that
\[ E(G) = \lambda_1 \left[ \text{tr} I + \frac{1}{2} \text{tr} \left( \frac{A^2}{\lambda_1^2} - I \right) \right] = \lambda_1 n + \left( \frac{1}{\lambda_1} \right) \sum_{i=1}^{n} k_i - \left( \frac{\lambda_1}{2} \right) n. \]
The result is now an immediate consequence of (15). \qed

It can be easily verified that
\[ E(G) \leq \sqrt{2mn} \leq \left( \frac{\lambda_1}{2} \right) n + \left( \frac{1}{\lambda_1} \right) m, \]
where the first bound is the well-known McClelland one \[9\]. However, we can systematically improve the bound found above by using the same approach used for its proof, as we will show in the next two results.

**Theorem 3.** Let \( G \) be a graph with \( n \) nodes, \( m \) edges, \( P_3 \) paths of three vertices and \( C_4 \) cycles of length four. Then,
\[ E(G) \leq \left( \frac{3\lambda_1}{8} \right) n + \left( \frac{6\lambda_1^3 - 1}{4\lambda_1^2} \right) m - \left( \frac{1}{2\lambda_1^2} \right) P_3 - \left( \frac{1}{\lambda_1^4} \right) C_4. \]

Proof. It is easy to see that
\[ \text{tr} (B^2) = \text{tr} \left( \frac{A^2}{\lambda_1^2} - I \right)^2 = \frac{1}{\lambda_1} \text{tr} A^4 - \frac{2}{\lambda_1^3} \text{tr} A^2 + \text{tr} I. \]

We can now obtain the traces of \( A^4 \) and \( A^2 \) in terms of the subgraphs contributing to them. It is known (see, e.g., \[3\] page 137) that
\[ \text{tr} A^4 = 2m + 4P_3 + 8C_4, \]
and of course
\[ \text{tr} A^2 = 2m. \]
Then, by plugging these two formulas into the expression for $\frac{\lambda_1}{8} \operatorname{tr}(B^2)$ we get

$$
\frac{\lambda_1}{8} \operatorname{tr}(B^2) = \left(\frac{\lambda_1}{8}\right) n + \left(\frac{1 - 4\lambda_1^2}{4\lambda_1^3}\right) m + \left(\frac{1}{2\lambda_1^3}\right) P_3 - \left(\frac{1}{\lambda_1^3}\right) C_4.
$$

Finally, by taking

$$
E(G) \leq \left(\frac{\lambda_1}{2}\right) n + \left(\frac{1}{\lambda_1}\right) - \frac{\lambda_1}{8} \operatorname{tr}(B^2)
$$

we obtain the result.

An important feature of this bound is that it clearly agrees with the chemical intuition. For instance, it is well known that conjugated $C_4$ cycles destabilize a molecule, due to their increase in the molecular energy. We recall that the energy $E(G)$ for a molecule is given in units of $\beta$, which is negative. Thus, both terms $P_3$ and $C_4$ make contributions that increase the total energy of a molecule.

We can improve the previous bound by using a similar approach.

**Theorem 4.** Let $G$ be a graph. Then,

$$
E(G) \leq \frac{5\lambda_1}{16} n + \frac{30\lambda_1^3 - 12\lambda_1^2 + 1}{16\lambda_1^3} m - \frac{5\lambda_1^3 - 3}{4\lambda_1^3} P_3 - \frac{7\lambda_1^2 - 12}{4\lambda_1^3} C_4 \\
+ \left(\frac{3}{2\lambda_1^3}\right) C_3 + \left(\frac{3}{4\lambda_1^3}\right) P_4 + \left(\frac{3}{2\lambda_1^3}\right) S_{1,3} + \left(\frac{9}{2\lambda_1^3}\right) D_4 + \left(\frac{3}{2\lambda_1^3}\right) F \\
+ \left(\frac{3}{2\lambda_1^3}\right) H + \left(\frac{3}{2\lambda_1^3}\right) C_6.
$$

where $C_n$ and $P_n$ represent cycles and paths with $n$ vertices, $S_{1,3}$ is the star subgraph with one central vertex and 3 pendant ones, and $D_4$ is the diamond graph, i.e., a graph consisting of $C_4$ in which an edge is added to one pair of nonadjacent vertices, $F$ is a subgraph consisting of one square with a pendant node and $H$ is a subgraph consisting of two triangles sharing a common node.

