ON THE ENERGY OF 3-CIRCULANT GRAPHS

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ABSTRACT. The energy of a graph G is defined as the sum of the absolute values of all the eigenvalues of the graph. In this paper, We consider the energy of the 3-circulant graphs, and obtain a computation formula, and establish new results for a certain class of circulant graphs. At the same time,we give a conjecture: The largest energy of circulant graphs relate with their components.

1. INTRODUCTION

All graphs considered in this paper are finite, simple and undirected. For notations and terminology, see[1],[2]. Given a graph G, define the energy of G, denoted by $E(G)$, is defined to be the sum of the absolute values of its eigenvalues. Hence if $A(G)$ is the adjacency matrix of G, and $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of $A(G)$, then

$$E(G) = \sum_{k=1}^{n} |\lambda_k|$$

The set $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ is the spectrum of G, which is denoted by Spec G. This notion is related to some applications of graph theory to chemistry and has been studied carefully in the literature([3],[4],[5]), and references therein. In particular, it is shown in [6] that

$$E(G) \leq \frac{n}{2}(\sqrt{n} + 1) \tag{1}$$

for any graph G with n vertices as well as that the bound (1) can be achieved for infinitely many graphs.

For the family of bipartite graphs a stronger bound $E(G) \leq \frac{n}{4}(\sqrt{2n} + 2)$ has been shown in [7]. Here we give an explicit construction of an infinite family of 3-circulant graphs which attain the bound (1) asymptotically.

2000 *Mathematics Subject Classification.* Primary 05C35; 05C50;

Key words and phrases. Energy of graphs; 3-Circulant graphs; formula; conjecture.

The author was supported in part by SRF of Hunan Provincial Education Department Grant #06C755,and Hunan Science and Technology Plan Project Grant#2008FJ3090.

We now recall that an n-vertex graph G is called hyper-energetic if $E(G) > 2(n-1)$. This concept has been introduced in [3], which is in relation to some problems of molecular chemistry.

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.

Recently several results have been obtained for the hyper-energetic circulant graphs [8]. In particular, it is well known that the complete n-vertex graph K_n satisfies $E(K\_n) = 2(n-1)$. In [9] a conjecture is made that the graphs obtained from K_n by removing a Hamiltonian circuit are not hyper-energetic. It fact, in [8] this conjecture has been shown to be wrong, even for a more general class of circulant graphs. Here we derive a somewhat stronger, albeit less explicit, lower bound on the energy of such graphs.

In this paper, we investigate the upper bound on 3-circulant graphs. Here we prove that if G is a 3-circulant graph on n vertices, then $E(G) < n + \sum_{p=0}^{n-1} |2\cos\frac{2ap\pi}{n}|$

In Section 2, we shall introduce the background on 3-circulant graphs. In Section 3, we shall quote some lemmas.In Section 4,we present a proof of Theorem 1.We also prove a similar result regarding Lemma 5.

2. Background on circulant graphs

Now,we consider the class of graphs called circulant graphs. Let S be any subset of $\{0,1,2,\cdots,n-1\}$ such that $S \equiv$-S mod n. A graph G with vertex set $\{0,1,2,\cdots,n-1\}$ is called a *circulant* graph if two vertices i and j are adjacent if and only if $(i-j)$ mod $n \in S$,[10].

The adjacency matrix $A(G)$ is a circulant matrix, i.e., $a_{i,j} = a_{i-1,j-1}$ with the subscript calculation done mod n.In other words, row $(i+1)$ of the matrix is a cyclic right shift one position from row (i).

We begin with the 3-circulant graphs. A 3-circulant is defined by a jump set $S = \{a, \frac{n}{2}, n-a\}$ with three elements. All 3-circulant graphs are 3-regular. Since the sum of the degree of the vertices must be two times the number of edges, 3-circulant graphs must have an even number of vertices. Therefore, in what follows we shall assume that n is even. Since S is a three-element subset of $\{0,1,2,\cdots,n-1\}$ such that $S \equiv -S$ mod n, it is clear that S must have the triple form $S = \{a, \frac{n}{2}, n-a\}$, a result of Broere [11] gives precise conditions on the connectivity of 3-circulant.

