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THE ENERGY OF INTEGRAL CIRCULANT GRAPHS WITH PRIME POWER ORDER

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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. Such a graph can be characterized by its vertex count n and a set $\mathcal{D}$ of divisors of n such that its vertex set is $\mathbb{Z}_n$ and its edge set is $\{\{a,b\} : a, b \in \mathbb{Z}_n, \gcd(a-b,n) \in \mathcal{D}\}$. For an integral circulant graph on p^s vertices, where p is a prime, we derive a closed formula for its energy in terms of n and $\mathcal{D}$. Moreover, we study minimal and maximal energies for fixed p^s and varying divisor sets $\mathcal{D}$.

1. INTRODUCTION

In this work, we study the energy of integral circulant graphs. These are a subclass of the important and well-researched class of circulant graphs (see Davis [**11**]) and play a role in quantum physics [**26**], [**6**]. Circulant graphs are characterized by the fact that every cyclic rotation of the vertex numbers yields a graph isomorphic to the original. For each vertex the relative "jump" distances to the adjacent vertices (in terms of vertex indices, computing modulo n) are the same. Thus, in order to describe a particular circulant graph, one only needs to record n and the set of jump distances. Integral circulant graphs are those circulant graphs that have only integer eigenvalues. Graphs with this spectral property are quite rare [**1**].

The circulant graphs are exactly the Cayley graphs $\mathrm{Cay}(\mathbb{Z}_n, S)$. The *Cayley graph* $\mathrm{Cay}(\Gamma, S)$ of a multiplicative group Γ with identity 1 and a set $S \subseteq \Gamma$ is

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defined to have vertex set Γ and edge set $\{\{a,b\}: \ a,b \in \Gamma, ab^{-1} \in S\}$. The set S is usually assumed to satisfy $1 \notin S$ and $S^{-1} = \{s^{-1}: \ s \in S\} = S$, which implies $\mathrm{Cay}(\Gamma, S)$ to be loop-free and undirected. The *unitary* Cayley graphs are the graphs $\mathrm{Cay}(\mathbb{Z}_n, U_n)$, where U_n is the unit group of $\mathbb{Z}_n$. Consequently, they have vertex set $\mathbb{Z}_n$ and edge set $\{\{a,b\}: \ a,b \in \mathbb{Z}_n, \ \gcd(a-b,n) = 1\}$. In the existing literature $\mathrm{Cay}(\mathbb{Z}_n, U_n)$ is often denoted by X_n.

According to a result by So [**28**], the integral circulant graphs can be characterized as follows: Given an integer n and a set $\mathcal{D}$ of positive divisors of n, define the graph $\mathrm{ICG}(n,\mathcal{D})$ to have vertex set $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$ and edge set $\{\{a,b\}: \ a,b \in \mathbb{Z}_n, \ \gcd(a-b,n) \in \mathcal{D}\}$. Every integral circulant graph can be represented by such a graph $\mathrm{ICG}(n,\mathcal{D})$ (observe that $n \in \mathcal{D}$ introduces a loop in the graph). By this characterization, it is easy to see that the integral circulant graphs arise as a natural generalization of the unitary Cayley graphs, which are exactly the integral circulant graphs $\mathrm{ICG}(n,\{1\})$. Following this point of view, the shorter term *gcd graphs* has sometimes been used for the integral circulant graphs [**15**], [**18**]. Both the class of integral circulant graphs and the subclass of unitary Cayley graphs have received increased research attention lately (see e.g. [**12**], [**8**], [**18**], [**25**], [**6**], [**7**], [**15**], [**2**], [**16**], [**22**], [**3**]).

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. This concept has been introduced in the 1970ies by Gutman [**13**], originally in the context of mathematical chemistry. Today the energy of graphs is mainly studied for genuine mathematical interest. With slight modification this notion can even be extended to arbitrary real rectangular matrices, cf. [**21**] and [**17**]. In [**10**] Brualdi gives a short survey on the graph energy.

There has been some recent work on the energy of unitary Cayley graphs. Balakrishnan [**4**] considered graphs $\mathrm{Cay}(\mathbb{Z}_n, U_n)$ for $n = p^s$ with $s \geq 1$ and showed $E(\mathrm{Cay}(\mathbb{Z}_{p^s}, U_{p^s})) = 2\varphi(p^s) = 2(p-1)p^{s-1}$, where φ is Euler's totient function. Ramaswamy and Veena [**25**] have extended this to arbitrary unitary Cayley graphs, by showing that $E(\mathrm{Cay}(\mathbb{Z}_n, U_n)) = 2^k\varphi(n)$ for $n = p_1^{s_1}\cdots p_k^{s_k}$ with distinct primes p_i and positive integers s_i. The same result has been obtained independently by Ilić [**15**].