**Proof.** It is easy to see that

$$
\operatorname{tr}(B^3) = \operatorname{tr}\left(\frac{A^2}{\lambda_1^3} - I\right)^3
$$

$$
= \frac{1}{\lambda_1^3}\operatorname{tr}A^6 - \frac{3}{\lambda_1^3}\operatorname{tr}A^4 + \frac{3}{\lambda_1^3}\operatorname{tr}A^2 - \operatorname{tr}I.
$$

The expression for $\operatorname{tr}A^6$ in terms of subgraphs (see [3, page 139]) is given by:

$$
\operatorname{tr}A^6 = 2m + 12P_3 + 24C_3 + 48C_4 + 12S_{1,3} + 6P_4 + 36D_4 + 12F + 24H + 12C_6.
$$
Then, by plugging these two formulas into the expression for $\frac{\lambda_1}{16} \text{tr} (B^3)$ we get

$$\frac{\lambda_1}{16} \text{tr} (B^3) = \left(\frac{1 - 6\lambda_1^2 - 6\lambda_1^4}{16\lambda_1^6}\right) m + \left(\frac{3 - 3\lambda_1^2}{4\lambda_1^4}\right) P_3 - m \left(\frac{12 - 3\lambda_1^2}{4\lambda_1^6}\right) C_4$$

$$+ \left(\frac{3}{4\lambda_1^4}\right) C_3 + \left(\frac{3}{8\lambda_1^6}\right) P_4 + \left(\frac{3}{4\lambda_1^4}\right) S_{1,3} + \left(\frac{9}{4\lambda_1^8}\right) D_4 + \left(\frac{3}{4\lambda_1^6}\right) F$$

$$+ \left(\frac{3}{2\lambda_1^4}\right) H + \left(\frac{3}{4\lambda_1^2}\right) C_6.$$

Then by taking

$$E(G) \leq m \left(\frac{3\lambda_1}{8}\right) n + \left(\frac{6\lambda_1^2 - 1}{4\lambda_1^2}\right) m - \left(\frac{1}{\lambda_1^2}\right) P_3 - \left(\frac{1}{\lambda_1^2}\right) C_4 + m \left(\frac{\lambda_1}{16}\right) \text{tr} (B^3),$$

we get the final result.

This result clearly indicates that subgraphs like $C_6$ contribute to decreasing the energy of a graph. In molecular systems this is an important result due to the well-known fact that benzenoid molecules, which are constructed on the basis of fusing together $C_6$ fragments, are very stable. However, the result shows also other fragments which contribute to the stabilization of conjugated molecular systems as the ones studied in the HMO context. This includes the fragment $P_4$ which obviously corresponds to the butadiene fragment and which is easily recognizable as a stabilizing fragment. Other fragments appear here in a more unexpected way, such as $C_3, D_4, F$ and $H$.

5. Bounding individual fragment contributions

One important consequence of the findings of this paper is that we can obtain bounds for the contribution of individual subgraphs to the total graph energy. For instance, suppose that we are interested in knowing how the subgraph $C_8$ contributes to $E(G)$. Then, we can do the following. We first identify the first spectral moment of the matrix $B$ in which $C_8$ contributes. That is, $C_8$ appears for the first time in the term $\lambda_1^2 \text{tr} A^8$ of $B^4$. Thus, let $\eta_G(C_8)$ be the contribution of the cycle of 8 nodes to the total energy of a graph $G$ and let $\eta_8(C_8)$ be the contribution of $C_8$ to the 8th spectral moment of $A$, i.e., $\eta_8(C_8) = 16$. Then,

$$\eta_G(C_8) \leq \lambda_1 \left(\frac{2 \cdot 4}{4}\right) \frac{(-1)^{4+1}}{2^{2-4}(2 \cdot 4 - 1)} \left(\frac{\eta_8(C_8)}{\lambda_1^8}\right) = -\left(\frac{5}{8\lambda_1^7}\right).$$

