Energy and NEPS of Graphs

Dragan Stevanović

Faculty of Science and Mathematics
Višegradska 33, 18000 Niš, Serbia and Montenegro

and

Faculty of Economics
Kamenička 6, 11000 Beograd, Serbia and Montenegro

Abstract

The energy of a graph is the sum of the absolute values of the eigenvalues of the graph. We study the energy of the non-complete extended \( p \)-sum (NEPS) of graphs, a very general composition of graphs which special case is the product of graphs. We show that the energy of the product of graphs is the product of the energy of graphs, and how this result may be used to construct arbitrarily large families of noncospectral connected graphs having the same number of vertices and the same energy. Further, unlike the product, we show that the energy of any other NEPS of graphs cannot be represented as a function of the energy of starting graphs.

MSC 2000 Classification: 05C50

Keywords: Energy of a graph; Equienergetic graphs; Product of graphs.

1 Introduction

In this paper we consider only simple graphs with at least two vertices. Let \( G \) be a graph and let \(|G|\) denotes the number of its vertices. The eigenvalues \( \lambda_1, \lambda_2, \ldots, \lambda_{|G|} \) of an adjacency matrix of \( G \) are called the eigenvalues of \( G \), and form the spectrum of \( G \). The energy \( E(G) \) of the graph \( G \) is defined as

\[
E(G) = \sum_{i=1}^{|G|} |\lambda_i|.
\]

In chemistry, the energy of a graph is intensively studied since it can be used to approximate the total \( \pi \)-electron energy of a molecule (see, e.g., [6, 7]). Recently, the concept of energy started to attract considerable attention of mathematicians involved in the study of spectral graph theory; for some recent mathematical works on the energy of graphs see [1, 9-18, 21].

1 The author gratefully acknowledges support from the Grant 1389 of the Serbian Ministry of Science, Technology and Development.
Here we are interested in studying energy of certain compositions of graphs. The *non-complete extended p-sum* (shortly NEPS) of graphs is a very general graph operation. Many graph operations are special cases of NEPS, to name just the sum, product and strong product of graphs. It is defined for the first time in [5], while the following definition is taken from [4, p. 66], with a minor modification.

**Definition 1** Let $B$ be a set of binary $n$-tuples, i.e. $B \subseteq \{0, 1\}^n \setminus \{(0, \ldots, 0)\}$ such that for every $i = 1, \ldots, n$ there exists $\beta \in B$ with $\beta_i = 1$. The non-complete extended $p$-sum (NEPS) of graphs $G_1, \ldots, G_n$ with basis $B$, denoted by NEPS($G_1, \ldots, G_n; B$), is the graph with the vertex set $V(G_1) \times \ldots \times V(G_n)$, in which two vertices $(u_1, \ldots, u_n)$ and $(v_1, \ldots, v_n)$ are adjacent if and only if there exists $(\beta_1, \ldots, \beta_n) \in B$ such that $u_i$ is adjacent to $v_i$ in $G_i$ whenever $\beta_i = 1$, and $u_i = v_i$ whenever $\beta_i = 0$.

Graphs $G_1, \ldots, G_n$ are called the *factors* of NEPS. The condition that for every $i = 1, \ldots, n$ there exists $\beta \in B$ with $\beta_i = 1$, which does not appear in the definition in [4, p. 66], implies that NEPS effectively depends on each $G_i$.

**Example** The product $G_1 \times G_2 \times \ldots \times G_n$ of graphs $G_1, G_2, \ldots, G_n$, also called direct product, is NEPS of these graphs with basis $B = \{(1, 1, \ldots, 1)\}$; the sum $G_1 + G_2 + \ldots + G_n$ of graphs $G_1, G_2, \ldots, G_n$, also called Cartesian product, is NEPS of these graphs with basis consisting of $n$-tuples of the form $(0, \ldots, 0, 1, 0, \ldots, 0)$ with 1 on $i$-th place, for each $i = 1, 2, \ldots, n$.

