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SOME BOUNDS ON VB-DOMINATING LAPLACIAN ENERGY OF A GRAPH

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Abstract. A block is a maximal connected subgraph of G that has no cut-vertices. A vertex v and block b are said to block dominate (b-dominate) each other if v is in the block b. A set $D \subseteq V$ is said to be a vertex block dominating set if every block in G is b-dominated by some vertex in D. The vertex block domination number $\gamma_{vb} = \gamma_{vb}(G)$ is the cardinality of the minimum vertex block dominating set of G. In this paper, we define the minimum vb-dominating Laplacian energy $LE_{vb}(G)$ and obtain some bounds on $LE_{vb}(G)$ in terms of existing graph parameters. Further, we compute $LE_{vb}(G)$ of alkanes. In addition to that, we find relationship between $LE_{vb}(G)$ and $E_{vb}(G)$.

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1. Introduction

The terminologies and notations used here are the same as in [10, 25]. A graph $G = (V, E)$ is a connected finite simple graph of order p and size q. Graph spectral theory has well-known applications in chemistry. One of the most intresting graph-spectrum-based quantities is the graph energy. In 1978, the idea of graph energy was proposed by Ivan Gutman [8]. A huge number of graph energy variants based on matrices apart from the adjacency matrix have been studied in [12, 21, 24, 13]. I. Gutman and B.Zhou [9] defined the Laplacian energy of a graph. The Laplacian matrix of G is denoted by $L = [l_{ij}]_{p\times p}$, where

$$l_{ij} = \begin{cases} -1 & \text{if } v_i \sim v_j \\ 0 & \text{if } v_i \nsim v_j \\ d(v_i) & \text{if } i = j. \end{cases}$$

Let $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of L. Then the Laplacian energy of G is defined as $LE(G) = \sum\limits_{i=1}^{p} |\varphi_i - \frac{2q}{p}|$.

A cut-vertex of a graph G is the vertex whose removal increases the number of components of G. A maximal connected subgraph of G that has no cut-vertices is a block. In 2013, P. G. Bhat et al. [2] initiated the study of vb-dominating sets. Let $\mathcal{B}(G)$ is the set of all blocks of a graph G and we denote $|\mathcal{B}(G)| = m$. A vertex $v \in V$ and a block $b \in B(G)$ are said to block

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dominate (b-dominate) each other if v is in the block b. A set $S \subseteq V$ is said to be a vertex-block dominating set (vb-dominating set) if every block in G is b-dominated by some vertex in S. The vertex block domination number $\gamma_{vb} = \gamma_{vb}(G)$ is the cardinality of the minimum vb-dominating set of G. Let $d_{vb}(u)$ denotes the vb degree of a vertex u in G, i.e, the number of blocks incident on u in G. In [23] it is proved that, for any connected graph G with p vertices and m blocks, $\sum\limits_{u \in V} d_{vb}(u) = p + m - 1$.
In a graph any two vertices vv-adjacent to each other if they are in same block. The point graph $P_G(G)$ of a graph G is a graph with $V(P_G(G)) = V(G)$ and any two vertices in $P_G(G)$ are adjacent if, and only if, they are vv-adjacent in G. The number of edges in the point graph is denoted by q_p [2]. Sayinath Udupa et al. [21] introduced minimum vv-dominating Laplacian matrix $L_{vv}(G)$ of a graph and studied its properties. Motivated by this we introduce vb-dominating Laplacian matrix $L_{vb}(G)$.

2. Minimum vertex-block dominating Laplacian energy

We denote a minimum vb-dominating set of a graph G as γ_{vb}-set. Now we define the minimum vb-dominating Laplacian matrix of G as follows, $L_{vb}(G) = [l_{ij}]$, where

$$l_{ij} = \begin{cases} -1 & \text{if } v_i \text{ and } v_j \text{ are vv-adjacent} \\ d_{vb}(v_i) - 1 & \text{if } i = j, v_i \in \gamma_{vb}\text{-set} \\ d_{vb}(v_i) & \text{if } i = j, v_i \notin \gamma_{vb}\text{-set} \\ 0 & \text{otherwise} \end{cases}$$

Note that $L_{vb}(G)$ is a $p \times p$ matrix. Let $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$. Then the minimum vb-dominating Laplacian energy is defined as,

$$LE_{vb}(G) = \sum_{i=1}^{p} \left| \varphi_i - \frac{2q_p}{p} \right|. \tag{1}$$

The minimum vb-dominating Laplacian matrix of a graph G is independent of the internal structure of the blocks in G.