Let us abbreviate $\mathcal{E}(n,\mathcal{D}) = E(\mathrm{ICG}(n,\mathcal{D}))$ and let $n = p_1^{s_1}\cdots p_k^{s_k}$ as above. Then, in the context of integral circulant graphs, the previous result reads as follows:

$$\mathcal{E}(n,\{1\}) = 2^k\varphi(n).$$

Ilić [**15**] has slightly generalized these results to some integral circulant graphs that are not unitary Cayley graphs:

$$\begin{aligned} &\mathcal{E}(n,\{1,p_i\}) = 2^{k-1}p_i\varphi(n/p_i), && \text{provided that } s_i = 1,\\ &\mathcal{E}(n,\{p_i,p_j\}) = 2^k\varphi(n), && \text{provided that } s_1 = \ldots = s_k = 1. \end{aligned}$$

In this paper we shall add to these results by proving an explicit formula for the energy $\mathcal{E}(n,\mathcal{D})$ for any prime power $n = p^s$ and any divisor set $\mathcal{D}$. The reason for the restriction of n to prime powers is the fact that, except for the special case $n = p_1p_2$ (cf. final section, last paragraph, or Ilić's results above), the energies of integral circulant graphs $\mathrm{ICG}(n,\mathcal{D})$ do not reveal any sign of multiplicative behaviour with respect to n and, therefore, severe complications arise for arbitrary n. Despite our restriction, now arbitrary divisor sets $\mathcal{D}$ are permitted − in contrast to the limitations of earlier results. It will be an easy corollary to our formula for the energy of $\mathrm{ICG}(p^s,\mathcal{D})$ to determine for fixed p^s the integral circulant graphs with minimal energy, simply by demonstrating that the corresponding divisor sets $\mathcal{D}$ are exactly the singletons. On the other hand, the graphs with maximal energy apparently behave in a much more irregular fashion, and a general specification seems to be difficult. Yet we provide explicit results for prime powers p^s with small exponents.

Sharp upper bounds in terms of n for the energy of an arbitrary graph with n vertices are known (cf. Koolen and Moulton [**19**]). Maximal energies to be found in special graph classes were studied by Balakrishnan [**4**] and Li et al. [**20**] for k-regular graphs, and by Shparlinksi [**27**] for circulant graphs. These investigations are motivated by the interesting question of hyperenergeticity. A graph G on n vertices is called *hyperenergetic* if its energy is greater than the energy of the complete graph on the same number of vertices, i.e. if $E(G) > E(K_n) = 2(n-1)$. It had once been conjectured that no hyperenergetic graphs exist, but since then many classes of hyperenergetic graphs have been discovered. One simple construction is due to Hou and Gutman. They show in [**14**] that if a graph G has more than $2n-1$ edges, then its line graph is necessarily hyperenergetic. It follows that $L(K_n)$ is hyperenergetic for all $n \geq 5$ (this fact seems to have been known before). Let us note in passing that a surprising fact about line graph energies is that k-th iterated line graphs ($k \geq 2$) of any two r-regular graphs ($r \geq 3$) with the same number of vertices actually have the same energies, as shown by Ramane et al. [**24**].

Actually, the class of circulant graphs contains a wealth of hyperenergetic members. Stevanović and Stanković have shown that, for fixed but arbitrary sets of jump distances, all circulants with this jump set are hyperenergetic, if only they have sufficiently many vertices [**29**]. Bounds on the average energy of circulants, depending on the number of vertices and the jump set size, have been given by Blackburn and Shparlinski [**9**]. As a special case of circulant graphs, almost all unitary Cayley graphs on n vertices have been shown to be hyperenergetic, see [**25**] by Ramaswamy and Veena. The necessary and sufficient condition is that n has at least 3 distinct prime divisors or that n is odd in case of only two prime divisors. We characterize all graphs $\mathrm{ICG}(p^s,\mathcal{D})$ that are hyperenergetic. Note that, according to Ramaswamy and Veena, for $\mathcal{D} = \{1\}$ there are none. It turns out that for each fixed prime power p^s ($p \geq 3$ and $s \geq 3$) the set of integral circulant graphs $\mathrm{ICG}(p^s,\mathcal{D})$ contains hyperenergetic elements, graphs with energy $2(p^s-1)$ just like the corresponding complete graph K_{p^s} as well as graphs with lower energy, which we shall call *hypoenergetic*.

2. THE ENERGY OF INTEGRAL CIRCULANT GRAPHS WITH FIXED DIVISOR SET

For an integer $n > 1$ and a non-empty set $\mathcal{D} \subseteq \{1 \le d \le n : \ d \mid n\}$ of divisors of n we denote by $\mathcal{E}(n, \mathcal{D})$ the energy of the integral circulant graph $\mathrm{ICG}(n, \mathcal{D})$. By the formula for the eigenvalues of integral circulant graphs obtained by Klotz and Sander [**18**], the energy of a integral circulant graph turns out to be a sum of Ramanujan sums, namely

$$\mathcal{E}(n,\mathcal{D}) = \sum_{k=1}^{n} \left| \sum_{d\in\mathcal{D}} \mu\Big(\frac{n}{(n,kd)}\Big) \cdot \frac{\varphi\left(\frac{n}{d}\right)}{\varphi\Big(\frac{n}{(n,kd)}\Big)} \right|, \tag{1}$$

where μ denotes Möbius' well-known function. We shall determine $\mathcal{E}(p^s, \mathcal{D})$ for arbitrary prime powers p^s and arbitrary divisor sets $\mathcal{D}$. Since it is customary to study only energies of loopless graphs, we shall assume that $p^s \notin \mathcal{D}$. However, our results can be easily adapted to deal with graphs containing loops as well.