One of the most important properties of NEPS of graphs, which is the basis of our study, is that its spectrum can be represented by the spectra of its factors (see, e.g., Theorem 2.23 in [4]).

**Theorem 1** The spectrum of NEPS($G_1, \ldots, G_n; B$) consists of all possible values $\Lambda$ given by

$$\Lambda = \sum_{\beta \in B} \lambda_1^{\beta_1} \cdots \lambda_n^{\beta_n},$$

where $\lambda_i$ is an arbitrary eigenvalue of $G_i$, $i = 1, \ldots, n$.

In the next section, we first show that the energy of the product of graphs is the product of the energy of graphs, and how this result may be used to construct arbitrarily large families of noncospectral graphs having the same energy. Then, unlike the product, we show that the energy of NEPS with any other basis cannot be represented as a function of the energy of its factors. Still, we can get an upper bound on the energy of NEPS in terms of the energy and the number of vertices of its factors.

## 2 Product of graphs

For $m \in \mathbb{N}$ let $[m] = \{1, 2, \ldots, m\}$ and for $m_1, m_2, \ldots, m_n \in \mathbb{N}$ let

$$[m_1, m_2, \ldots, m_n] = [m_1] \times [m_2] \times \ldots \times [m_n].$$
Theorem 2 For graphs \( G_1, G_2, \ldots, G_n \) it holds that
\[
E(G_1 \times G_2 \times \ldots \times G_n) = E(G_1) \cdot E(G_2) \cdot \ldots \cdot E(G_n).
\] (3)

Proof For \( i = 1, 2, \ldots, n \), let graph \( G_i \) has eigenvalues \( \lambda_{i,j} \), \( j = 1, 2, \ldots, |G_i| \). From (2) it follows that the eigenvalues of the product \( G_1 \times G_2 \times \ldots \times G_n \) are of the form \( \prod_{i=1}^{n} \lambda_{i,j_i} \) for \((j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]\) and we get
\[
E(G_1 \times G_2 \times \ldots \times G_n) = \sum_{(j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]} \prod_{i=1}^{n} \lambda_{i,j_i} = \prod_{i=1}^{n} \prod_{j_i \in [|G_i|]} \lambda_{i,j_i} = \prod_{i=1}^{n} E(G_i). \quad \blacksquare
\]

If \( G \) and \( H \) are two graphs for which the equality \( E(G) = E(H) \) holds, then \( G \) and \( H \) are called equienergetic. In view of (1), cospectral graphs are equienergetic. Further, union of a graph \( G \) and an arbitrary number of isolated vertices has the same energy as \( G \), while it is not cospectral to \( G \). Far less trivial case are pairs of non-cospectral connected equienergetic graphs. Finding examples of such graphs became of interest recently [1, 2, 19]. The smallest pair of non-cospectral connected equienergetic graphs with the same number of vertices are the pentagon and the four-sided pyramid, shown in Fig. 1, whose eigenvalues are \( 2, \sqrt{5} - 1, \sqrt{5} - 1, -\sqrt{5} + 1, -\sqrt{5} + 1, \sqrt{5} + 1, 0, 0, -\sqrt{5} + 1, -2 \), respectively.

Figure 1: The smallest pair of non-cospectral connected equienergetic graphs with the same number of vertices.

The first construction of infinitely many pairs of non-cospectral connected equienergetic graphs with the same number of vertices is described in [19]. Based on Theorem 2 we can give one more such construction. Let \( G \) be a pentagon, \( H \) a four-sided pyramid, and for each \( n \in \mathbb{N} \) and \( i = 1, 2, \ldots, n \), let
\[
G_{n,i} = G \times \ldots \times G \times H \times \ldots \times H.
\]