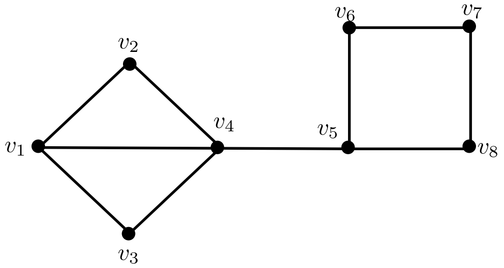


Figure 1. Graph G

Example 1. *Let G be a graph as shown in Figure 1 with a minimum vb-dominating set*
$B = \{v_4, v_5\}$. Then

$$L_{vb}(G) = \begin{bmatrix} 1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & 1 \end{bmatrix}$$

The minimum vb-dominating Laplacian eigenvalues of G *are* $-2.3028,$ $-1.7913, 1.3028, 2.0000, 2.0000, 2.0000, 2.0000$ *and 2.7913.Therefore, the minimum vb-dominating Laplacian energy of the graph* G *is* $LE_{vb}(G) = 18$*.*

3. BOUNDS FOR MINIMUM VB-DOMINATING LAPLACIAN ENERGY OF A GRAPH

Theorem 3.1. *Let* G *be a graph of order* p *and size* q *with* m *blocks and* $\varphi_1, \varphi_2, ..., \varphi_p$ *are the eigenvalues of* $L_{vb}(G)$*.Then*

(i) $\sum\limits_{i=1}^{p} \varphi_i = (p+m-1) - \gamma_{vb}$.

(ii) $\sum\limits_{i=1}^{p} \varphi_i^2 = 2q_p + \sum\limits_{i=1}^{p} (d_{vb}(v_i) - k_i)^2$.

Proof. (i) The sum of principal diagonal elements of $L_{vb}(G)$ is equal to $\sum\limits_{i=1}^{p} d_{vb}(v_i) - |\gamma_{vb} - set| = (p+m-1) - |\gamma_{vb}|$.

Also the sum of the Laplacian eigenvalues of $L_{vb}(G)$ is equal to the trace of $L_{vb}(G)$. Therefore, $\sum\limits_{i=1}^{p} \varphi_i = (p+m-1) - \gamma_{vb}$.

(ii) The sum of squares of the Laplacian eigenvalues of $L_{vb}(G)$ is the trace of $L_{vb}(G)^2$.

$$\text{Therefore, } \sum_{i=1}^{p} \varphi_i^2 = \sum_{i=1}^{p} \sum_{j=1}^{p} l_{ij} l_{ji}$$

$$= 2\sum_{i<j} (l_{ij})^2 + \sum_{i=1}^{p} (l_{ii})^2$$

$$= 2q_p + \sum_{i=1}^{p} (d_{vb}(v_i) - k_i)^2, \text{ where } k_i = \begin{cases} 1 & \text{if } v_i \in \gamma_{vb}\text{-set} \\ 0 & \text{if } v_i \notin \gamma_{vb}\text{-set} \end{cases}$$

and q_p is the number of edges in the point graph of G. □

$$\text{Let } R = q_p + \frac{1}{2} \sum_{i=1}^{p} (d_{vb}(v_i) - k_i)^2, \text{ where } k_i = \begin{cases} 1 & \text{if } v_i \in \gamma_{vb}\text{-set} \\ 0 & \text{if } v_i \notin \gamma_{vb}\text{-set.} \end{cases} \quad (2)$$

3.1. Lower bounds on $LE_{vb}(G)$.

Theorem 3.2. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. Then $LE_{vb}(G) \geq \frac{2R}{|\varphi_1|} - 2q_p$, where R is the expression defined as in* (2).

Proof. It is easy to observe that, for any graph $|\varphi_1||\varphi_i| \geq \varphi_i^2$, for all i, $1 \leq i \leq p$. Then,

$$|\varphi_1| \sum_{i=1}^{p} |\varphi_i| \geq \sum_{i=1}^{p} \varphi_i^2.$$

$$\text{This implies that, } \sum_{i=1}^{p} |\varphi_i| \geq \frac{2R}{|\varphi_1|}.$$

By taking $a = |\varphi_i|$ for all $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a| - |b| \leq |a - b|$, we get

$$|\varphi_i| - \left|\frac{2q_p}{p}\right| \leq \left|\varphi_i - \frac{2q_p}{p}\right|.$$

$$\text{This implies that, } \sum_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G).$$

$$\text{Therefore, } LE_{vb}(G) \geq \frac{2R}{|\varphi_1|} - 2q_p.$$

□

Lemma 3.3. *(* [17] *Ozeki's inequality)*
If $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, ..n$ be two sequences of real numbers such that $0 \leq m_1 \leq a_i \leq M_1$ and $0 \leq m_2 \leq b_i \leq M_2$ for every i, $1 \leq i \leq n$, then $\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - (\sum_{i=1}^{n} a_i b_i)^2 \leq \frac{n^2}{4}[M_1 M_2 - m_1 m_2]^2$.

Theorem 3.4. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. Then $LE_{vb}(G) \geq \sqrt{2Rp - \frac{p^2}{4}[|\varphi_1| - |\varphi_p|]^2} - 2q_p$, where R is the expression defined as in* (2).