Theorem 2.1. *Let p be a prime and s an arbitrary positive integer. Let $\mathcal{D}$ be a non-empty set of positive divisors d of p^s with $d < p^s$, i.e. $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ with $0 \le a_1 < a_2 < \ldots < a_r \le s-1$. Then*

$$\mathcal{E}(p^s,\mathcal{D}) = 2(p-1)\Bigg(p^{s-1}r - (p-1)\sum_{k=1}^{r-1}\sum_{i=k+1}^{r} p^{s-a_i+a_k-1}\Bigg).$$

Proof. By (1) we have

$$\begin{aligned}\mathcal{E}(p^s,\mathcal{D}) &= \sum_{k=1}^{p^s} \left| \sum_{d\in\mathcal{D}} \mu\left(\frac{p^s}{(p^s,kd)}\right) \cdot \frac{\varphi\left(\frac{p^s}{d}\right)}{\varphi\left(\frac{p^s}{(p^s,kd)}\right)} \right| \\ &= \sum_{k=1}^{p^s} \left| \sum_{i=1}^{r} \mu\left(\frac{p^s}{(p^s,kp^{a_i})}\right) \cdot \frac{\varphi\left(p^{s-a_i}\right)}{\varphi\left(\frac{p^s}{(p^s,kp^{a_i})}\right)} \right|.\end{aligned}$$

We partition the sum over k according to the greatest power of p dividing k, using the notation $p^j \| k$ to express that $p^j \mid k$ but $p^{j+1} \nmid k$. Hence

$$\begin{aligned}\mathcal{E}(p^s,\mathcal{D}) &= \sum_{j=0}^{s-1} \sum_{\substack{k=1\\ p^j\|k}}^{p^s} \left| \sum_{i=1}^{r} \mu\left(\frac{p^s}{(p^s,kp^{a_i})}\right) \cdot \frac{\varphi\left(p^{s-a_i}\right)}{\varphi\left(\frac{p^s}{(p^s,kp^{a_i})}\right)} \right| + \left| \sum_{i=1}^{r} \mu(1) \cdot \frac{\varphi\left(p^{s-a_i}\right)}{\varphi(1)} \right| \\ &= \sum_{j=0}^{s-1} \left(\frac{p^s}{p^j} - \frac{p^s}{p^{j+1}}\right) \left| \sum_{i=1}^{r} \mu\left(\frac{p^s}{p^{\min\{s,j+a_i\}}}\right) \cdot \frac{\varphi\left(p^{s-a_i}\right)}{\varphi\left(\frac{p^s}{p^{\min\{s,j+a_i\}}}\right)} \right| + \sum_{i=1}^{r} \varphi(p^{s-a_i})\end{aligned}$$

$$= p^{s-1}(p-1)\sum_{j=0}^{s-1}\frac{1}{p^j}\left|\sum_{i=1}^{r}\mu\Big(p^{s-\min\{s,j+a_i\}}\Big)\cdot\frac{\varphi\left(p^{s-a_i}\right)}{\varphi\left(p^{s-\min\{s,j+a_i\}}\right)}\right|+\sum_{i=1}^{r}\varphi(p^{s-a_i})\,.$$

Now our sum simplifies substantially by the fact that $\mu(n)$ vanishes for all positive integers n which are not squarefree. Consequently

$$\begin{aligned}\mathcal{E}(p^s,\mathcal{D}) &= p^{s-1}(p-1)\sum_{j=0}^{s-1}\frac{1}{p^j}\left|\sum_{\substack{i=1\\ j+a_i=s-1}}^{r}\mu(p)\cdot\frac{\varphi(p^{j+1})}{\varphi(p)}+\sum_{\substack{i=1\\ j+a_i\ge s}}^{r}\mu(1)\cdot\frac{\varphi(p^{s-a_i})}{\varphi(1)}\right| \\ &\quad+\sum_{i=1}^{r}\varphi(p^{s-a_i}) \\ &= p^{s-1}(p-1)\sum_{j=0}^{s-1}\frac{1}{p^j}\left|-\sum_{\substack{i=1\\ a_i=s-j-1}}^{r}p^j+\sum_{\substack{i=1\\ a_i\ge s-j}}^{r}\left(p^{s-a_i}-p^{s-a_i-1}\right)\right|+\sum_{i=1}^{r}\varphi(p^{s-a_i}) \\ &= p^{s-1}(p-1)\sum_{j=0}^{s-1}\left|-\sum_{\substack{i=1\\ a_i=s-j-1}}^{r}1+\sum_{\substack{i=1\\ a_i\ge s-j}}^{r}\left(p^{s-j-a_i}-p^{s-j-a_i-1}\right)\right|+\sum_{i=1}^{r}\varphi(p^{s-a_i}).\end{aligned}$$

We put $S_j := \left|-\sum\limits_{\substack{i=1\\ a_i=s-j-1}}^{r}1+\sum\limits_{\substack{i=1\\ a_i\ge s-j}}^{r}\left(p^{s-j-a_i}-p^{s-j-a_i-1}\right)\right|$ and have thus shown

$$\mathcal{E}(p^s,\mathcal{D}) = p^{s-1}(p-1)\sum_{j=0}^{s-1}S_j+\sum_{i=1}^{r}\varphi(p^{s-a_i}). \tag{2}$$

In order to evaluate S_j we distinguish several cases.

