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A Note on the Calculation of Vertex Energy of Graphs Based on Estrada-Benzi Approach

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Abstract

Consider a simple undirected connected graph G that has an adjacency matrix $\boldsymbol{A}$. For a vertex $i \in V(G)$, the vertex energy (VE) of i in G is $E_\pi(i) = |\boldsymbol{A}|_{ii}$, where $|\boldsymbol{A}| = (\boldsymbol{A}\boldsymbol{A}^*)^{1/2}$. Furthermore, the graph energy of G is $E_\pi(G) = \sum_{i=1}^{n} |\lambda_i| = \sum_{i=1}^{n} E_\pi(i)$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $\boldsymbol{A}$. This paper introduces new computational equations for the vertex energy of graphs based on an equitable partition strategy, star sets, and the Estrada-Benzi approach. Furthermore, this paper provides the VE bounds of the graphs using a multi-digraph that corresponds to the quotient graphs of G. Additionally, this study calculates the VE upper bounds of the vertex's maximum degree for the wheel, the friendship, and endohedral fullerenes graphs more accurately.

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1 Introduction

Let $G = (V(G),\ E(G))$ be a simple undirected connected graph and $\boldsymbol{A}$ denotes the adjacency matrices of G and d_u denotes the degree of vertex u for G. Assuming that $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $\boldsymbol{A}$, G's graph energy [2, 27] is defined as follows:

$$E_\pi(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The concept of graph energy originated from studying the entire energy of a π-electron molecule of conjugated hydrocarbons based on the Hückel molecular orbital (HMO) theory in chemistry [13, 32]. Hückel's graph energy chemical interpretation was used to interpret Gutman's graph energy definition in 1978 [28]. Many scholars have studied the bounds of graph energy [4,29] and characterized the extremal graph using graph energy [1,35]. Estrada and Benzi reveal that the weighted sum of even power traces belonging to the adjacency matrix can obtain any graph's energy [20]. The corresponding energy calculation formula, the Estrada-benzi approach, is given in [43]. Furthermore, graph energy can also measure network resilience [17, 45] and evaluate the centrality of a vertex in a complex network [33, 37, 39]. Graph energy has also been used in other studies in physics, chemistry, computer science, and mathematics [19, 21, 30, 36, 41].

Based on the study of graph energy and motivated by the noncommutative probability, the vertex energy, or energy of a vertex (VE) was developed [5, 6]. Specifically, for a vertex $i \in V(G)$, the VE of i in G is:

$$E_\pi(i) = |\boldsymbol{A}|_{ii},$$

where $|\boldsymbol{A}| = (\boldsymbol{A}\boldsymbol{A}^*)^{1/2}$. It is evident that graph energy and vertex energy have the following relationship:

$$E_\pi(G) = \sum_{i=1}^{n} E_\pi(i).$$

Several scholars studied the VE concept. For instance, Arizmendi and

Sigarreta studied VE under a class joining trees perspective [8]. Arizmendi [7] and Qiao et al. [47] obtained a Coulson-type integral formula for the VE of a graph. Arizmendi, Hidalgo, and Juárez-Romero [6] obtained a probability type formula of a graph's VE and provided the VE bounds. VE is also an index of centrality in complex networks [10]. The reader is referred to [31] for more VE-related studies.

Equitable partition was first presented in [9, 24] and is defined as follows. Consider G be a graph with n vertices, and τ is a V(G) partition with $V_1 \cup V_2 \cup \cdots \cup V_t$. If constants b_{ij} exist so that every vertex in the cell V_i has b_{ij} neighbors in the cell V_j for all $i, j \in \{1, 2, \ldots, t\}$, then τ is an equitable partition. Matrix $(b_{ij})_{t\times t}$ is the divisor matrix of τ. Given that the orbits of any group of automorphisms in G constitute an equitable partition, every graph G has equitable partitions [16]. Data clustering, chemical analysis, and control theory heavily rely on equitable partitions [3, 38, 44]. Given that the spectrum of $(b_{ij})_{t\times t}$ is contained in G [9], $\boldsymbol{C}$ is the characteristic matrix of τ, whose columns represent the characteristic vectors of $V_1, \ldots, V_t$.

The quotient graph G/τ of G associated with τ is a multi-digraph, with its vertices representing subsets of $\tau(V_1, \ldots, V_t)$, where the d_{ij} arcs range from V_i to V_j [34]. The present study is based upon an equitable partition τ such that $\forall i, j \in \{1, \ldots, t\}$ with $i \neq j$, $\forall x \in V_i$, $|N_G(x) \cap V_j| = d_{ij}$, and as a t-partition of the vertices of G [25]. If τ is equitable, the quotient graph's adjacency matrix is consistent with the division matrix $\boldsymbol{B}$ of G [48].

In [15, 16], the authors introduced the star set and star complement concepts. Specifically, let λ be an eigenvalue of G with multiplicity k. A star set for λ in G is a vertex subset $\mathbb{X} \subseteq V(G)$ satisfying $|\mathbb{X}| = k$ where λ is not an eigenvalue of the induced subgraph $G - \mathbb{X}$. In this scenario, $G - \mathbb{X}$ is the star complement for λ in G. As well known, any eigenvalue of any graph has star sets [14, 42]. The reader is referred to [11, 46] for further details.

Since the equitable partitions and star sets exist for any eigenvalue of any graph, this study utilized the equitable partitions, the star complement, and the Estrada-Benzi approach to formulate the graphs' VE. The formulations provided assist in calculating the VE of large graphs while utilizing the structures of smaller subgraphs. This study also provided the VE bounds of the graphs using the multi-digraph of G's quotient graph. Precisely, we calculated with high accuracy the upper bounds of the VE of the max degree of the vertex for the wheel, the friendship, and endohedral fullerenes graphs.

The rest of this study is organized as follows. Section 2 presents the VE calculation formulas in the context of the equitable partitions of the graphs, the star complements technique, and the Estrada-Benzi approach. Section 3 introduces the expressions for the graph energy of the graph estimations. Section 4 compares the vertex energy bounds of this paper to those presented in the current literature. Finally, Section 5 concludes this work.

2 Vertex energy calculations for graphs

Let $\boldsymbol{A}$ be the adjacency matrix of G, and $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ its eigenvalues. The Perron-Frobenius theorem states that $\rho(\boldsymbol{A}) = \lambda_1$, i.e., the spectral radius of $\boldsymbol{A}$. Let $\mathrm{Tr}(\boldsymbol{A})$ denote the trace of $\boldsymbol{A}$. Consider $\boldsymbol{I}$ be an identity matrix. For a graph G with an order of n with an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_t$, its characteristic $n \times t$ matrix has as columns the $V_1, \ldots, V_t$ characteristic vectors.