\[i \text{ times}\]
\[n-i \text{ times}\]
Then graphs $\mathcal{G}_{n,i}$, $i = 1, 2, \ldots, n$ form a family of $n$ mutually non-cospectral connected equienergetic graphs having the same number of vertices. Namely, each graph $\mathcal{G}_{n,i}$ has $5^n$ vertices and the energy equal to $(2\sqrt{5} + 2)^n$. Next, the largest eigenvalue of $\mathcal{G}_{n,i}$ is equal to $2^i(\sqrt{5}+1)^{n-1}$, and so no two of these graphs may be cospectral. Further, in [20] it was proven that NEPS($G_1, \ldots, G_n; B$) of connected graphs $G_1, G_2, \ldots, G_n$ is itself connected if and only if the rank of $B'$ over the binary field $GF_2$ is equal to $k$, where $k$ is the number of bipartite graphs among $G_1, G_2, \ldots, G_n$, and $B'$ consists of the $k$ columns of $B$ corresponding to the bipartite graphs. Since $G$ and $H$ are non-bipartite graphs, for each $\mathcal{G}_{n,i}$ we have $k = 0$ and $B' = \emptyset$, and thus the graph $\mathcal{G}_{n,i}$ is connected.

3 Other NEPS of graphs

After seeing a simple formula (3) for the energy of the product of graphs, one would expect that similar expressions exist for other NEPS of graphs. Quite surprisingly, this is not the case for any other NEPS of graphs.

\textbf{Theorem 3} Let $B$ be a basis of NEPS. Then there exists a function $f_B : \mathbb{R}^n \rightarrow \mathbb{R}$ such that

$$E(\text{NEPS}(G_1, G_2, \ldots, G_n; B)) = f_B(E(G_1), E(G_2), \ldots, E(G_n))$$

holds for any graphs $G_1$, $G_2$, \ldots, $G_n$ if and only if $B = \{(1, \ldots, 1)\}$.

\textbf{Proof} If the basis of NEPS is $\{(1, 1, \ldots, 1)\}$, then the result follows from Theorem 2. Now, suppose that for some basis $B \neq \{(1, 1, \ldots, 1)\}$ there exists a function $f_B : \mathbb{R}^n \rightarrow \mathbb{R}$ such that

$$E(\text{NEPS}(G_1, G_2, \ldots, G_n; B)) = f_B(E(G_1), E(G_2), \ldots, E(G_n))$$

holds for every $G_1, G_2, \ldots, G_n$. From the condition $B \neq \{(1, 1, \ldots, 1)\}$ it follows that the basis $B$ contains an $n$-tuple with a coordinate equal to 0. Without loss of generality, we may suppose that $B$ contains an $n$-tuple with 0 at the first coordinate. Let $B_0 = \{\beta \in B : \beta_1 = 0\}$ and $B_1 = \{\beta \in B : \beta_1 = 1\}$.

For $i = 1, 2, \ldots, n$, let graph $G_i$ has eigenvalues $\lambda_{i,j}$, $j = 1, 2, \ldots, |G_i|$. We have that

$$E(\text{NEPS}(G_1, G_2, \ldots, G_n; B))$$

$$= \sum_{(j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]} \left| \sum_{\beta \in B_{i=1}} \prod_{j=1}^n \lambda_{i,j}^\beta \right|$$

$$= \sum_{(j_2, \ldots, j_n) \in [|G_2|, \ldots, |G_n|]} \sum_{j_1 \in [|G_1|]} \left| \prod_{\beta \in B_{i=2}} \lambda_{i,j_1}^\beta \prod_{j=2}^n \lambda_{i,j}^\beta \right|$$

$$= \sum_{(j_2, \ldots, j_n) \in [|G_2|, \ldots, |G_n|]} \sum_{j_1 \in [|G_1|]} \left| \lambda_{1,j_1} \sum_{\beta \in B_{i=2}} \prod_{j=2}^n \lambda_{i,j}^\beta + \sum_{\beta \in B_{i=2}} \prod_{j=2}^n \lambda_{i,j_1}^\beta \right|$$

