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On Solutions of Fractional order Telegraph Partial Differential Equation by Crank-Nicholson Finite Difference Method

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Abstract

Three main tools to study graphs mathematically are to make use of the vertex degrees, distances and matrices. The classical graph energy was defined by means of the adjacency matrix in 1978 by Gutman and has a large number of applications in chemistry, physics and related areas. As a result of its importance and numerous applications, several modifications of the notion of energy have been introduced since then. Most of them are defined by means of graph matrices constructed by vertex degrees. In this paper we define another type of energy called q-distance energy by means of distances and matrices. We study some fundamental properties and also establish some upper and lower bounds for this new energy type.

Keywords: q-distance matrix, q-distance eigenvalues, q-distance energy, join of graphs, union of graphs
AMS 2010 codes: 05C07, 05C76, 05C90.

1 Introduction and preliminaries

Let G be a graph with n vertices and m edges and let $A = (a_{ij})$ be the adjacency matrix of G. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A in non-increasing order are called the eigenvalues of the graph G. As A is real symmetric, the

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eigenvalues of G are real with sum equal to zero. The energy $E(G)$ of G is defined by I. Gutman, [7], to be the sum of the absolute values of the eigenvalues of G, i.e.

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

For details on the mathematical aspects of the theory of graph energy, see the review [9], papers [4, 5, 8] and the references cited therein. The basic properties including various upper and lower bounds for the energy of a graph have been established in [16, 18], and the notion of graph energy has been found to have remarkable chemical applications in the molecular orbital theory of conjugated molecules, [6, 10]. In [11], a QSPR study is made for the energy of certain graph theoretical matrices. In [17], some graph operations are realized.

The distance matrix of G is the square matrix of order n whose (i, j)-th entry is the distance between the vertices v_i and v_j which is defined as the length of the shortest path between these two vertices. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of the distance matrix of G. The distance energy DE is defined by

$$DE = DE(G) := \sum_{i=1}^{n} |\mu_i|.$$

Detailed information on distance energy can be found in [3, 13, 14, 21]. The distance energy of the join of two given graphs can be found in [20]. In [19], a generalization of the distance notion is given.

Recently R. B. Bapat et al., [1], defined a new distance matrix, called as the q-distance matrix denoted by

$$A_q(G) = (q_{ij}).$$

For an indeterminate q, the entries q_{ij} of this new matrix are defined by

$$q_{ij} = \begin{cases} 1 + q + q^2 + \cdots + q^{k-1}, & \text{if } k = d_{ij}, \\ 0, & \text{if } i = j, \end{cases}$$

where $k = d_{ij}$ is the distance between the vertices v_i and v_j. Each entry of $A_q(G)$ is a polynomial in q. Observe that $A_q(G)$ is an entry-wise non-negative matrix for all $q \geq -1$.

The characteristic polynomial of $A_q(G)$ is defined by

$$f_n(G, \mu) = det(\mu I - A_q(G)).$$

The q-distance eigenvalues of the graph G are similarly the eigenvalues of $A_q(G)$. Since $A_q(G)$ is real and symmetric, its eigenvalues are also real numbers and we label them in non-increasing order $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. The q-distance energy of G is denoted by $E_q(G)$ and is defined by

$$E_q(G) = \sum_{i=1}^{n} |\mu_i|.$$

Note that the trace of $A_q(G) = 0$ and also if $q = 1$, then the q-distance energy coincides with distance energy of a graph.

Example 1. *Consider a crown graph S_6^0 as in Fig. 1.1.*

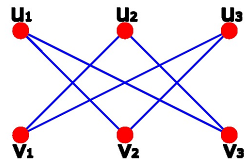

Figure 1.1 *The crown graph* S_0^6

As

$$A_q(S_6^0) = \begin{pmatrix} 0 & 1+q & 1+q & 1+q+q^2 & 1 & 1 \\ 1+q & 0 & 1+q & 1 & 1+q+q^2 & 1 \\ 1+q & 1+q & 0 & 1 & 1 & 1+q+q^2 \\ 1+q+q^2 & 1 & 1 & 0 & 1+q & 1+q \\ 1 & 1+q+q^2 & 1 & 1+q & 0 & 1+q \\ 1 & 1 & 1+q+q^2 & 1+q & 1+q & 0 \end{pmatrix},$$

the characteristic polynomial of S_0^6 *is*

$$(\mu+q^2-q+1)(\mu-q^2-3q-5)(\mu+q^2+2q+1)^2(\mu-q^2+1)^2.$$

Then the q-distance spectrum of S_6^0 *would be*

$$\begin{pmatrix} -q^2+q-1 & q^2+3q+5 & -q^2-2q-1 & q^2-1 \\ 1 & 1 & 2 & 2 \end{pmatrix}$$

and therefore the q-distance energy of S_6^0 *is found as*

$$\begin{aligned} E_q(S_6^0) &= |-(q^2-q+1)| + |q^2+3q+5| + 2\cdot|-(q^2+2q+1)| + 2\cdot|q^2-1| \\ &= q^2-q+1+q^2+3q+5+2q^2+4q+2+2q^2-2 \\ &= 6q^2+6q+6. \end{aligned}$$

2 Properties of the q-distance eigenvalues

Here we study some fundamental properties of the q-distance eigenvalues. We start with the following well-known lemmas:

Lemma 2. *Let G be a graph with the adjacency matrix A and the spectrum spec*$(G) = \{\mu_1, \mu_2, \ldots, \mu_n\}$. *Then it is well-known that*

$$det\ A = \prod_{i=1}^{n} \mu_i.$$

In addition, for any polynomial $P(x)$, *the value* $P(\mu)$ *is an eigenvalue of* $P(A)$ *and hence*

$$det\ P(A) = \prod_{i=1}^{n} P(\mu_i).$$

Lemma 3. *Let* $B = \begin{pmatrix} B_0 & B_1 \\ B_1 & B_0 \end{pmatrix}$ *be a symmetric 2 × 2 block matrix. Then the spectrum of B is the union of the spectra of* $B_0 + B_1$ *and* $B_0 - B_1$.

