A lower bound for the energy of symmetric matrices and graphs

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Abstract

The energy of a symmetric matrix is the sum of the absolute values of its eigenvalues. We introduce a lower bound for the energy of a symmetric partitioned matrix into blocks. This bound is related to the spectrum of its quotient matrix. Furthermore, we study necessary conditions for the equality. Applications to the energy of the generalized composition of a family of arbitrary graphs are obtained. A lower bound for the energy of a graph with a bridge is given. Some computational experiments are presented in order to show that, in some cases, the obtained lower bound is incomparable with the well known lower bound $2\sqrt{m}$, where m is the number of edges of the graph.

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1. Motivation and Main Goal

In this work we deal with an (n, m)-graph G which is an undirected simple graph with a vertex set $\mathcal{V}(G)$ of cardinality n and an edge set $\mathcal{E}(G)$ of cardinality m. The concept of energy of graphs appeared in Mathematical Chemistry and we review in this section its importance. In Chemistry *Molecular graphs* represent the structure of molecules.They are generated, in general, by the following rule: vertices stand for atoms and edges for bonds. A *matching* N in a graph G is a nonempty set of edges such that no two have a vertex in common. A *perfect matching* is a matching whose set of vertices (set of end vertices of the edges forming the matching) coincides with the set of vertices of G. There are two basic types of molecular graphs: those representing *saturated hydrocarbons* and those representing *conjugated* π *-electron systems*. In the second class, the molecular graph should have perfect matchings (called "Kekulé structure"). In the 1930s, Erich Hückel put forward a method for finding approximate solutions of the Schrödinger equation of a class of organic molecules, the so-called *conjugated hydrocarbons* (conjugated π-electron systems) which have a system of connected π-orbitals with *delocalized* π-electrons (electrons in a molecule that are not associated with a single atom or a covalent bond). Thus, the HMO (Hückel molecular orbital model) enables to describe approximately the behavior of the so-called π-electrons in a conjugated molecule, especially in conjugated hydrocarbons. For more details see [13] and the references therein. As usual we denote the adjacency matrix of G by $A(G)$. The eigenvalues of G are the eigenvalues of this matrix.

Following to HMO theory, the total π-electron energy, E_π, is a quantum-chemical characteristic of conjugated molecules that agrees with their thermodynamic properties. For conjugated hydrocarbons in their ground electronic states, E_π is calculated from the eigenvalues of the adjacency matrix of the molecular graph:

$$E_\pi = n\alpha + E\beta,$$

where n is the number of carbon atoms, α and β are the HMO carbon-atom coulomb and carbon-carbon resonance integrals, respectively. For the majority conjugated π-electron systems

$$E = \sum_{i=1}^{n} |\lambda_i| \,, \tag{1}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the underlying molecular graph. For molecular structure researches, E is a very interesting quantity. In fact, it is traditional to consider E as the total π-electron energy expressed in β-units. The spectral invariant defined by (1) is called the *energy* of the graph G, (see [9]). It is worth to be mentioned that in the contemporary literature, a plethora of upper bound for this invariant has been reported. On the other hand, lower bounds for energy are much fewer in number, probably because these are much more difficult to deduce. Of these (recently determined) lower bounds, the reader shoud be referred [1, 3, 11, 12, 14, 17].

Let $M = (M_{ij})$ be a partitioned matrix, we say that M has a symmetric partitioning if $M_{ij} = (M_{ji})^t$, for all $1 \leq i, j \leq k$. Note that a matrix with a symmetric partitioning is symmetric. The *energy of a symmetric matrix* is defined as the sum of the absolute values of its eigenvalues, see [15, 16].

Given a symmetric matrix that is partitioned into a block form, the matrix of the average row sums of the blocks of the original matrix is not necessarily a symmetric matrix. This matrix is known as the *quotient* matrix of the partitioned given matrix [10]. If each block of the matrix has constant row sum then the partitioning of M is called regular or equitable.

Taking into account these concepts we introduce the main goal of the paper, Theorem 1.1, that gives a lower bound for the energy of a symmetric matrix partitioned into blocks. This bound is related to the spectrum of its quotient matrix. It is worth to observe that the quotient matrix is not necessarily symmetric but it is diagonally similar to a symmetric one.

