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The maximal energy of classes of integral circulant graphs

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ABSTRACT

The energy of a graph is the sum of the moduli of the eigenvalues of its adjacency matrix. We study the energy of integral circulant graphs, also called gcd graphs, which can be characterized by their vertex count n and a set $\mathcal{D}$ of divisors of n in such a way that they have vertex set $\mathbb{Z}_n$ and edge set $\{\{a, b\} : a, b \in \mathbb{Z}_n, \gcd(a-b, n) \in \mathcal{D}\}$. For a fixed prime power $n = p^s$ and a fixed divisor set size $|\mathcal{D}| = r$, we analyse the maximal energy among all matching integral circulant graphs. Let $p^{a_1} < p^{a_2} < \cdots < p^{a_r}$ be the elements of $\mathcal{D}$. It turns out that the differences $d_i = a_{i+1} - a_i$ between the exponents of an energy maximal divisor set must satisfy certain balance conditions: (i) either all d_i equal $q := \frac{s-1}{r-1}$, or at most the two differences $[q]$ and $[q+1]$ may occur; (ii) there are rules governing the sequence $d_1, \ldots, d_{r-1}$ of consecutive differences. For particular choices of s and r these conditions already guarantee maximal energy and its value can be computed explicitly.

1. Introduction

Integral circulant graphs have attracted much research attention lately, in particular since more and more people have become aware that they play a role in quantum physics [24,6]. A characteristic property of circulant graphs is that their vertices can be numbered such that any cyclic rotation of the vertex numbering results in a graph isomorphic to the original graph. Circulant graphs have been the object of research for quite some time [9] and belong to the important family of Cayley graphs. The integral circulant graphs, having only integer eigenvalues, form a small but rather distinguished subclass since integral graphs are quite rare among graphs in general [1].

Given an integer n and a set $\mathcal{D}$ of positive divisors of n, the integral circulant graph $\mathrm{ICG}(n, \mathcal{D})$ is defined as the graph having vertex set $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$ and edge set $\{\{a, b\}: a, b \in \mathbb{Z}_n, \gcd(a-b, n) \in \mathcal{D}\}$. We consider only loopless gcd graphs, i.e. $n \notin \mathcal{D}$. For $|\mathcal{D}| = 1$ we obtain the subclass of so-called unitary Cayley graphs. Over the years, the general structural properties of integral circulant graphs have been well researched [11,7,26,18,2,3,19,12,10,4]. Due to the connection with quantum physics, emphasis has lately been placed on researching the energy of integral circulant graphs [25,16,17,21,5,20,22,23].

The *energy* $E(G)$ of a graph G on n vertices is defined as

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

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. Refer to [8,13,14] for general results on graph energy.

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Let us abbreviate $\mathcal{E}(n, \mathcal{D}) = E(\mathrm{ICG}(n, \mathcal{D}))$. Given a positive integer n, we consider

$$\mathcal{E}_{\min}(n) := \min\{\mathcal{E}(n, \mathcal{D}): \mathcal{D} \subseteq \{1 \le d < n: d \mid n\}\}$$

and

$$\mathcal{E}_{\max}(n) := \max\{\mathcal{E}(n, \mathcal{D}): \mathcal{D} \subseteq \{1 \le d < n: d \mid n\}\}.$$

Consider a prime power $n = p^s$ and a divisor set $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ with exponents $0 \le a_1 < \cdots < a_r \le s-1$. According to Theorem 2.1 in [22] we have

$$\mathcal{E}(p^s, \mathcal{D}) = 2(p-1)p^{s-1}\left(r - (p-1)h_p(a_1, \ldots, a_r)\right), \tag{1}$$

where

$$h_p(x) = h_p(x_1, \ldots, x_r) := \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{x_i - x_k}} \tag{2}$$

for $x = (x_1, \ldots, x_r) \in \mathbb{R}^r$. Observe that h_p has the symmetry property

$$h_p(s-1-a_r, \ldots, s-1-a_1) = h_p(a_1, \ldots, a_r) \tag{3}$$

for all integral exponents $0 \le a_1 < a_2 < \cdots < a_{r-1} < a_r \le s-1$. A straightforward consequence of (1) is that $\mathcal{E}_{\min}(p^s)$ is attained precisely for the singleton divisor sets $\mathcal{D} = \{p^t\}$ with $0 \le t \le s-1$ (cf. [22, Theorem 3.1]).

