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The energy of a graph☆

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Abstract

The energy, $E(G)$, of a simple graph G is defined to be the sum of the absolute values of the eigen values of G. If G is a k-regular graph on n vertices,then $E(G) \leqslant k + \sqrt{k(n-1)(n-k)} = B_2$ and this bound is sharp. It is shown that for each $\epsilon > 0$, there exist infinitely many n for each of which there exists a k-regular graph G of order n with $k < n - 1$ and $\frac{E(G)}{B_2} < \epsilon$. Two graphs with the same number of vertices are equienergetic if they have the same energy. We show that for any positive integer $n \geqslant 3$, there exist two equienergetic graphs of order $4n$ that are not cospectral.

AMS classification: 05C50

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1. Introduction

All graphs considered in this paper are finite, simple and undirected. For notations and terminology, see [2,5].

The energy, $E(G)$, of a graph G is defined to be the sum of the absolute values of its eigen values. Hence if $A(G)$ is the adjacency matrix of G, and $\lambda_1, \ldots, \lambda_n$ are the eigen values of $A(G)$, then $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The set $\{\lambda_1, \ldots, \lambda_n\}$ is the

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spectrum of G and denoted by Spec G. The totally disconnected graph K_n^c has zero energy while the complete graph K_n with the maximum possible number of edges (among graphs on n vertices) has energy 2(n-1). It was therefore conjectured in [7] that all graphs have energy at most 2(n-1). But then this was disproved in [10]. Graphs for which the energy is greater than 2(n-1) are called hyperenergetic graphs. If $E(G) \leqslant (2n-1)$, G is called non-hyperenergetic. Families of hyperenergetic and non-hyperenergetic graphs have been constructed in [8,10–12].

In theoretical chemistry, the π-electron energy of a conjugated carbon molecule, computed using the Hückel theory, coincides with the energy as defined here. Hence results on graph energy assume special significance.

In Section 2, we examine the nature of the energy of the graph $K_n - H$, where H is a Hamilton cycle of G. In Section 3, it is shown that there exist an infinite number of values of n for which k-regular graphs exist whose energies are arbitrarily small compared to the known sharp bound $k + \sqrt{k(n-1)(n-k)}$ for the energy of k-regular graphs on n vertices. In Section 4, the existence of equienergetic graphs not having the same spectrum is established.

2. Circulant graphs

Before proceeding to the main results, we make some observations on circulant graphs. First we give a lemma, whose proof is well-known.

Lemma 2.1. *If C is a circulant matrix of order n with first row $a_1, a_2, \ldots, a_n$, then the determinant of C is given by*

$$\det C = \prod_{0 \leqslant j \leqslant n-1} (a_1 + a_2\omega^j + a_3\omega^{2j} + \cdots + a_n\omega^{(n-1)j}),$$

whose ω is a primitive nth *root of unity.*

Let $S \subseteq \{1, 2, \ldots, n\}$ with the property that if $i \in S$, then $n - i \in S$. The graph G with vertex set $V = \{v_0, v_1, \ldots, v_{n-1}\}$ and in which v_i is adjacent to v_j iff $i - j \pmod{n} \in S$ is called a circulant graph since the adjacency matrix $A(G)$ of G is a circulant or order n with 1 in $(i+1)$th position of its first row iff $i \in S$ (and 0 in the remaining positions). Clearly G is $|S|$-regular. If $S = \{\alpha_1, \ldots, \alpha_k\} \subset \{1, 2, \ldots, n\}$, then the first row of $A(G)$ has 1 in the $\alpha_i + 1$th position, $1 \leqslant i \leqslant k$, and 0 in the remaining positions. Hence by Lemma 1, the eigen values of G are given by

$$\left\{\omega^{j\alpha_1} + \omega^{j\alpha_2} + \cdots + \omega^{j\alpha_k} : 0 \leqslant j \leqslant n-1, \omega = \text{ a primitive } n\text{th root of unity}\right\}.$$

Circulant graphs have been used in the study of graph decomposition problems [1,3].