We can now prove the following results on q-distance eigenvalues:

Theorem 4. *Let G be an (n,m) graph of diameter 2 with the q-distance eigenvalues $\mu_1,\mu_2,\dots,\mu_n$. Then*

$$\sum_{i=1}^{n} {\mu_i}^2 = 2m + (n^2-n-2m)(1+q)^2.$$

Proof. In a q-distance adjacency matrix $A_q(G)$, there are $2m$ elements equal to 1 and n^2-n-2m elements equal to $(1+q)$. Therefore

$$\begin{aligned}\sum_{i=1}^{n}\mu_i^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} q_{ij}q_{ji}\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}(q_{ij})^2\\ &= (2m)(1)^2+(n^2-n-2m)(1+q)^2\\ &= 2m+(n^2-n-2m)(1+q)^2.\end{aligned}$$

Theorem 5. *Let G be an (n,m) graph of diameter 2 and let μ_1 be its greatest q-distance eigenvalue. Then*

$$\mu_1 \geq \frac{n(n-1)(1+q)-2mq}{n}.$$

Proof. Let G be a connected graph of diameter 2 with its vertices labeled as $v_1,v_2,\dots,v_n$ and let d_i denote the degree of v_i. As G is of diameter 2, it is easy to observe that the i^{th} row of A_q consists of d_i times 1s and $n-d_i-1$ times 2s. Let $X=[1,1,1,\dots,1]$ be a vector containing only 1s. Then by the Rayleigh principle, we have

$$\begin{aligned}\mu_1 &\geq \frac{XA_qX^T}{XX^T}\\ &= \frac{\sum_{i=1}^{n}\big(d_i(1)+(n-d_i-1)(1+q)\big)}{n}\\ &= \frac{(2m+(n-1)n(1+q)-2m(1+q))}{n}\\ &= \frac{n(n-1)(1+q)-2mq}{n}.\end{aligned}$$

Theorem 6. *Let G be an r-regular graph of diameter 2 with $r,\mu_2,\dots,\mu_n$ as its eigenvalues. Then the q-distance eigenvalues of G are $-rq+(n-1)(1+q), -q\mu_2-(1+q), -q\mu_3-(1+q),\dots,-q\mu_n-(1+q)$.*

Proof. Let G be an r-regular graph with diameter 2 and adjacency matrix A. $\overline{A}$ is the adjacency matrix of $\overline{G}$. Then the q-distance adjacency matrix of G will be

$$A_q = A + (1+q)\overline{A}. \tag{1}$$

If $r,\mu_2,\dots,\mu_n$ are the eigenvalues of A with $r\geq\mu_2\geq\cdots\geq\mu_n$, then $n-1-r, -\mu_2-1, -\mu_3-1,\dots,-\mu_n-1$ are the eigenvalues of $\overline{A}$. By Eqn. (1), the theorem is proved.

Theorem 7. *Let G be a connected r-regular graph of diameter one or two with the adjacency matrix A and $spec(G)=\{r,\mu_2,\mu_3,\dots,\mu_n\}$. Then the product graph $H=G\times K_2$ is $(r+1)$-regular and of diameter 2 or 3 with $spec(H)=\{-rq(1+q)+2n(1+q)+q^2(n-1)-1, -q\mu_i(1+q)-(1+2q+q^2), -rq(1-q)+q^2(1-n)-1, -q\mu_i(1-q)-(1-q^2)\}$ for $i=1,2,3,\dots,n$.*

Proof. Since G is of diameter 1 or 2, its q-distance matrix is $A+(1+q)\overline{A}$. Then the q-distance matrix of H is of the form

$$\begin{pmatrix} A+(1+q)\overline{A} & J+qA+(q+q^2)\overline{A}\\ J+qA+(q+q^2)\overline{A} & A+(1+q)\overline{A}\end{pmatrix}.$$

By Lemma 3, the spectrum of H is the union of the spectra of $(1+q)A+(1+2q+q^2)\overline{A}+J$ and $(1-q)A+(1-q^2)\overline{A}-J$. If $r,\mu_2,\dots,\mu_n$ are the eigenvalues of A with $r\geq\mu_2\geq\cdots\geq\mu_n$ then $n-r-1,-\mu_2-1,-\mu_3-1,\dots,-\mu_n-1$ are the eigenvalues of $\overline{A}$. Also we know that $n,0,0,\dots,0$ are the eigenvalues of J. Therefore, the theorem follows.

3 Bounds for the q-distance energy

In this section, we find several bounds for the q-distance energy $E_q(G)$. The first one is a sequel of the work of McClelland's, [18].