Next, we present the relationship between divisor, adjacency, and characteristic matrices.

Lemma 2.1. *[24] Let τ be an equitable partition of graph G with divisor matrix $\boldsymbol{B}$ and characteristic matrix $\boldsymbol{C}$, then*

$$\boldsymbol{A}\boldsymbol{C} = \boldsymbol{C}\boldsymbol{B}.$$

Lemma 2.2. *[9, 48] If $\boldsymbol{A}$ is the adjacency matrix of a graph with an equitable partition, and $\boldsymbol{B}$ is the adjacency matrix of a divisor concerning the partition, then $\rho(\boldsymbol{A}) = \rho(\boldsymbol{B})$.*

Corollary 2.3 is obtained from Lemmas 2.1 and 2.2.

Corollary 2.3. *If τ is an equitable partition of graph G with divisor matrix*

B *and characteristic matrix* ***C****, then*

$$\left(\left(\frac{\boldsymbol{A}}{\rho(\boldsymbol{A})}\right)^k - \boldsymbol{I}\right)\boldsymbol{C} = \boldsymbol{C}\left(\left(\frac{\boldsymbol{B}}{\rho(\boldsymbol{B})}\right)^k - \boldsymbol{I}\right),$$

where k *is any positive integer.*

It is well known that the sum of the absolute values of the eigenvalues of the adjacency matrix of G equals $\mathrm{Tr}\,|\boldsymbol{A}|$, where $|\boldsymbol{A}| = (\boldsymbol{A}\boldsymbol{A}^*)^{1/2}$. In 2017, Estrada and Benzi [20] provided a new formula for calculating the value of $|\boldsymbol{A}|$:

$$|\boldsymbol{A}| = \sqrt{|\boldsymbol{A}^2|} = \lambda_1(\boldsymbol{A})\sqrt{\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})}\right)^2} = \lambda_1(\boldsymbol{A})\sqrt{\boldsymbol{I} + \left(\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})}\right)^2 - \boldsymbol{I}\right)}, \tag{1}$$

where $\lambda_1(\boldsymbol{A})$ represents the spectral radius, i.e., the largest eigenvalue of the graph's adjacency matrix. Hence, the graph energy is:

$$E_\pi(G) = \mathrm{Tr}\,|\boldsymbol{A}| = \lambda_1(\boldsymbol{A})\left(\sum_{k=0}^{\infty}\binom{\frac{1}{2}}{k}\mathrm{Tr}\left(\frac{\boldsymbol{A}^2}{\lambda_1^2(\boldsymbol{A})} - \boldsymbol{I}\right)^k\right). \tag{2}$$

Eq. (2) can be re-written as:

$$E_\pi(G) = \lambda_1(\boldsymbol{A})\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\mathrm{Tr}\left(\frac{\boldsymbol{A}^2}{\lambda_1^2(\boldsymbol{A})} - \boldsymbol{I}\right)^k\right). \tag{3}$$

The above formulas are also known as the Estrada-Benzi approach of graph energy, which can be used to calculate the vertex energy. The VE of i in G, where $i \in V(G)$ is a vertex, is calculated as follows:

$$E_\pi(i) = |\boldsymbol{A}|_{ii} = \lambda_1(\boldsymbol{A})\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(\frac{\boldsymbol{A}^2}{\lambda_1^2(\boldsymbol{A})} - \boldsymbol{I}\right)^k\right)_{ii}. \tag{4}$$

Next, VE is formulated using the graphs' equitable partitions, and the VE of G is calculated using the Estrada-Benzi approach with a smaller matrix.

Theorem 2.4. *Assuming* G *has an equitable partition* $V(G) = V_1 \cup V_2 \cup$

$\cdots \cup V_t$ *and* $V_1 = \{u\}$ *, then*

$$E_\pi(u) = \lambda_1(\boldsymbol{B}) \left(\left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I} \right)^k \right) \right)_{V_1 V_1},$$

where $\boldsymbol{B}$ *is the divisor matrix of the equitable partition.*

Proof. According to equation (1) and (2), we have

$$|\boldsymbol{A}| = \lambda_1(\boldsymbol{A}) \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})} \right)^2 - \boldsymbol{I} \right)^k.$$

Let $\boldsymbol{C}$ be the characteristic matrice of an equitable partition. Lemma 2.1, 2.2 and Corollary 2.3 asserts the following,

$$\begin{aligned} &\lambda_1(\boldsymbol{A}) \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})} \right)^2 - \boldsymbol{I} \right)^k \boldsymbol{C} \\ &= \lambda_1(\boldsymbol{B}) \boldsymbol{C} \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{\boldsymbol{B}}{\lambda_1(\boldsymbol{B})} \right)^2 - \boldsymbol{I} \right)^k \\ &= \lambda_1(\boldsymbol{B}) \boldsymbol{C} \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I} \right)^k \right). \end{aligned}$$

As $V_1 = \{u\}$, according to equation (1) and (2), we obtain

$$\begin{aligned} E_\pi(u) &= \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})} \right)^2 - \boldsymbol{I} \right)^k \right)_{uu} \\ &= \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} \left(\left(\frac{\boldsymbol{A}}{\lambda_1(\boldsymbol{A})} \right)^2 - \boldsymbol{I} \right)^k \boldsymbol{C} \right)_{uV_1} \\ &= \lambda_1(\boldsymbol{B}) \left(\boldsymbol{C} \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I} \right)^k \right) \right)_{uV_1} \end{aligned}$$

$$= \lambda_1(\boldsymbol{B}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I} \right)^k \right)_{V_1 V_1}.$$

■

Considering two vertex disjoint graphs G_1 and G_2, their joint graph $G_1 \otimes G_2$ has $V(G_1 \otimes G_2) = V(G_1) \cup V(G_2)$ and $E(G_1 \otimes G_2) = E(G_1) \cup E(G_2) \cup \{xy : x \in V(G_1) \text{ and } y \in V(G_2)\}$. Furthermore, if G_2 is a complete graph K_1, $G_1 \otimes K_1$ is also called a cone over G_1 [16].