3. Two examples

Example 3.1. Let G be the graph $K_n - H$, where $V(K_n) = \{1, 2, \ldots, n\}$ and $H = (123 \cdots n)$, a Hamilton cycle of K_n. Then $\lambda I - A(G)$ is a circulant with first row $(\lambda, 0, -1, \ldots - 1, 0)$, and hence

$$\begin{aligned}\text{Spectrum of } G = &\text{ the set of roots of } \det(\lambda I - A)\\ = &\{\omega^{2j} + \cdots + \omega^{(n-2)j} : 0 \leqslant j \leqslant n-1;\\ &\quad \omega = \text{ a primitive } n\text{th root of unity}\}\\ = &\{-1 - \omega^{j} - \omega^{(n-1)j}; 0 \leqslant j \leqslant n-1\}.\end{aligned}$$

Hence

$$E(G) = \sum_{j=0}^{n-1} |1 + \omega^{j} + \omega^{(n-1)j}| = \sum_{j=0}^{n-1} \left| 1 + 2\cos\frac{2\pi j}{n} \right|.$$

Computations show that for $4 \leqslant n \leqslant 100$, the graphs $K_n - H$ are non-hyperenergetic.

Open Problem 1

$K_n - H$ is non-hyperenergetic for $n \geqslant 4$.

Example 3.2. All subdivision graphs are non-hyperenergetic. Recall that the subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex on each edge of G.

Hence if G has n vertices and m edges, $S(G)$ has $m + n$ vertices and $2m$ edges. Now all graphs of order n with number of edges less than $2n - 2$ are non-hyperenergetic [8]. For all subdivision graphs of non-trivial graphs, we have

$$2m < 2|V(S(G))| - 2 = 2(m + n) - 2.$$

Hence all subdivision graphs are non-hyperenergetic.

4. Energy bounds

For a graph G on n vertices and having m edges, it is shown in [7] that

$$E(G) \leqslant \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} = B_1 \tag{1}$$

while if G is k-regular,

$$E(G) \leqslant k + \sqrt{k(n-1)(n-k)} = B_2. \tag{2}$$

Since $k = \frac{2m}{n}$ for a k-regular graph, the bound B_2 is an immediate consequence of the bound B_1. If $k = 3$, the upper bound $B_2 = 3 + \sqrt{2(n-1)(n-3)}$. But $B_2 \leqslant 2(n-1)$ is equivalent to $(n-4)^2 \geqslant 0$ which is true. Hence all cubic graphs are non-hyperenergetic. There are regular graphs for which the bound B_2 is attained. For example, for all complete graphs equality holds. In other words, the bounds B_1 and B_2 are both sharp. So the following question is pertinent:

Question 1. For any two positive integers n and k, $n-1 > k \geqslant 2$ and $\epsilon > 0$, does there exist a k-regular graph G with $\frac{E(G)}{B_2} > 1-\epsilon$, where $B_2 = k + \sqrt{k(n-1)(n-k)}$?

In the process of trying to tackle the above question, we have obtained the following result.

Theorem 4.1. *For each $\epsilon > 0$, there exist infinitely many n for each of which there exists a k-regular graph G of order n with $k < n-1$ and $\frac{E(G)}{B_2} < \epsilon$.*

In view of Theorem 4.1, we ask:

Open Problem 2

Given a positive integer $n \geqslant 3$, and $\epsilon > 0$, does there exist k-regular graph G of order n such that $\frac{E(G)}{B_2} > 1-\epsilon$ for some $k < (n-1)$?

Proof of Theorem 4.1. Let $\alpha_1, \alpha_2, \ldots, \alpha_k$ be the numbers less then n and prime to n so that $k = \phi(n)$ where ϕ is the Euler ϕ-function. Let G be the circulant graph of order n with $S = \{\alpha_1, \alpha_2, \ldots, \alpha_k\}$. Let $\lambda_j = \omega^{j\alpha_1} + \cdots + \omega^{j\alpha_k}$, $0 \leqslant j \leqslant n-1$, where ω is a primitive nth root of unity. Then the eigen values of G are $\lambda_1, \lambda_2, \ldots, \lambda_n$. We now want to compute $E(G) = \sum |\lambda_i|$, the energy of G. Set $Q_i = \omega^{\alpha_i}$, $1 \leqslant i \leqslant k$. Then $\lambda_j = \sum_{i=1}^{k} Q_i^j$. Now $Q_1, \ldots, Q_k$ are the roots of the cyclotomic polynomial [9].

$$\begin{aligned}\Phi_n(X) &= (X-Q_1)(X-Q_2)\cdots(X-Q_k)\\ &= X^k + a_1X^{k-1} + \cdots + a_k,\end{aligned} \tag{3}$$

where $a_1 = -\sum_{i=1}^{k} Q_i$ etc., and as is well-known, the coefficients a_i are all rational integers.

