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ON THE ENERGY OF REGULAR GRAPHS

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Abstract

The energy E of any n-vertex regular graph G of degree r , $r > 0$, is greater than or equal to n . Equality holds if and only if every component of G is isomorphic to the complete bipartite graph $K_{r,r}$. If G is triangle– and quadrangle–free, then $E \geq nr/\sqrt{2r-1}$. In particular, for any fullerene and nanotube with n carbon atoms, $1.34\,n \leq E \leq 1.73\,n$.

INTRODUCTION

Let G be a graph on n vertices, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues [1]. The *energy* of G is defined as [2]

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

Numerous results on graph energy are known; for details see the book [3], the recent reviews [4, 5], the recent papers [6–8], and the references cited therein. Curiously, however, almost no results concerning the energy of regular graphs were reported so far.[1]

In what follows we are concerned with regular graphs. Let G be such a graph, n the number of its vertices and r its degree (i. e., the degree of each of its vertices). Then G possesses $m = \frac{1}{2} nr$ edges. If $r = 0$, then all eigenvalues of G are equal to zero and, consequently, $E(G) = 0$. Therefore, in what follows, we assume that $r > 0$.

An upper bound for the energy of a regular graph is readily deduced from the McClelland inequality [12], i. e., from $E \leq \sqrt{2mn}$, namely:

$$E(G) \leq n \sqrt{r} \ .$$

A somewhat better upper bound is obtained by applying the Koolen–Moulton inequality [13, 14], i. e., $E \leq (2m/n) + \sqrt{(n-1)(2m - 4m^2/n^2)}$, namely:

$$E(G) \leq r + \sqrt{(n-1)(2m - r^2)} \ .$$

We now deduce a simple, yet best possible, lower bound for the energy of regular graphs, in terms of the parameters n and r.

A LOWER BOUND FOR THE ENERGY OF REGULAR GRAPHS

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the graph G, denote by M_k its k-th spectral moment,

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k$$

[1] Exceptionally, a spectral property of the iterated line graphs of regular graphs was established [9], by means of which pairs of non-cospectral equienergetic regular graphs could be constructed [9–11]. In [9] it was shown that if G is an n-vertex regular graph of degree r, $r \geq 3$, then the energy of its second iterated line graph (which is also a regular graph) depends only on the parameters n and r.

and recall [1] that $M_k(G)$ is equal to the number of self–returning walks of length k in G. In what follows we shall need the well known relation, $M_2 = 2m$, which in the case of regular graphs reduces to

$$M_2(G) = nr \tag{2}$$

as well as:

Lemma 1. *Let G be a regular graph on n vertices, of degree r , $r \geq 0$. Then*

$$M_4(G) \leq n\, r^3 \ . \tag{3}$$

Equality in (3) is attained if and only if every component of G is isomorphic to the complete bipartite graph $K_{r,r}$.

Proof. In the general case, a self–returning walk of length k, starting at some vertex v_0 goes through some vertices v_a, v_b, and v_c (in that order), and then ends at the vertex v_0. There are three types of such self–returning walks:

1: v_0, v_a, v_0, v_c, v_0, where v_a and v_c are either distinct or identical vertices;

2: v_0, v_a, v_b, v_a, v_0, where v_b is different from v_0;

3: v_0, v_a, v_b, v_c, v_0, where the four vertices v_0, v_a, v_b, v_c are mutually distinct, i. e., they form a quadrangle.

If G is a regular graph of degree r, then for a given vertex v_0 there are r^2 walks of type 1. To see this, note that it is possible to go from v_0 to one of its first neighbors (denoted by v_a) in r different ways. The next step (from v_a to v_0) is unique. The third step (from vertex v_0 to one of its first neighbors, denoted by v_c) can again be done in r different ways, whereas the fourth step (from v_c to v_0) is again unique. Therefore there are $r \times 1 \times r \times 1 = r^2$ self–returning walks of type 1.

In an analogous manner one verifies that there are $r(r-1)$ walks of type 2. This time for the first and second steps there are r and $r-1$ possibilities, respectively, whereas the third and fourth steps are unique.

The number of self–returning walks of type 3 depends both on the actual structure of the graph G and on the choice of the starting vertex v_0. It is possible to go from

v_0 to v_a in r different ways and from v_a to v_b in $r-1$ different ways. If v_0 and v_b are not adjacent, then it is possible to go from v_b to v_c also in $r-1$ different ways, which yields a total of $r \times (r-1) \times (r-1) = r(r-1)^2$ ways. If, however, v_0 and v_b are adjacent, which means that the vertices v_0, v_a, v_b form a triangle, then the number of walks v_0, v_a, v_b, v_c is smaller than $r(r-1)^2$.

Now, in order to be able to go from v_c to v_0 (thus closing a quadrangle) these two vertices need to be adjacent. Thus, whenever there is a pair of nonadjacent vertices (v_0, v_c), the number of walks of type 3 will be less than $r(r-1)^2$. In the absence of triangles, if v_0 and v_c are not adjacent, then the distance between them is 3.