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

Lemma 2.1. [12] *If A is an $n\times n$ circulant matrix with first row $[c_1, c_2, \cdots, c_n]$, then the eigenvalues of A are given by*

$$\lambda_p = \sum_{i=1}^{n} c_i \omega^{(i-1)p}, p = 0, 1, \cdots, n-1,$$

where $\omega = e^{\frac{2\pi i}{n}}$

Now, let us quote an example[9]. Let G be the graph $K\_n - H$, where $V(K\_n) = \{1, 2, \cdots, n\}$ and $H = (123\cdots n)$, a Hamilton cycle of K_n. Then $\lambda I - A(G)$ is a circulant matrix with first row $(\lambda, 0, -1, \cdots, -1, 0)$, hence the Spectrum of G=the set of roots of

$$\det(\lambda I - A) = \{\omega^{2j} + \cdots + \omega^{(n-2)j} : 0 \leq j \leq n-1\}$$

ω=a primitive n-th root of unity 1, and $\omega = \{-1 - \omega^j - \omega^{(n-1)j} : 0 \leq j \leq n-1\}$

$$\begin{aligned} E(G) &= \textstyle\sum_{j=0}^{n-1} |1 + \omega^j + \omega^{(n-1)j}| \\ &= \textstyle\sum_{j=0}^{n-1} |1 + 2\cos\frac{2\pi j}{n}| \end{aligned}$$

Computations show that for $4 \leq n \leq 100$, the graph $K\_n - H$ is non-hyper-energetic.

3. Some Lemmas

Any disconnected 3-circulant graphs G is made up of d isomorphic copies of connected 3-circulants $G_i, i = 1, 2, \cdots, d$, then $E(G) = \sum_{i=1}^{d} E(G_i)$. We give some lemmas.

Lemma 3.1. [10] *Let G be a circulant graph with n vertices formed by $S = \{s_1, \cdots, s_k\}$. If $d = gcd(s_1, \cdots, s_k, n)$, then G has d connected components each isomorphic to the circulant graph on $\frac{n}{d}$ vertices formed by $s' = \{\frac{s_1}{d}, \cdots, \frac{s_k}{d}\}$.*

We can apply the lemma to the 3-circulant case as follows.

Lemma 3.2. [10] *Let n be even and $S = \{a, \frac{n}{2}, n-a\}$. If $gcd(a, \frac{n}{2}, n) = d$. then the circulant graph with n vertices formed by S has d components each isomorphic to the circulant graph on $\frac{n}{d}$ vertices formed by $S' = \{\frac{a}{d}, \frac{n}{2d}, \frac{n-a}{d}\}$.*

A simple example illustrates this result, see Figure 1.

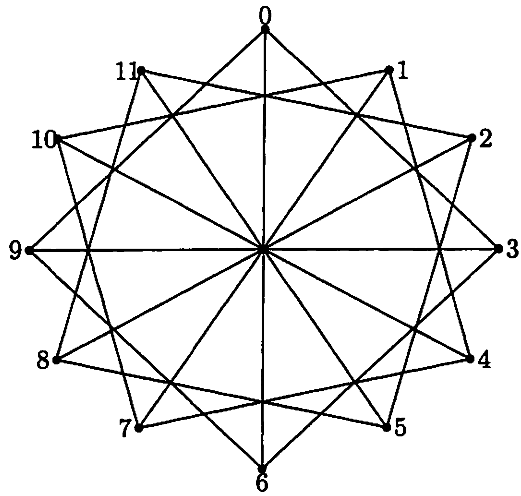

Figure 1. 3-circulant graph with 12 vertices formed by $S = \{3, 6, 9\}$

Let $n = 12$ and $S = \{3, 6, 9\}$. The $gcd(3, 6, 9) = 3$ indicating three connected components. Indeed the numberic vertices {1,4,7,10}, {2,5,8,11}, {3,6,9,12} form three subgraph isomorphic to K_4.