Theorem 8. *Let G be a simple (n,m) graph with diameter 2. If $P=|detA_q(G)|$, then*

$$\sqrt{2m+(n^2-n-2m)(1+q)^2+n(n-1)P^{\frac{2}{n}}}\leq E_q(G)\leq\sqrt{n(2m+(n^2-n-2m)(1+q)^2)}.$$

Proof. Recall that the Cauchy-Schwarz inequality states that

$$\Big(\sum_{i=1}^n a_ib_i\Big)^2\leq\Big(\sum_{i=1}^n a_i^2\Big)\Big(\sum_{i=1}^n b_i^2\Big).$$

If we substitute $a_i=1$ and $b_i=\mid\mu_i\mid$, then we obtain

$$\Big(\sum_{i=1}^n\mid\mu_i\mid\Big)^2\leq\Big(\sum_{i=1}^n 1\Big)\Big(\sum_{i=1}^n\mu_i^2\Big).$$

Hence by Theorem 4, we have

$$E_q^2(G)\leq n(2m+(n^2-n-2m)(1+q)^2)$$

and therefore we obtain

$$E_q(G)\leq\sqrt{n(2m+(n^2-n-2m)(1+q)^2)}.$$

Since the arithmetic mean is not smaller than the geometric mean, we have

$$\begin{aligned}\tfrac{1}{n(n-1)}\textstyle\sum_{i\neq j}\mid\mu_i\mu_j\mid &\geq\Big[\textstyle\prod_{i\neq j}\mid\mu_i\mu_j\mid\Big]^{\frac{1}{n(n-1)}}\\ &=\Big[\textstyle\prod_{i=1}^n\mid\mu_i\mid^{2(n-1)}\Big]^{\frac{1}{n(n-1)}}\\ &=\Big[\textstyle\prod_{i=1}^n\mid\mu_i\mid\Big]^{\frac{2}{n}}\\ &=\Big[\textstyle\prod_{i=1}^n\mu_i\Big]^{\frac{2}{n}}\\ &=|detA_q(G)|^{\frac{2}{n}}\\ &=P^{\frac{2}{n}}.\end{aligned}$$

Therefore

$$\sum_{i\neq j}\mid\mu_i\mu_j\mid\geq n(n-1)P^{\frac{2}{n}}.$$

Now consider

$$\begin{aligned}E_q^2(G)&=\Big(\textstyle\sum_{i=1}^n\mid\mu_i\mid\Big)^2\\ &=\textstyle\sum_{i=1}^n\mid\mu_i\mid^2+\sum_{i\neq j}\mid\mu_i\mid\mid\mu_j\mid.\end{aligned}$$

Therefore, by Theorem 4, we obtain

$$E_q^2(G) \geq 2m + (n^2 - n - 2m)(1+q)^2 + n(n-1)P^{\frac{2}{n}}$$

and hence

$$E_q(G) \geq \sqrt{2m + (n^2 - n - 2m)(1+q)^2 + n(n-1)P^{\frac{2}{n}}}.$$

Now, we find another bound for $E_q(G)$ which is a sequel to the work of Koolen and Moulton's, [12].

Theorem 9. *If G is an (n,m) graph with diameter 2 so that*

$$\frac{n(n-1)(1+q) - 2mq}{n} \geq 1,$$

then

$$E_q(G) \leq \frac{n(n-1)(1+q) - 2mq}{n} + \sqrt{(n-1)\left[(2m + (n^2 - n - 2m)(1+q)^2 - \left(\frac{n(n-1)(1+q) - 2mq}{n}\right)^2\right]}.$$

Proof. By substituting $a_i = 1$ and $b_i = \mid \mu_i \mid$ in Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=2}^{n} \mid \mu_i \mid\right)^2 \leq \sum_{i=2}^{n} 1 \sum_{i=2}^{n} \mu_i^2 [E_q(G) - \mu_1]^2 \leq (n-1)(2m + (n^2 - n - 2m)(1+q)^2).$$

Hence

$$E_q(G) \leq \mu_1 + \sqrt{(n-1)(2m + (n^2 - n - 2m)(1+q)^2 - \mu_1^2)}.$$

Let

$$f(x) = x + \sqrt{(n-1)(2m + (n^2 - n - 2m)(1+q)^2 - x^2)}.$$

Then for a decreasing function $f(x)$, the fact $f'(x) \leq 0$ implies that

$$1 - \frac{x(n-1)}{\sqrt{(n-1)(2m + (n^2 - n - 2m)(1+q)^2 - x^2)}} \leq 0.$$

From this we obtain

$$x \geq \sqrt{\frac{2m + (n^2 - n - 2m)(1+q)^2}{n}}.$$

Therefore the function $f(x)$ is decreasing in the interval

$$\left(\sqrt{\frac{2m + (n^2 - n - 2m)(1+q)^2}{n}}, \sqrt{2m + (n^2 - n - 2m)(1+q)^2}\right).$$

Clearly the number $(n(n-1)(1+q) - 2mq)/n$ belongs to that interval and since $\mu_1 \geq (n(n-1)(1+q) - 2mq)/n$, we have $(n(n-1)(1+q) - 2mq)/n \leq \mu_1 \leq \sqrt{2m + (n^2 - n - 2m)(1+q)^2}$. By Lemma 5.3, we can write $f(\mu_1) \leq f\Big((n(n-1)(1+q) - 2mq)/n\Big)$. Hence

$$E_q(G) \leq f(\mu_1) \leq f\Big((n(n-1)(1+q) - 2mq)/n\Big)$$

implying the result.

