MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **92** (2024) 105–131
ISSN: 0340–6253
doi: 10.46793/match.92-1.105D

On Second Zagreb Energy of Graphs

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(Received July 7, 2023)

Sažetak

Chemical structures are transformed into real numbers employing topological indices, which enable numerical computations to substitute pricey wet lab experiments. The spectral properties of topological indices can be investigated by appropriate modification of adjacency matrix. Gutman and Trinajstic, pioneers in the field of chemical graph theory, presented the Zagreb indices, which have governed topological indices research since 1972. The modified adjacency matrix associated to the second Zagreb index (M_2) is studied in this work. The second Zagreb energy (ZE_2) is generated from this matrix. The application potential of ZE_2 is explored by investigating its efficiency in modelling physico-chemical properties of molecules and isomer discrimination. We aim to set up crucial bounds of spectral radius and spread with identifying extremal graphs. Moreover, the ZE_2 energy is investigated for numerous special graphs including regular, semi-regular and chain graphs. We construct a divisor type matrix to estimate the M_2-spectrum and ZE_2 energy of the chain graph.

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1 Introduction

Throughout this article, we consider G as a graph of order n and size m. Here, $V(G)$ and $E(G)$ represent the set of all vertices and edges, respectively of the graph G. If two vertices u_i and u_j are connected, then we consider it as $u_iu_j \in E(G)$. Let $N_G(u_i)$ be the total number of vertices adjacent to the vertex u_i. The degree of a vertex u_i is represented as d_i which is equal to $|N_G(u_i)|$.

The spectral graph theory [4] can be thought of as an approach to employ linear algebra, in particular the well developed theory of matrix to explore numerous secrets of discrete mathematics and its applications. An important and leading tool in this area of research is the adjacency matrix. For a graph G, its adjacency matrix is denoted as $A(G)$, whose (i,j)-th entry is given by

$$a_{ij} = \begin{cases} 1, & if\ u_iu_j \in E(G), \\ 0, & otherwise. \end{cases}$$

Now, the characteristic polynomial is $\Phi_A(G,\lambda) = \det(\lambda I_n - A(G))$, where I_n represents the identity matrix of order $n \times n$. Since $A(G)$ is real symmetric matrix, its all eigenvalues are real, and we can arrange them as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The set $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is known as the A-spectrum of G which is denoted by $Sp(A(G))$. If $\{\lambda_1, \lambda_2, \ldots, \lambda_k\}$ be the set of distinct A-eigenvalues of G with multiplicities $\{l_1, l_2, \ldots, l_k\}$, then the spectrum of $A(G)$ can be written as

$$Sp(A(G)) = \begin{pmatrix} \lambda_1 & \lambda_2 & ... & \lambda_k \\ l_1 & l_2 & ... & l_k \end{pmatrix}.$$

The greatest eigenvalue λ_1 is called the spectral radius and the difference $\lambda_1 - \lambda_n$ is known as the spread. In 1978, Gutman proposed a striking concept of graph energy [19] to estimate the total π-electron energy of conjugated hydrocarbon. For any graph G, the graph energy is formulated as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1}$$

The survey article [18] by Gutman and Ramane provides detail information on graph energy and for more discussion, see [15, 16, 20, 29]. Promising investigations of this quantity from theoretical and application point of view [43] led to the introduction of several energy variants including extended energy [45], Laplacian energy [21, 23], distance energy [10, 13], and so on. The topological indices [34] are numerical graph invariants that characterizes the molecular topology of chemical compounds. It plays crucial role in quantitative structure property relationship (QSPR) [25] analysis to model different properties and activities of molecules. The idea of topological indices was initiated in 1947, when Harold Wiener presented the well-known Wiener index [12] for estimating boiling point of alkanes. Later, significant proportion of mathematical chemistry research was performed on indices based on different graph parameters [25]. The degree-based indices were spread through the most commonly used Zagreb indices [22], which are formulated as

$$M_1(G) = \sum_{u_iu_j \in E(G)} d_i + d_j, \qquad M_2(G) = \sum_{u_iu_j \in E(G)} d_i\, d_j.$$

Since the last few years, researchers have focused on exploring the spectral properties of topological indices by appropriate modification of the adjacency matrix $A(G)$ [31]. The degree based indices can be represented as $\sum_{u_iu_j \in E(G)} F\,(d_i,\, d_j)$, where F is a suitable symmetric function. For instance, in case of M_2, $F\,(d_i,\, d_j) = d_i d_j$. Now, corresponding to each such index, we can extend the adjacency matrix [14], whose (i, j)-th element is

$$\mathbf{a}_{ij} = \begin{cases} F\,(d_i,\, d_j)\,, & if\ u_iu_j \in E(G), \\ 0, & otherwise. \end{cases}$$

This extended matrix produces numerous energy variants defined analogously to (1) for varying F. Some of these variants are ABC energy [42], Randić energy [17], Zagreb energy [28, 33, 39], geometric-arithmetic energy [26], NDe energies [40], harmonic energy [37] and so on. In 2018, Rad, Jahanbani and Gutman [33] put forward the energies corresponding to first and second Zagreb indices. They extensively investigated about the first

Zagreb energy. However, the energy variant associated to the M_2 index has been largely remained unexplored. The present work is an attempt to unveil the application potential and mathematical features of the second Zagreb energy. The extended adjacency matrix associated with the second Zagreb index, named as M_2-matrix, is defined as $\Omega(G) = \Big(b_{ij}\Big)$, where

$$b_{ij} = \begin{cases} d_i\, d_j, & if\ u_i u_j \in E(G), \\ 0, & otherwise. \end{cases}$$

The characteristic polynomial of $\Omega(G)$ is $\Phi_\Omega(G, \nu) = \det(\nu I_n - \Omega(G))$. As $\Omega(G)$ is real symmetric, its eigenvalues are possible to be expressed as $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$. The set $\{\nu_1, \nu_2, \ldots, \nu_n\}$ is known as the M_2-spectrum, which is denoted as $Sp(\Omega(G))$. We call the maximum eigenvalue ν_1 as the M_2-spectral radius, and the difference $\nu_1 - \nu_n$ is known as the M_2-spread of G. Now, the second zagreb energy of G is denoted as $ZE_2(G)$, which is defined as

$$ZE_2(G) = \sum_{i=1}^{n} |\nu_i|. \tag{2}$$

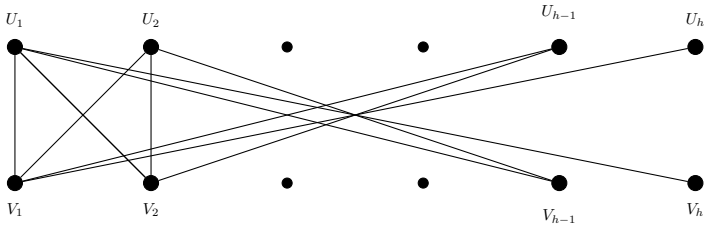
The central theme of this work is to explore the application potential and mathematical features of ZE_2 energy. The role of ZE_2 in structure-property modelling and isomer discrimination is investigated. Numerous tight bounds of the M_2 spectral radius and M_2-spread are derived with characterizing extremal graphs. The ZE_2 energy is investigated for different special graphs, including regular, semi-regular and chain graphs. A divisor type matrix is put forward to determine the M_2-spectrum and ZE_2 energy of the chain graph.