Lemma 3.3. [6] *If $2m \geq n$ and G is a graph on n vertices with m edges, then the inequality*

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)[2m - (\frac{2m}{n})^2]} \qquad (2)$$

holds. Moreover, equality holds in (2) if and only if G is either $\frac{n}{2}K\_2$, K_n, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{n-1}}$.

Lemma 3.4. [9] *For each $\epsilon > 0$, there exist infinitely many n for each of which there exist a k-regular graph G of order n with $k < n-1$ and $\frac{E(G)}{B_2} < \epsilon$. where $B_2 = k + \sqrt{k(n-1)(n-k)}$*

4. Main results

Given a 3-circulant graph G with the triple form $\{a, \frac{n}{2}, n-a\}$, its energy not only is related with n, but also concerns with a. For fixed n the energy of G changes with a. For example, we take $n = 12$, $a = 1, 2, 3, 4, 5$, respectively, where a is the correlation constant. It is obvious that all the 3-circulant graphs have the form {1,6,11}, $\{2, 6, 10\}$,

$\{3,6,9\}$, {4,6,8}, $\{5,6,7\}$, respectively. According to the the direct calculation, we readily obtain the energy of 3-circulant graphs, which embraces $16.92, 16.00, 18.00, 12.00, 16.92$. In view of this,we clearly show that the 3-circulant graph with three connected components and the form $\{3,6,9\}$ has maximal energy. This gives evidence for the following conjecture: Among all the circulant graphs on n vertices the one with largest energy has maximal number of components.

Now we shall investigate the energy of 3-circulant graphs, we obtained the following theorem.

Theorem 4.1. *Suppose that G is a 3-circulant with form $\{a, \frac{n}{2}, n-a\}$, where a is a positive integer and $1 \leq a \leq \frac{n}{2}$, then the inequality $E(G) = \sum_{p=0}^{n-1} |\lambda_p|$ holds.*

Proof. Let A is the adjacency matrix of G with first row $\{c_1, c_2, \cdots, c_n\}$, with the exception of $\{c_a, c_{\frac{n}{2}}, c_{n-a}\}$, the others all be zeros. By lemma 1, We have

$$\begin{aligned}
\lambda_p &= c_a\omega^{(a-1)p} + c_{\frac{n}{2}}\omega^{(\frac{n}{2}-1)p} + c_{n-a}\omega^{(n-a-1)p} \\
&= \omega^{(a-1)p} + \omega^{(\frac{n}{2}-1)p} + \omega^{(n-a-1)p} \\
&= \exp\tfrac{2\pi}{n}(a-1)pi + \exp\tfrac{2\pi}{n}(\tfrac{n}{2}-1)pi + \exp\tfrac{2\pi}{n}(n-a-1)pi \\
&= \cos\tfrac{2(a-1)p\pi}{n} + i\sin\tfrac{2(a-1)p\pi}{n} + (-1)^p\{\cos\tfrac{2p\pi}{n} - i\sin\tfrac{2p\pi}{n}\} \\
&\quad + \cos\tfrac{2(a+1)p\pi}{n} - i\sin\tfrac{2(a+1)p\pi}{n} \\
&= 2\cos\tfrac{2ap\pi}{n}\{\cos\tfrac{2p\pi}{n} - i\sin\tfrac{2p\pi}{n}\} + (-1)^p(\cos\tfrac{2p\pi}{n} - i\sin\tfrac{2p\pi}{n}) \\
&= (2\cos\tfrac{2ap\pi}{n} + (-1)^p)(\cos\tfrac{2p\pi}{n} - i\sin\tfrac{2p\pi}{n})
\end{aligned}$$

Hence

$$\begin{aligned}
E(G) &= \sum_{p=0}^{n-1} |\lambda_p| \\
&= \sum_{p=0}^{n-1} |2\cos\tfrac{2ap\pi}{n} + (-1)^p||\cos\tfrac{2p\pi}{n} - i\sin\tfrac{2p\pi}{n}| \qquad \square \\
&= \sum_{p=0}^{n-1} |2\cos\tfrac{2ap\pi}{n} + (-1)^p| \leq n + \sum_{p=0}^{n-1} |2\cos\tfrac{2ap\pi}{n}|
\end{aligned}$$

Thus, we can compute precisely the energy $E(G)$, if only we know the values of n and a.