Theorem 1.1. *Let M be a $n \times n$ symmetric matrix, partitioned into blocks, as in (6). For $1 \leq i \leq k$, let n_i be the order of the square diagonal block M_{ii} of M. Let $\overline{M}$ be the quotient matrix of M, then*

$$E(M) \geq E\left(\Phi \overline{M} \Phi^{-1}\right), \tag{2}$$

where $\Phi = diag\left(\sqrt{n_1}, \ldots, \sqrt{n_k}\right)$. If equality holds then the partitioning into blocks of M is regular, the nullity of M is at least $n - k$ and $trace\,(M) = trace\left(\overline{M}\right)$.

2. Notation and Outline

We introduce now some notation. If $e \in \mathcal{E}(G)$ has end vertices u and v we say that u and v are neighbors and we denote this edge by uv. Sometimes (by convenience), after the labeling of the vertices of G, the edge $v_i v_j$ is written by ij. A graph with no edges (but at least one vertex) is called *empty graph.* For $u_i \in \mathcal{V}(G)$, the number of vertices adjacent to u_i is denoted by $d(u_i)$ or d_i, and it is called the vertex degree of u_i, where i is the label of u_i. A *q-regular* graph G is a graph where every vertex has degree q. The complete graph of order n is an $(n-1)$-regular graph with n vertices and it is denoted by K_n. A graph is *bipartite* if its vertex set can be split into two nonempty subsets X and Y such that each edge of G has one end vertex in X and the other in Y. The pair (X, Y) is called a *bipartition* of G. We denote $G\,(X, Y)$ any graph with bipartition (X, Y). A bipartite graph $G\,(X, Y)$ is *complete* if each vertex of X is adjacent to all vertices of Y. We denote $K_{p,q}$ the *complete bipartite* graph with bipartition (X, Y) such that $|X| = p$ and $|Y| = q$.

For a real symmetric matrix M, let us denote by $\lambda_i(M)$ the i-th largest eigenvalue of M. The spectrum of M (the multiset of the eigenvalues of M) is represented by $\sigma(M)$.

We denote the $r \times s$ zero block matrix by $\mathbf{O}_{r\times s}$. The matrices $\mathbb{J}_{n_1 n_2}$, and I_n represent the all ones matrix and the identity matrix of orders $n_1 \times n_2$ and n, respectively. If $n_2 = 1$ we use $\mathbb{J}_{n_1}$ instead $\mathbb{J}_{n_1 1}$. Note that $\mathbb{J}_n$ is the all ones vector column of order n. For the remaining basic terminology and notation used throughout the paper we refer to the book [7].

In what follows we describe the outline of the paper. In [2], by using the Cauchy-Schwarz inequality in appropriate way, it was obtained a sharp and improved upper bound for the energy of bipartite graphs and for large family of graphs, namely those graphs whose adjacency matrix is partitioned into a block form with constant row sums. In this paper our aim is to present a lower bound for the energy of a graph G whose adjacency matrix, $A(G)$ is partitioned into a block form in terms of its quotient matrix. To this goal we prove that the quotient matrix is diagonally similar to a symmetric matrix whose energy is a lower bound for the energy of the original one. Moreover, we obtain necessary conditions for the equality. Applications to the energy of the *generalized composition* of a family of graphs [6, 18] are obtained. In addition, we present an explicit formula to the mentioned lower bound in the case of a graph with two isomorphic components connected by a bridge. Then, we compare the obtained lower bound with the well known lower bound $2\sqrt{m}$, where m is the number of edges of the graph, [5, 13].

3. Generalized Composition of Graphs

In this section we recall the definition of Generalized Composition of graphs. Let G_1 and G_2 be two vertex-disjoint graphs. The *join of* G_1 and G_2 is the graph $G_1 \vee G_2$ such that $\mathcal{V}(G_1 \vee G_2) = \mathcal{V}(G_1) \cup \mathcal{V}(G_2)$ and $\mathcal{E}(G_1 \vee G_2) = \mathcal{E}(G_1) \cup \mathcal{E}(G_2) \cup \{ij : i \in \mathcal{V}(G_1) \text{ and } j \in \mathcal{V}(G_2)\}$. A generalization of the join operation was introduced in [6, 18] as follows:

Consider a family of k graphs, $\mathcal{F} = \{G_1, \ldots, G_k\}$, where each graph G_i has order n_i, for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Each vertex $v_i \in \mathcal{V}(H)$ is assigned to the graph $G_i \in \mathcal{F}$. The *H-join* or *Generalized Composition* of $G_1, \ldots, G_k$ is the graph $G = H[G_1, \ldots, G_k]$ such that $\mathcal{V}(G) = \bigcup_{i=1}^{k} \mathcal{V}(G_i)$ and edge set:

$$\mathcal{E}(G) = \left(\bigcup_{i=1}^{k} \mathcal{E}(G_i)\right) \cup \left(\bigcup_{uw \in \mathcal{E}(H)} \{ij : i \in \mathcal{V}(G_u), j \in \mathcal{V}(G_w)\}\right).$$

The following example shows how does it works the Generalized Composition of the three graphs K_3, K_2, C_4, with $H = P_3$, [6].