Bapat and Pati, [2], proved that if the graph energy is a rational number, then it is an even integer. A similar result for q-distance energy can be given as follows:

Lemma 10. *Let G be an (n,m) graph. If the q-distance energy $E_q(G)$ of G is a rational number, then*

$$E_q(G) \equiv \mid 0 \mid \pmod{2}.$$

Proof. Proof is similar to Theorem 5.4 of [15].

4 Join of two graphs

One of the ways of studying graphs is to make use of smaller graphs usually those subgraphs whose own are the components of the given graph. Similarly to this idea, many graph operations, sometimes called graph products, are defined to make the necessary calculations on some given graphs by means of similar calculations on some smaller graphs. In this section, we shall study one of the most practical of these products, called the join, of two graphs and calculate the q-distance energy of it. Other operations can be applied similarly to obtain some other properties.

Definition 1. The join of two graphs G_1 and G_2 denoted by $G_1 \nabla G_2$ is a larger graph obtained from G_1 and G_2 by joining each vertex of G_1 to all the vertices of G_2.

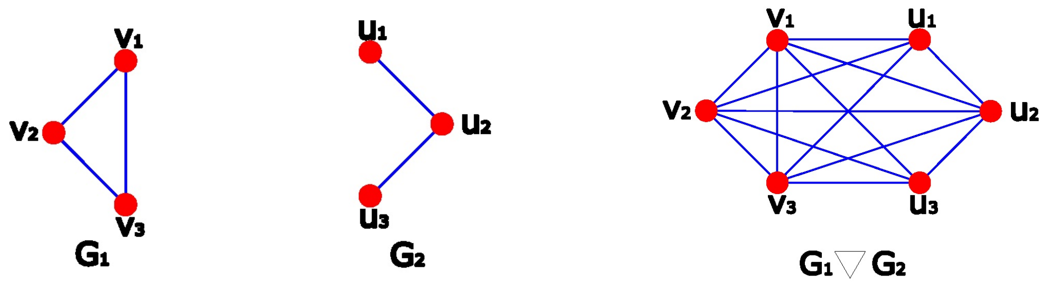

Figure 4.1 Join of two graphs

Theorem 11. *Let G_1 be an r_1-regular graph on n_1 vertices having diam$(G_1) \leq 2$ and G_2 be an r_2-regular graph on n_2 vertices having diam$(G_2) \leq 2$. Let further $\phi(G_1 : \mu)$ and $\phi(G_2 : \mu)$ be the q-distance characteristic polynomials of G_1 and G_2, respectively. Then the q-distance characteristic polynomial of the q-distance matrix of $G_1 \nabla G_2$ is*

$$\frac{(\mu-(1+q)(n_1-1)+r_1q)(\mu-(1+q)(n_2-1)+r_2q)-n_1n_2}{(\mu-(1+q)(n_1-1)+r_1q)(\mu-(1+q)(n_2-1)+r_2q)}\phi(G_1:\mu)\phi(G_2:\mu). \tag{2}$$

Proof. Let us assume that $v_1, v_2, \ldots, v_{n_1}$ be the vertices of the graph G_1 and $u_1, u_2, \ldots, u_{n_2}$ be the vertices of the graph G_2. Let q_{ij} denote the q-distance between the vertices v_i and v_j in G_1 and q'_{ij} denote the q-distance between the vertices u_i and u_j in G_2. In G_1, every vertex is at distance 1 from r_1 vertices and at distance $1+q$ from the remaining n_1-1-r_1 vertices. Therefore for $i = 1, 2, 3, \ldots, n_1$, we can write

$$\begin{aligned}\sum_{j=1}^{n_1} q_{ij} &= 1(r_1)+(1+q)(n_1-1-r_1)\\ &= r_1+(1+q)(n_1-1)-r_1-r_1q\\ &= (1+q)(n_1-1)-r_1q\end{aligned}$$

and similarly, for $i = 1,2,3,\ldots,n_2$, we have

$$\sum_{j=1}^{n_2} q'_{ij} = (1+q)(n_2-1)-r_2q.$$

Let $E_q(G_1 \nabla G_2)$ be the q-distance adjacency matrix of the join graph $G_1 \nabla G_2$. Then this matrix $A_q(G_1 \nabla G_2)$ has the form

$$\begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n_1} \\ u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{n_1} \end{array}
\begin{array}{c}
\begin{array}{cccccccccc} v_1 & v_2 & v_3 & \dots & v_{n_1} & u_1 & u_2 & u_3 & \dots & u_{n_2} \end{array} \\
\left(\begin{array}{ccccc|ccccc}
0 & q_{12} & q_{13} & \dots & q_{1n_1} & 1 & 1 & 1 & \dots & 1 \\
q_{21} & 0 & q_{23} & \dots & q_{2n_1} & 1 & 1 & 1 & \dots & 1 \\
q_{31} & q_{32} & 0 & \dots & q_{3n_1} & 1 & 1 & 1 & \dots & 1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
q_{n_11} & q_{n_12} & q_{n_13} & \dots & 0 & 1 & 1 & 1 & \dots & 1 \\
\hline
1 & 1 & 1 & \dots & 1 & 0 & q'_{12} & q'_{13} & \dots & q'_{1n_2} \\
1 & 1 & 1 & \dots & 1 & q'_{21} & 0 & q'_{23} & \dots & q'_{2n_2} \\
1 & 1 & 1 & \dots & 1 & q'_{31} & q'_{32} & 0 & \dots & q'_{3n_2} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
1 & 1 & 1 & \dots & 1 & q'_{n_21} & q'_{n_22} & q'_{n_23} & \dots & 0
\end{array}\right)_{(n_1+n_2)\times(n_1+n_2)}
\end{array}.$$