We apply Newton's method [4] to compute the eigen values λ_j. Consider

$$\begin{aligned}
&(1-Q_1y)(1-Q_2y)\cdots(1-Q_ky)\\
&\quad = 1-\left(\sum_i Q_i\right)y+\left(\sum_{i<j} Q_iQ_j\right)y^2-\cdots\\
&\quad = 1+a_1y+a_2y^2+\cdots+a_ky^k.
\end{aligned}$$

Taking logarithmic differentiation (w.r.t. y), we get

$$\sum_{i=1}^{k}\frac{-Q_i}{1-Q_iy}=\frac{a_1+2a_2y+3a_3y^2+\cdots+ka_ky^{k-1}}{1+a_1y+a_2y^2+\cdots+a_ky^k}.$$

This gives

$$\begin{aligned}
&\sum_{i=1}^{k}-Q_i\left(\sum_{j=0}^{\infty}Q_i^jy^j\right)(1+a_1y+a_2y^2+\cdots+a_ky^k)\\
&\quad = a_1+2a_2y+3a_3y^2+\cdots+ka_ky^{k-1}\\
&\quad \Rightarrow \left[\sum_{j=0}^{\infty}\left(\sum_{i=1}^{k}-Q_i^{j+1}\right)y^j\right][1+a_1y+a_2y^2+\cdots+a_ky^k]\\
&\quad = \left[\sum_{j=0}^{\infty}-\lambda_{j+1}y^j\right][1+a_1y+a_2y^2+\cdots+a_ky^k]\\
&\quad = (-\lambda_1-\lambda_2y-\lambda_3y^2-\cdots)[1+a_1y+a_2y^2+\cdots+a_ky^k]\\
&\quad = a_1+2a_2y+3a_3y^2+\cdots+ka_ky^{k-1}. \qquad (4)
\end{aligned}$$

Eq. (4) gives the following recurrence equations:

$$-\lambda_r-\lambda_{r-1}a_1-\lambda_{r-2}a_2-\cdots-\lambda_1a_{r-1}=ra_r \text{ or } 0 \qquad (5)$$

according to whether $r \leqslant k$ or $r > k$.

Hence if we know the a_i's (that is, if we know the cyclotomic polynomial $\Phi_n(X)$), then the λ_i's can be computed recursively.

We now take $n=p^r$, $r \geqslant 1$, and p, a prime. Then $k=\phi(n)=p^r-p^{r-1}$. Now the cyclotomic polynomial $\Phi_n(X)$ is given by [9]

$$\Phi_n(X)=\prod_{d|n}(X^d-1)^{\mu(n/d)} \qquad (6)$$

where μ stands for the Möbius function defined by

$$\mu(m)=\begin{cases}1 & \text{if } m=1,\\ 0 & \text{if } m \text{ contains a square greater than 1},\\ (-1)^r & \text{if } m \text{ is a product of } r \text{ distinct primes.}\end{cases}$$

Hence

$$\begin{aligned}\Phi_{p^r}(X) &= \prod_{d|n}(X^d - 1)^{\mu(p^r/d)}\\ &= (X^{p^r} - 1)^{\mu(1)}(X^{p^{r-1}} - 1)^{\mu(p)}\\ &= (X^{p^r} - 1)/(X^{p^{r-1}} - 1)\\ &= X^{(p-1)p^{r-1}} + X^{(p-2)p^{r-1}} + \cdots + X^{p^{r-1}} + 1. \end{aligned} \tag{7}$$

From (3)

$$\begin{aligned}\Phi_{p^r}(X) = {} & X^{(p-1)p^{r-1}} + a_1 X^{(p-1)p^{r-1}-1} + a_2 X^{(p-1)p^{r-1}-2}\\ & + \cdots + a_{p^{r-1}} X^{(p-2)p^{r-1}} + \cdots + a_{2p^{r-1}} X^{(p-3)p^{r-1}}\\ & + \cdots + a_{(p-2)p^{r-1}} X^{p^{r-1}} + \cdots + a_{(p-1)p^{r-1}}. \end{aligned} \tag{8}$$

(Recall that $k = \phi(p^r) = (p-1)p^{r-1}$.)