Bearing the above in mind, we conclude that $r^2 + r(r-1) + r(r-1)^2$ is an upper bound for the number of self–returning walks of length 4, starting as some vertex v_0 of a regular graph of degree r. Therefore,

$$M_4(G) \leq n \left[r^2 + r(r-1) + r(r-1)^2 \right]$$

which directly leads to (3).

Equality in (3) will be attained if in the graph G there are no triangles and no two vertices are at distance greater than two. It is immediate to see that complete bipartite graphs are the only connected graphs having these properties. Of these only $K_{r,r}$ is regular od degree r. Lemma 1 follows. □

Corollary 2. *If G is same as in Lemma 1, but triangle– and quadrangle–free, then $M_4(G) = n\,[r^2 + r(r-1)]$.*

Theorem 3. *Let G be a regular graph on n vertices, of degree r , $r > 0$. Then*

$$E(G) \geq n \ . \tag{4}$$

Equality in (4) is attained if and only if every component of G is isomorphic to the complete bipartite graph $K_{r,r}$.

Proof. Our starting point is the inequality

$$E \geq \frac{(M_2)^2}{\sqrt{M_2\, M_4}} \tag{5}$$

that has been deduced in [6], used in [7], and discussed in detail in [8]. Evidently, the inequality (5) remains valid if the term M_4 is replaced by its upper bound. Using the upper bound (3) and taking into account (2), we immediately arrive at (4).

¿From Lemma 1 we see that equality in (4) may happen at most for the graphs whose all components are $K_{r,r}$. Because the only two non-zero eigenvalues of $K_{r,r}$ are r and $-r$ [1], we see that $E(K_{r,r}) = 2r$, which is just equal to the number of vertices of $K_{r,r}$.

Therefore, for the graphs whose all components are isomorphic to $K_{r,r}$ equality in (4) indeed happens. □

Corollary 4. *If G is same as in Theorem 3, but triangle– and quadrangle–free, then*

$$E(G) \geq \frac{nr}{\sqrt{2r-1}} \ .$$

A LOWER BOUND FOR THE ENERGY OF SEMIREGULAR BIPARTITE GRAPHS

Let G be a semiregular bipartite graph, consisting of n_a vertices of one color (say white), all having degree r_a, and n_b vertices of the other color (say black), all having degree r_b. Note that such graph has $\frac{1}{2}\,(n_a\,r_a + n_b\,r_b)$ edges, and therefore

$$M_2(G) = n_a\,r_a + n_b\,r_b \ .$$

By means of a reasoning fully analogous to that used in the proof of Lemma 1, we conclude that the number of self–returning walks of length 4, starting and ending at some white vertex of G is greater than or equal to $(r_a)^2 + r_a\,(r_b - 1) + r_a\,(r_b - 1)(r_a - 1)$. The same estimate for a black vertex is $(r_b)^2 + r_b\,(r_a - 1) + r_b\,(r_a - 1)(r_b - 1)$. Therefore,

$$\begin{aligned} M_4(G) &\leq n_a \left[(r_a)^2 + r_a\,(r_b - 1) + r_a\,(r_b - 1)(r_a - 1)\right] \\ &+ n_b \left[(r_b)^2 + r_b\,(r_a - 1) + r_b\,(r_a - 1)(r_b - 1)\right] \\ &= (n_a\,r_a + n_b\,r_b)\,r_a\,r_b \ . \end{aligned}$$

When the above relations for M_2 and M_4 are substituted back into (5), we arrive at:

Theorem 5. *Let G be a semiregular graph with parameters as specified above. Then*

$$E(G) \geq n_a \sqrt{\frac{r_a}{r_b}} + n_b \sqrt{\frac{r_b}{r_a}} \ . \tag{6}$$

Equality in (6) is attained if and only if every component of G is isomorphic to the complete bipartite graph K_{r_a,r_b} .

APPLICATION TO FULLERENES AND NANOTUBES

Fullerenes and nanotubes are represented by graphs that are regular of degree 3. Species of this kind usually do not contain triangles and quadrangles [15–17]. Therefore, Corollaries 2 and 4 applicable and we get:

Theorem 6. *The energy E of the molecular graph of a fullerene or a nanotube with n carbon atoms is bounded as:*

$$\frac{3}{\sqrt{5}} n < E < \sqrt{3}\, n \ . \tag{7}$$

or, what is the same, $1.34\, n \leq E \leq 1.73\, n$.

We see that the energy varies within a remarkable narrow interval, especially if one bears in mind that the bounds (7) are not the best possible.

Strictly speaking, the quantity E in formula (7) needs not necessarily coincide with the HMO total π-electron energy of the fullerenes and/or nanotubes. Namely, the quantity E, as defined via Eq. (1), coincides with the HMO total π-electron energy provided that all bonding MOs are occupied and all antibonding MOs are empty [3, 5]. Because of the presence of five-membered rings (especially in fullerenes) this condition may be, and usually is, violated, so that a few bonding MOs remain empty. Even in such cases, the difference between E and HMO total π-electron energy is insignificant, compared to the other drastic approximations committed within the HMO approach. Anyway, in our opinion the main chemical implication of Theorem 6 is that the gross part of the total π-electron energy of fullerenes and nanotubes is determined solely by their carbon–atom content and depends very little on other structural features.

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