Let $\phi(G_1 \nabla G_2 : \mu)$ denote the q-distance characteristic polynomial of $G_1 \nabla G_2$; i.e.,

$$\phi(G_1 \nabla G_2 : \mu) = |\mu - E_q(G_1 \nabla G_2)|.$$

This polynomial is equal to the following determinant

$$\left|\begin{array}{ccccc|ccccc}
\mu & -q_{12} & -q_{13} & \dots & -q_{1n_1} & -1 & -1 & -1 & \dots & -1 \\
-q_{21} & \mu & -q_{23} & \dots & -q_{2n_1} & -1 & -1 & -1 & \dots & -1 \\
-q_{31} & -q_{32} & \mu & \dots & -q_{3n_1} & -1 & -1 & -1 & \dots & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-q_{n_11} & -q_{n_12} & -q_{n_13} & \dots & \mu & -1 & -1 & -1 & \dots & -1 \\
\hline
-1 & -1 & -1 & \dots & -1 & \mu & -q'_{12} & -q'_{13} & \dots & -q'_{1n_2} \\
-1 & -1 & -1 & \dots & -1 & -q'_{21} & \mu & -q'_{23} & \dots & -q'_{2n_2} \\
-1 & -1 & -1 & \dots & -1 & -q'_{31} & -q'_{32} & \mu & \dots & -q'_{3n_2} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-1 & -1 & -1 & \dots & -1 & -q'_{n_21} & -q'_{n_22} & -q'_{n_23} & \dots & \mu
\end{array}\right|_{(n_1+n_2)\times(n_1+n_2)}.$$

Applying the row operations $R'_{n_1+2} = R_{n_1+2} - R_{n_1+1}$; $R'_{n_1+3} = R_{n_1+3} - R_{n_1+1}$; $\cdots$; $R'_{n_1+n_2} = R_{n_1+n_2} - R_{n_1+1}$ to the above determinant, we see that the determinant becomes

$$\left|\begin{array}{ccccc|ccccc}
\mu & -q_{12} & -q_{13} & \dots & -q_{1n_1} & -1 & -1 & -1 & \dots & -1 \\
-q_{21} & \mu & -q_{23} & \dots & -q_{2n_1} & -1 & -1 & -1 & \dots & -1 \\
-q_{31} & -q_{32} & \mu & \dots & -q_{3n_1} & -1 & -1 & -1 & \dots & -1 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-q_{n_11} & -q_{n_12} & -q_{n_13} & \dots & \mu & -1 & -1 & -1 & \dots & -1 \\
\hline
-1 & -1 & -1 & \dots & -1 & \mu & -q'_{12} & -q'_{13} & \dots & -q'_{1n_2} \\
0 & 0 & 0 & \dots & 0 & -q'_{21}-\mu & \mu+q'_{12} & -q'_{23}+q'_{13} & \dots & -q'_{2n_2}+q'_{1n_2} \\
0 & 0 & 0 & \dots & 0 & -q'_{31}-\mu & -q'_{32}+q'_{12} & \mu+q'_{13} & \dots & -q'_{3n_2}+q'_{1n_2} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \dots & 0 & -q'_{n_21}-\mu & -q'_{n_22}+q'_{12} & -q'_{n_23}+q'_{13} & \dots & \mu+q'_{1n_2}
\end{array}\right|.$$

Applying the column operation $C'_{n_1+1} = C_{n_1+1} + C_{n_1+2} + \cdots + C_{n_1+n_2}$, using the fact that $q'_{ij} = q'_{ji}$ and the equations above, the same determinant becomes

$$\left|\begin{array}{cccc|ccccc}
\mu & -q_{12} & \dots & -q_{1n_1} & -n_2 & -1 & -1 & \dots & -1 \\
-q_{21} & \mu & \dots & -q_{2n_1} & -n_2 & -1 & -1 & \dots & -1 \\
-q_{31} & -q_{32} & \dots & -q_{3n_1} & -n_2 & -1 & -1 & \dots & -1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-q_{n_1 1} & -q_{n_1 2} & \dots & \mu & -n_2 & -1 & -1 & \dots & -1 \\
\hline
-1 & -1 & \dots & -1 & \mu-(1+q)(n_2-1)-r_2 q & -q'_{12} & -q'_{13} & \dots & -q'_{1n_2} \\
0 & 0 & \dots & 0 & 0 & \mu+q'_{12} & -q'_{23}+q'_{13} & \dots & -q'_{2n_2}+q'_{1n_2} \\
0 & 0 & \dots & 0 & 0 & -q'_{32}+q'_{12} & \mu+q'_{13} & \dots & -q'_{3n_2}+q'_{1n_2} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \dots & 0 & 0 & -q'_{n_2 2}+q'_{12} & -q'_{n_2 3}+q'_{13} & \dots & \mu+q'_{1n_2}
\end{array}\right|$$