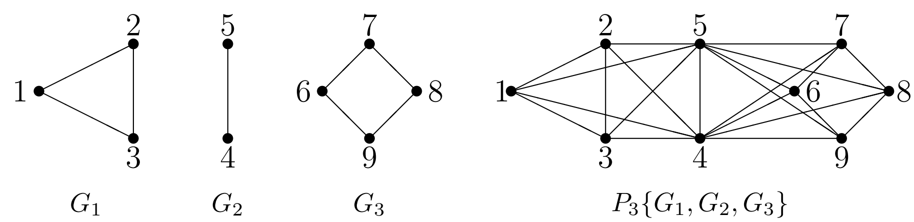

Figure 1: The H-join of $\mathcal{F} = \{K_3, K_2, C_4\}$, with $H = P_3$.

4. Proof of the Main Theorem

This section is devoted to establish a lower bound for the energy of a matrix M with symmetric partitioning in terms of the spectrum of its quotient matrix, (see [10]). To obtain our lower bound we use the concept of interlacing of real numbers, ([10]). Consider two non-increasing sequences of real numbers $\alpha_1 \geq \cdots \geq \alpha_n$ and $\beta_1 \geq \cdots \geq \beta_k$ with $k < n$. The second sequence is said to *interlace* the first one whenever

$$\alpha_i \geq \beta_i \geq \alpha_{n-k+i}, \quad \text{for } 1 \leq i \leq k. \tag{3}$$

The interlacing is called tight if there exists an integer ℓ with $1 \leq \ell \leq k$ such that

$$\beta_i = \alpha_i, \quad \text{for } 1 \leq i \leq \ell \tag{4}$$

and

$$\beta_i = \alpha_{n-k+i}, \quad \text{for } 1 + \ell \leq i \leq k. \tag{5}$$

If $k = n - 1$ the interlacing becomes

$$\alpha_1 \geq \beta_1 \geq \alpha_2 \geq \beta_2 \geq \cdots \geq \alpha_{n-1} \geq \beta_{n-1} \geq \alpha_n,$$

which clarifies the name. We consider the $n \times n$ matrix M with a symmetric partitioning given by:

$$M = \begin{pmatrix} M_{11} & M_{12} & \dots & & M_{1k} \\ M_{21} & M_{22} & & & M_{2k} \\ \vdots & & \ddots & \ddots & \vdots \\ & & \ddots & & \\ M_{k1} & \dots & & & M_{kk} \end{pmatrix}. \tag{6}$$

where the block M_{ij} has order $n_i \times n_j$. Then, the *quotient matrix* $\overline{M} = (m_{ij})$ of M is the $k \times k$ matrix where

$$m_{ij} = \frac{1}{n_i} \left(\mathbb{J}_{n_i}^t M_{ij} \mathbb{J}_{n_j} \right), \qquad \text{for } 1 \leq i, j \leq k. \tag{7}$$

The partitioning into blocks of M is called regular (or equitable) if each block M_{ij} of M has constant row sum. Note that in this case $\overline{M}$ corresponds to the row sums matrix. If M is regularly partitioned, by Lemma 2.3.1 in [4], the eigenvalues of $\overline{M}$ are eigenvalues of M.

Theorem 4.1. *[10]Suppose $\overline{M}$ the quotient matrix of a partitioned symmetric matrix M then the eigenvalues of $\overline{M}$ interlace the eigenvalues of M. Moreover, if the interlacing is tight, then the partition of M is regular. On the other hand, if the M is regularly partitioned, then the eigenvalues of $\overline{M}$ are eigenvalues of M.*

The next proof corresponds to the proof of the main theorem referred at Section 1.