The negative sign indicates that an octacycle increases the energy of the graph. In the case of molecules treated under the HMO scheme, it is well known that cycles with $4n$ atoms destabilize the molecule, which is exactly the result obtained here. Of course, to improve this bound it is necessary to find the contributions of this subgraph to higher moments of the matrix $B$, but in this way it is at least possible to obtain bounds and to analyze the chemical impact of such fragments in a molecule.
6. Numerical results

In this section we show some numerical results on the different bounds obtained in this paper for simple graphs of importance in chemistry. The goal of these bound is not to obtain good approximations of the graph energy for these graphs. Indeed, the direct calculation of the energy for these graphs is easier than the calculation of the bounds. Our goal is to show how the incorporation of certain subgraphs into the bounds improves them and providing a structural interpretation of the graph energy for such graphs. In all cases we compare our bounds with the one of McClelland [9], which is simple and remarkably good in approaching the graph energy.

First we study a series of cycle graphs $C_n$ for $3 \leq n \leq 10$. In Table 1 we give the values of the energy and the results of bounding it with the three bounds obtained here as well as by McClelland’s one. As can be seen even for such simple graphs the current approach needs to incorporate terms coming from the tr$A^6$ in order to improve McClelland’s bound. In this type of graphs, a few of the subgraphs contributing to (27) are not present, e.g., $S_{1,3}$, $D_4$, $F$, $H$, and some of the others only appear in specific graphs, such as $C_3$, $C_4$, and $C_6$. Thus, the main improvement in this bound in relation to the other two comes from the better account of the contributions of $n$, $m$ and $P_3$ and the newly introduced contribution of $P_4$.

| $n$ | $E(G)$ | $\sqrt{2mn}$ | [16] | [21] | [27] |
|-----|--------|---------------|------|------|------|
| 3   | 4.000  | 4.243         | 4.5  | 4.219| 4.113|
| 4   | 4.000  | 5.657         | 6    | 5.500| 5.250|
| 5   | 6.472  | 7.071         | 7.5  | 7.031| 6.836|
| 6   | 8.000  | 8.485         | 9    | 8.438| 8.277|
| 7   | 8.988  | 9.899         | 10.5 | 9.844| 9.570|
| 8   | 9.657  | 11.314        | 12   | 11.250| 10.938|
| 9   | 11.517 | 12.728        | 13.5 | 12.656| 12.305|
| 10  | 12.944 | 14.142        | 15   | 14.062| 13.672|

Table 1. Values of the energy $E(G)$ and their estimation using McClelland’s bound $\sqrt{2mn}$ as well as the bounds obtained in this work for the cycle graphs $C_n$ with different number of nodes.

As a second example we study a series of fullerene graphs having from 20 to 540 nodes. The results are given in Table 2. Here again, it is necessary to go beyond the contribution of tr$A^4$ to make improvements over McClelland’s bound. Here the main contributions to this improvement are made by $n$, $m$, $P_3$, $P_4$, $S_{1,3}$, and $C_6$. Notice, that the contributions of $C_5$ are only captured after the consideration of tr$A^{10}$, which is not studied here. It can be then said that the energy of fullerenes is bounded by the following specific expression:

$$
\[
E(G) \leq \left(\frac{5\lambda_1}{16}\right)n + \left(\frac{30\lambda_1^4 - 12\lambda_1^2 + 1}{16\lambda_1^2}\right)m - \left(\frac{5\lambda_2^2 - 3}{4\lambda_1^2}\right)P_3 \\
+ \left(\frac{3}{4\lambda_1^2}\right)P_4 + \left(\frac{3}{2\lambda_1^2}\right)S_{1,3} + \left(\frac{3}{2\lambda_1^2}\right)C_6.
\]

(33)

7. Conclusions

The main conclusion of this work is that the graph energy is a weighted sum of the traces of even powers of the adjacency matrix. The potential advantages of this finding is that new techniques can be designed to bound the energy of graphs, in which the specific contribution of subgraphs can be obtained. This is of great importance in chemistry where the search for additive rules for molecular properties is a golden rule for understanding such properties in structural terms. Finally, we hope that the new findings reported here might allow to better understand certain properties of the graph energy in certain families of graphs.

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