

Kneser Graphs and their Complements are Hyperenergetic

S. AKBARI^{a,b}, F. MOAZAMI^b, S. ZARE^b

^a*Institute for Studies in Theoretical Physics and Mathematics,*

P. O. Box 19395-5746, Tehran, Iran

^b*Department of Mathematical Sciences, Sharif University of Technology,*

P. O. Box 11365-9415, Tehran, Iran

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Abstract

A graph G of order n is called hyperenergetic if $E(G) > 2n - 2$, where $E(G)$ is the energy of G . In this paper it is shown that Kneser graph $K_{n:r}$ is hyperenergetic for any naturals n and $r \geq 2$ with $n \geq 2r + 1$. Also we prove that for $r \geq 2$, the complement of Kneser graph, $E(\overline{K_{n:r}})$, is hyperenergetic.

*E-mail addresses: s_akbari@sharif.edu (S. Akbari), sa_zare.f@yahoo.com (S. Zare), farokhlagha_moazami@yahoo.com (F. Moazami).

I. Introduction

Let G be a graph with n vertices, m edges and eigenvalues $\lambda_1, \dots, \lambda_n$. The *energy* of G is defined as $E(G) = |\lambda_1| + \dots + |\lambda_n|$. We call n the order of G . The energy of a graph has recently been much studied in the mathematical-chemistry literature, for instance see, [1], [4], [5], [6], [7].

In the theory of conjugated molecules the total π -electron energy and various “resonance energies” derived from it, plays an outstanding role, for more details see [8]. The graph G is said to be *hyperenergetic* if its energy exceeds the energy of K_n ; that is, if $E(G) > 2n - 2$. Otherwise, G is called *non-hyperenergetic*. The concept of *hyperenergeticity* was introduced first by I. Gutman, see [11]. In [12], I. Gutman conjectured that $E(G) \leq 2n - 2$ holds for all graphs with n vertices.

This conjecture is false. The first counterexample was found in 1986 using Cvetkovics’s computer system graphs, see [3]. In 1998, by means of Monte Carlo construction of graphs with n vertices and $1, 2, \dots, \frac{n(n-1)}{2}$ edges, it became clear that among graph with large number of edges there are numerous species whose energies are greater than $2(n - 1)$. Almost in the same time the Indian mathematician Walinkar with coworkers communicated the first systematic construction of such graphs. It has been prove that for every $n \geq 8$, there exists a hyperenergetic graph of order n , see Corollary 7.8 of [9]. Hyperenergetic graphs are important because molecular graphs with maximum energy pertain to maximality stable π -electron systems.

The line graph $L(G)$ of a graph G is constructed by taking the edges of G as vertices of $L(G)$, and joining two vertices in $L(G)$, whenever the corresponding edges in G have a common vertex. In [13] it is shown that if a graph of order n has more

than $2n - 1$ edges, then its line graph is hyperenergetic. Thus the line graph of every k -regular graph with $k > 3$ is hyperenergetic. Recently a very large number of papers on hyperenergetic graphs has been published, for instance see [9, 10, 11, 13, 15].

The *Kneser graph* $K_{n:r}$ is the graph whose vertices are the r -subsets of an n -set, with two vertices adjacent if and only if the sets are disjoint. In [14] it is shown that the eigenvalues of the Kneser graph $K_{n:r}$ are $(-1)^i \binom{n-r-i}{r-i}$ with multiplicity $\binom{n}{i} - \binom{n}{i-1}$, for $i = 0, 1, \dots, r$. Thus $E(K_{n:r}) = \sum_{i=0}^r \left(\binom{n}{i} - \binom{n}{i-1} \right) \binom{n-r-i}{r-i}$.

We begin with the following lemma.

Lemma 1. *If $n = 2r + 1$, then $E(K_{n:r}) = 2^{2r}$. Thus for $r \geq 4$, the Kneser graph $K_{n:r}$ is hyperenergetic.*

Proof. We have

$$E(K_{n:r}) = \sum_{i=0}^r \left(\binom{n}{i} - \binom{n}{i-1} \right) \binom{n-r-i}{r-i}.$$

This follows that for $n = 2r + 1$,

$$\begin{aligned} E(K_{n:r}) &= \sum_{i=0}^r \binom{2r+1}{i} (r+1-i) - \sum_{i=0}^r \binom{2r+1}{i-1} (r+1-i) = \\ &= (r+1) \binom{2r+1}{r} - r \binom{2r+1}{r} + \sum_{i=0}^r \binom{2r+1}{i-1} = \sum_{i=0}^r \binom{2r+1}{i} = \\ &= \sum_{i=0}^r \binom{2r+1}{i} + \sum_{i=r+1}^{2r+1} \binom{2r+1}{2r+1-i} - \sum_{i=r+1}^{2r+1} \binom{2r+1}{2r+1-i} = 2^{2r+1} - \sum_{i=0}^r \binom{2r+1}{i}. \end{aligned}$$

Therefore we obtain that $E(K_{n:r}) = 2^{2r}$.

Now, by induction on r , it is not hard to see that

$$2^{2r} > 2 \binom{2r+1}{r} - 2.$$

□

In the next theorem we show that almost all Kneser graphs are hyperenergetic.

Theorem 1. *For any natural numbers, $r \geq 2$ and $n \geq 2r + 2$, the Kneser graph $K_{n,r}$ is hyperenergetic.*

Proof. If $r = 2$, then we have $E(K_{n,2}) = 2(n - 1)(n - 3)$. By assumption $n \geq 6$ and so $2(n - 1)(n - 3) > 2\binom{n}{2} - 1$.