Proof. (Proof of Theorem 1.1) Suppose that M is the matrix in (6) with eigenvalues $\alpha_1 \geq \cdots \geq \alpha_n$ and let $\beta_1 \geq \cdots \geq \beta_k$ with $k < n$, the eigenvalues of $\overline{M}$. Let $\ell = \max\limits_{1 \leq i \leq k} \{i : \beta_i \geq 0\}$. Therefore, $\ell \leq k$ and if $\ell < k$ then $\beta_\ell \geq 0$ and $\beta_{\ell+1} < 0$. By Theorem 4.1, as the eigenvalues of $\overline{M}$ interlace the eigenvalues of M, in particular

$$\alpha_i \geq \beta_i, \text{ for } 1 \leq i \leq \ell,$$

we have $|\alpha_i| = \alpha_i \geq |\beta_i|$, for $1 \leq i \leq \ell$. Again, from Theorem 4.1, for $\ell + 1 \leq i \leq k$ we have

$$0 > \beta_i \geq \alpha_{n-k+i}.$$

In consequence, for $\ell+1 \leq i \leq k$ we have $|\alpha_{n-k+i}| \geq |\beta_i|$. Furthermore, if $i \geq \ell+1$, then $n-k+i \geq n-k+\ell+1 \geq \ell+1$, then

$$\{\alpha_i : 1 \leq i \leq \ell\} \cap \{\alpha_{n-k+i} : \ell+1 \leq i \leq k\} = \emptyset$$

and

$$\Upsilon = \{\alpha_i : 1 \leq i \leq \ell\} \cup \{\alpha_{n-k+i} : \ell+1 \leq i \leq k\} \subseteq \{\alpha_i : 1 \leq i \leq n\}.$$

Considering all together

$$\sum_{i=1}^{k} |\beta_i| = \sum_{i=1}^{\ell} |\beta_i| + \sum_{i=\ell+1}^{k} |\beta_i| \leq \sum_{i=1}^{\ell} |\alpha_i| + \sum_{i=\ell+1}^{k} |\alpha_{n-k+i}| \leq E(M).$$

Note that $\sigma\left(\Phi\overline{M}\Phi^{-1}\right) = \sigma\left(\overline{M}\right) = \{\beta_i : 1 \leq i \leq k\}$. Next, it will be shown that the $k \times k$ matrix $\Phi\overline{M}\Phi^{-1} = (\nu_{ij})$ is symmetric. Recall that the (i,j) entry of $\overline{M}$, m_{ij} verifies $n_i m_{ij} = \mathbb{J}_{n_i}^t M_{ij} \mathbb{J}_{n_j}$, hence

$$n_j m_{ji} = \mathbb{J}_{n_j}^t M_{ji} \mathbb{J}_{n_i} = \mathbb{J}_{n_j}^t M_{ij}^t \mathbb{J}_{n_i} = n_i m_{ij}.$$

Then

$$\nu_{ij} = \frac{\sqrt{n_i} m_{ij}}{\sqrt{n_j}} = \frac{\sqrt{n_i}\sqrt{n_i} m_{ij}}{\sqrt{n_i n_j}} = \frac{n_i m_{ij}}{\sqrt{n_i n_j}} = \frac{n_j m_{ji}}{\sqrt{n_i n_j}} = \frac{\sqrt{n_j} m_{ji}}{\sqrt{n_i}} = \nu_{ji}.$$

Hence,

$$E(M) \quad \geq \quad E\left(\Phi\overline{M}\Phi^{-1}\right).$$

For the equality case, all the above inequalities are satisfied as equalities and, in this case ℓ is such that (4) and (5) hold. Thus the partitioning of M is regular as the interlacing is tight. Since, the condition $\sum_{\alpha_j \notin \Upsilon} |\alpha_j| = 0$ must be hold too, $|\alpha_j| = 0$ (hence $\alpha_j = 0$) for all $\alpha_j \notin \Upsilon$, then the nullity of the matrix M must be at least $n-k$ implying that the range of M is at most equal to k. If equality holds then

$$\begin{aligned}
trace(\overline{M}) &= \sum_{i=1}^{k} \beta_i \\
&= \sum_{i=1}^{\ell} \beta_i + \sum_{i=\ell+1}^{k} \beta_i \\
&= \sum_{i=1}^{\ell} \alpha_i + \sum_{i=\ell+1}^{k} \alpha_{k+i} = \sum_{i=1}^{n} \alpha_i - \sum_{\alpha_j \notin \Upsilon} \alpha_j \\
&= \sum_{i=1}^{n} \alpha_i = trace(M).
\end{aligned}$$

■

5. A Lower Bound for the Energy of some Graphs

In [6], a complete characterization of the spectrum of the H-join of *regular* graphs was obtained. In this case it was given a labeling of the vertices of the H-join graph which led to a partitioning of the adjacency matrix of the graph into a block form. Using this labeling we obtain a lower bound for the energy of the H-join of any family of graphs.