Case 1: $j = s-a_k-1$ for some $k\in\{1,2,\dots,r\}$.

Then

$$S_{s-a_k-1} = \left|-1+\sum_{\substack{i=1\\ a_i\ge a_k+1}}^{r}\left(p^{a_k-a_i+1}-p^{a_k-a_i}\right)\right| = \left|-1+\sum_{i=k+1}^{r}\left(p^{a_k-a_i+1}-p^{a_k-a_i}\right)\right|, \tag{3}$$

where the last sum is empty for $k=r$, hence vanishes. We have

$$\begin{aligned}\sum_{i=k+1}^{r}\left(p^{a_k-a_i+1}-p^{a_k-a_i}\right) &= (p-1)\cdot p^{a_k-a_{k+1}}\sum_{i=k+1}^{r}p^{a_{k+1}-a_i} \\ &\le (p-1)\cdot p^{a_k-a_{k+1}}\sum_{i=0}^{\infty}p^{-i} = p^{a_k-a_{k+1}+1}\le 1.\end{aligned}$$

With (3) this yields for $1 \le k \le r$

$$S_{s-a_k-1} = 1 - \sum_{i=k+1}^{r} (p^{a_k-a_i+1} - p^{a_k-a_i}) = 1 - (p-1) \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}}. \tag{4}$$

Case 2: $s - a_k \le j \le s - a_{k-1} - 2$ for some fixed $k \in \{2, 3, \ldots, r\}$.

First notice that the interval for j is empty if $a_k = a_{k-1} + 1$. Otherwise any j lying in the interval satisfies

$$a_{k-1} + 1 \le s - j - 1 \le a_k - 1. \tag{5}$$

This means that for such j the first sum in the definition of S_j is empty, hence

$$S_j = \sum_{\substack{i=1 \\ a_i \ge s-j}}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}) = \sum_{i=k}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}),$$

using (5) once again. We conclude

$$\begin{aligned}
\sum_{j=s-a_k}^{s-a_{k-1}-2} S_j &= \sum_{j=s-a_k}^{s-a_{k-1}-2} \sum_{i=k}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}) \\
&= \sum_{i=k}^{r} (p^{s-a_i} - p^{s-a_i-1}) \sum_{j=s-a_k}^{s-a_{k-1}-2} p^{-j} \\
&= (p-1) \sum_{i=k}^{r} p^{s-a_i-1} \cdot \frac{1}{p^{s-a_k}} \sum_{j=0}^{a_k-a_{k-1}-2} p^{-j} \\
&= (p-1) \sum_{i=k}^{r} p^{-(a_i-a_k+1)} \frac{p}{p-1} \left(1 - \frac{1}{p^{a_k-a_{k-1}-1}}\right),
\end{aligned}$$

where the formula for the innermost geometric sum also holds if it is empty, i.e. in case $a_k = a_{k-1} + 1$. Consequently we have for $2 \le k \le r$

$$\sum_{j=s-a_k}^{s-a_{k-1}-2} S_j = \left(1 - \left(\frac{1}{p}\right)^{a_k-a_{k-1}-1}\right) \sum_{i=k}^{r} \frac{1}{p^{a_i-a_k}}. \tag{6}$$

Case 3: $0 \le j \le s - a_r - 2$.

By definition of S_j we have

$$\sum_{j=0}^{s-a_r-2} S_j = \sum_{j=0}^{s-a_r-2} \sum_{\substack{i=1 \\ a_i \ge s-j}}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}) = 0, \tag{7}$$

since the inner sum is empty because of $s - j \ge a_r + 2$.

Case 4: $s-a_1 \le j \le s-1$.

Here we have

$$\sum_{j=s-a_1}^{s-1} S_j = \sum_{j=s-a_1}^{s-1} \sum_{\substack{i=1 \\ a_i \ge s-j}}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}) = \sum_{j=s-a_1}^{s-1} \sum_{i=1}^{r} (p^{s-j-a_i} - p^{s-j-a_i-1}),$$

since $s-j \le a_1$ in the innermost sum. For that reason we obtain similarly as before

$$\sum_{j=s-a_1}^{s-1} S_j = \left(1 - \left(\frac{1}{p}\right)^{a_1}\right) \sum_{i=1}^{r} \frac{1}{p^{a_i - a_1}}, \tag{8}$$

which again is also satisfied in the case of an empty sum, i.e. for $a_1 = 0$.

Putting (4), (6), (7) and (8) together and setting $a_0 := -1$, we get from (2)

$$\begin{aligned}
\mathcal{E}(p^s, \mathcal{D}) &= p^{s-1}(p-1) \sum_{j=0}^{s-1} S_j + \sum_{i=1}^{r} \varphi(p^{s-a_i}) \\
&= p^{s-1}(p-1) \sum_{k=1}^{r} \left(1 - (p-1) \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}}\right) \\
&\quad + p^{s-1}(p-1) \sum_{k=1}^{r} \left(1 - \left(\frac{1}{p}\right)^{a_k - a_{k-1} - 1}\right) \sum_{i=k}^{r} \frac{1}{p^{a_i - a_k}} \\
&\quad + \sum_{i=1}^{r} (p^{s-a_i} - p^{s-a_i-1}).
\end{aligned}$$

