Available online at www.sciencedirect.com
SCIENCE DIRECT®

Linear Algebra and its Applications 414 (2006) 378–382

LINEAR ALGEBRA AND ITS APPLICATIONS

www.elsevier.com/locate/laa

On the energy of some circulant graphs

Igor Shparlinski *

Department of Computing, Macquarie University, Sydney, NSW 2109, Australia

Received 5 October 2005; accepted 17 October 2005
Available online 7 December 2005
Submitted by R.A. Brualdi

Abstract

We give an explicit construction of circulant graphs of very high energy. This construction is based on Gauss sums. We also show the Littlewood conjecture can be used to establish new result for a certain class of circulant graphs.

AMS classification: 05C35; 05C50; 11T24; 42A05

Keywords: Energy of graphs; Circulant graphs; Gauss sums; Littlewood conjecture

1. Introduction

Given a graph $\mathscr{G}$ with n vertices and eigenvalues $\lambda_0, \ldots, \lambda_{n-1}$, we define its *energy* as

$$E(\mathscr{G}) = \sum_{j=0}^{n-1} |\lambda_j|.$$

This notion is related to some applications of graph theory to chemistry and has been studied intensively in the literature, see [1,3,5,6,9–12,15,17] and references therein. In particular, it is shown in [9] that

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

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

* Tel.: +61 2 9850 9585; fax: +61 2 9850 9551.
E-mail address: igor@comp.mq.edu.au

0024-3795/$ - see front matter
doi:10.1016/j.laa.2005.10.020

For the family of bipartite graphs a stronger bound

$$E(\mathscr{G}) \leqslant \frac{n}{4}(\sqrt{2n}+2)$$

has been shown in [10]. Here we give an explicit construction of an infinite family of circulant graphs which attain the bound (1) asymptotically.

We now recall that an n-vertex graph $\mathscr{G}$ is called *hyperenergetic* if $E(\mathscr{G}) > 2(n-1)$. This concept has been introduced in [4] in relation to some problems of molecular chemistry.

Recently several results have been obtained for the hyperenergetic circulant graphs, see [1,17]. In particular, it is well known that the complete n-vertex graph $\mathscr{K}_n$ satisfies $E(\mathscr{K}_n) = 2(n-1)$. In [1] a conjecture is made that the graphs obtained from $\mathscr{K}_n$ by removing a Hamiltonian circuit are not hyperenergetic. It fact, in [17] this conjecture has been shown to be wrong for this and an even more general class of circulant graphs. Here we derive a somewhat stronger, albeit less explicit, lower bound on the energy of such graph.

Our proofs follow almost immediately from two classical number theoretic results, the formula for the absolute value of *Gauss sums*, see [13, Chapter 5] and the *Littlewood conjecture*, which has been independently settled by Konyagin [8] and McGehee et al. [14], see also [16].

2. Background on circulant graphs

For an integer $n \geqslant 1$ we let $\mathbb{Z}_n$ denote the residue ring modulo n, which we assume to be represented by the integers $\{1, \dots, n\}$.

Given a subset $\mathscr{S} \subseteq \{1, \dots, \lfloor n/2 \rfloor\}$ an indirected n-vertex *circulant graph* $\mathscr{C}_n(\mathscr{S})$ is a graph whose vertices are labeled by elements of $\mathbb{Z}_n$ and the vertices $i, j \in \mathbb{Z}_n$, are connected if and only if either $j - i \in \mathscr{S}$ (certainly we compute $i - j$ in $\mathbb{Z}_n$ and also treat $\mathscr{S}$ as a subset of $\mathbb{Z}_n$).

We also define $\overline{\mathscr{C}}_n(\mathscr{S})$ as the complement of $\mathscr{C}_n(\mathscr{S})$, which is clearly is also a circulant graph. Moreover

$$\overline{\mathscr{C}}_n(\mathscr{S}) = \mathscr{C}_n(\mathscr{R}),$$

where

$$\mathscr{R} = \{1, \dots, \lfloor n/2 \rfloor\} \setminus \mathscr{S}. \tag{2}$$

Let us define $\mathbf{e}(z) = \exp(2\pi \iota z)$ where $\iota = \sqrt{-1}$. Then, it is well known that for $\mathscr{S} \subseteq \{1, \dots, \lfloor n/2 \rfloor\}$, the eigenvalues of the graph $\mathscr{G}_n(\mathscr{S})$ are given by

$$\lambda_j(\mathscr{S}) = \sum_{s \in \mathscr{S} \cup -\mathscr{S}} \mathbf{e}(js/n), \quad j = 0, 1, \dots, n-1. \tag{3}$$