Next we propose a previous conjecture:

Among 3-circulant graphs with n vertices, $E(G)$ is maximal energy for the graph G', where G' has the largest components.

Whether this conjecture is correct or not, let us look at the *Table*1 below:

Clearly,Table 1 gives further evidence for this conjecture.

This table shows the fact that the 3-circulant graph has many case components as $n = 4K, k \in \mathbb{N}_+$. In particular, it embraces the largest number

Table 1: The relation n and energy

Vertices	$S = \{a, \frac{n}{2}, n-a\}$	Components	Energy
8	{1,4,7}	1	11.64
	{2,4,6}	2	12
	{3,4,5}	1	11.64
10	{1,5,9}	1	14.88
	{2,5,8}	1	14.42
	{3,5,7}	1	14.88
	{4,5,6}	1	14.42
12	{1,6,11}	1	16.92
	{2,6,10}	2	16
	{3,6,9}	3	18
	{4,6,8}	2	12
	{5,6,7}	1	16.92
14	{1,7,13}	1	20.42
	{2,7,12}	1	20.20
	{3,7,11}	1	20.42
	{4,7,10}	1	20.20
	{5,7,9}	1	20.42
	{6,7,8}	1	20.20
16	{1,8,15}	1	23.05
	{2,8,14}	2	23.28
	{3,8,13}	1	23.05
	{4,8,12}	4	24
	{5,8,11}	1	23.05
	{6,8,10}	2	23.28
	{7,8,9}	1	23.05
18	{1,9,17}	1	25.04
	{2,9,16}	1	25.65
	{3,9,15}	3	24
	{4,9,14}	1	25.65
	{5,9,13}	1	25.04
	{6,9,12}	3	18
	{7,9,11}	1	25.04
	{8,9,10}	1	25.65
20	{1,10,19}	1	28.78
	{2,10,18}	2	29.76
	{3,10,17}	1	28.78
	{4,10,16}	2	28.84
	{5,10,15}	5	30

Table 1(cont.)

Vertices	$S=\{a,\frac{n}{2},n-a\}$	Components	Energy
20	{6,10,14}	2	29.76
	{7,10,13}	1	28.78
	{8,10,12}	2	28.84
	{9,10,11}	1	28.78
22	{1,11,21}	1	31.83
	{2,11,20}	1	31.64
	{3,11,19}	1	31.83
	{4,11,18}	1	31.64
	{5,11,17}	1	31.83
	{6,11,16}	1	31.64
	{7,11,15}	1	31.83
	{8,11,14}	1	31.64
	{9,11,13}	1	31.83
	{10,11,12}	1	31.64

of components with the form $S=\{k,2k,3k\}$, and have k components, then $E(G)$ have maximal value,i.e.,$E(G)=kE(K\_4)=6k$. $E(G)$ depends on the number of components; we can discover this from above *Table* 1. On the contrary, for $n=4k+2, k\in\mathrm{N}_+$, the energy of 3-circulant graph does not have positive ratio to its components,i.e.,that is, the more number of components, its energy is not greater.

As we have seen from *Table* 1 that the energy of 3-circulant graph is maximal with form $S=\{1,\frac{n}{2},n-1\}$, for $n=4k+2, k\in\mathrm{N}_+$. However, there are exceptions, for instance, $n=18$, the energy of the 3-circulant graph is maximal with form $S=\{2,9,16\}$,but not form $S=\{1,9,17\}$. Therefore, further study is required to determine which kind of energy is the largest.

Acknowledgments The author would like to express his gratitude to Professor R.A.Brualdi for his kind advice and encouragement. Thanks to the referee for his useful comments and suggestions.

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