If $r = 3$, then by an easy calculation we find that $E(K_{n,3}) = \frac{4}{3}(n - 1)(n - 3)(n - 5)$. Now, since $n \geq 8$, we have $E(K_{n,3}) > 2\binom{n}{3} - 1$.

Now we consider two following cases:

Case 1. $2r + 2 \leq n \leq 3r - 1$. Since the following inequality holds

$$\binom{n-r}{r} \geq \binom{n-r-1}{r-1} \geq \dots \geq n - 2r + 1 \geq 3 \tag{1}$$

we have

$$\begin{aligned} E(K_{n,r}) &= \sum_{i=0}^r \left[\binom{n}{i} - \binom{n}{i-1} \right] \binom{n-r-i}{r-i} \\ &\geq 3 \sum_{i=0}^{r-1} \left[\binom{n}{i} - \binom{n}{i-1} \right] + \binom{n}{r} - \binom{n}{r-1} \\ &= \binom{n}{r} + \frac{2r}{n-r+1} \binom{n}{r}. \end{aligned}$$

Because of $n \leq 3r - 1$, we have $\frac{2r}{n-r+1} \geq 1$. So $E(K_{n,r}) \geq 2\binom{n}{r} > 2\left(\binom{n}{r} - 1\right)$.

Case 2. $n \geq 3r - 1, r \geq 4$. It is easy to see that

$$\binom{n}{i} - \binom{n}{i-1} \geq \frac{1}{2} \binom{n}{i}.$$

Therefore

$$E(K_{n,r}) \geq \frac{1}{2} \sum_{i=0}^r \binom{n}{i} \binom{n-r-i}{r-i}.$$

It is not hard to see that

$$\binom{n}{r-2} \binom{n-2r+2}{2} \geq 3 \binom{n}{r-1}.$$

For the proof of the above inequality it is sufficient to show that

$$\frac{r-1}{2} \frac{(n-2r+2)(n-2r+1)}{n-r+2} \geq 3.$$

Since $\frac{r-1}{2} \geq \frac{3}{2}$ and $\frac{(n-2r+2)(n-2r+1)}{n-r+2} \geq 2$, the above inequality holds.

Thus

$$E(K_{n:r}) \geq \frac{1}{2} \left(\binom{n}{r} + \binom{n}{r-1} (n-2r+4) \right).$$

We claim that $\binom{n}{r-1} (n-2r+4) \geq 3 \binom{n}{r}$.

To prove the above inequality it is enough to show that $n(r-3) - 2r^2 + 7r - 3 \geq 0$. Since $n \geq 3r - 1$ we have $n(r-3) - 2r^2 + 7r - 3 \geq r^2 - 3r \geq 0$. Hence we conclude that

$$E(K_{n:r}) \geq 2 \binom{n}{r} > 2 \left(\binom{n}{r} - 1 \right).$$

□

Lemma A. [2, p. 56] If G is regular graph of degree k of order n , then

$$P_{\overline{G}}(\lambda) = (-1)^n \frac{\lambda - n + k + 1}{\lambda + k + 1} P_G(-\lambda - 1),$$

which \overline{G} is complement of G .

By Lemma A the complement of Kneser graph, $\overline{K_{n:r}}$, has eigenvalues $\lambda_0 = \binom{n}{r} - \binom{n-r}{r} - 1$ and $\lambda_i = -1 - (-1)^i \binom{n-r-i}{r-i}$ with multiplicity $\binom{n}{i} - \binom{n}{i-1}$, for $i = 1, \dots, r$.

Now using the previous lemma we prove that the complement of Kneser graphs are hyperenergetic.

Theorem 2. *The complement of the Kneser graph for $r \geq 2$ is hyperenergetic .*

Proof. If $r = 2$, then $E(\overline{K_{n:2}}) = L(K_n)$. Therefore by Proposition 7.2 of [9], $E(\overline{K_{n:2}})$ is hyperenergetic. Let $r = 3$, it is not hard to see that $E(\overline{K_{n:3}}) = n(n - 3)(n - 4)$, so $E(\overline{K_{n:3}}) > 2\binom{n}{3} - 1$. Now suppose that $r > 3$ we have

$$E(\overline{K_{n:r}}) = \binom{n}{r} - \binom{n-r}{r} - 1 + \sum_{i=1}^r \left(\binom{n}{i} - \binom{n}{i-1} \right) \binom{n-r-i}{r-i} + \sum_{i=1}^{\lfloor \frac{r}{2} \rfloor} \left(\binom{n}{2i} - \binom{n}{2i-1} \right) - \sum_{i=0}^{\lceil \frac{r}{2} \rceil - 1} \left(\binom{n}{2i+1} - \binom{n}{2i} \right).$$

If r is even, then we have

$$E(\overline{K_{n:r}}) = E(K_{n:r}) - 2\binom{n-r}{r} + 2\sum_{i=1}^r (-1)^i \binom{n}{i}$$

and if r is odd, then

$$E(\overline{K_{n:r}}) = E(K_{n:r}) - 2\binom{n-r}{r} + 2\sum_{i=1}^{r-1} (-1)^i \binom{n}{i}.$$

Thus by Theorem 1, it is sufficient to show that for even r , $-2\binom{n-r}{r} + 2\sum_{i=1}^r (-1)^i \binom{n}{i} \geq 0$ and for odd r , $-2\binom{n-r}{r} + 2\sum_{i=1}^{r-1} (-1)^i \binom{n}{i} \geq 0$. By induction on r one can easily see that $\sum_{i=0}^r (-1)^i \binom{n}{i} = (-1)^r \binom{n-1}{r}$. Now, the proof is complete.

□

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