Theorem 5.1. *Let $\mathcal{F} = \{G_1, \ldots, G_k\}$ be a family of k graphs, where each graph G_i has n_i vertices and m_i edges for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{v_1, \ldots, v_k\}$. Let $G = H[G_1, \ldots, G_k]$ be the H-join of $G_1, \ldots, G_k$. Moreover, consider the $\frac{k(k-1)}{2}$-tuple of scalars*

$$\rho = (\rho_{12}, \rho_{13}, \ldots, \rho_{1k}, \rho_{23}, \ldots, \rho_{2k}, \ldots, \rho_{k-1k}) \tag{8}$$

assigned to H and to the family $\mathcal{F}$, such that

$$\rho_{\ell q} = \rho_{q\ell} = \begin{cases} \sqrt{n_\ell n_q} & \text{if } \ell q \in \mathcal{E}(H), \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

for $1 \leq \ell \leq k-1$ and $\ell + 1 \leq q \leq k$. Denote by $C(\rho)$ the next matrix

$$C(\rho) = \begin{pmatrix} \frac{2m_1}{n_1} & \rho_{12} & \cdots & \rho_{1k-1} & \rho_{1k} \\ \rho_{12} & \frac{2m_2}{n_2} & \cdots & \rho_{2k-1} & \rho_{2k} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{1k} & \rho_{2k} & \cdots & \rho_{k-1k} & \frac{2m_k}{n_k} \end{pmatrix}. \tag{10}$$

Then

$$E(G) \geq E(C(\rho)). \tag{11}$$

Equality holds if and only if the compound graphs $G_1, \ldots, G_k$ are empty graphs.

Proof. For $1 \leq i \leq k$, let $A_i = A(G_i)$ and $A(H) = (h_{ij})$ is the $k \times k$, adjacency $(0,1)$-matrix of H. Following the labeling of the graph in [6], the adjacency matrix of G becomes

$$\begin{pmatrix} A_1 & h_{12}\mathbb{J}_{n_1 n_2} & \ldots & h_{1k}\mathbb{J}_{n_1 n_k} \\ h_{12}\mathbb{J}_{n_2 n_1} & A_2 & \ldots & h_{2k}\mathbb{J}_{n_2 n_k} \\ \vdots & \vdots & \ddots & \vdots \\ h_{k1}\mathbb{J}_{n_k n_1} & h_{k2}\mathbb{J}_{n_k n_2} & \ldots & A_k \end{pmatrix}$$

and the the quotient matrix is

$$\overline{A} = \begin{pmatrix} \frac{2m_1}{n_1} & h_{12}n_2 & \ldots & h_{1k-1}n_{k-1} & h_{1k}n_k \\ h_{12}n_1 & \frac{2m_2}{n_2} & \ldots & h_{2k-1}n_{k-1} & h_{2k}n_k \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ h_{1k}n_1 & h_{2k}n_2 & \ldots & h_{k-1k}n_{k-1} & \frac{2m_k}{n_k} \end{pmatrix}.$$

Let $\Phi = diag\left(\sqrt{n_1}, \ldots, \sqrt{n_k}\right)$. The result follows from Theorem 1.1 and noticing that $C(\rho) = \Phi\overline{A}\Phi^{-1}$. If equality holds, by the equality case of Theorem 1.1, $trace\left(\overline{A}\right) = 0$, implying that the compound graphs $G_1, \ldots, G_k$ must be the empty graphs of orders $n_1, \ldots, n_k$, respectively. On the other hand, if $G_1, \ldots, G_k$ are empty subgraphs of G, by the result in [6] the spectrum of G is the union of the spectrum of $C(\rho)$ and $n-k$ null eigenvalues. Then the nullity of $A(G)$ must be at least $n-k$, thus the equality case follows. ■

6. A lower bound for graphs with a bridge

In this section we present a lower bound for the energy of graphs with a bridge. Using a particular partitioning of the adjacency matrix of the graph, we compared the obtained lower bound with the well known lower bound for the energy of a graph $2\sqrt{m}$, were m is its number of edges, [13], showing that they are incomparable. Some specific notation used throughout this section is introduced. By a nontrivial subset of vertices of G we mean a nonempty proper subset X of $\mathcal{V}(G)$. The induced subgraph with a nontrivial vertex set $X \subset \mathcal{V}(G)$ is denoted by $\langle X \rangle$.