Theorem 2.5. *Let $H = G \otimes K_1$ be a graph, where G is a d-regular graph with n vertices, then the VE of vertex $u \in K_1$ in H is*

$$E_\pi(u) = \frac{d + \sqrt{d^2 + 4n}}{2} - \sum_{k=1}^{\infty} \binom{2k}{k} \frac{1}{4(2k-1)} \left(\frac{d^k \left(\sqrt{d^2+4n}\right)^{k-1}}{\left(d + \sqrt{d^2+4n}\right)^{2k-2}} \right).$$

Proof. The graph H has an equitable partition $V(H) = \{u\} \cup V(G)$, and the divisor matrix of this equitable partition is $\boldsymbol{B} = \begin{pmatrix} 0 & n \\ 1 & d \end{pmatrix}$. Let

$$\boldsymbol{P} = \begin{pmatrix} \frac{-d+\sqrt{d^2+4n}}{2} & -\frac{d+\sqrt{d^2+4n}}{2} \\ 1 & 1 \end{pmatrix},$$

and

$$\boldsymbol{P}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{d^2+4n}} & \frac{d+\sqrt{d^2+4n}}{2\sqrt{d^2+4n}} \\ -\frac{1}{\sqrt{d^2+4n}} & \frac{-d+\sqrt{d^2+4n}}{2\sqrt{d^2+4n}} \end{pmatrix},$$

we have

$$\boldsymbol{B} = \boldsymbol{P} \begin{pmatrix} \frac{d+\sqrt{d^2+4n}}{2} & 0 \\ 0 & \frac{d-\sqrt{d^2+4n}}{2} \end{pmatrix} \boldsymbol{P}^{-1}.$$

Then the eigenvalues of divisor matrix $\boldsymbol{B}$ are $\lambda_1(\boldsymbol{B}) = \frac{d+\sqrt{d^2+4n}}{2}$ and $\lambda_2(\boldsymbol{B}) = \frac{d-\sqrt{d^2+4n}}{2}$.

$$\boldsymbol{B}^2 = \boldsymbol{P} \begin{pmatrix} \frac{2d^2+4n+2d\sqrt{d^2+4n}}{4} & 0 \\ 0 & \frac{2d^2+4n-2d\sqrt{d^2+4n}}{4} \end{pmatrix} \boldsymbol{P}^{-1}.$$

According to Theorem 2.4, the vertex u of VE is

$$\begin{aligned}
E_\pi(u) &= \lambda_1(\boldsymbol{B})\left(\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})}-\boldsymbol{I}\right)^k\right)\right)_{11}\\
&= \lambda_1(\boldsymbol{B})\left(I+\sum_{k=1}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(\boldsymbol{P}\begin{pmatrix}0 & 0\\ 0 & t^k\end{pmatrix}\boldsymbol{P}^{-1}\right)\right)_{11}\\
&= \lambda_1(\boldsymbol{B})\left(I+\sum_{k=1}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\begin{pmatrix}t_1 & t_2\\ t_3 & t_4\end{pmatrix}\right)_{11}\\
&= \frac{d+\sqrt{d^2+4n}}{2}-\sum_{k=1}^{\infty}\binom{2k}{k}\frac{1}{4(2k-1)}\left(\frac{d^k\left(\sqrt{d^2+4n}\right)^{k-1}}{\left(d+\sqrt{d^2+4n}\right)^{2k-2}}\right),
\end{aligned}$$

where $t=-\frac{4d\sqrt{d^2+4n}}{\left(d+\sqrt{d^2+4n}\right)^2}$, $t_1=\frac{2^{2k-1}(-d)^k\left(\sqrt{d^2+4n}\right)^{k-1}}{\left(d+\sqrt{d^2+4n}\right)^{2k-1}}$,
$t_2=-\frac{n(-4d)^k\left(\sqrt{d^2+4n}\right)^{k-1}}{\left(d+\sqrt{d^2+4n}\right)^{2k-1}}$, $t_3=-\frac{(-4d)^k\left(\sqrt{d^2+4n}\right)^{k-1}}{\left(d+\sqrt{d^2+4n}\right)^{2k-1}}$,
$t_4=\frac{2^{2k-1}(-d)^k\left(\sqrt{d^2+4n}\right)^{k-1}\left(-d+\sqrt{d^2+4n}\right)}{\left(d+\sqrt{d^2+4n}\right)^{2k}}$.

■

Next, we calculate the VE for a friendship graph by Theorem 2.5.

Example 2.6. *The* $F_m = K_1 \otimes \underbrace{(K_2 \cup K_2 \cdots K_2)}_{m}$ *graph is also called the friendship graph with* $2m+1$ *vertex. The spectra of* F_m *are* $\{\frac{1\pm\sqrt{8m+1}}{2}, -1^{[m]}, 1^{[m-1]}\}$ *[6]. From Theorem 2.5, the VE of the vertex of degree* $2m$ *in* F_m *is:*

$$\frac{1+\sqrt{8m+1}}{2}-\sum_{k=1}^{\infty}\binom{2k}{k}\frac{1}{4(2k-1)}\left(\frac{\left(\sqrt{8m+1}\right)^{k-1}}{\left(1+\sqrt{8m+1}\right)^{2k-2}}\right).$$

The graph energy of F_m *is*

$$E\left(F_m\right)=2m-1+\frac{1+\sqrt{8m+1}}{2}+\frac{\sqrt{8m+1}-1}{2}=2m-1+\sqrt{8m+1}.$$

All vertices of degree 2 in F_m *share the same VE and therefore, a* *vertice's energy of degree 2 in F_m is:*

$$1+\frac{\sqrt{8m+1}-3}{4m}+\frac{1}{2m}\sum_{k=0}^{\infty}\binom{2k}{k}\frac{1}{4(2k-1)}\left(\frac{\left(\sqrt{8m+1}\right)^{k-1}}{\left(1+\sqrt{8m+1}\right)^{2k-2}}\right).$$

This is consistent with the result in [6].

Remark 1. *The reader is referred to [12] for further research on the cones' spectra over regular graphs (e.g., $tC_m \otimes K_1$ and $tK_m \otimes K_1$). Theorem 2.5 provides the VE of cones over regular graphs (networks).*

A vertex subset is a star set based on the criterion below.