2 Preliminaries

We consider δ, Δ to be the minimum and maximum degrees, respectively. If $d_{u_i} = r$ for all $u_i \in V(G)$ for some natural number r, then G is r-regular. P_n, C_n, K_n and S_n are known as path, cycle, complete and star graphs, respectively. Let G be bipartite graph with partition of vertex set

as $V(G) = V_1 \cup V_2$. If $|V_1| = \alpha$, $|V_2| = \beta$ and all vertices belonging to the same vertex set have equal degree, then G is known as (α, β)-semiregular bipartite. We use $K_{m,n}$ to represent the complete bipartite graph whose vertices are partitioned into two sets having m, n vertices. To represent strongly regular graph of n vertices, we consider $G_s(n, r, \mathrm{a}, \mathrm{b})$. It is an r regular graph having following property: if $u_i u_j \in E\Big(G_s(n, r, \mathrm{a}, \mathrm{b})\Big)$, then $|N_G(u_i) \cap N_G(u_j)| = a$, else $|N_G(u_i) \cap N_G(u_j)| = b$.

A graph is referred to as a chain graph if it is bipartite and the neighbourhoods of each colour class's vertices form a chain with respect to inclusion. This is a $\{2K_2, C_3, C_5\}$ -free graphs. Chain graphs are sometimes called double nested graphs [7]. See current articles [1,3] for mathematical characteristics of chain graphs. A chain graph or double nested graph is denoted as $G = (U, V; E)$, where vertex set of this graph contains two colour classes and each of them are separated into h non-empty sets, i.e., $U = \cup_{i=1}^{h} U_i$ and $V = \cup_{i=1}^{h} V_i$. Each vertex in U_i is connected to all vertices of $\cup_{k=1}^{h+1-i} V_k$. Let $N_G(u)$ be the set of all neighbours of a vertex u. Thus, if $u^{'} \in U_{i+1}$, $u^{''} \in U_i$, $w^{'} \in V_{i+1}$ and $w^{''} \in V_i$, then $N_G(u^{'}) \subset N_G(u^{''})$, $N_G(w^{'}) \subset N_G(w^{''})$ and this clarifies the property of double nesting (see Figure : 1).



Slika 1. The structure of chain graph.

Consider $n_i = |U_i|$ and $m_i = |V_i|$ for $i = 1, 2, ..., h$. Then G can be symbolised as

$$DNG(n_1, n_2, n_3, ..., n_h; m_1, m_2, m_3, ..., m_h).$$

Let $\alpha_t = \sum_{i=1}^{t} m_i$ and $\beta_j = \sum_{i=1}^{j} n_i$ for $1 \leq t, j \leq h$. The sum degree of vertices

in U_i and V_i are defined as $d_{U_i} = n_i\,\alpha_{h+1-i}$ and $d_{V_i} = m_i\,\beta_{h+1-i}$ respectively. Now order and size of G is $n = \alpha_h + \beta_h$ and $m = \sum_{i=1}^{h} n_i\,\alpha_{h+1-i} = \sum_{i=1}^{h} m_i\,\beta_{h+1-i}$, respectively.

Let $L = (l_{i,j}) \in \mathbb{R}^{m\times n}$ and $M \in \mathbb{R}^{r\times s}$. Then the Kronecker product of the matrix L and M is $rm \times sn$ block matrix, which is defined as

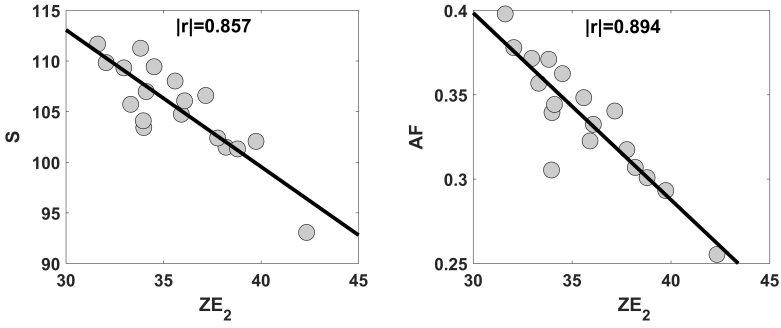
$$L \otimes M = \begin{pmatrix} l_{11}M & l_{12}M & \cdots & l_{1n}M \\ l_{12}M & l_{21}M & \cdots & l_{2n}M \\ \vdots & \vdots & \ddots & \vdots \\ l_{1n}M & l_{2n}M & \cdots & l_{mn}M \end{pmatrix}.$$

Proposition 1. *[36] Let L and M be two matrices of sizes m and n, respectively. If $\epsilon_1, \epsilon_2, \cdots, \epsilon_m$ are the eigenvalues of L and $\sigma_1, \sigma_2, \cdots, \sigma_n$ are eigenvalues of M. Then the eigenvalues of $L \otimes M$ are given as $\epsilon_i\,\sigma_j$ where $i = 1, 2, \cdots, m$ and $j = 1, 2, \cdots, n$.*

3 Chemical significance

The present section is directed towards investigating the usefulness of second Zagreb energy ZE_2. To explore an invariant's predictive potential, Randić and Trinajstić [32] propose correlating theoretical invariants with experimental physico-chemical properties of a benchmark dataset. The octane isomer data set is considered in this work, since they represent sufficiently large and structurally diverse group of alkanes for basic investigation [24,32]. The ZE_2 energy is found to correlate well with entropy (S) and acentric factor (AF) of octanes. The linear fitting of such correlations are displayed in Figure 2, which indicates that linear regression model can be formed to predict S and AF by ZE_2.

The scatter plot in Figure 2 is divided into some clusters that are closely similar to the second Zagreb index M_2. Thus, we consider the following



(a) (b)

Slika 2. Correlation of ZE_2 with (a) entropy and (b) acentric factor for octane isomers.

regression models:

$$P = c_1 TI + c_2, \tag{3}$$

$$P = d_1 TI + d_2 M_2 + d_3, \tag{4}$$

From Table 1, one can say that the data variances for S and AF are almost

Tabela 1. The outcomes of evaluation of the model (3) in case of ZE_2.