Given a graph G and $u \in \mathcal{V}(G)$, nontrivial subset of vertices X, let $N_X(u) := X \cap N(u)$. The cardinality of $N_X(u)$ is $d_X(u)$. In what follows $n_1, n_2 \geq 2$.

Definition 6.1. *Let (n_1, m_1) and (n_2, m_2) be the number of vertices and edges of two disjoint graphs G_1 and G_2, respectively. An (n_1+n_2, m_1+m_2+1)-graph G, with the extra edge v_1v_2 (the bridge), is called a graph with a bridge if results from the the graphs G_1 and G_2, by connecting v_1 to v_2.*

For a graph with a bridge v_1v_2 with $v_1 \in \mathcal{V}(G_1)$ and $v_2 \in \mathcal{V}(G_2)$, the labeling of the vertices is the following:

1. We start labeling the set of vertices of $X_1 = \mathcal{V}(G_1) \setminus \{v_1\}$;
2. Next, we use the labels n_1 and $n_1 + 1$ to v_1 and v_2, respectively;
3. Finally, the labels $n_1 + 2$ to $n_1 + n_2$ are used for the vertices in $X_2 = \mathcal{V}(G_2) \setminus \{v_2\}$.

Using the above labeling of the vertices, the adjacency matrix of G, takes the form

$$A(G) = \begin{pmatrix} A_{11} & x & 0 & 0 \\ x^t & 0 & 1 & 0 \\ 0 & 1 & 0 & y^t \\ 0 & 0 & y & A_{22} \end{pmatrix}, \tag{12}$$

where

$$A_{11} = A(\langle X_1 \rangle), \quad A_{22} = A(\langle X_2 \rangle)$$

and

$$A(G_1) = \begin{pmatrix} A_{11} & x \\ x^t & 0 \end{pmatrix}, \quad A(G_2) = \begin{pmatrix} 0 & y^t \\ y & A_{22} \end{pmatrix}.$$

In order to apply Theorem 1.1 to the adjacency matrix in (12) the following averages are presented:

$$d_1 = \tfrac{d_{X_1}(v_1)}{n_1 - 1}, \quad d_2 = \tfrac{d_{X_2}(v_2)}{n_2 - 1}, \tag{13}$$

and

$$f_1 = \tfrac{1}{n_1 - 1} \textstyle\sum_{v \in X_1} d_{X_1}(v), \quad f_2 = \tfrac{1}{n_2 - 1} \textstyle\sum_{v \in X_2} d_{X_2}(v). \tag{14}$$

The next theorem gives a lower bound for the energy of a graph obtained from two others connecting two vertices by a bridge.

Theorem 6.2. *Let G_1 an (n_1, m_1)-graph and G_2 an (n_2, m_2)-graph be two disjoint graphs. Let $v_1 \in \mathcal{V}(G_1)$ and $v_2 \in \mathcal{V}(G_2)$. Let G the $(n_1 + n_2, m_1 + m_2 + 1)$-graph obtained from the previous two with the bridge $v_1 v_2$. Let*

$$B = \begin{pmatrix} f_1 & \sqrt{n_1 - 1}\, d_1 & 0 & 0 \\ \sqrt{n_1 - 1}\, d_1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{n_2 - 1}\, d_2 \\ 0 & 0 & \sqrt{n_2 - 1}\, d_2 & f_2 \end{pmatrix},$$

where d_1, d_2, f_1 and f_2 are defined as in (13) and (14), respectively. Then

$$E(G) \geq E(B). \tag{15}$$

In particular, if $G_2 \simeq G_1$,

$$E(G) \geq \gamma,$$

where

$$\gamma = \sqrt{(f_1 - 1)^2 + 4d_1^2 (n_1 - 1)} + \sqrt{(f_1 + 1)^2 + 4d_1^2 (n_1 - 1)}. \tag{16}$$