In [23] divisor sets $\mathcal{D}$ producing graphs with maximal energy $\mathcal{E}_{\max}(p^s)$ were studied. Equivalently, exponent tuples $(a_1, \ldots, a_r)$ minimizing h_p had to be found. By the result cited above, such minimizers satisfy $r \ge 2$, and they obviously must have the entries $a_1 = 0$ and $a_r = s-1$. Accordingly, a corresponding $a = (a_1, \ldots, a_r)$ lies in the set

$$A(s, r) := \{(a_1, \ldots, a_r) \in \mathbb{Z}^r: 0 = a_1 < a_2 < \cdots < a_{r-1} < a_r = s-1\},$$

and such an a is called an *admissible* exponent tuple.

Hence the quest for minimizers of h_p is only interesting in case $r \ge 3$, which we shall assume in the sequel. It was shown by the use of methods from convex optimization that, for fixed s and r, the function h_p becomes almost minimal if only $0 = a_1 < a_2 < \cdots < a_{r-1} < a_r = s-1$ are chosen in nearly equidistant positions [23, Theorem 4.2]. Note here that perfect equidistance can only be achieved if $(r-1) \mid (s-1)$ because the a_i are integers. It is the purpose of this article to use combinatorial instead of analytic arguments in order to refine the earlier approximative results.

The nearly equidistant positioning just mentioned indicates that the key to maximizing the energy lies in considering the successive exponent differences. Hence, for a given $a \in A(s, r)$, we define its *delta vector* as

$$\delta(a) := (\delta_1(a), \delta_2(a), \ldots, \delta_{r-1}(a)) \in \mathbb{N}^{r-1}$$

with $\delta_j(a) := a_{j+1} - a_j$ $(1 \le j \le r-1)$. Obviously, we have $\sum_{j=1}^{r-1} \delta_j(a) = s-1$. Thus, introducing

$$D(s, r) := \left\{(d_1, \ldots, d_{r-1}) \in \mathbb{N}^{r-1}: \sum_{j=1}^{r-1} d_j = s-1\right\},$$

the function

$$\delta: \begin{cases} A(s, r) \longrightarrow D(s, r) \\ (a_1, a_2, \ldots, a_r) \mapsto (a_2 - a_1, a_3 - a_2, \ldots, a_r - a_{r-1}) \end{cases}$$

is 1–1 with its inverse

$$\delta^{-1}: \begin{cases} D(s, r) \longrightarrow A(s, r) \\ (d_1, d_2, \ldots, d_{r-1}) \mapsto (0, d_1, d_1 + d_2, \ldots, d_1 + d_2 + \cdots + d_{r-2,s-1}). \end{cases}$$

The mentioned divisor set structure becomes apparent by restrictions on the delta vector $\delta(a)$ corresponding to an energy maximal exponent tuple a as follows:

First, the set $\{\delta_j(a): j = 1, \ldots, r-1\}$ of differences is either a singleton or has only two elements that are successive positive integers. Second, the distribution of the differences must satisfy certain balance conditions, in the sense that the differences of the value occurring less often than the other must be distributed somewhat "evenly" between the other difference values.

In some cases, these restriction will already characterize the delta vectors, and consequently the divisor set(s) imposing maximal energy on the corresponding class of integral circulant graphs. In other words, for some fixed s and r, we will be able to determine precisely

$$\min h_p := \min\{h_p(a): a \in A(s, r)\}$$

along with all admissible a satisfying $h_p(a) = \min h_p$.