Proof. We choose $a_i = |\varphi_i|$, $b_i = 1$, for all i, $i = 1, 2, ..., p, m_1 = |\varphi_p|$ $M_1 = |\varphi_1|$ and $m_2 = M_2 = 1$ in Lemma 3.3. Then,

$$\sum_{i=1}^{p} |\varphi_i|^2 \sum_{i=1}^{p} 1 - \left(\sum_{i=1}^{p} |\varphi_i|\right)^2 \leq \frac{p^2}{4}[|\varphi_1| - |\varphi_p|]^2.$$

$$\text{That is, } \sqrt{\sum_{i=1}^{p} |\varphi_i|^2 \sum_{i=1}^{p} 1 - \frac{p^2}{4}[|\varphi_1| - |\varphi_p|]^2} \leq \sum_{i=1}^{p} |\varphi_i|.$$

$$\text{This implies that, } \sqrt{2Rp - \frac{p^2}{4}[|\varphi_1| - |\varphi_p|]^2} \leq \sum_{i=1}^{p} |\varphi_i|.$$

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ...p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a| - |b| \leq |a - b|$, we get

$$|\varphi_i| - \left|\frac{2q_p}{p}\right| \leq \left|\varphi_i - \frac{2q_p}{p}\right|.$$

$$\text{That is, } \sum_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G).$$

$$\text{Therefore, } LE_{vb}(G) \geq \sqrt{2Rp - \frac{p^2}{4}[|\varphi_1| - |\varphi_p|]^2} - 2q_p.$$

□

Lemma 3.5. [14] *Let $a = (a_i)$ and (b_i), $i = 1, 2, ..., n$ be two sequences of real numbers such that $a \leq a_i \leq A < \infty$ and $b \leq b_i \leq B < \infty$ where $a, b, A, B \in R$. Then $\left|n \sum\limits_{i=1}^{n} a_i b_i - \sum\limits_{i=1}^{n} a_i \sum\limits_{i=1}^{n} b_i\right| \leq n^2 \alpha(n)(A - a)(B - b)$, where $\alpha(n) = \frac{1}{4}\left[1 - \frac{(-1)^{n+1}+1}{2n^2}\right]$. Further, equality holds if and only if $a_1 = a_2 = ... = a_n$ or $b_1 = b_2 = ... = b_n$.*

Theorem 3.6. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. Then $LE_{vb}(G) \geq \sqrt{2Rp - p^2\alpha(p)(|\varphi_1| - |\varphi_p|)^2} - 2q_p$, where R is the expression defined as in (2) and $\alpha(p) = \frac{1}{4}\left[1 - \frac{(-1)^{p+1}+1}{2p^2}\right]$.*

Proof. We choose $a_i = |\varphi_i|$, $b_i = |\varphi_i|$, for all i, $i = 1, 2, ..., p$, $a = b = |\varphi_p|$ and $A = B = |\varphi_1|$ in Lemma 3.5. Then,

$$\left|p \sum_{i=1}^{p} |\varphi_i|^2 - \sum_{i=1}^{p} |\varphi_i| \sum_{i=1}^{p} |\varphi_i|\right| \leq p^2\alpha(p)\left(|\varphi_1| - |\varphi_p|\right)^2,$$

$$\text{where } \alpha(p) = \frac{1}{4}\left[1 - \frac{(-1)^{p+1}+1}{2p^2}\right].$$

$$\text{This implies that, } \left|2Rp - \left(\sum_{i=1}^{p} |\varphi_i|\right)^2\right| \leq p^2\alpha(p)\left(|\varphi_1| - |\varphi_p|\right)^2.$$

Using Cauchy-Schwarz inequality $\left(\sum\limits_{i=1}^{n} a_i b_i\right)^2 \leq \sum\limits_{i=1}^{n} a_i^2 \sum\limits_{i=1}^{n} b_i^2$, choose $a_i = 1$ and $b_i = |\varphi_i|$, for all i, $i = 1, 2, ...p$, then, $2Rp \geq \left(\sum\limits_{i=1}^{p} |\varphi_i|\right)^2$.

$$\text{Therefore, } \sqrt{2Rp - p^2\alpha(p)\left(|\varphi_1| - |\varphi_p|\right)^2} \leq \sum_{i=1}^{p} |\varphi_i|.$$

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a| - |b| \leq |a - b|$, we get,

$$|\varphi_i| - \left|\frac{2q_p}{p}\right| \leq \left|\varphi_i - \frac{2q_p}{p}\right|.$$

This implies that, $\sum\limits_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G)$.

$$\text{Therefore, } LE_{vb}(G) \geq \sqrt{2Rp - p^2\alpha(p)(|\varphi_1| - |\varphi_p|)^2} - 2q_p,$$

where $\alpha(p) = \frac{1}{4}\left[1 - \frac{(-1)^{p+1}+1}{2p^2}\right]$. □

Lemma 3.7. [11] *Suppose* a_i *and* b_i, $i = 1, 2, .., n$ *are positive real numbers. Then* $\sum\limits_{i=1}^{n} a_i^2 \sum\limits_{i=1}^{n} b_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum\limits_{i=1}^{n} a_ib_i\right)^2$, *where* $M_1 = max\{a_1, a_2, ..., a_n\}, M_2 = max\{b_1, b_2, ..., b_n\}, m_1 = min\{a_1, a_2, ..., a_n\}$ *and* $m_2 = min\{b_1, b_2, ..., b_n\}$.