Lemma 2.7. *[14, 42] Consider $\mathbb{X}$ be a vertex subset in graph G and $\boldsymbol{A}=\begin{pmatrix}\boldsymbol{A}_{\mathbb{X}} & \boldsymbol{W}^{\top}\\ \boldsymbol{W} & \boldsymbol{F}\end{pmatrix}$, where $\boldsymbol{A}_{\mathbb{X}}$ is the subgraph's adjacency matrix induced by $\mathbb{X}$. Then $\mathbb{X}$ is a star set for an eigenvalue $\lambda(\boldsymbol{A})$ of G if and only if $\lambda(\boldsymbol{A})$ is not an eigenvalue of $\boldsymbol{F}$ and*

$$\lambda(\boldsymbol{A})\boldsymbol{I}-\boldsymbol{A}_{\mathbb{X}}=\boldsymbol{W}^{\top}(\lambda\boldsymbol{I}-\boldsymbol{F})^{-1}\boldsymbol{W}.$$

Below is the Estrada-Benzi formula for graph energy, which utilizes a star set of graphs.

Theorem 2.8. *Consider $\mathbb{X}$ a star set for an eigenvalue $\lambda(\boldsymbol{A})$ of graph G, and $\boldsymbol{A}=\begin{pmatrix}\boldsymbol{A}_{\mathbb{X}} & \boldsymbol{W}^{\top}\\ \boldsymbol{W} & \boldsymbol{F}\end{pmatrix}$, where $\boldsymbol{A}_{\mathbb{X}}$ is the subgraph's adjacency matrix induced by $\mathbb{X}$. Consider $r=\frac{\lambda^2(\boldsymbol{A})-\lambda_1^2(\boldsymbol{A})}{\lambda_1^2(\boldsymbol{A})}$, $\boldsymbol{Q}=\boldsymbol{F}-\lambda(\boldsymbol{A})\boldsymbol{I}$, $\boldsymbol{C}=\boldsymbol{Q}^{-1}\boldsymbol{W}\boldsymbol{W}^{\top}+\boldsymbol{Q}$ and $\boldsymbol{Z}=\frac{(\boldsymbol{C}+\lambda(\boldsymbol{A})\boldsymbol{I})^2-\lambda_1^2(\boldsymbol{A})\boldsymbol{I}}{\lambda_1^2(\boldsymbol{A})}$. Then,*
(1) *For any vertex $u\in\mathbb{X}$,*

$$E_{\pi}(u)=\lambda_1(\boldsymbol{A})\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(r^k+\sum_{v_1,v_2\in N_u(\widetilde{\mathbb{X}})}(\boldsymbol{P})_{v_1v_2}\right)\right),$$

where $\boldsymbol{P}=\boldsymbol{C}^{-1}\left(\boldsymbol{Z}^k-r^k\boldsymbol{I}\right)\boldsymbol{Q}^{-1}$, $N_u(\widetilde{\mathbb{X}})$ is the set of all neighbors of u in $\widetilde{\mathbb{X}}=V(G)\backslash\mathbb{X}$.

(2) *For any* $v \in \widetilde{\mathbb{X}} = V(G)\backslash\mathbb{X}$,

$$E_\pi(v) = \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\boldsymbol{T} + \boldsymbol{Z}^k \right) \right)_{vv},$$

where $\boldsymbol{T} = \boldsymbol{Q}^{-1}\boldsymbol{W}\boldsymbol{W}^\top\boldsymbol{C}^{-1}\left(r^k\boldsymbol{I} - \boldsymbol{Z}^k\right)$.

Proof. By Lemma 2.7, we obtain

$$\begin{aligned} \boldsymbol{A} - \lambda(\boldsymbol{A})\boldsymbol{I} &= \begin{pmatrix} \boldsymbol{A}_X - \lambda(\boldsymbol{A})\boldsymbol{I} & \boldsymbol{W}^\top \\ \boldsymbol{W} & \boldsymbol{Q} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ -\boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{0} & \boldsymbol{W}^\top \\ \boldsymbol{0} & \boldsymbol{C} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} \end{pmatrix}, \end{aligned}$$

where

$$\boldsymbol{C} = \boldsymbol{Q}^{-1}\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{Q} = \boldsymbol{Q}^{-1}\left(\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{Q}^2\right).$$

Since $\boldsymbol{W}\boldsymbol{W}^\top + \boldsymbol{Q}^2$ is positive definite, $\boldsymbol{C}$ is nonsingular. Hence,

$$\boldsymbol{A} - \lambda(\boldsymbol{A})\boldsymbol{I} = \boldsymbol{S} \begin{pmatrix} \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{C} \end{pmatrix} \boldsymbol{S}^{-1},$$

where

$$\begin{aligned} \boldsymbol{S} &= \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ -\boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{W}^\top\boldsymbol{C}^{-1} \\ \boldsymbol{0} & \boldsymbol{I} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{I} & \boldsymbol{W}^\top\boldsymbol{C}^{-1} \\ -\boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} - \boldsymbol{Q}^{-1}\boldsymbol{W}\boldsymbol{W}^\top\boldsymbol{C}^{-1} \end{pmatrix}, \end{aligned}$$

$$\begin{aligned} \boldsymbol{S}^{-1} &= \begin{pmatrix} \boldsymbol{I} & -\boldsymbol{W}^\top\boldsymbol{C}^{-1} \\ \boldsymbol{0} & \boldsymbol{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{I} - \boldsymbol{W}^\top\boldsymbol{C}^{-1}\boldsymbol{Q}^{-1}\boldsymbol{W} & -\boldsymbol{W}^\top\boldsymbol{C}^{-1} \\ \boldsymbol{Q}^{-1}\boldsymbol{W} & \boldsymbol{I} \end{pmatrix}. \end{aligned}$$

According to equation (1) and (2), we have

$$
\begin{aligned}
|\boldsymbol{A}| &= \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(\frac{\boldsymbol{A}^2}{\lambda_1^2(\boldsymbol{A})} - \boldsymbol{I} \right)^k \right) \\
&= \lambda_1(\boldsymbol{A}) \boldsymbol{S} \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \begin{pmatrix} r^k \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Z}^k \end{pmatrix} \right) \boldsymbol{S}^{-1} \\
&= \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \begin{pmatrix} \boldsymbol{M}_1 & \boldsymbol{M}_2 \\ \boldsymbol{M}_3 & \boldsymbol{M}_4 \end{pmatrix} \right),
\end{aligned}
$$