$$= \left|\begin{array}{cccccc}
\mu & -q_{12} & -q_{13} & \cdots & -q_{1n_1} & -n_2 \\
-q_{21} & \mu & -q_{23} & \cdots & -q_{2n_1} & -n_2 \\
-q_{31} & -q_{32} & \mu & \cdots & -q_{3n_1} & -n_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-q_{n_1 1} & -q_{n_1 2} & q_{n_1 3} & \cdots & \mu & -n_2 \\
-1 & -1 & -1 & \cdots & -1 & \mu-(1+q)(n_2-1)+r_2 q
\end{array}\right| |B|,$$

where

$$|B| = \left|\begin{array}{cccc}
\mu+q'_{12} & -q'_{23}+q'_{13} & \cdots & -q'_{2n_2}+q'_{1n_2} \\
-q'_{32}+q'_{12} & \mu+q'_{13} & \cdots & -q'_{3n_2}+q'_{1n_2} \\
\vdots & \vdots & \vdots & \vdots \\
-q'_{n_2 2}+q'_{12} & -q'_{n_2 3}+q'_{12} & \cdots & \mu+q'_{1n_2}
\end{array}\right|_{(n_2-1)\times(n_2-1)}.$$

Applying the row operations $R'_2 = R_2 - R_1, R'_3 = R_3 - R_1, \cdots, R'_{n_1} = R_{n_1} - R_1$, the above determinant transforms to

$$\left|\begin{array}{cccccc}
\mu & -q_{12} & -q_{13} & \cdots & -q_{1n_1} & -n_2 \\
-q_{21}-\mu & \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} & 0 \\
-q_{31}-\mu & -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-q_{n_{11}}-\mu & -q_{n_{12}}+q_{12} & -q_{n_{13}}+q_{13} & \cdots & \mu+q_{1n_1} & 0 \\
-1 & -1 & -1 & \cdots & -1 & \mu-(1+q)(n_2-1)+r_2 q
\end{array}\right| |B|.$$

Applying the column operation $C'_1 = C_1 + C_2 + \cdots + C_{n_1}$ and using the above equations, the determinant becomes

$$\begin{vmatrix} \mu-(1+q)(n_1-1)+r_1q & -q_{12} & -q_{13} & \cdots & -q_{1n_1} & -n_2 \\ 0 & \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} & 0 \\ 0 & -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \\ 0 & -q_{n_{12}}+q_{12} & -q_{n_{13}}+q_{13} & \cdots & \mu+q_{1n_1} & 0 \\ -n_1 & -1 & -1 & \cdots & -1 & \mu-(1+q)(n_2-1)+r_2q \end{vmatrix} |B|.$$

Expanding it along the first column C_1, we obtain

$$\phi(G_1 \nabla G_2 : \mu) = \left\{(\mu-(1+q)(n_1-1)+r_1q)\Delta_1 - (-1)^{n_1} n_1 \Delta_2\right\}|B|, \tag{3}$$

where

$$\Delta_1 = \begin{vmatrix} \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} & 0 \\ -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -q_{n_{12}}+q_{12} & -q_{n_{13}}+q_{13} & \cdots & \mu+q_{1n_1} & 0 \\ -1 & -1 & \cdots & -1 & \mu-(1+q)(n_1-1)+r_2q \end{vmatrix}$$

$$= (\mu-(1+q)(n_1-1)+r_2q)|A|(-1)^{n_1+n_2}$$

$$= (\mu-(1+q)(n_1-1)+r_2q)|A|$$

and

$$\Delta_2 = \begin{vmatrix} -q_{12} & -q_{13} & \cdots & -q_{1n_1} & -n_2 \\ \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} & 0 \\ -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -q_{n_{12}}+q_{12} & -q_{n_{13}}+q_{13} & \cdots & \mu+q_{1n_1} & 0 \end{vmatrix}$$

$$= (-1)^{-n_1+1}(-n_2)|A|$$

$$= n_2(-1)^{n_1}|A|.$$

Therefore we have

$$\begin{aligned} \phi(G_1 \nabla G_2 : \mu) = {} & ((\mu-(1+q)(n_1-1)+r_1q)(\mu-(1+q)(n_2-1)+r_2q)|A|) \\ & -(-1)^{n_1} n_1 n_2 (-1)^{n_1}|A|)|B|, \end{aligned}$$

i.e.

$$\begin{aligned} \phi(G_1 \nabla G_2 : \mu) = |A||B|[&(\mu-(1+q)(n_1-1)+r_1q) \\ & \cdot(\mu-(1+q)(n_2-1)+r_2q) - n_1n_2] \end{aligned}$$

where

$$|A| = \begin{vmatrix} \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} \\ -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} \\ \vdots & \vdots & \vdots & \vdots \\ -q_{n_{12}}+q_{12} & -q_{n_{13}}+q_{13} & \cdots & \mu+q_{1n_1} \end{vmatrix}.$$

Clearly

$$|A| = \frac{1}{(\mu-(1+q)(n_1-1)+r_1q)} \times \begin{vmatrix} \mu-(1+q)(n_1-1)+r_1q & -q_{12} & -q_{13} & \cdots & -q_{1n_1} \\ 0 & \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} \\ 0 & -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & -q_{n_12}+q_{12} & -q_{n_13}+q_{13} & \cdots & \mu+q_{1n_1} \end{vmatrix}.$$