Theorem 3.8. *Let* G *be a graph with* p *vertices and* $\varphi_1, \varphi_2, ..., \varphi_p$ *be the eigenvalues of* $L_{vb}(G)$ *with* $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. *If* $L_{vb}(G)$ *is non-singular matrix, then* $LE_{vb}(G) \geq \frac{2\sqrt{2Rp}\sqrt{|\varphi_1||\varphi_p|}}{|\varphi_1|+|\varphi_p|} - 2q_p$, *where* R *is the expression defined as in* (2).

Proof. Let $a_i = |\varphi_i|$, $b_i = 1$, for all i, $i = 1, 2, ..., p$ and $M_1 = |\varphi_1|$, $m_1 = |\varphi_p|$, and $m_2 = M_2 = 1$. Then by using Lemma 3.7, we get

$$\sum_{i=1}^{p} |\varphi_i|^2 \sum_{i=1}^{p} 1 \leq \frac{1}{4}\left(\sqrt{\frac{|\varphi_1|}{|\varphi_p|}} + \sqrt{\frac{|\varphi_p|}{|\varphi_1|}}\right)^2 \left(\sum_{i=1}^{p} |\varphi_i|\right)^2.$$

$$\text{That is, } \frac{4(2Rp)}{\left(\sqrt{\frac{|\varphi_1|}{|\varphi_p|}} + \sqrt{\frac{|\varphi_p|}{|\varphi_1|}}\right)^2} \leq \left(\sum_{i=1}^{p} |\varphi_i|\right)^2.$$

$$\text{This implies that, } \frac{2\sqrt{2Rp}\sqrt{|\varphi_1||\varphi_p|}}{|\varphi_1| + |\varphi_p|} \leq \sum_{i=1}^{p} |\varphi_i|.$$

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a| - |b| \leq |a - b|$, we get,

$$|\varphi_i| - \left|\frac{2q_p}{p}\right| \leq \left|\varphi_i - \frac{2q_p}{p}\right|.$$

This implies that, $\sum\limits_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G)$.

$$\text{Therefore, } LE_{vb}(G) \geq \frac{2\sqrt{2Rp}\sqrt{|\varphi_1||\varphi_p|}}{|\varphi_1| + |\varphi_p|} - 2q_p.$$

□

Lemma 3.9. *([3] Bhatia and Davis's bound on variance)*
Let $a_1, a_2, ..., a_k$ be real numbers such that $a \leq a_i \leq A$, for all i, $i = 1, 2, ..., k$ and $\varphi = \frac{\sum_{i=1}^{k} a_i}{k}$. Then $\sum_{i=1}^{k} a_i^2 \leq k[\varphi(A+a) - Aa]$, equality holds if and only if each a_i is either A or a.

Theorem 3.10. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. Then $LE_{vb}(G) \geq \frac{2R+p|\varphi_1||\varphi_p|}{|\varphi_1|+|\varphi_p|} - 2q_p$, where R is the expression defined as in (2).*

Proof. We choose $a_i = |\varphi_i|$, for all i, $i = 1, 2..., p$, $a = |\varphi_p|$, $A = |\varphi_1|$ and $\varphi = \frac{\sum_{i=1}^{p} |\varphi_i|}{p}$ in Lemma 3.9. Then,

$$\sum_{i=1}^{p} |\varphi_i|^2 \leq p\left(\frac{\sum_{i=1}^{p} |\varphi_i|}{p}(|\varphi_1| + |\varphi_p| - |\varphi_1||\varphi_p|)\right).$$

$$\text{That is, } 2R \leq \sum_{i=1}^{p} |\varphi_i| \left[|\varphi_1| + |\varphi_p|\right] - p|\varphi_1||\varphi_p|.$$

$$\text{This implies that, } \frac{2R + p|\varphi_1||\varphi_p|}{|\varphi_1| + |\varphi_p|} \leq \sum_{i=1}^{p} |\varphi_i|.$$

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a| - |b| \leq |a - b|$ we get,

$$|\varphi_i| - \left|\frac{2q_p}{p}\right| \leq \left|\varphi_i - \frac{2q_p}{p}\right|.$$

$$\text{This implies that, } \sum_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G).$$

$$\text{Therefore, } LE_{vb}(G) \geq \frac{2R + p|\varphi_1||\varphi_p|}{|\varphi_1| + |\varphi_p|} - 2q_p.$$

□

Note that the above result coincides with Theorem 3.2 if one of the eigenvalue of $L_{vb}(G)$ is 0.