We thus obtain

$$\begin{aligned}
\frac{\mathcal{E}(p^s, \mathcal{D})}{p^{s-1}(p-1)} &= \sum_{k=1}^{r} \left(1 - (p-1) \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}}\right) \\
&\quad + \sum_{k=1}^{r} \left(1 - \left(\frac{1}{p}\right)^{a_k - a_{k-1} - 1}\right) \sum_{i=k}^{r} \frac{1}{p^{a_i - a_k}} + \sum_{i=1}^{r} \frac{1}{p^{a_i}} \\
&= r - (p-1) \sum_{k=1}^{r} \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}} \\
&\quad + \sum_{k=1}^{r} \sum_{i=k}^{r} \frac{1}{p^{a_i-a_k}} - p \sum_{k=1}^{r} \sum_{i=k}^{r} \frac{1}{p^{a_i - a_{k-1}}} + \sum_{i=1}^{r} \frac{1}{p^{a_i}} \\
&= r - (p-1) \sum_{k=1}^{r} \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}} \\
&\quad + \sum_{k=1}^{r} \left(1 + \sum_{i=k+1}^{r} \frac{1}{p^{a_i-a_k}}\right) - p \sum_{l=0}^{r-1} \sum_{i=l+1}^{r} \frac{1}{p^{a_i-a_l}} + \sum_{i=1}^{r} \frac{1}{p^{a_i}}
\end{aligned}$$

$$
\begin{aligned}
&= 2r - (p-2)\sum_{k=1}^{r}\sum_{i=k+1}^{r}\frac{1}{p^{a_i-a_k}}\\
&\quad - p\left(\sum_{l=1}^{r}\sum_{i=l+1}^{r}\frac{1}{p^{a_i-a_l}} + \sum_{i=1}^{r}\frac{1}{p^{a_i-a_0}}\right) + \sum_{i=1}^{r}\frac{1}{p^{a_i}}\\
&= 2r - (2p-2)\sum_{k=1}^{r}\sum_{i=k+1}^{r}\frac{1}{p^{a_i-a_k}}.
\end{aligned}
$$

This completes the proof of the theorem. □

Let us remark on connectivity. A Cayley graph $\mathrm{Cay}(\Gamma, S)$ with $S=\{s_1,\ldots,s_r\}$ is connected if and only if S generates Γ. This means a graph $\mathrm{ICG}(n,\mathcal{D})$ with $\mathcal{D} = \{d_1,\ldots,d_r\}$ is connected if and only if $\gcd(n, d_1,\ldots,d_r) = 1$ (cf. [**28**]). For $n = p^s$ this is equivalent to $1 \in \mathcal{D}$, which translates to the condition $a_1 = 0 < a_2 < \ldots < a_r \le s-1$. Clearly, the energies of graph components add up, so we could restrict ourselves to connected graphs. However, we shall generally permit $a_1 > 0$, since there is virtually no extra complexity introduced by this.

We now present some easy consequences of Theorem 2.1, i.e. for simple integral circulant graphs. The straightforward proof of the following corollary is left to the reader.

Corollary 2.1. *Let p be a prime and s an arbitrary positive integer.*

(i) *For $r = 1$, i.e. $\mathcal{D} = \{p^t\}$ with some non-negative integer $t \le s-1$, we have $\mathcal{E}(p^s,\mathcal{D}) = 2(p-1)p^{s-1}$.*

(ii) *For $\mathcal{D} = \{1, p^{s-1}\}$, i.e. $s \ge r = 2$ and $a_1 = 0$, $a_2 = s-1$, we have $\mathcal{E}(p^s,\mathcal{D}) = 2(p-1)(2p^{s-1} - p + 1)$.*

(iii) *For $\mathcal{D} = \{1, p, p^2, \ldots, p^{r-1}\}$ with $r \le s$, i.e. $a_i = i-1$ $(1 \le i \le r)$, we have $\mathcal{E}(p^s,\mathcal{D}) = 2(p^s - p^{s-r})$.*

Our formula in Theorem 2.1 makes it obvious that $\mathcal{E}(p^s,\mathcal{D})$ is always an integer divisible by $2(p-1)$. This is in line with the work of Bapat and Pati [**5**] who showed that the energy of any graph is never an odd integer (see also [**23**]).

Recalling our introductory remarks on hyperenergeticity we observe that for each fixed p^s, $p \ge 3$ and $s \ge 3$, there exist lots of integral circulant graphs which are hyperenergetic, but some are not. In fact, the integral circulant graphs in Corollary 2.1(ii), for instance, are apparently hyperenergetic for all primes $p \ge 3$ and all $s \ge 3$. Since the graph with $r = s$ in Corollary 2.1(iii) happens to be the complete graph K_{p^s}, we also have integral circulant graphs on the edge of hyperenergeticity. Finally, the integral circulant graphs in Corollary 2.1(iii) with $r < s$ as well as those in Corollary 2.1(i) are even hypoenergetic, i.e. there energy lies below that of the corresponding complete graph K_{p^s}.

As an easy consequence of Theorem 2.1 we obtain the following characterisation of the hyperenergetic integral circulant graphs $\mathrm{ICG}(p^s,\mathcal{D})$.