From Eqs. (7) and (8), we have

$$a_{p^{r-1}} = a_{2p^{r-1}} = \cdots = a_{(p-1)p^{r-1}} = 1$$

while the remaining a_j's are zero. These when substituted in Eq. (5) yield:

$$\lambda_1 = 0; \quad \lambda_2 = 0; \ldots; -\lambda_{p^{r-1}} - \lambda_{p^{r-1}-1}a_1 - \cdots - \lambda_1 a^{p^{r-1}-1} = p^{r-1}a_{p^{r-1}}$$

(and hence $\lambda_{p^{r-1}} = -p^{r-1}$);

$$-\lambda_{p^{r-1}+1} - \lambda_{p^{r-1}}a_1 - \lambda_{p^{r-1}-1}a_2 \cdots - \lambda_1 a^{p^{r-1}} = (p^{r-1}+1)a_{p^{r-1}+1}$$

(and hence $\lambda_{p^{r-1}+1} = 0$); ...;

$$-\lambda_{2p^{r-1}} - \lambda_{2p^{r-1}-1}a_1 - \cdots - \lambda_{p^{r-1}}a_{p^{r-1}} - \cdots - \lambda_1 a^{2p^{r-1}-1} = 2p^{r-1}a_{2p^{r-1}}$$

and hence $-\lambda_{2p^{r-1}} + p^{r-1} = 2^{p^{r-1}}$, and therefore $\lambda_{2p^{r-1}} = -p^{r-1}$ and so on. Thus

$$\lambda_{p^{r-1}} = \lambda_{2p^{r-1}} = \cdots = \lambda_{(p-1)p^{r-1}} = -p^{r-1}$$

while

$$\begin{aligned}\lambda_{p^r} &= \sum_{j=1}^{k} Q_j^{p^r} = \sum_{j=1}^{k}(\omega^{\alpha_j})^{p^r} = \sum_{j=1}^{k}(\omega^{p^r})^{\alpha_j}\\ &= \sum_{j=1}^{k} 1 = k = (p-1)p^{r-1}. \end{aligned} \tag{9}$$

Thus from (9)

$$E(G) = \sum_{i=1}^{n}|\lambda_i| = \sum_{i=1}^{p-1}|\lambda_{ip^{r-1}}| + |\lambda_{p^r}|$$

$$= (p-1)p^{r-1} + p^{r-1}(p-1)$$
$$= 2(p-1)p^{r-1}.$$

Now the bound B_2 for $E(G)$ is given by

$$B_2 = k + \sqrt{k(n-1)(n-k)}, \text{ (where } n = p^r \text{ and } k = (p-1)p^{r-1})$$
$$= (p-1)p^{r-1} + \sqrt{(p-1)p^{r-1}(p^r-1)(p^r-(p^r-p^{r-1}))}.$$

Hence

$$\frac{E(G)}{B_2} = \frac{2}{1+\sqrt{1+p+p^2+\cdots+p^{r-1}}} \to 0$$

either as $p \to \infty$ or as $r \to \infty$.

This proves that there are $\phi(n)$-regular graphs of order n for infinitely many n whose energies are much smaller compared to the bound B_2. □

5. Equienergetic graphs

In this section, we establish the existence of equienergetic non-cospectral graphs.

Definition 5.1. Two graphs of the same order are called equienergetic (resp. cospectral) if they have the same energy (resp. spectrum).

Naturally, two cospectral graphs are equienergetic.

We now recall the definitions of the tensor product of two graphs and two matrices.

Definition 5.2. The tensor product of two graphs G_1 and G_2 is the graph $G_1 \otimes G_2$ with vertex set $V(G_1) \times V(G_2)$ and in which the vertices (u_1, u_2) and (v_1, v_2) are adjacent iff $u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$.

Definition 5.3. The tensor product $A \otimes B$ of the $r \times s$ matrix $A = (a_{ij})$ and the $t \times u$ matrix $B = (b_{ij})$ is defined as the $rt \times su$ matrix got by replacing each entry a_{ij} of A by the double array $a_{ij}B$.

