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 [†]

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.

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I. Introduction

Let G be a graph with n vertices, m edges and eigenvalues $\lambda_1, \ldots, \lambda_n$. The *energy of G* is defined as $E(G) = |\lambda_1| + \cdots + |\lambda_n|$. We call n the order of G. In chemistry, the energy of a graph is intensively studied since it can be used to approximate, the total π-electron energy of molecule.

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 [3]. 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 [6]. In [7] 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 [2]. In 1998, by means of Monte Carlo construction of graphs with n vertices and $1, 2, ..., \frac{n(n-1)}{2}$ edges, it became clear that among graph with large number of edges

[*] Corresponding author. Fax: +98-21-6005117.

[†] *E-mail addresses*: s_akbari@sharif.edu (S. Akbari), sa_zare_f@yahoo.com (S. Zare), farokhlagha_moazami@yahoo.com (F. Moazami).

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 [4]. 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 [8] 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 [4, 5, 6, 8, 10].

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 [9] 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 $i = 0, 1, \ldots, r$. Thus $E(K_{n:r}) = \sum_{i=0}^{r}(\binom{n}{i}-\binom{n}{i-1})\binom{n-r-i}{r-i}$.

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 $n = 2r+1$,

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

$$(r+1)\binom{2r+1}{r} - r\binom{2r+1}{r} + \sum_{i=0}^{r}\binom{2r+1}{i-1} = \sum_{i=0}^{r}\binom{2r+1}{i} =$$

$$\sum_{i=0}^{r}\binom{2r+1}{i} + \sum_{i=r+1}^{2r+1}\binom{2r+1}{2r+1-i} - \sum_{i=r+1}^{2r+1}\binom{2r+1}{2r+1-i} = 2^{2r+1} - \sum_{i=0}^{r}\binom{2r+1}{i}.$$

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

$$\binom{n-r}{r} \geq \binom{n-r-1}{r-1} \geq \cdots \geq n-2r+1 \geq 3 \qquad (1)$$

we have

$$E(K_{n:r}) = \sum_{i=0}^{r} \left(\binom{n}{i} - \binom{n}{i-1} \right) \binom{n-r-i}{r-i} \geq 3 \sum_{i=0}^{r-1} \left(\binom{n}{i} - \binom{n}{i-1} \right) + \binom{n}{r} - \binom{n}{r-1} =$$

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

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

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

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

□

Lemma A. [1, 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 $i = 1, \ldots, r$.

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 [4], $E(\overline{K_{n:2}})$ 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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