Applying the operation $C_1' = C_1-(C_2+C_3+\cdots+C_{n_1})$, the determinant becomes

$$|A| = \frac{1}{\mu-(1+q)(n_1-1)+r_1q} \times \begin{vmatrix} \mu & -q_{12} & -q_{13} & \cdots & -q_{1n_1} \\ -\mu-q_{21} & \mu+q_{12} & -q_{23}+q_{13} & \cdots & -q_{2n_1}+q_{1n_1} \\ -\mu-q_{n_31} & -q_{32}+q_{12} & \mu+q_{13} & \cdots & -q_{3n_1}+q_{1n_1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -\mu-q_{n_11} & -q_{n_12}+q_{12} & -q_{n_13}+q_{13} & \cdots & \mu+q_{1n_1} \end{vmatrix}.$$

Applying the operations $R' = R_2+R_1; R_3' = R_3+R_1; \cdots ; R_n' = R_{n_1}+R_1$, we have

$$\begin{aligned} |A| &= \frac{1}{\mu-(1+q)(n_1-1)+r_1q} \times \begin{vmatrix} \mu & -q_{12} & -q_{13} & \cdots & -q_{1n_1} \\ -q_{21} & \mu & -q_{23} & \cdots & -q_{2n_1} \\ -q_{31} & -q_{32} & \mu & \cdots & -q_{3n_1} \\ \vdots & \vdots & \vdots & \vdots & \\ -q_{n_11} & -q_{n_12} & -q_{n_13} & \cdots & \mu \end{vmatrix} \\ &= \frac{1}{\mu-(1+q)(n_1-1)+r_1q}\phi(G_1;\mu). \end{aligned}$$

Similarly,

$$|B| = \frac{1}{\mu-(1+q)(n_2-1)+r_2q}\phi(G_2;\mu).$$

By substituting these values in the above equation, we have the required result.

Theorem 12. *Let G_1 and G_2 be r_1- and r_2-regular graphs with n_1 and n_2 vertices, respectively. If $diam(G_1) \leq 2$ and $diam(G_2) \leq 2$, then*

$$E_q(G_1 \bigtriangledown G_2) = \begin{cases} E_q(G_1)+E_q(G_2), & \text{if } RK \geq n_1n_2, \\ E_q(G_1)+E_q(G_2)-(R+K)+\sqrt{(R+K)^2-4(RK-n_1n_2)}, & \text{if } RK < n_1n_2, \end{cases}$$

where $R = (1+q)(n_1-1)-r_1q$ and $K = (1+q)(n_2-1)-r_2q$.

Proof. From Theorem 2, we have

$$\phi(G_1\nabla G_2;\mu) = \frac{((\mu-(1+q)(n_1-1)+r_1q)(\mu-(1+q)(n_2-1)+r_2q)-n_1n_2))}{(\mu-(1+q)(n_1-1)+r_1q)(\mu-(1+q)(n_2-1)+r_2q)}\phi(G_1;\mu)\phi(G_2;\mu)$$

implying that

$$\phi(G_1\nabla G_2;\mu) = \frac{((\mu-R)(\mu-K)-n_1n_2)\phi(G_1;\mu)\phi(G_2;\mu)}{(\mu-R)(\mu-K)},$$

where $R = (1+q)(n_1-1) - r_1 q$ and $K = (1+q)(n_2-1) - r_2 q$; i.e.,

$$(\mu - R)(\mu - K)\phi(G_1 \nabla G_2; \mu) = ((\mu - R)(\mu - K) - n_1 n_2)\phi(G_1; \mu)\phi(G_2; \mu).$$

That is,

$$(\mu - R)(\mu - K)\phi(G_1 \nabla G_2; \mu) = (\mu^2 - (R+K)\mu + RK - n_1 n_2)\phi(G_1; \mu)\phi(G_2; \mu).$$

Let

$$P_1(\mu) = (\mu - R)(\mu - K)\phi(G_1 \nabla G_2; \mu)$$

and

$$P_2(\mu) = (\mu^2 - (R+K)\mu + RK - n_1 n_2)\phi(G_1; \mu)\phi(G_2; \mu).$$

The roots of the equation $P_1(\mu) = 0$ are R, K and $q-$distance eigenvalues of $G_1 \nabla G_2$. Therefore, the sum of the absolute values of the roots of $P_1(\mu) = 0$ is

$$R + K + E_q(G_1 \nabla G_2) \tag{4}$$

and similarly the roots of the equation $P_2(\mu) = 0$ are $q-$distance eigenvalues of G_1 and G_2 and hence

$$\frac{R+K+\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2}, \quad \frac{R+K-\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2}.$$

Therefore, the sum of the absolute values of the roots of $P_2(\mu) = 0$ is

$$\begin{aligned} E_q(G_1) + E_q(G_2) + \left| \frac{R+K+\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2} \right| \\ + \left| \frac{R+K-\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2} \right|. \end{aligned}$$

Since $P_1(\mu) = P_2(\mu)$, from above equations, we get,

$$\begin{aligned} R + K + E_q(G_1 \nabla G_2) = {} & E_q(G_1) + E_q(G_2) \\ & + \left| \frac{R+K+\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2} \right| \\ & + \left| \frac{R+K-\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2} \right|. \end{aligned}$$