It is easy to check that for any two graphs G_1, and G_2 with adjacency matrices $A(G_1)$ and $A(G_2)$ respectively, the adjacency matrix $A(G_1 \otimes G_2)$ of $(G_1 \otimes G_2)$ is given by

$$A(G_1 \otimes G_2) = A(G_1) \otimes A(G_2).$$

Our next lemma is well-known. For the sake of completeness, we present its proof.

Lemma 5.4. *If A is a matrix of order r with spectrum $\{\lambda_1, \ldots, \lambda_r\}$, and B, a matrix of order s with spectrum $\{\mu_1, \mu_2, \ldots, \mu_s\}$ then the spectrum of $(A \otimes B)$ is $\{\lambda_i \mu_j : 1 \leqslant i \leqslant r; 1 \leqslant j \leqslant s\}$.*

Proof. Let X and Y be eigen vectors corresponding to the eigen values λ and μ of A and B respectively. Then $AX = \lambda X$ and $BY = \mu Y$. Now for any four matrices P, Q, R and S, $(P \otimes Q)(R \otimes S) = PR \otimes QS$ whenever the products PR and QS are defined. Hence $(A \otimes B)(X \otimes Y) = AX \otimes BY = \lambda X \otimes \mu Y = \lambda\mu(X \otimes Y)$. As $X \otimes Y$ is a non-zero vector, $\lambda\mu$ is an eigen value of $A \otimes B$. Conversely, any eigen value of $A \otimes B$ is of the form $\lambda_i \mu_j$ for some i and j. To see this, we note that $A \otimes B = (A \otimes I_s)(I_r \otimes B) = (I_r \otimes B)(A \otimes I_s)$. In other words, $A \otimes B$ is a product of two commuting matrices. Now the spectrum of $I_r \otimes B$ is the spectrum of B repeated r times. A similar statement applies for the spectrum of $A \otimes I_s$. Now if C and D are two commuting matrices of order t, with spectra $\{\alpha_1, \ldots, \alpha_t\}$ and $\{\beta_1, \ldots, \beta_t\}$ respectively, then each of the t eigen values of CD is of the form $\alpha_i \beta_j$ for some i and j [6].

This proves the result. □

Corollary 5.5. *If G_1 and G_2 are any two graphs,*

$$E(G_1 \otimes G_2) = E(G_1)E(G_2).$$

Proof. Let the spectra of G_1 and G_2 be $\{\lambda_1, \ldots, \lambda_r\}$ and $\{\mu_1, \ldots, \mu_t\}$ respectively. Then $E(G_1 \otimes G_2) = \sum_{i,j} |\lambda_i \mu_j| = \sum_{i=1}^{r} |\lambda_i| \cdot \sum_{j=1}^{s} |\mu_j| = E(G_1)E(G_2)$. □

Corollary 5.6. *For any non-trivial graph G, $E(G) > 1$.*

Proof. Suppose $E(G) < 1$. Then $E(G \otimes \cdots \otimes G(\text{p times})) = E(G)^p \to 0$ as $p \to \infty$. Hence the graph $G \otimes G \otimes \cdots (p \text{ times}) \to$ The totally disconnected graph, which is absurd. The same argument would show that not all the eigen values of a graph G can be of absolute value less than 1. Consequently, if $E(G) = 1$, then the absolute values of all the eigen values of G must be less than 1, a contradiction. □

Theorem 5.7. *There exist (non-isomorphic) equienergetic graphs that are not cospectral.*

Proof. Let G be a non-trivial graph of order n. Since the sum of the eigen values of G is zero, G has at least two distinct values. Let $H_1 = G \otimes K_2 \otimes k_2$ and $H_2 = G \otimes C_4$, where C_4 is the cycle of length 4. Then, by Corollary 5.5, $E(H_1) = E(H_2) = 4E(G)$, since $E(K_2) = 2$ and $E(C_4) = 4$. H_1 and H_2 are both of order $4n$. Thus H_1 and H_2 are equienergetic. The spectrum of H_1 is (Spec(G) repeated twice) $\cup$ ($-$Spec(G) repeated twice) while Spec(H_2) is (2 Spec(G)$\cup$($-$2 Spec(G)$\cup$ (0 repeated $2n$ times). Consequently, H_1 and H_2 are not cospectral. (Further, H_1 and

H_2 have maximum degrees Δ and 2Δ respectively, where Δ is the maximum degree of G. Hence H_1 and H_2 are non-isomorphic.) $\square$

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