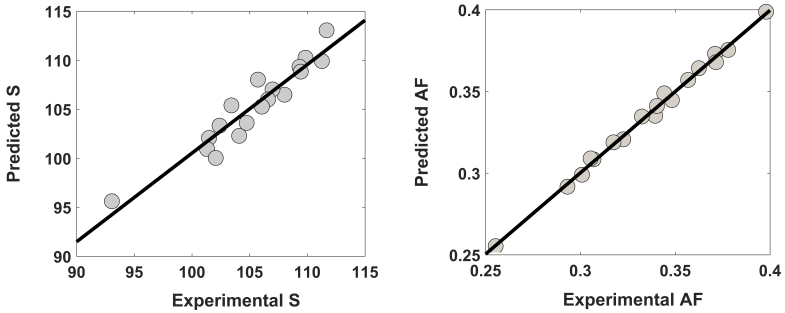
Properties	c_1	c_2	r^2	$RMSE$	F	SF
S	-1.352	153.649	0.734	2.264	44.162	5.63×10^{-6}
AF	-0.011	0.731	0.799	0.0154	63.949	5.57×10^{-7}

73%, 80%, respectively. A remarkable improvement in structure-property modelling is noticed when M_2 is considered as second predictor variable in model (4). The findings generated by (4) are reported in Table 2.

Tabela 2. The outcomes of evaluation of the model (4) in case of ZE_2.

Properties	d_1	d_2	d_3	R^2	$RMSE$	F	SF
S	0.678	-1.544	128.66	0.904	1.361	70.583	2.34×10^{-8}
AF	0.006	-0.013	0.521	0.99	0.002	1427.982	7.68×10^{-18}

The ZE_2 explains 90% and 99% of data variance for entropy and acentric factor, respectively. The errors of the model are also reduced. From F and SF values, the models can be stated to be reliable. The predicted and experimental properties are shown in Figure 3, which indicates well alignment between experimental and predicted data.



Slika 3. Relation between experimental and predicted properties for octane isomers.

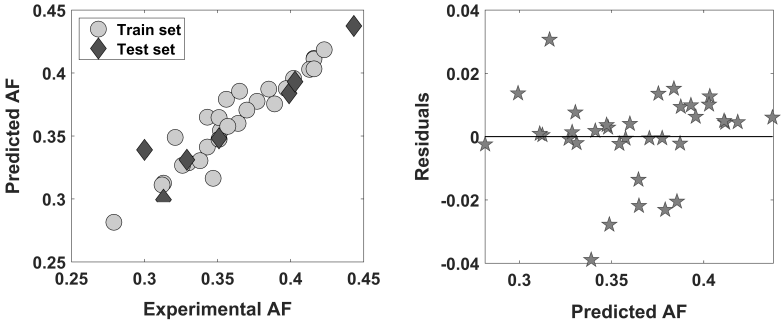
In view of all parameters, it is evident that the performance of ZE_2 is notable for AF compared to S. To appropriately investigate a constructed model, external validation plays crucial role. Nonane isomers are taken into account for external validation of the model (4) for AF. We compile experimental AF values from the chemical database [6]. The data set is divided into training and test sets in the ratio 80 : 20 by means of python scikit-learn module. We employ the training set to construct the model, the parameters of which are listed in Table 3.

Tabela 3. The outcomes of evaluation of model (4) for nonane isomer training data set.

Property	d_1	d_2	d_3	R^2	$RMSE$	F	SF
AF	0.006	-0.014	0.608	0.91	0.0124	132.2	5.06×10^{-14}

It yields considerable predictive ability of ZE_2 on training set. The coefficient of determination is 91%. The behaviour of predicted AF by ZE_2 and M_2 against experimental values are shown in Figure 4 (a). Residual points of model are randomly scattered around zero line in Figure 4 (b),

which ensure that the model fits the data well. In case of test set, the data variance is 88%, which makes the external validation meaningful.



(a) (b)

Slika 4. Relation between experimental and predicted properties for octane isomers.

In addition to remarkable predictive potential, an efficient descriptor should discriminate isomeric structures. The discrimination potency of a descriptor is crucial in coding and computer processing of various molecules. Konstantinova [5] presented the sensitivity, a measure of isomer discrimination, whose formulation is as follows:

$$S_{TI} = \frac{N - N_{TI}}{N},$$

N, N_{TI} are the count of isomers and number of them that cannot be separated by the descriptor TI, accordingly. The discrimination potential of a descriptor is directly proportional to S_{TI}. The S_{TI} values of some mostly utilised descriptors and ZE_2 for octane, nonane and decane isomers are listed in Table 4, which yields that the ZE_2 energy outperforms well-known descriptors in isomer discrimination.

Tabela 4. S_{TI} values of molecular descriptors for octane, nonane and decane isomers.

	M_1	F	M_2	ISI	SDD	SCI	RR	R	ZE_2
S_I for octane	0.333	0.389	0.722	0.722	0.889	0.889	0.889	0.889	**1.000**
S_I for nonane	0.2	0.229	0.457	0.686	0.686	0.8	0.8	0.8	**1.000**
S_I for decane	0.107	0.133	0.28	0.547	0.547	0.64	0.653	0.667	**1.000**

4 Bounds for Ω-spectral radious

This section presents some crucial bounds for the maximum eigenvalue of $\Omega(G)$ for a graph G. Let us consider the k-th spectral moment of $\Omega = \Omega(G)$ as $\Upsilon_k = \sum_{i=1}^{n} (\nu_i)^k$. We immediately have $\Upsilon_k = trace(\Omega^k)$. For the sake of simplification, the $M_2(G)$ value of an edge u_iu_j is formulated as $M_2(u_iu_j) = d_i\, d_j$. After employing some derivations on the elements of Ω, we clearly obtain the following result.

Lemma 1. *For a graph G having n vertices, we have*

$$\Upsilon_0 = n,\ \Upsilon_1 = 0,\ \Upsilon_2 = 2 \sum_{u_iu_j \in E(G)} \Big(M_2(u_iu_j) \Big)^2.$$

Lemma 2. *[27] If B be an $n \times n$ symmetric matrix with $p \times p$ leading submatrix B_p, then*

$$\nu_{n-i+1}(B) \leq \nu_{p-i+1}(B_p) \leq \nu_{p-i+1}(B) \tag{5}$$

where $i = 1, 2, ..., p$ and $\nu_i(B)$ be the i-th largest eigenvalue of B.

If G be r-regular, then $\Omega(G) = r^2A(G)$ and $\lambda_1(G) = r$. Thus, $\nu_1(G) = r^2\lambda_1(G) = r^3$ and $\nu_i(G) = r^2\lambda_i(G)$ for $i = 2, 3, ..., n$. If $G \cong K_n$, then $\nu_1 = (n-1)^3$ and $\nu_i(G) = -r^2$ for $i = 2, 3, ..., n$ as $\lambda_1(G) = (n-1)^3$ and $\lambda_i = -1$ for $i = 2, 3, ..., n$.