Case 1: If $RK \geq n_1 n_2$, the last equation reduces to

$$\begin{aligned} R + K + E_q(G_1 \nabla G_2) = {} & E_q(G_1) + E_q(G_2) \\ & + \frac{R+K+\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2} \\ & + \frac{R+K-\sqrt{(R+K)^2 - 4(RK - n_1 n_2)}}{2}, \end{aligned}$$

and therefore

$$R + K + E_q(G_1 \nabla G_2) = E_q(G_1) + E_q(G_2) + R + K$$

implying that

$$E_q(G_1 \nabla G_2) = E_q(G_1) + E_q(G_2).$$

Case 2: If $RK < n_1n_2$, this time the last equation above reduces to

$$\begin{aligned} R+K+E_q(G_1\nabla G_2) &= E_q(G_1)+E_q(G_2) \\ &+ \frac{R+K+\sqrt{(R+K)^2-4(RK-n_1n_2)}}{2} \\ &+ \frac{R+K-\sqrt{(R+K)^2-4(RK-n_1n_2)}}{2}. \end{aligned}$$

Hence we get

$$R+K+E_q(G_1\nabla G_2) = E_q(G_1)+E_q(G_2)+\sqrt{(R+K)^2-4(RK-n_1n_2)}$$

and finally

$$E_q(G_1\nabla G_2) = E_q(G_1)+E_q(G_2)-(R+K)+\sqrt{(R+K)^2-4(RK-n_1n_2)}.$$

5 Brief summary and conclusion

Energy is a very important subject of graph theory with many applications in physics and chemistry. Similarly to the classical graph energy, there are a few other types of energy in graphs which are similarly defined by means of some other matrices. In this paper, we have defined a new type of energy called q-distance energy. As the distances are calculated between the vertices of the graph representing the atoms in the corresponding molecule, the q-distance energy is expected to have applications in chemistry due to its effect on the intermolcecular forces which affect the graph energy. The q-distance energy has been obtained for the join of two graphs. Similar studies can be made for other graph operations. Also, we have established lower and upper bounds for this new energy.

References

[1] R. B. Bapat, A. K. Lal, S. Pati, (2006), A q-analogue of the distance matrix of a tree, Linear Algebra and its Applications, 416 (2–3), 799–814

[2] R. B. Bapat, S. Pati, (2011), Energy of a graph is never an odd integer, Bull. Kerala Math. Assoc., 1, 129-132

[3] G. Caporossi, E. Chasset, B. Furtula, (2009), Some conjectures and properties on distance energy, Les Cahiers du GERAD, G-2009-64, 1-7

[4] D. Cvetković, I. Gutman (eds.), (2009), Applications of Graph Spectra, Beograd: Matematicki institut SANU

[5] D. Cvetković, I. Gutman (eds.), (2011), Selected Topics on Applications of Graph Spectra, Beograd: Matematicki institut SANU

[6] A. Graovac, I. Gutman, N. Trinajstić, (1977), Topological Approach to the Chemistry of Conjugated Molecules, Springer, Berlin

[7] I. Gutman, (1978), The Energy of a Graph, Ber. Math-Statist. Sekt. Forschungsz. Graz, 103, 1-22

[8] I. Gutman, (2001), The Energy of a Graph: Old and New Results, ed. by A. Betten, A. Kohnert, R. Laue, A. Wassermann, Algebraic Combinatorics and Applications, Springer, Berlin, 196-211

[9] I. Gutman, X. Li, J. Zhang, (2009), Graph Energy, ed. by M. Dehmer, F. Emmert-Streib, Analysis of Complex Networks. From Biology to Linguistics, Wiley - VCH, Weinheim, 154-174

[10] I. Gutman, O. E. Polansky, (1986), Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin

[11] S. M. Hosamani, B. B. Kulkarni, R. G. Boli, V. M. Gadag, (2017), QSPR Analysis of Certain Graph Theoretical Matrices and Their Corresponding Energy, Appl. Maths and Nonlin. Sciences, 2 (1), 131-150

[12] J. H. Koolen, V. Moulton, (2001), Maximal Energy Graphs, Adv. Appl. Math., 26, 47-52

[13] G. Indulal, (2009), Sharp Bounds on the Distance Spectral Radius and the Distance Energy of Graphs, Lin. Algebra Appl., 430, 106-113

[14] G. Indulal, I. Gutman, A. Vijayakumar, (2008), On Distance Energy of Graphs, MATCH Commun. Math. Comput. Chem., 60, 461-472

[15] M. R. R. Kanna, B. N. Dharmendra, G. Sridhara, (2013), Minimum dominating energy of a graph, International Journal of Pure and Applied Mathematics, 85 (4), 707-718

[16] H. Liu, M. Lu, F. Tian, (2007), Some Upper Bounds for the Energy of Graphs, Journal of Mathematical Chemistry, 41 (1), 45-57

[17] V. Lokesha, T. Deepika, P. S. Ranjini, I. N. Cangul, (2017), Operations of Nanostructures via SDD, ABC4 and GA5 indices, Appl. Maths and Nonlin. Sciences, 2 (1), 173-180

[18] B. J. McClelland, (1971), Properties of the latent roots of a matrix: The estimation of π-electron energies, J. Chem. Phys., 54, 640-643

[19] A. R. Nizami, A. Perveen, W. Nazeer, M. Baqir, (2018), WALK POLYNOMIAL: A New Graph Invariant, Appl. Maths and Nonlin. Sciences, 3 (1), 321-330

[20] H. S. Ramane, I. Gutman, D. S. Revankar, (2008), Distance equienergetic graphs, MATCH Commun. Math. Comput. Chem., 60, 473-484

[21] H. S. Ramane, D. S. Revankar, I. Gutman, S. B. Rao, B. D. Acharya, H. B. Walikar, (2008), Bounds for the distance energy of a graph, Kragujevac J. Math., 31, 59-68