In particular, if $\mathscr{R}$ is given by (2), then we easily see that

$$\lambda_0(\mathscr{S}) = 2\#\mathscr{S} - \delta(\mathscr{S}) \quad \text{and} \quad \lambda_0(\mathscr{R}) = n - 2\#\mathscr{S} - 1 + \delta(\mathscr{S}), \tag{4}$$

where $\delta(\mathscr{S}) = 1$ if $n/2 \in \mathscr{S}$ and $\delta(\mathscr{S}) = 0$ otherwise. Also

$$\lambda_j(\mathscr{S}) + \lambda_j(\mathscr{R}) = \sum_{s=1}^{n-1} \mathbf{e}(js/n) = -1, \quad j = 1, \dots, n-1. \tag{5}$$

3. Highly energetic circulants

Let p be a prime number. We denote by $\mathscr{Q}_p$ the set of all quadratic residues modulo p in the set $\{1, \dots, (p-1)/2\}$.

Theorem 1. *For any prime* $p \equiv 1 \pmod 4$, *we have*

$$E(\mathscr{C}_p(\mathscr{Q}_p)) \geqslant \frac{(p-1)(p^{1/2}+1)}{2}.$$

Proof. Since -1 is a quadratic residue modulo $p \equiv 1 \pmod 4$, we see that $\mathscr{Q}_p \cup -\mathscr{Q}_p$ is the set of all $(p-1)/2$ quadratic residues modulo p. Therefore, by (4) we obtain $\lambda_0(\mathscr{Q}_p) = (p-1)/2$. Also, from (3) we derive that for $j = 1, \ldots, p-1$ we have

$$|\lambda_j(\mathscr{Q}_p)| = \sum_{s \in \mathscr{Q}_p \cup -\mathscr{Q}_p} \mathbf{e}(js/p) = \frac{1}{2}\sum_{u=1}^{p-1} \mathbf{e}(ju^2/p)$$

since for every quadratic residue s the congruence $s \equiv u^2 (\mathrm{mod}\ p)$ has exactly two solutions. Recalling the properties of Gauss sums, see [13, Theorems 5.15 and 5.33], we see that

$$\sum_{u=1}^{p-1} \mathbf{e}(ju^2/p) = \sum_{u=0}^{p-1} \mathbf{e}(ju^2/p) - 1 = \begin{cases} p^{1/2} - 1, & \text{if } j \in \mathscr{Q}_p; \\ -p^{1/2} - 1, & \text{otherwise}; \end{cases}$$

for $j = 1, \ldots, p-1$. Therefore

$$|\lambda_j(\mathscr{Q}_p)| = \begin{cases} (p^{1/2}+1)/2, & \text{if } j \in \mathscr{Q}_p; \\ (p^{1/2}-1)/2, & \text{otherwise}; \end{cases} \qquad j = 1, \ldots, p-1$$

and after simple calculations the result follows. $\square$

4. Circulants with fixed links and the Littlewood conjecture

As we have remarked, it has been conjectured in [1] that the graphs obtained from the complete n-vertex graph $\mathscr{K}_n$ by removing a Hamiltonian circuit, that is, the graphs $\overline{\mathscr{C}}_n(\{1\})$, are not hyperenergetic. This conjecture has turned out to be wrong and in fact it is shown in [17] that the following limit exists and also that

$$\liminf_{n \to \infty} E(\overline{\mathscr{C}}_n(\mathscr{S}))/n > 2$$

for any fixed set $\mathscr{S} = \{s_1, \ldots, s_m\}$ of $m \geqslant 1$ distinct positive integers. Here we show that in fact more is true for these graphs and also for their complements $\mathscr{C}_n(\mathscr{S})$.

Let us define the constants κ_r, $r = 1, 2, \ldots$, by the equation

$$\kappa_r = \inf_{\#\mathscr{U}=r} \frac{1}{2\pi} \int_0^1 \left| \sum_{u \in \mathscr{U}} \mathbf{e}(\alpha u) \right| \mathrm{d}\alpha,$$

where the infimum is taken over all r-element sets $\mathscr{U}$ of integers. We recall that the famous Littlewood conjecture, which has been proved by Konyagin [8] and McGehee et al. [14], asserts that

$$\kappa_r > C \log r, \tag{6}$$

where $C > 0$ is an absolute constant. Moreover, Stegeman [16] has proved that one can take

$$C = \frac{4}{\pi^3}, \tag{7}$$

while is expected that in fact (6) holds for any $C < 4/\pi^2$, provided that r is large enough.