Now we identify graphs for which the the eigenvalues of $\Omega(G)$ coincide except Ω-spectral radious.

Lemma 3. *For a graph G having n vertices, we have $\nu_2 = \nu_3 = \cdots = \nu_n$ iff $G \cong \overline{K}_n$ or $G \cong K_n$.*

Dokaz. For $G \cong \overline{K}_n$, it is obvious that $\nu_1 = \nu_2 = \cdots = \nu_n = 0$. For $G \cong K_n$, we obtain $\nu_2 = \nu_3 = \cdots = \nu_n = -(n-1)^2$. Otherwise, $G \ncong \overline{K}_n$ and $G \ncong K_n$. Since $G \ncong \overline{K}_n$, then G has at least one edge and hence $\nu_1 > 0$ and $\nu_n < 0$ as $\sum_{i=1}^{n} \nu_i = 0$. Again $G \ncong K_n$ implies that there are at least two vertices in G that are not adjacent. Without maintaining uniformity, One may draw the conclusion that v_1 is not connected with v_2. Let $\Omega(G)_2$ be the leading 2×2 submatrix of $\Omega(G)$ corresponding to the vertices v_1 and v_2. Then $\nu_1(\Omega(G)_2) = \nu_2(\Omega(G)_2) = 0$. By Lemma 2, we immediately have

$$\nu_2(G) \geq \nu_2(\Omega(G)_2) = 0,$$

a contradiction to the fact $\nu_2 = \nu_3 = \cdots = \nu_n < 0$. This completes the proof. ■

Theorem 2. *For a graph G of order n with second zagreb index $M_2(G)$, we obtain*

$$\frac{2M_2(G)}{n} \leq \nu_1 \leq \sqrt{\left(1 - \frac{1}{n}\right) \Upsilon_2},$$

where Υ_2 is given in Lemma 1. The right equality holds iff $G \cong \overline{K}_n$ or $G \cong K_n$ and left equality occurs iff G is regular.

Dokaz. **Lower Bound:** Let $\mathbf{e} = (1, 1, \ldots, 1)^t \in \mathbb{R}^n$. Then by Rayleigh-Ritz principle, we find

$$\nu_1(G) = \max_{\mathbf{x} \in \mathbb{R}^n} \left\{ \frac{\mathbf{x}^t\, \Omega(G)\, \mathbf{x}}{\mathbf{x}^t\ \mathbf{x}} : \mathbf{x} \neq \mathbf{0} \right\} \geq \frac{\mathbf{e}^t\, \Omega(G)\ \mathbf{e}}{\mathbf{e}^t\, \mathbf{e}} = \frac{2M_2(G)}{n}.$$

Let G be r-regular. Then $2m = n\, r$ and hence $M_2(G) = r^2 m = \frac{nr^3}{2}$. Note that $\Omega(G) = r^2\, A(G)$. As $\lambda_1(G) = r$, one can easily find

$$\nu_1(G) = r^2\, \lambda_1(G) = r^3 = \frac{2M_2(G)}{n}.$$

Upper Bound: Since $\sum_{i=1}^{n} \nu_i = 0$, by Cauchy-Schwarz inequality, we obtain

$$\nu_1^2 = \left(-\sum_{i=2}^{n} \nu_i \right)^2 \leq (n-1) \sum_{i=2}^{n} \nu_i^2,$$

that is,

$$n\,\nu_1^2 \leq (n-1) \sum_{i=1}^{n} \nu_i^2 = (n-1)\,\Upsilon_2.$$

from which the required result follows. The equality appears iff $\nu_2 = \nu_3 = \cdots = \nu_n$, i.e., iff $G \cong \overline{K}_n$ or $G \cong K_n$, by Lemma 3. ■

Corollary. *For a graph G of n vertices with maximum degree Δ and second zagreb index $M_2(G)$, we have*

$$\nu_1(G) \leq \sqrt{\frac{2(n-1)\Delta^2\, M_2(G)}{n}},$$

where equality appears iff $G \cong \overline{K}_n$ or $G \cong K_n$.

Dokaz. For any edge $u_i u_j \in E(G)$,

$$\frac{d_i + d_j}{2} \geq \sqrt{d_i d_j}$$

i.e.,

$$d_i d_j \leq \Delta^2, \tag{6}$$

with equality appears iff $d_k = \Delta$ for all $u_k \in V(G)$. Using the above result,

we get

$$\Upsilon_2 = 2 \sum_{u_i u_j \in E(G)} (d_i d_j)^2 \leq 2\Delta^2 \sum_{u_i u_j \in E(G)} d_i\, d_j = 2\Delta^2\, M_2(G).$$

Now using Theorem 2, we attain the desired outcome. Also, the equality occurs iff $G \cong \overline{K}_n$ or $G \cong K_n$. ■

Lemma 4. *[9] If B be a symmetric $n \times n$ matrix with spectral radius μ_1 then for any $\mathbf{x} \in R^n$ $(\mathbf{x} \neq \mathbf{0})$,*

$$\mathbf{x}^T B\mathbf{x} \leq \mu_1 \mathbf{x}^T \mathbf{x}$$

where the equality holds iff μ_1 the largest eigenvalue of B is represented by the eigenvector $\mathbf{x}$.

Theorem 3. *For a graph G with maximum and minimum degrees Δ and δ, respectively, we have*

$$\lambda_1 \delta^2 \leq \nu_1 \leq \lambda_1 \Delta^2 \tag{7}$$

where both equalities occur iff G is regular.

Dokaz. Let $\mathbf{x} = (x_1, x_2, ..., x_n)^t$ be an unit eigenvector corresponding to the eigenvalue λ_1 of $A(G)$. Therefore, we have,

$$A(G)\mathbf{x} = \lambda_1 \mathbf{x}, \text{ that is, } \lambda_1 = \mathbf{x}^t A(G)\mathbf{x} = 2 \sum_{u_i u_j \in E(G)} x_i x_j. \tag{8}$$

For any $u_i u_j \in E(G)$, we have

$$M_2(u_i u_j) = d_i \, d_j \geq \delta^2$$

where equality appears iff $d_i = d_j = \delta$, that is, iff $d_k = \delta$ for any vertex $u_k \in V(G)$. Using this result with Lemma 4, we get

$$\nu_1 \geq \mathbf{x}^t \, \Omega(G) \, \mathbf{x} = 2 \sum_{u_i u_j \in E(G)} M_2(u_i u_j) \, x_i x_j \geq 2\delta^2 \sum_{u_i u_j \in E(G)} x_i x_j = \lambda_1 \, \delta^2$$

by (8) Also, the above equality occurs iff G is a regular graph.