Lemma 3.11. [4] *Let $a_1 \geq a_2 \geq ... \geq a_n > 0$ be real numbers. Then $\sum_{i=1}^{n} a_i - n\left(\prod_{i=1}^{n} |a_i|\right)^{\frac{1}{n}} \geq (\sqrt{a_1} - \sqrt{a_n})^2$ with equality if $a_2 = a_3 = ... = a_{n-1} = \sqrt{a_1 a_n}$.*

Theorem 3.12. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$. If $L_{vb}(G)$ is non-singular matrix, then $LE_{vb}(G) \geq pK^{\frac{1}{p}} + \left(\sqrt{|\varphi_1| - |\varphi_p|}\right)^2 - 2q_p$, where $K = \prod_{i=1}^{p} |\varphi_i|$.*

Proof. We choose $a_i = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ in Lemma 3.11. Then,

$$\sum_{i=1}^{p} |\varphi_i| - p \left(\prod_{i=1}^{p} |\varphi_i| \right)^{\frac{1}{p}} \geq \left(\sqrt{|\varphi_1| - |\varphi_p|} \right)^2 .$$

This implies that, $\displaystyle\sum_{i=1}^{p} |\varphi_i| \geq pK^{\frac{1}{p}} + \left(\sqrt{|\varphi_1| - |\varphi_p|} \right)^2$, where $K = \displaystyle\prod_{i=1}^{p} |\varphi_i|$.

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left| \frac{2q_p}{p} \right|$ in the triangular inequality $|a| - |b| \leq |a - b|$, we get,

$$|\varphi_i| - \left| \frac{2q_p}{p} \right| \leq \left| \varphi_i - \frac{2q_p}{p} \right| .$$

This implies that, $\displaystyle\sum_{i=1}^{p} |\varphi_i| - 2q_p \leq LE_{vb}(G)$.

Therefore, $LE_{vb}(G) \geq pK^{\frac{1}{p}} + \left(\sqrt{|\varphi_1| - |\varphi_p|} \right)^2 - 2q_p$, where $K = \displaystyle\prod_{i=1}^{p} |\varphi_i|$.

□

3.2. Upper bounds on $LE_{vb}(G)$.

Lemma 3.13. [5] *Let $p = (p_i)$, $q = (q_i)$ be two sequence of non-negative real numbers and $a = (a_i)$, $b = (b_i)$, $c = (c_i)$, $d = (d_i)$ be sequences of real numbers, $i = 1, 2, ..., n$. Then*

$$\sum_{i=1}^{n} p_i a_i^2 \sum_{i=1}^{n} q_i b_i^2 + \sum_{i=1}^{n} p_i c_i^2 \sum_{i=1}^{n} q_i d_i^2 \geq 2 \sum_{i=1}^{n} p_i a_i c_i \sum_{i=1}^{n} q_i b_i d_i .$$

If (p_i) and (q_i) are sequences of positive numbers, then the equality holds if and only if $a_i b_j = c_i d_j$ for any $i, j \in \{1, ..., n\}$.

Theorem 3.14. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$. Then $LE_{vb}(G) \leq \sqrt{\frac{p^2+4R^2}{2}} + 2q_p$, where R is the expression defined as in (2).*

Proof. We choose $a_i = b_i = p_i = q_i = 1$ and $c_i = d_i = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ in Lemma 3.13. Then,

$$\sum_{i=1}^{p} 1 \sum_{i=1}^{p} 1 + \sum_{i=1}^{p} |\varphi_i|^2 \sum_{i=1}^{p} |\varphi_i|^2 \geq 2 \sum_{i=1}^{p} |\varphi_i| \sum_{i=1}^{p} |\varphi_i| .$$

That is, $p^2 + (2R)^2 \geq 2 \left(\displaystyle\sum_{i=1}^{p} |\varphi_i| \right)^2$.

This implies that, $\displaystyle\sum_{i=1}^{p} |\varphi_i| \leq \sqrt{\frac{p^2 + 4R^2}{2}}$.

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a - b| \leq |a| + |b|$, we get

$$\left|\varphi_i - \frac{2q_p}{p}\right| \leq |\varphi_i| + \left|\frac{2q_p}{p}\right|.$$

$$\text{This implies that, } \sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right| \leq \sum_{i=1}^{p}|\varphi_i| + 2q_p.$$

$$\begin{aligned}\text{Therefore, } LE_{vb}(G) &\leq \sum_{i=1}^{p}|\varphi_i| + 2q_p \\ &\leq \sqrt{\frac{p^2+4R^2}{2}} + 2q_p.\end{aligned}$$

□

Theorem 3.15. *Let G be a graph with p vertices and φ_i, $i = 1, 2, ..., p$ be the eigenvalues of $L_{vb}(G)$. Then $LE_{vb}(G) \leq \sqrt{\frac{p^2}{2} + \frac{(2Rp+4q_p^2-4q_p(p+m-1-\gamma_{vb}))^2}{2p^2}}$, where R is the expression defined as in* (2).