Corollary 2.2. *Let p be a prime and s an arbitrary positive integer. Then* $\mathrm{ICG}(p^s, \mathcal{D})$ *with* $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$, $0 \le a_1 < a_2 < \ldots < a_r \le s-1$, *is hyperenergetic if and only if*

$$\sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}} < \frac{1}{p-1} \left(r - \frac{p^s - 1}{p^{s-1}(p-1)} \right).$$

3. INTEGRAL CIRCULANT GRAPHS WITH MINIMAL OR MAXIMAL ENERGY

In the preceding section we have seen that the class of integral circulant graphs stretches over a wide range from low-energetic to high-energetic graphs. As a further application of our formula for the energy of a integral circulant graph with prime power order we take a look at graphs with extremal energy. For fixed p^s the integral circulant graph(s) $\mathrm{ICG}(p^s, \mathcal{D})$ with minimal energy will be described most readily by identifying the corresponding divisor sets $\mathcal{D}$ as the singletons. The graphs with maximal energy, however, do not reveal any noticeable pattern, and a general specification seems to be out of reach. Yet we shall provide results for prime powers p^s with small exponents.

For simplicity we restrict ourselves to simple graphs from now on, although integral circulant graphs with loops could be incorporated without any further problems. Accordingly, we define

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

as well as

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

for any given positive integer n. A set $\mathcal{D} \subseteq \{1 \le d < n : \ d \mid n\}$ will be called *n-minimal* if $\mathcal{E}(n, \mathcal{D}) = \mathcal{E}_{\min}(n)$, and *$n$-maximal* if $\mathcal{E}(n, \mathcal{D}) = \mathcal{E}_{\max}(n)$.

We shall easily see in the next theorem that the sets $\mathcal{D} = \{p^t\}$ in Corollary 2.1(i) are exactly the p^s-minimal sets of divisors. Consequently, there is a unique *connected* integral circulant graph on p^s vertices with minimal energy, namely the respective unitary Cayley graph. This does not hold in general, as can be seen for $n = 6$, where $\mathcal{D} = \{1, 3\}$ is the unique minimizing divisor set.

Theorem 3.1. *Let p be a prime and s an arbitrary positive integer. Then*

$$\mathcal{E}_{\min}(p^s) = 2(p-1)p^{s-1},$$

and the p^s-minimal sets of divisors are exactly the sets $\mathcal{D} = \{p^t\}$ with $t = 0, 1, \ldots, s-1$.

Proof. By Corollary 2.1(i) we know that $\mathcal{E}(p^s, \mathcal{D}) = 2(p-1)p^{s-1}$ for each $\mathcal{D} = \{p^t\}$, $t = 0, 1, \ldots, s-1$, i.e. for each possible set $\mathcal{D}$ having $r = 1$ elements. Therefore, it suffices to show that $\mathcal{E}(p^s, \mathcal{D}) > 2(p-1)p^{s-1}$ for $r \ge 2$.

For $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ with $0 \le a_1 < a_2 < \ldots < a_r \le s-1$ and $r \ge 2$ we have

$$\sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}} < \sum_{k=1}^{r-1} \sum_{j=1}^{\infty} \frac{1}{p^j} = \frac{r-1}{p-1}.$$

Hence Theorem 2.1 implies $\mathcal{E}(p^s, \mathcal{D}) > 2(p-1)p^{s-1}$. $\square$

We now turn our attention to $\mathcal{E}_{\max}(p^s)$. For given $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$, $0 \le a_1 < \ldots < a_r \le s-1$, we have by Theorem 2.1

$$\mathcal{E}(p^s, \mathcal{D}) = 2(p-1)p^{s-1} \left(r - (p-1) h_p(a_1, \ldots, a_r) \right), \tag{9}$$

where

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

for arbitrary real numbers $x_1, \ldots, x_r$. In order to evaluate $\mathcal{E}_{\max}(p^s)$ we first want to determine

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

For that reason we define for integers $1 \le r \le s+1$

$$\begin{aligned} m_p(s, r) &:= \min \{ h_p(a_1, \ldots, a_r) : 0 \le a_1 < a_2 < \cdots < a_r \le s \text{ with } a_i \in \mathbb{Z} \} \\ &= \min \{ h_p(0, a_2, \ldots, a_{r-1}, s) : 0 < a_2 < \cdots < |1 a_{r-1} < s \text{ with } a_i \in \mathbb{Z} \}, \end{aligned} \tag{10}$$

the latter identity being a consequence of the structure of h_p. It is clear from (9) that

$$\mathcal{E}_{\max}(p^s, r) = 2(p-1)p^{s-1} \left(r - (p-1) m_p(s-1, r) \right). \tag{11}$$

Later on it remains to compute

$$\mathcal{E}_{\max}(p^s) = \max \{ \mathcal{E}_{\max}(p^s, r) : \ 1 \le r \le s \}. \tag{12}$$

Note that it follows from (10), thus $1 \in \mathcal{D}$, and an earlier remark that graphs $\mathrm{ICG}(p^s, \mathcal{D})$ with maximum energy are necessarily connected.

Proposition 3.1. *Let p be a prime. Then*

(i) $m_p(s, 2) = \dfrac{1}{p^s}$ *for all integers $s \ge 1$, and the minimum is attained only for $a_1 = 0$ and $a_2 = s$.*

(ii) $m_p(s, 3) = \dfrac{1}{p^{[s/2]}} + \dfrac{1}{p^s} + \dfrac{1}{p^{s-[s/2]}}$ *for all integers $s \ge 2$. The minimum is only obtained for $a_1 = 0$, $a_2 = [s/2]$ (or, alternatively, for $a_2 = [s/2] + 1$ if s is odd) and $a_3 = s$.*

Proof. (i) is clear by (10).