Let $\mathbf{y} = (y_1, y_2, \ldots, y_n)^t$ be a unit eigenvector associated to the eigenvalue ν_1 of $\Omega(G)$. Then by Lemma 4, we evaluate

$$\nu_1 = \mathbf{y}^t \, \Omega(G) \, \mathbf{y} \quad = \quad 2 \sum_{u_i u_j \in E(G)} M_2(u_i u_j) \, y_i y_j \leq 2 \, \Delta^2 \sum_{u_i u_j \in E(G)} y_i y_j.$$

i.e.,

$$\nu_1 \leq \lambda_1 \Delta^2,$$

by (6). The above equality occurs iff G is regular. ■

Corollary. *For a graph G with maximum and minimum degrees Δ and δ, respectively, we have*

$$\delta^3 \leq \nu_1(G) \leq \Delta^3$$

with both equalities occur iff G is regular.

Dokaz. Note that $\delta \leq \lambda_1(G) \leq \Delta$. Now employing Theorem 3, we get the above result, and both equalities occur iff G is regular. ■

Corollary. *If G is a graph with maximum degree Δ and minimum degree δ, then we have*

$$\frac{2m\,\delta^2}{n} \leq \nu_1(G) \leq \Delta^2\sqrt{(2m-n+1)}$$

where left hand equality occurs iff G is regular, and right hand equality appears iff $G \cong S_n$ or $G \cong K_n$.

Dokaz. We have $\lambda_1 \geq 2m/n$ [41]. Using this fact in Theorem 3, we get the lower bound. The left equality appears iff G is regular.

We also have, $\lambda_1 \leq \sqrt{2m-n+1}$ where equality appears iff $G \cong S_n$ or $G \cong K_n$ [44]. This result in combination with Theorem 3 yields the required upper bound. Moreover, the right equality appears iff $G \cong S_n$ or $G \cong K_n$. ■

We call the difference $\nu_1 - \nu_n$ as the M_2-spread of G. Now we intend to determine an upper bound of this spread in the following theorem.

Theorem 4. *For a connected graph G having $n\,(\geq 2)$ vertices, we have*

$$\nu_1 - \nu_n \leq \frac{n}{n-1}\nu_1 + \sqrt{\frac{n-2}{n-1}\Upsilon_2 - \frac{n^2-2n}{(n-1)^2}\nu_1^2}\ . \tag{9}$$

Equality appears iff G is complete or complete bipartite.

Dokaz. From Lemma 1, we have

$$\Upsilon_2 - \nu_1^2 - \nu_n^2 = \sum_{i=2}^{n-1} \nu_i^2.$$

Now using Cauchy Schwartz inequality, we get

$$\Upsilon_2 - \nu_1^2 - \nu_n^2 \geq \frac{\left(\nu_1 + \nu_n\right)^2}{n-2}, \tag{10}$$

where equality appears iff $\nu_2 = \nu_3 = \cdots = \nu_{n-1}$. From (10), one can deduce that

$$(n-1)\nu_n^2 + 2\nu_1\nu_n + (n-1)\nu_1^2 - \Upsilon_2(n-2) \leq 0. \tag{11}$$

Now equality in (11) yields $\nu_n = -\frac{\nu_1}{n-1} \pm \sqrt{\frac{n-2}{n-1}\Upsilon_2 - \frac{n^2-2n}{(n-1)^2}\nu_1^2}$, which in combination with (11) implies that

$$\nu_1 - \nu_n \leq \frac{n}{n-1}\nu_1 + \sqrt{\frac{n-2}{n-1}\Upsilon_2 - \frac{n^2-2n}{(n-1)^2}\nu_1^2},$$

where equality occurs iff $\nu_2 = \nu_3 = \cdots = \nu_{n-1}$.

Claim: $\nu_2 = \nu_3 = \cdots = \nu_{n-1}$ iff G is complete or complete bipartite. Now, we prove the above claim. Let $\nu_2 = \nu_3 = \cdots = \nu_{n-1}$. For $G \cong K_n$, we have $\nu_2 = \nu_3 = \cdots = \nu_{n-1} = -(n-1)^2$. Now, if $G \ncong K_n$, then the proof of Lemma 3 yields that $\nu_2(G) \geq 0$. If possible, consider $\nu_2(G) > 0$. Then $\nu_i(G) > 0 \ \forall \ i = 1, 2, ..., n-1$. Since $\nu_1(G) \geq |\nu_n(G)|$, we immediately have $\Upsilon_1 \neq 0$, a contradiction. Consequently, $\nu_i(G) = 0$ for all $i = 2, ..., n-1$. Thus, G is bipartite and it possesses three distinct M_2-eigenvalues. Consequently, the diameter of G is atmost 2, and hence it is complete bipartite. One can easily establish the converse part of the claim by determining the M_2-spectrum of complete and complete bipartite graphs. This completes the proof. ■

Corollary. *For a graph G having $n\,(\geq 2)$ vertices and maximum degree Δ, we obtain*

$$\nu_1 - \nu_n \leq \frac{\Delta^2}{(n-1)}\left(n\Delta + \sqrt{n(n-2)(n-1-\Delta)\Delta}\right). \tag{12}$$

The equality appears iff $G \cong K_n$ and $G \cong K_{\frac{n}{2}\,\frac{n}{2}}$.

Dokaz. From (9), we define $f(x) = \frac{n}{n-1}x + \sqrt{\frac{n-2}{n-1}\,\Upsilon_2 - \frac{n^2-2n}{(n-1)^2}\,x^2}$. Now, we get

$$f^{'}(x) = \frac{n}{n-1} - \frac{(n^2-2n)x}{(n-1)\sqrt{(n-1)(n-2)\Upsilon_2 - (n^2-2n)x^2}}.$$

One can easily verify that $f(x)$ is increasing on $x \leq \sqrt{\frac{(n-2)(n-1)\Upsilon_2}{(2n^2-6n+4)}}$. Note that $x \leq \Delta^3$ with equality appears iff G is regular.
Consequently, $f(x) \leq f(\Delta^3)$, where equality appears iff G is regular. Therefore, we get

$$\nu_1 - \nu_n \leq \frac{n\Delta^3}{(n-1)} + \sqrt{\frac{n-2}{n-1}\Upsilon_2 - \frac{(n^2-2n)\Delta^6}{(n-1)^2}}\ . \tag{13}$$

Moreover, it is clear that $\Upsilon_2 \leq n\Delta^5$ with equality occures iff G is regular. Applying this fact on (13), the desired result follows immediately, where the equality occurs iff $G \cong K_n$ and $G \cong K_{\frac{n}{2}\,\frac{n}{2}}$.