where $\boldsymbol{M}_1 = r^k \boldsymbol{I} + \boldsymbol{W}^\top \boldsymbol{C}^{-1} \left(\boldsymbol{Z}^k - r^k \boldsymbol{I} \right) \boldsymbol{Q}^{-1} \boldsymbol{W}$,
$\boldsymbol{M}_2 = \boldsymbol{W}^\top \boldsymbol{C}^{-1} \left(\boldsymbol{Z}^k - r^k \boldsymbol{I} \right)$,
$\boldsymbol{M}_3 = r^k \boldsymbol{Q}^{-1} \boldsymbol{W} \boldsymbol{W}^\top \boldsymbol{C}^{-1} \boldsymbol{Q}^{-1} \boldsymbol{W} - \boldsymbol{Q}^{-1} \boldsymbol{W} \boldsymbol{W}^\top \boldsymbol{C}^{-1} \boldsymbol{Z}^k \boldsymbol{Q}^{-1} \boldsymbol{W} + \boldsymbol{Z}^k \boldsymbol{Q}^{-1} \boldsymbol{W} - r^k \boldsymbol{Q}^{-1} \boldsymbol{W}$,
$\boldsymbol{M}_4 = \boldsymbol{Q}^{-1} \boldsymbol{W} \boldsymbol{W}^\top \boldsymbol{C}^{-1} \left(r^k \boldsymbol{I} - \boldsymbol{Z}^k \right) + \boldsymbol{Z}^k$.

Therefore, we can obtained the VE of G as follows:

(1) For any vertex $u \in \mathbb{X}$, we have

$$
\begin{aligned}
E_\pi(u) &= |\boldsymbol{A}|_{uu} \\
&= \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(r^k + \sum_{v_1, v_2 \in N_u(\widetilde{\mathbb{X}})} (\boldsymbol{P})_{v_1 v_2} \right) \right),
\end{aligned}
$$

where $\boldsymbol{P} = \boldsymbol{C}^{-1} \left(\boldsymbol{Z}^k - r^k \boldsymbol{I} \right) \boldsymbol{Q}^{-1}$, $N_u(\widetilde{\mathbb{X}})$ is the set of all neighbours of u in $\widetilde{\mathbb{X}} = V(G) \backslash \mathbb{X}$.

(2) For any vertex $v \in \widetilde{\mathbb{X}}$, we have

$$
E_\pi(v) = \lambda_1(\boldsymbol{A}) \left(\sum_{k=0}^{\infty} \binom{2k}{k} \frac{(-1)^{k+1}}{2^{2k}(2k-1)} \left(T + Z^k \right) \right)_{vv},
$$

where $\boldsymbol{T} = \boldsymbol{Q}^{-1} \boldsymbol{W} \boldsymbol{W}^\top \boldsymbol{C}^{-1} \left(r^k \boldsymbol{I} - \boldsymbol{Z}^k \right)$.

■

An example of the calculation of theorem 2.8 is given as follows.

Example 2.9. *Figure 1 illustrates the vertices of the Peterson graph. It*

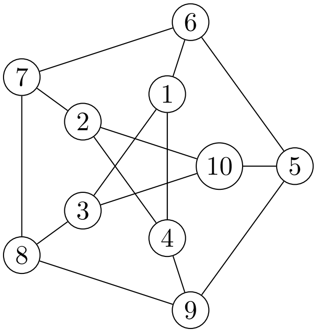

Figure 1. Label of the Petersen graph

has eigenvalue -2 with multiplicity 4 (see [16]), and it is the block matrix of the adjacency matrix as follows:

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_{\mathbb{X}} & \boldsymbol{W}^{\top} \\ \boldsymbol{W} & \boldsymbol{F} \end{pmatrix},$$

where

$$\boldsymbol{A}_{\mathbb{X}} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{W}^{\top} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\boldsymbol{F} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}.$$

Given that -2 is not $\boldsymbol{F}$'s eigenvalue, the set of vertices $\mathbb{X} = \{6, 7, 8, 9\}$ is a star set for eigenvalue -2. Using Theorem 2.8, which defines $\boldsymbol{C}$, $\boldsymbol{Q}$ can be calculated.

$$
\boldsymbol{Q} = \begin{pmatrix} \frac{4}{3} & -\frac{1}{3} & 1 & 1 & -\frac{1}{3} & -\frac{5}{3} \\ -\frac{1}{3} & \frac{4}{3} & 0 & -1 & -\frac{2}{3} & \frac{2}{3} \\ 1 & 0 & 2 & 1 & -1 & -2 \\ 1 & -1 & 1 & 2 & 0 & -2 \\ -\frac{1}{3} & -\frac{2}{3} & -1 & 0 & \frac{4}{3} & \frac{2}{3} \\ -\frac{5}{3} & \frac{2}{3} & -2 & -2 & \frac{2}{3} & \frac{10}{3} \end{pmatrix}
$$

and

$$
\boldsymbol{C} = \boldsymbol{Q}^{-1}\boldsymbol{W}\boldsymbol{W}^{\top} + \boldsymbol{Q} = \begin{pmatrix} 4 & 1 & 1 & 1 & 1 & 1 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 1 & 1 & 4 & 1 & 1 & 1 \\ 1 & 1 & 1 & 4 & 1 & 1 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ -1 & -1 & -1 & -1 & -1 & 2 \end{pmatrix}.
$$

Allow $\boldsymbol{Z}$ *be a matrix as defined in Theorem 2.8. For any* $i \in \{6,7,8,9\}$ *and* $j \in \{1,2,3,4,5,10\}$ *by Theorem 2.8, then* $r = \frac{-5}{9}$*, we have*

$$
\begin{aligned}
E_{\pi}(i) &= 3\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(\left(\frac{-5}{9}\right)^{k} + \sum_{v_1,v_2\in N_u(\widetilde{\mathbb{X}})}(\boldsymbol{P})_{v_1v_2}\right)\right) \\
&\approx 1.6,
\end{aligned}
$$

and

$$
\begin{aligned}
E_{\pi}(j) &= 3\left(\sum_{k=0}^{\infty}\binom{2k}{k}\frac{(-1)^{k+1}}{2^{2k}(2k-1)}\left(\boldsymbol{T} + \boldsymbol{Z}^{k}\right)\right)_{vv} \\
&\approx 1.6.
\end{aligned}
$$

3 Bounds of the vertex energy based on the quotient graph

In this section, we obtain some bounds for the VE of G by multi-digraph corresponding to quotient graphs of G, in terms of different parameters associated with the structure of the digraph. The order of these digraphs is generally much smaller than the order of the original graph, so these bounds are more practical.