4
Let \( j = (j_2, \ldots, j_n) \) and let
\[
A_j = \sum_{\beta \in B_1} \prod_{i=2}^{n} \lambda_{i,j_i}^\beta \quad \text{and} \quad B_j = \sum_{\beta \in B_0} \prod_{i=2}^{n} \lambda_{i,j_i}^\beta.
\]

Then
\[
E(\text{NEPS}(G_1, G_2, \ldots, G_n; B)) = \sum_{j \in [G_1], \ldots, G_n]} \sum_{j \in [G_1] | H, \gamma} |\lambda_{1,j_1} A_j + B_j|.
\] (4)

Let \( m \geq 2 \). The complete graph \( K_{m+1} \) has a simple eigenvalue \( m \) and an eigenvalue \(-1\) with multiplicity \( m \), and its energy is \( 2m \). The complete bipartite graph \( K_{m,m} \) has simple eigenvalues \( m \) and \(-m\), and an eigenvalue \( 0 \) with multiplicity \( 2m - 2 \), and its energy is also \( 2m \). Thus, since \( E(K_{m+1}) = 2m = E(K_{m,m}) \) we must have that
\[
E(\text{NEPS}(K_{m+1}, G_2, \ldots, G_n; B)) = E(\text{NEPS}(K_{m,m}, G_2, \ldots, G_n; B)).
\] (5)

From (4) it follows that
\[
E(\text{NEPS}(K_{m+1}, G_2, \ldots, G_n; B)) = \sum_{j \in [G_2], \ldots, G_n]} |mA_j + B_j| + m| - A_j + B_j|
\]
and
\[
E(\text{NEPS}(K_{m,m}, G_2, \ldots, G_n; B)) = \sum_{j \in [G_2], \ldots, G_n]} |mA_j + B_j| + (2m - 2)|B_j| + | - mA_j + B_j|.
\]

For each \( j \in [G_2], \ldots, G_n] \) it holds that
\[
m| - A_j + B_j| = | - mA_j + mB_j| = |(-mA_j + B_j) + (m - 1)B_j| \\
\leq | - mA_j + B_j| + (m - 1)|B_j| \leq | - mA_j + B_j| + (2m - 2)|B_j|.
\] (6)

Adding \( |mA_j + B_j| \) to both sides of previous inequality and summing over all \( j \in [G_2], \ldots, G_n] \), we get
\[
E(\text{NEPS}(K_{m+1}, G_2, \ldots, G_n; B)) \leq E(\text{NEPS}(K_{m,m}, G_2, \ldots, G_n; B)).
\] (7)

Further, each graph \( G_i, i = 2, \ldots, n \), has at least two vertices, and therefore it has a positive principal eigenvalue. Without loss of generality, we may suppose that the principal eigenvalue of \( G_i \) is \( \lambda_{i,1} \). Then the product \( \prod_{i=2}^{n} \lambda_{i,j_i}^\beta \) is positive for each binary \( n \)-tuple \( \beta \). Since the set \( B_0 \) is not empty, we get that \( B_{(1,1,\ldots,1)} \) is positive and that the strong inequality holds in (6) for \( j = (1,1,\ldots,1) \). Thus, the strong inequality also holds in (7), which is in contradiction with (5).

Thus, the energy of NEPS is not representable as a function of the energy of its factors, except for the product of graphs. However, we can bound the energy of NEPS by a function of the energy and the number of vertices of its factors.
where

The meaning of NEPS$\{G_1, G_2, \ldots, G_n; B\}$ holds that

$$E(\text{NEPS}(G_1, G_2, \ldots, G_n; B)) \leq \sum_{\beta \in B}^{n} \prod_{i=1}^{n} E(G_i), \quad (8)$$