■

5 Second Zagreb energy for some special graphs

In this section, we aim to derive explicit expressions of ZE_2 energy for some special graphs including regular, semi-regular and chain graphs.

Lemma 5. *[2] For a connected $G_s(n, r, a_1, b_1)$, we have*

$$Sp(A(G_s(n,r,a_1,b_1))) = \left\{ r, \underbrace{\beta_1, \ldots, \beta_1}_{m_1}, \underbrace{\beta_2, \ldots, \beta_2}_{m_2} \right\},$$

where,

$$\beta_1 = \frac{a_1 - b_1 + \sqrt{(a_1-b_1)^2 + 4(r-b_1)}}{2}, \qquad \beta_2 = \frac{a_1 - b_1 - \sqrt{(a_1-b_1)^2 + 4(r-b_1)}}{2},$$

$$m_1 = \frac{1}{2}\left(n - 1 - \frac{2r + (n-1)(a_1-b_1)}{\sqrt{(a_1-b_1)^2 + 4(r-b_1)}}\right), \quad m_2 = \frac{1}{2}\left(n - 1 + \frac{2r + (n-1)(a_1-b_1)}{\sqrt{(a_1-b_1)^2 + 4(r-b_1)}}\right).$$

Theorem 5. *For a graph G of order $n \geq 3$ having no isolated vertices, we have*

(*i*) *$ZE_2(G) = r^2\,\mathcal{E}(G)$, when G is r-regular. Particularly, $ZE_2(K_n) = 2(n-1)^3$ and $ZE_2(C_n) = 8\sum_{i=0}^{n-1}\left|\cos\left(\frac{2\pi i}{n}\right)\right|$. When G is connected $G_s(n, r, a_1, b_1)$, we have*

$$ZE_2(G) = r^2\left(r + \frac{2(n-1)(r-b_1) - r\,(a_1-b_1)}{\sqrt{(a_1-b_1)^2 + 4(r-b_1)}}\right).$$

(*ii*) *$ZE_2(G) = \alpha\,\beta\,\mathcal{E}(G)$, when G is (α, β)-semiregular bipartite. Particularly, $ZE_2(K_{p,q}) = 2\,pq\sqrt{pq}$, where $p + q = n$. Also we have $ZE_2(S_n) = 2\,(n-1)\sqrt{n-1}$.*

Dokaz. (*i*) Let G be r-regular. Then, we have $\Omega(G) = r^2 A(G)$. Consequently, $\nu_i = r^2\lambda_i$ $(1 \leq i \leq n)$, which implies that $ZE_2(G) = r^2\,\mathcal{E}(G)$. For K_n, $\mathcal{E}(K_n) = 2(n-1)$, which gives $ZE_2(K_n) = 2(n-1)^3$. Also, for C_n we have $\mathcal{E}(C_n) = \sum_{i=0}^{n-1}\left|2\cos\left(\frac{2\pi i}{n}\right)\right|$. Therefore, $ZE_2(C_n) = 8\sum_{i=0}^{n-1}\left|\cos\left(\frac{2\pi i}{n}\right)\right|$. When G is connected $G_s(n, r, a, b)$, then in view of Lemma 5, we immediately obtain $\nu_1 = r^3$, $\nu_2 = \nu_3 = \ldots = \nu_{m_1+1} = r^2\,\beta_1$, $\nu_{m_1+2} = \nu_{m_1+3} = \cdots = \nu_n = r^2\,\beta_2$, from which the desired $ZE_2(G)$ energy follows from Lemma 5.

(*ii*) Note that $\Omega(G) = rs\,A(G)$ and $\nu_i = rs\,\lambda_i,\ i = 1, 2, \ldots, n$, when G is (α, β)-semiregular bipartite. Thus, $ZE_2(G) = \alpha\,\beta\,\mathcal{E}(G)$. In particular, $\mathcal{E}(K_{p,q}) = 2\sqrt{pq}$, which yields $ZE_2(K_{p,q}) = 2\,pq\sqrt{pq}$. As $S_n \cong K_{1,n-1}$, we have $ZE_2(S_n) = 2\,(n-1)\sqrt{n-1}$. ■

5.1 Chain graph

This section aims to investigate the M_2-spectrum and ZE_2 energy of chain graph.

If a graph G has k vertices possessing similar neighbours and t eigenvalues equal to 0, then $t \geq k-1$ [30]. As a consequence of this result, we have following result.

Lemma 6. *Let G be a graph with vertices $\{u_1, u_2, \cdots, u_k\}$ having same set of neighbors. Then G has at least $k-1$ M_2-eigenvalues equal to 0.*

Consider a set of positive numbers $\mathbf{p} = \{p_1, p_2, \cdots, p_n\}$. Now, we define P_k to be the average of product of k-element subset of $\mathbf{p}$, i.e., $P_1 = \dfrac{1}{n}(p_1 + p_2 + \cdots + p_n)$, $P_2 = \frac{1}{\frac{1}{2}n(n-1)}(p_1p_2 + p_1p_3 + \cdots + p_1p_n + p_2p_3 + \cdots + p_{n-1}p_n)$, $\ldots$, $P_n = p_1p_2\cdots p_n$.

Lemma 7. *[35] For positive real numbers $p_1, p_2, \cdots, p_n$, we have*

$$P_1 \geq P_2^{\frac{1}{2}} \geq P_3^{\frac{1}{3}} \geq \cdots \geq P_n^{\frac{1}{n}}\ .$$

Equality holds iff $p_1 = p_2 = \cdots = p_n$.

From the definition of $\Omega(G)$ and the construction of chain graph, we can obtain the M_2-matrix of chain graph G. By Lemma 6, we have the eigenvalue 0 with multiplicity $\sum_{i=1}^{h}(m_i + n_i - 2)$ of M_2-matrix. Here we construct a divisor type matrix to generate the non-zero M_2 -spectrum for chain graph. It is defined as

$$\mathcal{D} = \begin{pmatrix} \mathbf{0} & \mathcal{P} \\ \mathcal{Q} & \mathbf{0} \end{pmatrix}$$