Theorem 2. *For any fixed set* $\mathscr{S} = \{s_1, \ldots, s_m\}$ *of* $m \geqslant 1$ *distinct positive integers, we have*

$$\lim_{n\to\infty} E(\overline{\mathscr{C}}_n(\mathscr{S}))/n \geqslant 1 + \kappa_{2m}.$$

Proof. We have

$$E(\overline{\mathscr{C}}_n(\mathscr{S})) = \sum_{j=0}^{n-1} |\lambda_j(\mathscr{R})|,$$

where $\mathscr{R}$ is given by (2). Assuming that $n > 2m$, by (4) and (5), we derive

$$E(\overline{\mathscr{C}}_n(\mathscr{S})) = n - 2m - 1 + \sum_{j=1}^{n-1} |1 + \lambda_j(\mathscr{S})|.$$

Since

$$f(\alpha) = \left|1 + \sum_{s\in\mathscr{S}\cup-\mathscr{S}} \mathbf{e}(\alpha s)\right|$$

is a continuous function of α, we see that by (3) that

$$\begin{aligned}
\frac{1}{n-1}\sum_{j=1}^{n-1} |1 + \lambda_j(\mathscr{S})| &= \frac{1}{n-1}\sum_{j=1}^{n-1} \left|\sum_{s\in\mathscr{S}\cup-\mathscr{S}\cup\{0\}} \mathbf{e}(js/n)\right| \\
&= \int_0^1 \left|\sum_{s\in\mathscr{S}\cup-\mathscr{S}\cup\{0\}} \mathbf{e}(\alpha s)\right| d\alpha + o(1) \\
&\geqslant \kappa_{2m+1} + o(1)
\end{aligned}$$

which finishes the proof. $\square$

In particular, we see from (6), (7) and Theorem 2 that

$$\lim_{n\to\infty} E(\overline{\mathscr{C}}_n(\mathscr{S}))/n > 1 + \frac{4}{\pi^3}\log(2m).$$

Certainly the same arguments also apply that under the conditions of Theorem 2 we have

$$\lim_{n\to\infty} E(\mathscr{C}_n(\mathscr{S}))/n \geqslant \kappa_{2m} > \frac{4}{\pi^3}\log(2m).$$

5. Remarks

It is easy to see that the bound (6) is tight up to the value of the constant. For example, it is attained for the set $\mathscr{U} = \{1, \ldots, r\}$. However for some sets $\mathscr{U}$ satisfying some additional properties it can be improved. Typically for such special sets $\log r$ can be replaced with $r^{1/2}$, see [2,7] and references therein. Accordingly, one can improve Theorem 2 for sets $\mathscr{S}$ satisfying some special properties.

There is also a reverse link between graph theory and number theory. For example, Lemma 2.4 of [15] generalises a result of [7].

Acknowledgments

The author is very grateful to Ivan Gutman for many useful discussions and encouragement. During the preparation of this paper, the author was supported in part by ARC grant DP0556431.

References

[1] R. Balakrishnan, The energy of a graph, Linear Algebra Appl. 387 (2004) 287–295.
[2] M.Z. Garaev, Upper bounds for the number of solutions of a diophantine equation, Trans. Amer. Math. Soc. 357 (2005) 2527–2534.
[3] I. Gutman, The energy of a graph, Ber. Math.-Stat. Sekt. Forschungszent. Graz 103 (1978) 1–22.
[4] I. Gutman, Hyperenergetic molecular graphs, J. Serb. Chem. Soc. 64 (1999) 199–205.
[5] I. Gutman, The energy of a graph: old and new results, Algebraic Combinatorics and Applications (Gößweinstein, 1999), Springer, Berlin, 2001, pp. 196–211.
[6] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total pi-electron energy on molecular topology, J. Serb. Chem. Soc. 70 (2005) 441–456.
[7] A.A. Karatsuba, An estimate of the L_1-norm of an exponential sum, Mat. Zametki 64 (1998) 401–404 (in Russian).
[8] S.V. Konyagin, On the Littlewood problem, Izv. Akad. Nauk SSSR Ser. Mat. 45 (1981) 243–265 (in Russian).
[9] J.H. Koolen, V. Moulton, Maximal energy graphs, Adv. Appl. Math. 26 (2001) 47–52.
[10] J.H. Koolen, V. Moulton, Maximal energy bipartite graphs, Graphs Combin. 19 (2003) 131–135.
[11] F. Li, B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, MATCH Commun. Math. Comput. Chem. 54 (2005) 379–388.
[12] W. Liu, X. Guo, H. Li, On the extremal energies of trees with a given maximum degree, MATCH Commun. Math. Comput. Chem. 54 (2005) 363–378.
[13] R. Lidl, H. Niederreiter, Finite Fields, Cambridge University Press, Cambridge, 1997.
[14] O.C. McGehee, L. Pigno, B. Smith, Hardy's inequality and the L^1 norm of exponential sums, Ann. Math. 113 (1981) 613–618.
[15] J. Rada, A. Tineo, Upper and lower bounds for the energy of bipartite graphs, J. Math. Anal. Appl. 289 (2004) 446–455.
[16] J.D. Stegeman, On the constant in the Littlewood problem, Math. Ann. 261 (1982) 51–54.
[17] D. Stevanović, I. Stanković, Remarks on hyperenergetic circulant graphs, Linear Algebra Appl. 400 (2005) 345–348.