Allow H be a multi-digraph corresponding to quotient graphs of G. Let $\pi : u_0, u_1, \ldots, u_l$ be a sequence of vertices, where (u_{k-1}, u_k) forms an arc or self-loop in H for any $1 \leq k \leq l$. π is a directed path of length l from u_0 to u_l, and π is a directed closed path if $u_0 = u_l$. Allow $\omega_j^{(u_i)}$ be the number of directed closed paths of length j associated with the vertex $v_i \in V(H)$. The sequence $\left(\omega_j^{(u_1)}, \omega_j^{(u_2)}, \ldots, \omega_j^{(u_n)}\right)$ is a directed closed paths sequence of length j in H [22, 23].

Next, the approximate VE for G is estimated using the Estrada-Benzi approach. Consider Theorem 2.5, and let $\boldsymbol{B}$ be the weighted adjacent matrix of the quotient graph H that corresponds to an equitable partition. Moreover, let

$$\boldsymbol{M} = \frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I},$$

where all eigenvalues in the interval $[-1, 0]$ of $\boldsymbol{M}$, then $\boldsymbol{M}$ is a negative semidefinite matrix. Furthermore,

$$\boldsymbol{M}_{ii} = \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)_{ii} = \frac{\omega_2^{(i)}}{\lambda_1^2(\boldsymbol{B})} - 1,$$

where $\omega_2^{(i)}$ is directed closed paths of length 2, associated with the vertex i of the quotient graph H. Clearly, these diagonal terms are all nonpositive. The following result is proven using Theorem 2.4.

Theorem 3.1. *Suppose that G has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_t$, if $V_1 = \{u\}$, then*

$$E_\pi(u) \leq \frac{\omega_2^{(u)}}{2\lambda_1(\boldsymbol{B})} + \frac{\lambda_1(\boldsymbol{B})}{2}.$$

Proof. It is easy to see that

$$E_\pi(u) \leq \lambda_1(\boldsymbol{B}),$$

and that

$$E_\pi(u) = \lambda_1(\boldsymbol{B})\left(\boldsymbol{I} + \frac{1}{2}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right) - \left(\frac{1}{8}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^2 - \frac{1}{16}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^3 + \cdots\right)\right)_{uu},$$

which implies that

$$E_\pi(u) \leq \lambda_1(\boldsymbol{B})\left(\boldsymbol{I} + \frac{1}{2}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)\right)_{uu} = \frac{\omega_2^{(u)}}{2\lambda_1(\boldsymbol{B})} + \frac{\lambda_1(\boldsymbol{B})}{2}.$$

■

The VE of some transitive graphs (e.g., Hypercube graph and Complete graph) and some large symmetries graphs (e.g., Friendship graph and Complete bipartite graph) are studied in [6]. Theorem 3.1 can be used for this kind of graph to calculate and estimate an upper bound of the graph energy of G more conveniently.

Corollary 3.2. *Assuming that G with order n has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u_1\}, V_2 = \{u_2\}, \cdots, V_s = \{u_s\}$ $(s \leq k)$ and $E_\pi(u_g) = E_\pi(u_t)$ $(g \in 1, 2, \ldots, s,\ t \in s+1, \cdots, k,\ u_t \in V_t)$, then*

$$E_\pi(G) \leq \frac{\lambda_1(\boldsymbol{B})}{2} n + \frac{\sum_{i=1}^{k} c_i \omega_2^{(u_i)}}{2\lambda_1(\boldsymbol{B})},$$

where c_i denote the number of vertices in V_i. In particular, $c_i = 1$ for $i = 1, 2, \ldots, s$.

If any $c_i = 1$, then $E_\pi(G) \leq \frac{m}{2\lambda_1(B)} + \frac{\lambda_1(B)}{2} n$, where m be the edges of G. This result is consistent with [20]. Below, we give a more accurate estimate than Theorem 3.1.

Theorem 3.3. *Suppose that G has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u\}$, then*

$$E_\pi(u) \leq \frac{3\lambda_1(\boldsymbol{B})}{8} + \frac{3}{4\lambda_1(\boldsymbol{B})}\omega_2^{(u)} - \frac{1}{8\lambda_1^3(\boldsymbol{B})}\omega_4^{(u)}.$$

Proof. It is easy to see that

$$M^2 = \left(\frac{B^2}{\lambda_1^2(B)} - I\right)^2 = \frac{1}{\lambda_1^4(B)}B^4 - \frac{2}{\lambda_1^2(B)}B^2 + I.$$

Then, we have

$$\begin{aligned} E_\pi(u) &\le \lambda_1(B)\left(I + \frac{1}{2}\left(\frac{B^2}{\lambda_1^2(B)} - I\right) - \frac{1}{8}\left(\frac{B^2}{\lambda_1^2(B)} - I\right)^2\right)_{uu} \\ &= \left(\frac{3\lambda_1(B)}{8}I + \frac{3}{4\lambda_1(B)}B^2 - \frac{1}{8\lambda_1^3(B)}B^4\right)_{uu} \\ &= \frac{3\lambda_1(B)}{8} + \frac{3}{4\lambda_1(B)}\omega_2^{(u)} - \frac{1}{8\lambda_1^3(B)}\omega_4^{(u)}. \end{aligned}$$

■

Corollary 3.4. *Assuming that G with order n has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u_1\}, V_2 = \{u_2\}, \cdots, V_s = \{u_s\}$ $(s \le k)$ and $E_\pi(u_g) = E_\pi(u_t)$ $(g \in 1, 2, \ldots, s,\ t \in s+1, \cdots, k,\ u_t \in V_t)$, then*

$$E_\pi(G) \le \frac{3\lambda_1(B)}{8}n + \frac{3\sum_{i=1}^{k} c_i\omega_2^{(u_i)}}{4\lambda_1^2(B)} - \frac{\sum_{i=1}^{k} c_i\omega_4^{(u_i)}}{8\lambda_1^3(B)},$$

where c_i denote the number of vertices in V_i. In particular, $c_i = 1$ for $i = 1, 2, \ldots, s$.

If any $c_i = 1$, this result is consistent with that of reference [20].

Later theorems 3.5, 3.7, Corollaries 3.6, and 3.8 give more accurate upper bounds for vertex energy and graph energy based on the Estrada-Benzi approach in theorem 2.4. Although these results are easy to obtain, these upper bounds significantly improve the calculation accuracy of vertex energy.