Proof. The quotient matrix of $A(G)$ in (12) is given by

$$\overline{A} = \begin{pmatrix} f_1 & d_1 & 0 & 0 \\ (n_1 - 1)\, d_1 & 0 & 1 & 0 \\ 0 & 1 & 0 & (n_2 - 1)\, d_2 \\ 0 & 0 & d_2 & f_2 \end{pmatrix}.$$

Following the proof of Theorem 1.1, let $\Phi = diag\left(\sqrt{n_1 - 1}, 1, 1, \sqrt{n_2 - 1}\right)$. Then

$$B := \Phi \overline{A} \Phi^{-1} = \begin{pmatrix} f_1 & \sqrt{n_1 - 1}\, d_1 & 0 & 0 \\ \sqrt{n_1 - 1}\, d_1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{n_2 - 1}\, d_2 \\ 0 & 0 & \sqrt{n_2 - 1}\, d_2 & f_2 \end{pmatrix}.$$

By Theorem 1.1 we obtain the inequality in (15). If $G_1 \simeq G_2$ the matrix $B = \Phi \overline{A} \Phi^{-1}$ takes the form

$$B = \begin{pmatrix} T & JSJ \\ S & JTJ \end{pmatrix},$$

where

$$T=\begin{pmatrix} \frac{f_1}{\sqrt{n_1-1}\,d_1} & \sqrt{n_1-1}\,d_1 \\ & 0 \end{pmatrix}, \quad S=\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

and J is the square matrix with ones along the antidiagonal and zeros elsewhere. Following [8], the spectrum of $\Phi\overline{A}\Phi^{-1}$ is the union of the spectrum of $R_1 = T + JS$ and $R_2 = T - JS$, respectively. As

$$R_1=\begin{pmatrix} \frac{f_1}{\sqrt{n_1-1}\,d_1} & \sqrt{n_1-1}\,d_1 \\ & 1 \end{pmatrix}, \quad R_2=\begin{pmatrix} \frac{f_1}{\sqrt{n_1-1}\,d_1} & \sqrt{n_1-1}\,d_1 \\ & -1 \end{pmatrix},$$

then

$$\sigma\left(\Phi\overline{A}\Phi^{-1}\right)=\left\{\frac{f_1+1}{2}\pm\sqrt{\frac{(f_1-1)^2}{4}+d_1^2\,(n_1-1)},\frac{f_1-1}{2}\pm\sqrt{\frac{(f_1+1)^2}{4}+d_1^2\,(n_1-1)}\right\}.$$

As

$$d_1^2\,(n_1-1)\geq f_1, \quad f_1+d_1^2\,(n_1-1)\geq 0$$

we have

$$\frac{(f_1-1)^2}{4}+d_1^2\,(n_1-1)\geq\frac{(f_1+1)^2}{4}, \quad \frac{(f_1+1)^2}{4}+d_1^2\,(n_1-1)\geq\frac{(f_1-1)^2}{4}.$$

Therefore, and by (2), we obtain the following lower bound for the energy of G:

$$E\,(G)\geq\sqrt{(f_1-1)^2+4d_1^2\,(n_1-1)}+\sqrt{(f_1+1)^2+4d_1^2\,(n_1-1)}=\gamma.$$

■

Recall the particular case when G_1 is a (n_1, m_1)-graph and $G_2 \simeq G_1$. Let $v_1 \in \mathcal{V}\,(G_1)$ and $v_2 \in \mathcal{V}\,(G_2)$ be the copy of the vertex v_1 by the isomorphism between G_1 and G_2. Let G be the $(2n_1, 2m_1+1)$-graph obtained by connecting v_1 to v_2. Then, the (n,m)-graph G satisfies

$$\begin{aligned} m &= 1+(n_1-1)\,f_1+2d_{X_1}\,(v_1) \\ &= 1+(n_1-1)\,f_1+2\,(n_1-1)\,d_1. \end{aligned}$$

.

In the next table, we present some computational experiments to compare the lower bound in (16) to the well known lower bound

$$\beta = 2\sqrt{m},$$

for the graph G, (see [13]).

n_1	f_1	d_1	m	γ	β
8	6	1	57	**16.0551**	15.0997
10	8	1	91	**20.0362**	19.0788
10	6	1	73	17.0298	**17.0880**
10	4	1	55	14.5185	**14.8324**
10	0	1	19	**12.1655**	8.7178
9	0	1	17	**11.4891**	8.2462
9	6	1	65	**16.5498**	16.1245

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