Proof. We choose $a_i = b_i = p_i = q_i = 1$ and $c_i = d_i = \left|\varphi_i - \frac{2q_p}{p}\right|$, for all i, $i = 1, 2, ..., p$ in Lemma 3.13. Then,

$$\sum_{i=1}^{p}1\sum_{i=1}^{p}1 + \sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|^2\sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|^2 \geq 2\sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|\sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|.$$

$$\text{That is, } p^2 + \left(\sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|^2\right)^2 \geq 2\left(\sum_{i=1}^{p}\left|\varphi_i - \frac{2q_p}{p}\right|\right)^2.$$

This implies that,

$$2(LE_{vb}(G))^2 \leq p^2 + \left(\sum_{i=1}^{p}\varphi_i^2 + \sum_{i=1}^{p}\frac{4q_p^2}{p^2} - \frac{4q_p}{p}\sum_{i=1}^{p}\varphi_i\right)^2.$$

Thus,

$$LE_{vb}(G) \leq \sqrt{\frac{p^2}{2} + \frac{(2Rp+4q_p^2-4q_p(p+m-1-\gamma_{vb}))^2}{2p^2}}.$$

□

Lemma 3.16. [5] *Let $x = (x_i)$ and $y = (y_i)$, $i = 1, 2..., n$ be two sequences of real numbers and $z = (z_i)$ and $w = (w_i)$, $i = 1, 2, ..., n$ be two sequences of non-negative real numbers. Then $\sum_{i=1}^{n} w_i \sum_{i=1}^{n} z_i x_i^2 + \sum_{i=1}^{n} z_i \sum_{i=1}^{n} w_i y_i^2 \geq 2\sum_{i=1}^{n} z_i x_i \sum_{i=1}^{n} w_i y_i$. If z_i and w_i are positive, then the equality holds if and only if $x = y = k$, where k is a constant.*

Theorem 3.17. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$. Then $LE_{vb}(G) \leq R + \frac{p}{2} + 2q_p$, where R is the expression defined as in* (2).

Proof. We choose $x_i = |\varphi_i|$ and $w_i = y_i = z_i = 1$, for all i, $i = 1, 2, ..., p$ in Lemma 3.16. Then,

$$\sum_{i=1}^{p} 1 \sum_{i=1}^{p} |\varphi_i|^2 + \sum_{i=1}^{p} 1 \sum_{i=1}^{p} 1 \geq 2 \sum_{i=1}^{p} |\varphi_i| \sum_{i=1}^{p} 1.$$

$$\text{That is, } p \sum_{i=1}^{p} |\varphi_i|^2 + p^2 \geq 2p \sum_{i=1}^{p} |\varphi_i|.$$

$$\text{Hence, } \frac{2R+p}{2} \geq \sum_{i=1}^{p} |\varphi_i|.$$

By taking $a = |\varphi_i|$, for all i, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a - b| \leq |a| + |b|$, we get,

$$\left|\varphi_i - \frac{2q_p}{p}\right| \leq |\varphi_i| + \left|\frac{2q_p}{p}\right|.$$

$$\text{This implies that, } \sum_{i=1}^{p} \left|\varphi_i - \frac{2q_p}{p}\right| \leq \sum_{i=1}^{p} |\varphi_i| + 2q_p.$$

$$\text{Therefore, } LE_{vb}(G) \leq \frac{2R+p}{2} + 2q_p.$$

□

Theorem 3.18. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$. Then $LE_{vb}(G) \leq R + \frac{2q_p^2}{p} - \frac{2q_p}{p}(p + m - 1 - \gamma_{vb}) + \frac{p}{2}$, where M is the expression defined as in* (2).

Proof. We choose $x_i = |\varphi_i - \frac{2q_p}{p}|$, and $w_i = y_i = z_i = 1$, for all i, $i = 1, 2, ..., p$ in Lemma 3.16. Then,

$$\sum_{i=1}^{p} 1 \sum_{i=1}^{p} |\varphi_i - \frac{2q_p}{p}|^2 + \sum_{i=1}^{p} 1 \sum_{i=1}^{p} 1 \geq 2 \sum_{i=1}^{p} |\varphi_i - \frac{2q_p}{p}| \sum_{i=1}^{p} 1.$$

$$\text{That is, } p \sum_{i=1}^{p} |\varphi_i - \frac{2q_p}{p}|^2 + p^2 \geq 2p \sum_{i=1}^{p} |\varphi_i - \frac{2q_p}{p}|.$$

$$\text{This implies that, } \sum_{i=1}^{p} \varphi_i^2 + \frac{4q_p^2}{p^2} \sum_{i=1}^{p} 1 - \frac{4q_p}{p} \sum_{i=1}^{n} \varphi_i + p \geq 2 \sum_{i=1}^{p} |\varphi_i - \frac{2q_p}{p}|.$$

$$\text{Thus, } \; 2R + \frac{4q_p^2}{p} - \frac{4q_p}{p}(p + m - 1 - \gamma_{vb}) + p \geq 2LE_{vb}(G).$$

$$\text{Therefore, } R + \frac{2q_p^2}{p} - \frac{2q_p}{p}(p + m - 1 - \gamma_{vb}) + \frac{p}{2} \geq LE_{vb}(G).$$

□

Lemma 3.19. [1, 18] *Let $a = (a_i)$ and $x = (x_i)$, $i = 1, 2, ..., n$ be two sequences of positive real numbers and for $r \geq 0$, $\sum\limits_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum\limits_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum\limits_{i=1}^{n} a_i\right)^{r}}$, equality if and only if $\frac{x_1}{a_1} = \frac{x_2}{a_2} = ... = \frac{x_n}{a_n}$.*