(ii) We need to consider $h_p(0,a_2,s) = \frac{1}{p^{a_2}} + \frac{1}{p^s} + \frac{1}{p^{s-a_2}}$. By simple analysis one finds the minimum of $1/p^x + 1/p^{s-x}$ for real x to be at $x = s/2$. Since a_2 is an integer, our minimum is attained for $a_2 = [s/2]$ (or, alternatively, for $a_2 = [s/2]+1$ in case s is odd). □

The determination of $m_p(s,r)$ in general seems not to be so easy, even for $r = 4$. This topic will be further discussed in the concluding section.

Theorem 3.2. *Let p be a prime. Then*

(i) $\mathcal{E}_{\max}(p) = 2(p-1)$ *with the only p-maximal set $\mathcal{D} = \{1\}$.*

(ii) $\mathcal{E}_{\max}(p^2) = 2(p-1)(p+1)$ *with the only p^2-maximal set $\mathcal{D} = \{1,p\}$.*

(iii) $\mathcal{E}_{\max}(p^3) = 2(p-1)(2p^2-p+1)$ *with the only p^3-maximal set $\mathcal{D} = \{1,p^2\}$, except for the prime $p = 2$ for which $\mathcal{D} = \{1,2,4\}$ is also 2^3-maximal.*

(iv) $\mathcal{E}_{\max}(p^4) = 2(p-1)(2p^3+1)$ *with the only p^4-maximal sets $\mathcal{D} = \{1,p,p^3\}$ and $\mathcal{D} = \{1,p^2,p^3\}$.*

Proof. (i) In this case $\mathcal{D} = \{1\}$ is the only possible divisor set. Therefore Corollary 2.1(i) implies

$$\mathcal{E}_{\max}(p) = \mathcal{E}(p,\{1\}) = 2(p-1).$$

(ii) By Corollary 2.1(i) we have $\mathcal{E}(p^2,\{p^{a_1}\}) = 2(p-1)p$ for $a_1 \in \{1,p\}$. By Corollary 2.1(ii) we know that

$$\mathcal{E}(p^2,\{1,p\}) = 2(p-1)p(2-(p-1)m_p(1,2)) = 2(p-1)(p+1).$$

Since $\{1\}$, $\{p\}$ and $\{1,p\}$ are the only possible divisor sets, (ii) is proven.

(iii) Again by Corollary 2.1(i) we get $\mathcal{E}(p^3,\{p^{a_1}\}) = 2(p-1)p^2$ for $a_1 \in \{1,p,p^2\}$. It follows from Corollary 2.1(iii) that

$$\mathcal{E}(p^3,\{1,p,p^2\}) = 2(p-1)(p^2+p+1).$$

It remains to look at divisor sets with exactly two elements. By (11) and Proposition 3.1(i) we have

$$\max_{|\mathcal{D}|=2} \mathcal{E}(p^3,\mathcal{D}) = 2(p-1)p^2(2-(p-1)m_p(2,2)) = 2(p-1)(2p^2-p+1),$$

and the maximum is attained only for $\mathcal{D} = \{1,p^2\}$. Comparison of the energies completes the proof of (iii).

(iv) As before $\mathcal{E}(p^4,\{p^{a_1}\}) = 2(p-1)p^3$ for $a_1 \in \{1,p,p^2,p^3\}$. By (11) and Proposition 3.1(i) we obtain

$$\max_{|\mathcal{D}|=2} \mathcal{E}(p^4,\mathcal{D}) = 2(p-1)p^3(2-(p-1)m_p(3,2)) = 2(p-1)(2p^3-p+1),$$

and with Proposition 3.1(ii) we get

$$\max_{|\mathcal{D}|=3} \mathcal{E}(p^4, \mathcal{D}) = 2(p-1)p^3(3-(p-1)m_p(3,3)) = 2(p-1)(2p^3+1)$$

where the maximum is attained only for $\mathcal{D} = \{1, p, p^3\}$ and $\mathcal{D} = \{1, p^2, p^3\}$. Finally $\mathcal{E}(p^4, \{1, p, p^2, p^3\}) = 2(p-1)(p^3+p^2+p+1)$, by Corollary 2.1(iii). Comparing all the cases yields the desired result. □

4. CONCLUDING REMARKS AND OPEN PROBLEMS

Proposition 3.1 indicates how to approach $\mathcal{E}_{\max}(p^s)$ with arbitrary exponent s. The problem is to determine $m_p(s-1, r)$ in general, i.e. to choose integers $0 \leq a_1 \leq a_2 \leq \ldots \leq a_r \leq s-1$ in such a way that

$$h_p(a_1, \ldots, a_r) = \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}}$$

becomes minimal. It is obvious that we have to pick $a_1 = 0$ and $a_r = s-1$. According to a remark made in section 2, this incidentally means that graphs $\mathrm{ICG}(p^s, \mathcal{D})$ with maximal energy are per se connected.