Theorem 3.5. *Suppose that G has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u\}$, then*

$$E_\pi(u) \le \frac{5\lambda_1(B)}{16} + \frac{15}{16\lambda_1(B)}\omega_2^{(u)} - \frac{5}{16\lambda_1^3(B)}\omega_4^{(u)} + \frac{1}{16\lambda_1^5(B)}\omega_6^{(u)}.$$

Proof. It is easy to see that

$$\boldsymbol{M}^3 = \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^3 = \frac{1}{\lambda_1^6(\boldsymbol{B})}\boldsymbol{B}^6 - \frac{3}{\lambda_1^4(\boldsymbol{B})}\boldsymbol{B}^4 + \frac{3}{\lambda_1^2(\boldsymbol{B})}\boldsymbol{B}^2 - \boldsymbol{I}.$$

Then we have

$$\begin{aligned}
E_\pi(u) &\le \lambda_1(\boldsymbol{B})\left(\boldsymbol{I} + \frac{1}{2}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right) - \frac{1}{8}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^2 + \right.\\
&\qquad \left.\frac{1}{16}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^3\right)_{uu}\\
&= \left(\frac{5\lambda_1(\boldsymbol{B})}{16}\boldsymbol{I} + \frac{15}{16\lambda_1(\boldsymbol{B})}\boldsymbol{B}^2 - \frac{5}{16\lambda_1^3(\boldsymbol{B})}\boldsymbol{B}^4 + \frac{1}{16\lambda_1^5(\boldsymbol{B})}\boldsymbol{B}^6\right)_{uu}\\
&= \frac{5\lambda_1(\boldsymbol{B})}{16} + \frac{15}{16\lambda_1(\boldsymbol{B})}\omega_2^{(u)} - \frac{5}{16\lambda_1^3(\boldsymbol{B})}\omega_4^{(u)} + \frac{1}{16\lambda_1^5(\boldsymbol{B})}\omega_6^{(u)}.
\end{aligned}$$

■

Corollary 3.6. *Assuming that G with order n has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u_1\}, V_2 = \{u_2\}, \cdots, V_s = \{u_s\}$ $(s \le k)$ and $E_\pi(u_g) = E_\pi(u_t)$ $(g \in 1, 2, \ldots, s,\ t \in s+1, \cdots, k,\ u_t \in V_t)$, then*

$$E_\pi(G) \le \frac{5\lambda_1(\boldsymbol{B})}{16}n + \frac{15\sum_{i=1}^k c_i\omega_2^{(u_i)}}{16\lambda_1(\boldsymbol{B})} - \frac{5\sum_{i=1}^k c_i\omega_4^{(u_i)}}{16\lambda_1^3(\boldsymbol{B})} + \frac{\sum_{i=1}^k c_i\omega_6^{(u_i)}}{16\lambda_1^3(\boldsymbol{B})}.$$

where c_i denote the number of vertices in V_i. In particular, $c_i = 1$ for $i = 1, 2, \ldots, s$.

If any $c_i = 1$, this result is consistent with that of reference [20].

Theorem 3.7. *Suppose that G has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u\}$, then*

$$E_\pi(u) \le \frac{15\lambda_1(\boldsymbol{B})}{64} + \frac{5\omega_2^{(u)}}{8\lambda_1(\boldsymbol{B})} - \frac{25\omega_4^{(u)}}{32\lambda_1^3(\boldsymbol{B})} + \frac{3\omega_6^{(u)}}{8\lambda_1^5(\boldsymbol{B})} - \frac{5\omega_8^{(u)}}{64\lambda_1^7(\boldsymbol{B})}.$$

Proof. It is easy to see that

$$\begin{aligned}\boldsymbol{M}^4 &= \left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^4 \\ &= \frac{1}{\lambda_1^8(\boldsymbol{B})}\boldsymbol{B}^8 - \frac{4}{\lambda_1^6(\boldsymbol{B})}\boldsymbol{B}^6 + \frac{6}{\lambda_1^4(\boldsymbol{B})}\boldsymbol{B}^4 - \frac{4}{\lambda_1^2(\boldsymbol{B})}\boldsymbol{B}^2 + \boldsymbol{I}.\end{aligned}$$

We have

$$\begin{aligned}E_\pi(u) &\le \lambda_1(B)\Bigg(I + \frac{1}{2}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right) - \frac{1}{8}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^2 + \\ &\quad \frac{1}{16}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^3 - \frac{5}{64}\left(\frac{\boldsymbol{B}^2}{\lambda_1^2(\boldsymbol{B})} - \boldsymbol{I}\right)^4\Bigg)_{uu} \\ &= \Bigg(\frac{15\lambda_1(\boldsymbol{B})}{64}\boldsymbol{I} + \frac{5}{8\lambda_1(\boldsymbol{B})}\boldsymbol{B}^2 - \frac{25}{32\lambda_1^3(\boldsymbol{B})}\boldsymbol{B}^4 + \frac{3}{8\lambda_1^5(\boldsymbol{B})}\boldsymbol{B}^6 - \\ &\quad \frac{5}{64\lambda_1^5(\boldsymbol{B})}\boldsymbol{B}^6\Bigg)_{uu} \\ &= \frac{15\lambda_1(\boldsymbol{B})}{64} + \frac{5}{8\lambda_1(\boldsymbol{B})}\omega_2^{(u)} - \frac{25}{32\lambda_1^3(\boldsymbol{B})}\omega_4^{(u)} + \frac{3}{8\lambda_1^5(\boldsymbol{B})}\omega_6^{(u)} - \\ &\quad \frac{5}{64\lambda_1^7(\boldsymbol{B})}\omega_8^{(u)}.\end{aligned}$$

■

Corollary 3.8. *Assuming that G with order n has an equitable partition $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, if $V_1 = \{u_1\}, V_2 = \{u_2\}, \cdots, V_s = \{u_s\}$ $(s \le k)$ and $E_\pi(u_g) = E_\pi(u_t)$ $(g \in 1, 2, \ldots, s,\ t \in s+1, \cdots, k,\ u_t \in V_t)$, then*

$$E_\pi(G) \le \frac{15\lambda_1(\boldsymbol{B})}{64}n + \frac{5\sum_{i=1}^k c_i\omega_2^{(u_i)}}{8\lambda_1(\boldsymbol{B})} - \frac{25\sum_{i=1}^k c_i\omega_4^{(u_i)}}{32\lambda_1^3(\boldsymbol{B})} +$$

$$\frac{3\sum_{i=1}^k c_i\omega_6^{(u_i)}}{8\lambda_1^5(\boldsymbol{B})} - \frac{5\sum_{i=1}^k c_i\omega_8^{(u_i)}}{64\lambda_1^7(\boldsymbol{B})},$$

where c_i denote the number of vertices in V_i. In particular, $c_i = 1$ for $i = 1, 2, \ldots, s$.