Theorem 3.20. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$. Then $LE_{vb}(G) \leq \sqrt{2Rp + 4q_p^2 - 4q_p(p + m - 1 - \gamma_{vb})}$, where R is the expression defined as in* (2)*.*

Proof. We choose $x_i = \left|\varphi_i - \frac{2q_p}{p}\right|$, $a_i = 1$, for all i, $i = 1, 2, ..., p$ and $r = 1$ in Lemma 3.19. Then,

$$\sum_{i=1}^{p} \left|\varphi_i - \frac{2q_p}{p}\right|^2 \geq \frac{\left(\sum\limits_{i=1}^{p} \left|\varphi_i - \frac{2q_p}{p}\right|\right)^2}{p}.$$

$$\text{This implies that, } (LE_{vb}(G))^2 \leq p\left[\sum_{i=1}^{p} \varphi_i^2 + \frac{4q_p^2}{p^2}\sum_{i=1}^{p} 1 - \frac{4q_p}{p}\sum_{i=1}^{p}\varphi_i\right].$$

$$\text{Therefore, } LE_{vb}(G) \leq \sqrt{2Rp + 4q_p^2 - 4q_p(p + m - 1 - \gamma_{vb})}.$$

□

Lemma 3.21. *(* [15]*) Let $a_1, a_2, ...a_m$ be positive real numbers with the property $0 < r \leq a_i \leq R < +\infty$. Then $m\sum\limits_{i=1}^{m} a_i^2 - \left(\sum\limits_{i=1}^{m} a_i\right)^2 \geq \frac{m}{2}(R - r)^2$.*

Theorem 3.22. *Let G be a graph with p vertices and $\varphi_1, \varphi_2, ..., \varphi_p$ be the eigenvalues of $L_{vb}(G)$ with $|\varphi_1| \geq |\varphi_2| \geq ... \geq |\varphi_p|$.If $L_{vb}(G)$ is non-singular matrix, then $LE_{vb}(G) \leq \sqrt{2Rp - \frac{p}{2}(|\varphi_1| - |\varphi_p|)^2} + 2q_p$, where R is the expression defined as in* (2)*.*

Proof. We choose $a_i = |\varphi_i|$, for all i, $i = 1, 2, ...p$, $r = |\varphi_p|$, $R = |\varphi_1|$ in Lemma 3.21. Then,

$$p\sum_{i=1}^{p} |\varphi_i|^2 - \left(\sum_{i=1}^{p} |\varphi_i|\right)^2 \geq \frac{p}{2}\left(|\varphi_1| - |\varphi_p|\right)^2.$$

$$\text{That is, } 2Rp - \left(\sum_{i=1}^{p} |\varphi_i|\right)^2 \geq \frac{p}{2}\left(|\varphi_1| - |\varphi_p|\right)^2.$$

$$\text{This implies that, } \sum_{i=1}^{p} |\varphi_i| \leq \sqrt{2Rp - \frac{p}{2}(|\varphi_1| - |\varphi_p|)^2}.$$

By taking $a = |\varphi_i|$, $i = 1, 2, ..., p$ and $b = \left|\frac{2q_p}{p}\right|$ in the triangular inequality $|a - b| \leq |a| + |b|$, we get,

$$\left|\varphi_i - \frac{2q_p}{p}\right| \leq |\varphi_i| + \left|\frac{2q_p}{p}\right|.$$

$$\text{This implies that, } \sum_{i=1}^{p} \left|\varphi_i - \frac{2q_p}{p}\right| \leq \sum_{i=1}^{p} |\varphi_i| + 2q_p.$$

$$\text{Therefore, } LE_{vb}(G) \leq \sqrt{2Rp - \frac{p}{2}(|\varphi_1| - |\varphi_p|)^2} + 2q_p.$$

□

4. RELATIONSHIP BETWEEN MINIMUM VB-DOMINATING ENERGY AND MINIMUM VB-DOMINATING LAPLACIAN ENERGY

S. Udupa et al. [24] introduced the minimum *vb*-dominating energy $E_{vb}(G)$ of a graph G corresponding to minimum *vb*-dominating matrix $A_{vb}(G)$.

Remark 4.1.

[22] *Let I_n be the unit matrix of order n. Then the Laplacian energy can be expressed also as $LE(G) = \sum_{i=1}^{n} |\gamma_i|$ where γ_i, $i = 1, 2, ..., n$ are eigenvalues of the matrix $L(G) - \frac{2m}{n} I_n$.*

Let $A_{vb}(G)$ be the minimum vb-dominting matrix with $\lambda_1, \lambda_2, ...\lambda_p$ eigenvalues and $D_{vb}(G)$ be the diagonal matrix of order p whose $(i,i)^{th}$ entry is d_{ivb}, where d_{ivb} is the vb-degree of i^{th} vertex of G, for all i, $1 \leq i \leq p$, $i = 1, 2, ..., p$. Then,

$$L_{vb}(G) = D_{vb}(G) - A_{vb}(G). \tag{3}$$

The minimum vb-dominating Laplacian energy (1) can also be expressed as

$$LE_{vb}(G) = \sum_{i=1}^{p} |\gamma_i|, \tag{4}$$

where γ_i, $i = 1, 2, ..., p$ are the eigenvalues of the matrix $L_{vb}(G) - \left(\frac{2q_p}{p}\right) I_p$, where I_p be the unit matrix of order p.