where

$$\mathcal{P} = \begin{pmatrix} n_1\alpha_h\,\beta_h & n_1\alpha_h\,\beta_{h-1} & \cdots & n_1\alpha_h\,\beta_2 & n_1\alpha_h\,\beta_1 \\ n_2\alpha_{h-1}\,\beta_h & n_2\alpha_{h-1}\,\beta_{h-1} & \cdots & n_2\alpha_{h-1}\,\beta_2 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ n_{h-1}\alpha_2\,\beta_h & n_{h-1}\alpha_2\,\beta_{h-1} & \cdots & 0 & 0 \\ n_h\alpha_1\,\beta_h & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathcal{Q} = \begin{pmatrix} m_1\alpha_h\,\beta_h & m_1\alpha_{h-1}\,\beta_h & \cdots & m_1\alpha_2\,\beta_h & m_1\alpha_1\,\beta_h \\ m_2\alpha_h\,\beta_{h-1} & m_2\alpha_{h-1}\,\beta_{h-1} & \cdots & m_2\alpha_2\,\beta_{h-1} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ m_{h-1}\alpha_h\,\beta_2 & m_{h-1}\,\alpha_{h-1}\beta_2 & \cdots & 0 & 0 \\ m_h\alpha_h\,\beta_1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Note that, $\mathcal{D}^2 = \begin{pmatrix} \mathcal{PQ} & \mathbf{0} \\ \mathbf{0} & \mathcal{QP} \end{pmatrix}$. The spectra of $\mathcal{PQ}$ and $\mathcal{QP}$ are the same. Therefore, $\nu_1(G) = \sqrt{\nu_1(\mathcal{PQ})}$. The (i,j)-th entry of $\mathcal{PQ}$ is given by

$$p_{ij} = \begin{cases} n_i\,\alpha_{h+1-i}\;\alpha_{h+1-j}\sum\limits_{k=1}^{h+1-j} m_k(\beta_{h+1-k})^2, & for\ \ \mathrm{i}{\leq}\mathrm{j} \\ \\ n_i\alpha_{h+1-j}\;\alpha_{h+1-i}\sum\limits_{k=1}^{h+1-i} m_k(\beta_{h+1-k})^2, & for\ \ \mathrm{i}{>}\mathrm{j} \end{cases}$$

Let R_i and $R_i^{'}$ are the sums of the entries of i-th row of $\mathcal{PQ}$ and $\mathcal{QP}$. Then

$$R_i = n_i\,\alpha_{h+1-i}\sum_{k=1}^{h+1-i}\sum_{j=k}^{h} m_k(\beta_{h+1-k})^2\alpha_j \ \text{and}\ R_i^{'} = m_i\,\beta_{h+1-i}\sum_{k=1}^{h+1-i}\sum_{j=k}^{h} n_k(\alpha_{h+1-k})^2\beta_j.$$

Lemma 8. *[38] Let A be an $n \times n$ non-negative matrix and $\rho(A)$ be the largest eigenvalue of A. If R_i be the i-th row sum of this matrix. Then*

$$\min_i \sqrt{\frac{1}{R_i}\sum_{t=1}^{h} a_{it}\sum_{j=1}^{h} a_{tj}R_j} \leq \rho(A) \leq \max_i \sqrt{\frac{1}{R_i}\sum_{t=1}^{h} a_{it}\sum_{j=1}^{h} a_{tj}R_j}.$$

Theorem 6. *Let $\nu_1(G)$ be the largest eigenvalue for a connected chain graph G. Then*

$$\nu_1(G) \leq \sqrt[4]{\frac{\sum_{p=1}^{h}\left[\alpha_{h+1-p}\left(\sum_{k=1}^{h+1-p} m_k(\beta_{h+1-k})^2\right)\sum_{j=1}^{h} n_p\,\alpha_{h+1-p}\;\alpha_{h+1-j}\sum_{t=1}^{h+1-j} m_t(\beta_{h+1-t})^2 R_j\right]}{\sum_{k=1}^{h}\sum_{j=k}^{h} m_k(\beta_{h+1-k})^2\alpha_j}}$$

Dokaz. Employing Lemma 8 on matrix $\mathcal{PQ}$, we obtain

$$\min_i \sqrt{\frac{1}{R_i}\sum_{t=1}^{h} p_{it}\sum_{j=1}^{h} p_{tj}R_j} \leq \nu_1(\mathcal{PQ}) \leq \max_i \sqrt{\frac{1}{R_i}\sum_{t=1}^{h} p_{it}\sum_{j=1}^{h} p_{tj}R_j}\ .$$

The maximum value of the above expression is attained at $i = 1$. Consequently,

$$\nu_1(\mathcal{PQ}) \leq \sqrt{\frac{1}{R_1}\sum_{t=1}^{h} p_{1t}\sum_{j=1}^{h} p_{tj}R_j},$$

which implies the required result by considering the fact $\nu_1(G) = \sqrt{\nu_1(\mathcal{PQ})}$. ■

Lemma 9. *A graph G is bipartite iff its M_2-spectrum is symmetric about the origin on the real line.*

Dokaz. Let G be bipartite. Them $\Omega(G)$ is congruent to $\begin{pmatrix} 0 & M \\ M^t & 0 \end{pmatrix}$. Let ν be a characteristic value of $\Omega(G)$ with multiplicity α. Then $M\,v = \nu\,u$ and $M^t\,u = \nu\,v$, where $\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigen vector corresponding to ν. Now, one can obtain that $\begin{pmatrix} u \\ -v \end{pmatrix}$ is also an eigenvector of $\Omega(G)$ with eigenvalue $-\nu$. Consequently, α linearly independent eigenvectors corresponding to ν will generate α linearly independent eigenvectors of $-\nu$, i.e., algebraic multiplicities of ν and $-\nu$ are same. Hence, the first part is done.
Conversely, suppose $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$ be the eigenvalues of $\Omega(G)$ with the property $\nu_i = -\nu_{n-i+1}$, $1 \leq i \leq n$. Thus for any odd positive number α, we have $\sum_{i=1}^{n} \nu_i^{\alpha} = 0$. It is clear that $trace\,(\Omega^{\alpha}) = \sum_{i=1}^{n} \nu_i^{\alpha} = 0$. If G contains a cycle of odd length α, then the diagonal elements of Ω^{α}, i.e., $\Omega(i,\,i)$ for

each i-th vertex belonging to the odd cycle are positive. Consequently, $trace\,(\Omega^{\alpha}) > 0$, since all diagonal entries of Ω^{α} are non-negative. Thus, we arrive at a contradiction to the fact that G has an odd cycle. Evidently, G is bipartite. ■

Theorem 7. *Let $G \cong G(n_1, n_2, \cdots, n_h; m_1, m_2, \cdots, m_h)$ be a chain graph of order n. Then*

$$ZE_2(G) \geq 2\sqrt{\sum_{i=1}^{h}(h+1-i)\,m_i\,n_i\left(\alpha_i\,\beta_i\right)^2 + h(h-1)\prod_{i=1}^{h}\left[\left(m_i\,n_i\right)^{1/h}\left(\alpha_i\,\beta_i\right)^{2/h}\right]}$$

with equality occurs iff $G \cong K_{n_1,m_1}$ where $(n_1 + m_1 = n)$.