Proof For $i = 1, 2, \ldots, n$, let graph $G_i$ has eigenvalues $\lambda_{i,j}$, $j = 1, 2, \ldots, |G_i|$. The eigenvalues of NEPS$\{G_1, G_2, \ldots, G_n; B\}$ are of the form $\sum_{\beta \in B}^{n} \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i}$ for $(j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]$ and we have that

$$E(\text{NEPS}(G_1, G_2, \ldots, G_n; B)) = \sum_{(j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]} \left| \sum_{\beta \in B}^{n} \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} \right|$$

$$\leq \sum_{(j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]} \left| \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} \right|$$

$$= \sum_{\beta \in B}^{n} \left| \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} \right|$$

$$= \sum_{\beta \in B}^{n} \prod_{i=1}^{n} \sum_{j \in [|G_i|]} |\lambda_{i,j}^{\beta_i}|$$

$$= \sum_{\beta \in B}^{n} \prod_{i=1}^{n} \left\{ E(G_i), \quad \beta_i = 1 \right\} \quad |G_i|, \quad \beta_i = 0$$

$$= \sum_{\beta \in B}^{n} \prod_{i=1}^{n} E(G_i).$$

If $B = \{(1, 1, \ldots, 1)\}$, then the equality holds in (8) by Theorem 2.

Next, suppose that there exist graphs $G_1, G_2, \ldots, G_n$ and a basis $B$ such that the equality holds in (8). Then for each $j = (j_1, j_2, \ldots, j_n) \in [|G_1|, |G_2|, \ldots, |G_n|]$ it must hold that

$$\left| \sum_{\beta \in B}^{n} \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} \right| = \sum_{\beta \in B}^{n} \left| \prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} \right|,$$

i.e. the products $\prod_{i=1}^{n} \lambda_{i,j}^{\beta_i}$ are of the same sign for every $\beta \in B$. Let $a_{i,j}$ be the sign of $\lambda_{i,j}$, defined by

$$a_{i,j} = \left\{ \begin{array}{ll} 0, & \lambda_{i,j} \geq 0 \\ 1, & \lambda_{i,j} < 0 \end{array} \right.$$
so that $\lambda_{i,j} = (-1)^{a_{i,j}} |\lambda_{i,j}|$. Let $a_j = (a_{1,j}, a_{2,j}, \ldots, a_{n,j})$. We get that

$$\prod_{i=1}^{n} \lambda_{i,j}^{\beta_i} = \prod_{i=1}^{n} (-1)^{a_{i,j}} |\lambda_{i,j}| = (-1)^{\sum_{i=1}^{n} a_{i,j}} \prod_{i=1}^{n} |\lambda_{i,j}| = (-1)^{a_j} \prod_{i=1}^{n} |\lambda_{i,j}|,$$

where $a_j$ and $\beta$ are considered as vectors in $GF_2^n$ and $a_j \beta$ is their scalar product over the field $GF_2$. Thus, for each $j \in \{|G_1|, |G_2|, \ldots, |G_n|\}$ the products $\prod_{i=1}^{n} \lambda_{i,j}^{\beta_i}$ are of the same sign for every $\beta \in B$ if and only if $a_j \beta$ has a constant value for every $\beta \in B$.

Since every graph with at least two vertices has both a positive and a negative eigenvalue, the condition that $j$ takes all values from $\{|G_1|, |G_2|, \ldots, |G_n|\}$ implies the condition that $a_j$ takes all values from $GF_2^n$. Now, we can conclude that the equality holds in (8) only if for each $\alpha \in GF_2^n$ the scalar product $a_j \beta$ has a constant value for every $\beta \in B$. Taking value $\alpha = (0, \ldots, 0, 1, 0, \ldots, 0)$ with 1 on $i$-th place for $i = 1, 2, \ldots, n$, it follows that $\beta_i$ has a constant value for every $\beta \in B$, and so we get that $B$ contains exactly one element. Since by definition of NEPS for every $i = 1, \ldots, n$ there must exist $\beta \in B$ with $\beta_i = 1$, we see that it must hold $B = \{(1, 1, \ldots, 1)\}$. \[\Box\]

References