Remark 4.2.

Let A, B, and C be two real square matrices of order n, such that $A+B = C$. Then $\sum_{i=1}^{n} s_i(A) + \sum_{i=1}^{n} s_i(B) \geq \sum_{i=1}^{n} s_i(C)$ ([6] Ky Fan theorem). Also, $E(C) \leq E(A) + E(B)$ [19]. Further, equality holds if and only if, there exists an orthogonal matrix P such that PA and PB are both positive semidefinite matrices.

W. So et al. [22] proved that for a graph G of order n and size m with vertex degrees $d_1, d_2, ..., d_n$, and average vertex degree $\overline{d} = \frac{\sum_{i=1}^{n} d_i}{n}$, $LE(G) \leq E(G) \sum_{i=1}^{n} |d_i - \overline{d}|$, where d_i is degree of vertices present in graph G and $\overline{d}$ is average vertex degree.

Theorem 4.3. *Let G be a graph of order p and size q with vertices $u_1, u_2, ..., u_p$. Then $LE_{vb}(G) \leq E_{vb}(G) + \sum_{i=1}^{p} \left| d_{vb}(u_i) - \overline{d_{vv}} \right|$, where $\overline{d_{vv}}$ is average vv-degree of vertices.*

Proof. We rewrite (3) as,

$$\left(L_{vb}(G) - \left(\frac{2q_p}{p}\right) I_p \right) = (-A_{vb}(G)) + \left(D_{vb}(G) - \left(\frac{2q_p}{p}\right) I_p \right).$$

Using (4), Remark 4.2 and the fact that $D_{vb}(G) - \left(\frac{2q_p}{p}\right) I_p$ is a diagonal matrix whose eigenvalues are $d_{vb}(u_i) - \overline{d_{vv}}$, $i = 1, 2, ..., p$. We get, the desired result. □

5. Minimum vb-dominating Laplacian energy of Alkanes

Alkanes are saturated hydrocarbons with an open hydrocarbon chain. These compounds have the empirical formula C_nH_{2n+2}. They are made up entirely of hydrogen and carbon. Each hydrogen atom has one bond, whereas each carbon atom has four. [7].

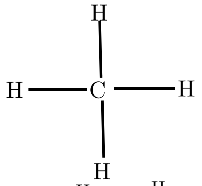
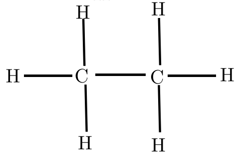
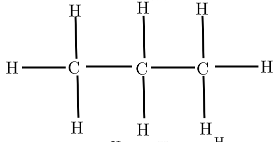
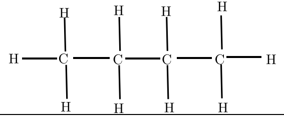
Name	**Structure**
Methane	
Ethane	
Propane	
Butane	

Table 1. Structure of Alkanes

and so on.

Example 2. *The molecular graph of methane is depicted in Figure 2.*

Note that $A = \{v_2\}$ is minimum vb-dominating set in G. The minimum vb-dominating Laplacian matrix for methane is as follows.

$$L_{vb}(G) = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & -1 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{bmatrix}$$

We have -0.2361, 1.0000, 1.0000, 1.0000 and 4.2361 are eigenvalues of $L_{vb}(G)$. The minimum vb-dominating Laplacian energy of methane is approximately equal to 6. If we similarly calculate the minimum vb-dominating Laplacian energy of ethane, propane, butane and remaing alkanes, we get the values approximately 11, 16, 21 and so on. Using these patterns, the following observations are made:

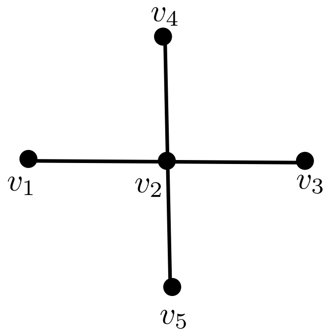


FIGURE 2. Graph G.

(i) The cardinality of minimum vb-dominating set γ_{vb} is same as that of number of carbon atoms present in alkanes.
(ii) Minimum vb-dominating Laplacian energy is approximately equal to $5\gamma_{vb} + 1$.

Remark 5.1.

(i) Molecular graph of any alkane is a tree [20]*.*
(ii) In a tree since each edge is a block, the minimum vb-Laplacian energy is same as that of Laplacian minimum covering energy [13]*.*

Note that for a tree T, Theorem 4.3 can be written as, $LE_{vb}(T) \leq E_{vb}(T) + \sum\limits_{i=1}^{p} |d_i - d|$, where d_i is degree of vertices and d is average degree of vertices. By Remark 5.1 (i) this property holds for Alkanes.

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