Remark 2. *In a directed graph, the number of directed closed paths with a vertex of length l can also be calculated by directed rooted subgraphs* *containing the vertex. Generally, a closed path containing a point of length l corresponds to more types of radical subgraph structures than a closed-directed path containing the vertex. This means that when expanding a series of the same order, the vertex energy calculated using quotient graphs may converge faster than the original graph.*

4 Numerical results

In order to reveal the advantages and disadvantages of calculating vertex energy between the quotient graph, we use the friendship graph F_m, the wheel graph W_n, and the endohedral fullerenes graph $K_1 \otimes \mathbf{C}_n$.

First, we give the real value of VE in the center vertex for F_m and compare the upper bound of this paper and the upper bound for the vertex energy in [6] (Proposition 3.2), as reported in Table 1. Then, we compare the upper bounds of the center vertex on W_n, as listed in Table 2.

Table 1. Values of the $VE(G)$ and some bounds be obtained for F_m with maximum degree node

Graph	$VE(G)$	$\sqrt{d_i}$ [6]	Thm. (3.1)	Thm. (3.3)	Thm. (3.5)	Thm. (3.7)
F_3	2.4	2.450	2.500	2.431	2.411	2.405
F_4	2.785	2.828	2.873	2.809	2.791	2.788
F_5	3.123	3.162	3.202	3.143	3.129	3.126
F_6	3.428	3.464	3.5	3.445	3.433	3.430
F_7	3.708	3.742	3.775	3.723	3.712	3.709
F_8	3.969	4	4.031	3.982	3.972	3.970
F_9	4.213	4.243	4.272	4.225	4.216	4.214
F_{10}	4.445	4.472	4.5	4.455	4.447	4.445

Table 2. Values of the $VE(G)$ and some bounds be obtained for W_n with maximum degree node

Graph	$VE(G)$	$\sqrt{d_i}$ [6]	Thm. (3.1)	Thm. (3.3)	Thm. (3.5)	Thm. (3.7)
W_3	1.5	1.732	2	1.778	1.679	1.624
W_4	1.789	2	2.236	2.023	1.931	1.883
W_5	2.041	2.236	2.449	2.244	2.159	2.115
W_6	2.268	2.450	2.646	2.447	2.367	2.328
W_7	2.475	2.649	2.828	2.635	2.561	2.525
W_8	2.667	2.828	3	2.813	2.742	2.709
W_9	2.846	3	3.162	2.979	2.913	2.883
W_{10}	3.015	3.162	3.317	3.139	3.075	3.047

Endohedral fullerenes are an intriguing group of molecules where atoms or small clusters (known as endohedral species) are enclosed within the empty interior of fullerenes, like the buckyball ($\mathbf{C}_{60}$) or other carbon nanostructures [18, 26, 40]. The encapsulated species' interaction with the fullerene cage leads to interesting chemical, physical, and electronic properties. Some simple fullerene embedding, defined as the cone of fullerene $\mathbf{C}_x$ (x is an even number greater than or equal to 20, except for 22), is defined as $K_1 \otimes \mathbf{C}_x$. The central nodes of these embedded fullerene graph classes are considered the atlas, and we provide the upper bound comparison of these central nodes, as reported in Table 3.

Table 3. Values of the $VE(G)$ and some bounds be obtained for $K_1 \otimes \mathbf{C}_n$ with maximum degree node

Graph	$VE(G)$	$\sqrt{d_i}$ [6]	Thm. (3.1)	Thm. (3.3)	Thm. (3.5)	Thm. (3.7)
$K_1 \otimes \mathbf{C}_{20}$	4.240	4.472	4.717	4.442	4.342	4.296
$K_1 \otimes \mathbf{C}_{24}$	4.684	4.899	5.123	4.860	4.769	4.728
$K_1 \otimes \mathbf{C}_{26}$	4.892	5.099	5.315	5.058	4.969	4.931
$K_1 \otimes \mathbf{C}_{28}$	5.091	5.291	5.5	5.247	5.162	5.127
$K_1 \otimes \mathbf{C}_{30}$	5.283	5.477	5.679	5.431	5.349	5.315
$K_1 \otimes \mathbf{C}_{32}$	5.468	5.657	5.852	5.609	5.529	5.498
$K_1 \otimes \mathbf{C}_{36}$	5.821	6	6.185	5.949	5.875	5.846
$K_1 \otimes \mathbf{C}_{50}$	6.917	7.071	7.228	7.015	6.954	6.933
$K_1 \otimes \mathbf{C}_{60}$	7.605	7.746	7.890	7.689	7.634	7.616
$K_1 \otimes \mathbf{C}_{76}$	8.592	8.718	8.846	8.660	8.614	8.600
$K_1 \otimes \mathbf{C}_{80}$	8.821	8.944	9.069	8.887	8.842	8.828
$K_1 \otimes \mathbf{C}_{180}$	13.333	13.416	13.500	13.365	13.341	13.335
$K_1 \otimes \mathbf{C}_{240}$	15.420	15.492	15.564	15.444	15.425	15.421

It can be seen from Tables 1-3 that the upper bound calculated by the Estrada-Benzi approach is well approximated close to the real value, demonstrating that the upper bound accuracy of Theorem 3.7 in the test graph set is accurate enough. Moreover, the upper bound provided by Theorem 3.3 in most number graphs is better than the one of Proposition 3.2 in [6]. In addition, since the above test atlas satisfies the conditions of Theorem 2.5, we can also manually calculate the values by Theorem 2.5.

5 Concluding remarks

Graph energy is associated with the total energy of π-electrons and linearly combines the energy related to the carbon atom's skeletal structure. Estrada and Benzi interpreted the energy in structural terms by considering the subgraphs and fragments of the underlying graph. The authors studied the contribution of subgraphs to the total energy of graphs and proposed an efficient computing method based on an even-order trace of the adjacency matrix. Their method is also suitable for solving the vertex energy of graphs. This paper generalizes the Estrada-Benzi approach, and given that every graph G contains equitable partitions and star complements, we derive some new equations for calculating vertex energy. Compared with the graph G's adjacency matrix used by the Estrada-Benzi approach to calculate the vertex energy, the formula used in this paper can obtain the vertex energy from a smaller matrix. The relation between the vertex energy and quotient graphs is also given. Furthermore, we obtained certain bounds for the graph energy based on a multi-digraph corresponding to quotient graphs of G. Future research will consider VE formulas for digraphs and approximating VE using other graph parameters.

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