Dokaz. In view of Lemma 6, it is evident that 0 is an eigenvalue of $\Omega(G)$ with multiplicity $\sum_{i=1}^{h}(m_i+n_i-2)$ and non-zero eigenvalues can be generated from the divisor type matrix $\mathcal{D}$, where

$$\mathcal{D} = \begin{pmatrix} \mathbf{0} & \mathcal{P} \\ \mathcal{Q} & \mathbf{0} \end{pmatrix}.$$

Let $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_{2h}$ be eigenvalues of $\mathcal{D}$. Then from (2) we have

$$ZE_2(G) = \sum_{i=1}^{2h} |\nu_i| \tag{14}$$

Since, G is a bipartite graph then by Lemma 9, ν_i is an eigenvalue of G iff -ν_i is also an eigenvalue of G. Then from (14) we have,

$$ZE_2(G) = 2\sum_{i=1}^{h} \nu_i. \tag{15}$$

Consequently,

$$\sum_{i=1}^{2h}\nu_i^2 = trace\left(\mathcal{D}^2\right) = 2\sum_{i=1}^{h}\sum_{j=1}^{h+1-i} n_i\,m_j\,\alpha_{h+1-i}^2\,\beta_{h+1-j}^2$$

i.e.,

$$\sum_{i=1}^{h}\nu_i^2=\sum_{i=1}^{h}\sum_{j=1}^{h+1-i} n_i\,m_j\,\alpha_{h+1-i}^2\,\beta_{h+1-j}^2$$

Now, we intend to derive an explicit expression of $\det(\mathcal{D})$.

Note that

$$\det(\mathcal{D})=\begin{vmatrix}\mathbf{0} & \mathcal{P}\\ \mathcal{Q} & \mathbf{0}\end{vmatrix}$$

$$=\prod_{i=1}^{h} m_i n_i \alpha_i \beta_i \begin{vmatrix} & & \mathbf{0} & & & \alpha_h & \alpha_h & \cdots & \alpha_h & \alpha_h\\ & & & & & \alpha_{h-1} & \alpha_{h-1} & \cdots & \alpha_{h-1} & 0\\ & & & & & \vdots & \vdots & \ddots & \vdots & \vdots\\ & & & & & \alpha_2 & \alpha_2 & \cdots & 0 & 0\\ & & & & & \alpha_1 & 0 & 0 & 0 & 0\\ \hline \beta_h & \beta_{h-1} & \cdots & \beta_2 & \beta_1 & & & & & \\ \beta_h & \beta_{h-1} & \cdots & \beta_2 & 0 & & & & & \\ \vdots & \vdots & \ddots & \vdots & \vdots & & & \mathbf{0} & & \\ \beta_h & \beta_{h-1} & \cdots & 0 & 0 & & & & & \\ \beta_h & 0 & 0 & 0 & 0 & & & & & \end{vmatrix}$$

$$=(-1)^h\prod_{i=1}^{h} m_i\,n_i\,(\alpha_i\,\beta_i)^2$$

Consequently,

$$\prod_{i=1}^{2h}\nu_i=\det(\mathcal{D})=(-1)^h\prod_{i=1}^{h} m_i\,n_i\,(\alpha_i\,\beta_i)^2\,,$$

which immediately implies that

$$(-1)^h\left(\prod_{i=1}^{h}\nu_i\right)^2=(-1)^h\prod_{i=1}^{h} m_i\,n_i\,(\alpha_i\,\beta_i)^2\,,$$

which again indicates that

$$\prod_{i=1}^{h}\nu_i = \left(\prod_{i=1}^{h}\alpha_i\,\beta_i\right)\left(\prod_{i=1}^{h}m_i\,n_i\right)^{1/2}$$

From Lemma 7, we have

$$\frac{1}{\frac{1}{2}h(h-1)}\sum_{1\le i<j\le h}\nu_i\,\nu_j \ge \left(\prod_{i=1}^{h}\nu_i\right)^{2/h}, \tag{16}$$

that is,

$$2\sum_{1\le i<j\le h}\nu_i\,\nu_j \ge h(h-1)\left(\prod_{i=1}^{h}\alpha_i\,\beta_i\right)^{2/h}\left(\prod_{i=1}^{h}m_i\,n_i\right)^{1/h},$$

with equality holds iff $\nu_1 = \nu_2 = \cdots = \nu_h$. Using this result in (15), we obtain

$$\begin{aligned}
ZE_2(G) &= 2\sqrt{\sum_{i=1}^{h}\nu_i^2 + 2\sum_{1\le i<j\le h}\nu_i\,\nu_j} \\
&= 2\sqrt{\sum_{i=1}^{h}\sum_{j=1}^{h+1-i} n_i\,m_j\,\alpha_{h+1-i}^2\,\beta_{h+1-j}^2 + 2\sum_{1\le i<j\le h}\nu_i\,\nu_j} \\
&\ge 2\sqrt{\sum_{i=1}^{h}(h+1-i)\,m_i\,n_i\left(\alpha_i\,\beta_i\right)^2 + h(h-1)\prod_{i=1}^{h}\left[\left(m_i\,n_i\right)^{1/h}\left(\alpha_i\,\beta_i\right)^{2/h}\right]}.
\end{aligned}$$

First we take $h = 1$. Then $G \cong K_{n_1,m_1}$, $(n_1 + m_1 = n)$, we have $Sp(G) = \left\{\pm(n_1m_1)^{3/2}, \underbrace{0,\ldots,0}_{n-2}\right\}$ and $ZE_2(G) = 2\,(n_1m_1)^{3/2}$. Hence, the equality holds in Theorem 7. Next we consider that $h \ge 2$. From the definition of chain graph, $G(1,1;1,1)$, i.e., P_4 is an induced subgraph of G. Lemma 2 yields that $\nu_2(G) \ge \nu_2(P_4) \approx 0.8284 > 0$. Again we know that, $\nu_1(G) > \nu_2(G)$, as G is connected. Thus in relation (16), strict inequality occurs for $h \ge 2$. Hence for $h \ge 2$, only inequality appears strictly in Theorem 7. ■

6 Concluding remarks

In this work, we have examined the usefulness of the second Zagreb energy by explaining the structure-property ability and isomer-discrimination proficiency. The ZE_2 has been found to model entropy and acentric factor with powerful accuracy. In case of AF, the performance is surprising. The constructed model has been successfully validated with external data set. The isomer discrimination ability of ZE_2 has also been observed to be surprising compared to existing mostly used indices. Tight bounds for M_2-spectral radius and spread have been derived with characterizing the extremal graphs. The ZE_2 energy has been studied for different special graphs, such as regular, semi-regular and chain graphs. A divisor type matrix has been constructed to estimate the M_2-spectrum and ZE_2 energy of the chain graph.

***Acknowledgment*:** This work was supported by the Post-doctoral Research Program of Sungkyunkwan University (2023).

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