A first guess, guided by some vague concept of symmetry, suggests to select $a_1, a_2, \ldots, a_{r-1}, a_r$ equidistant in the interval $[0, s-1]$, as we did in case $r = 3$ (cf. Prop. 3.1(ii)). Let us support this intuition by an informal analytic argument for the case $r = 4$. In order to minimize $h_p(0, a_2, a_3, s-1)$, we first fix a_3 and find by differentiation that

$$\frac{\partial h_p(0, a_2, a_3, s-1)}{\partial a_2} = 0$$

is satisfied for

$$a_2 = \frac{a_3}{2} - \frac{1}{2\log p} \log\left(1 + \frac{1}{p^{s-1-a_3}}\right),$$

hence $a_2 \approx \frac{a_3}{2}$ for large p. We observe that

$$h_p(0, a_2, a_3, s-1) = h_p(0, s-1-a_3, s-1-a_2, s-1),$$

which yields that $s-1-a_3 \approx \frac{s-1-a_2}{2}$ by the argument above. Putting everything together, we obtain $a_3 \approx \frac{2}{3}(s-1)$ and $a_2 \approx \frac{1}{3}(s-1)$.

The difficulty with the corresponding choice $a_i := \frac{(i-1)(s-1)}{r-1}$ $(1 \leq i \leq r)$ in general is the requirement that our a_i have to be integers. One would assume that an integral minimizer of h_p can be found in the vicinity of this choice.

For example, consider $n = p^s = 2^{12}$:

$(0, a_2, a_3, 11)$	$h_p(0, a_2, a_3, 11)$	$\mathcal{E}(2^{12}, \mathcal{D})$
$(0, 3.\overline{6}, 7.\overline{3}, 11)$	*0.2491250473*	*15363.58381*
$(0, 3, 7, 11)$	0.2622070312	15310
$(0, 3, 8, 11)$	0.2895507812	15198
$(0, 4, 7, 11)$	0.2661132812	15294
$(0, 4, 8, 11)$	0.2622070312	15310
$(0, 2, 7, 11)$	0.3540039062	14934
$(0, 3, 6, 11)$	0.3012695312	15150

The first line in the table evaluates h_p for the equidistant choice of rational exponents $a_i := \frac{(i-1)(s-1)}{r-1}$. Here we formally calculate the energy according to (9) (as the original equation (1) makes no sense in this relaxed context). The next group of entries explores the integral vicinity of $(0, 3.\overline{6}, 7.\overline{3}, 11)$ by means of rounding, whereas the bottom group strays even farther. The table contents indicate what can be verified by considering all valid tuples, namely, that $(0, 3, 7, 11)$ and $(0, 4, 8, 11)$ yield $m_p(11, 4)$ and $\mathcal{E}_{\max}(2^{12}, 4)$. Moreover, these tuples can be derived from the equidistant approximate tuple by suitable rounding.

Interestingly, it turns out that in general even for real a_i their equidistant positioning does not necessarily yield the real minimum of h_p. This phenomenon crops up for $r \geq 4$. In our example $n = 2^{12}$, we have $\min h_p(a_1, \ldots, a_4) = 0.2489650992\ldots = h_p(0, 3.629295009\ldots, 7.370704991\ldots, 11)$, the corresponding energy being approximately 15364.23895.

As another example, take $n = 3^{11}$. Then $h_p\left(0, \frac{10}{3}, \frac{20}{3}, 10\right) \approx 0.783760$ whereas the minimum of $h_p(0, a, b, 10)$ is approximately 0.783704 and is achieved for $a \approx 3.32557502$ and $b \approx 6.67442498$.

One way of proceeding further would be to be satisfied with simply taking nearest integers of the equidistant exponent tuple and derive approximate energy formulae. To this end, it would be beneficial to gain further insight into the structure of divisor sets $\mathcal{D}$ producing integral circulant graphs $\mathrm{ICG}(p^s, \mathcal{D})$ whose energy is equal or at least close to $\mathcal{E}_{\max}(p^s)$. This should be an object of future research.

If one thinks about extending any of the results already obtained to arbitrary n, then the most desirable situation would be if $\mathcal{E}_{\max}(n)$ exhibited multiplicative behaviour with respect to n. For the simple case $n = pq$ with distinct odd primes p, q this is indeed true. By considering the few possible divisor sets and using the results of [**25**] and [**15**] mentioned in the introduction, one easily finds that $\mathcal{E}_{\max}(pq) = \mathcal{E}_{\max}(p)\mathcal{E}_{\max}(q)$. However, we could not detect anything similar for more complex n. Given distinct primes p and $q \neq 2$, direct use of formula (1) yields e.g. that $\mathcal{E}_{\max}(p^2q) = 2\,(4p^2q - 6pq + 3q - 5p^2 + 8p - 4)$, not looking closely related to $\mathcal{E}_{\max}(p^2) = 2(p-1)(p+1)$ and $\mathcal{E}_{\max}(q) = 2(q-1)$ according to Theorem 3.2. Hence, it remains a major open question if it is at all possible to find a closed formula for the energy $\mathcal{E}(n, \mathcal{D})$ of integral circulant graphs with arbitrary n and $\mathcal{D}$.

Still, the case $n = p^s$ may turn out to be a valuable building block in settling this question. An answer would incorporate our Theorem 2.1 as well as the scattered results found in [**25**] and [**15**], forecited in the introduction.

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