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RELATIONS BETWEEN ENERGY OF GRAPHS AND WIENER, HARARY INDICES

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Abstract. Harary and Wiener indices are distance-based topological index. In this paper, we study the relations of graph energy $\varepsilon(G)$ and its Harary index $\mathrm{H}(G)$ and Wiener index $\mathrm{W}(G)$. Moreover, for a given graph G we study the lower bound of $\frac{\mathrm{H}(G)}{\varepsilon(G)}$ and $\frac{\mathrm{W}(G)}{\varepsilon(G)}$ in terms of the number of vertices of G.

1. Introduction

Let $G = (V, E)$ be a undirected simple graph with vertex set V and edge set E. The energy of a graph is the sum of the absolute values of eigenvalues of its adjacency matrix A_G and introduced by Gutman [4]. In other words, if G is a graph over n vertices and A_G is a matrix with $[a_{ij}] = 1$ whenever $ij \in E$, otherwise $[a_{ij}] = 0$, and $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is the set of eigenvalues of A_G, then energy of G is defined as

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

The energy of a graph is well-studied notion and attracts many authors in spectral graph theory. We refer the book [9] for an excellent survey in graph energy. In [1], the authors introduced the vertex energy of a graph which led further studies for energy bounds for a graph. The energy of a vertex v_i with respect to G over n vertices, is denoted by $\varepsilon_G(v_i)$, and defined as

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$$\varepsilon_G(v_i) = |A_G|_{ii} \text{ for } i = 1, 2, \ldots, n,$$

where $|A_G| = (A_G A_G^*)^{\frac{1}{2}}$ with A_G is adjacency matrix of G.

So the energy of a graph G is the sum of the each vertex energies of G,

$$\varepsilon(G) = \varepsilon_G(x_1) + \varepsilon_G(x_2) + \cdots + \varepsilon_G(x_n), \tag{1.1}$$

this allows a refinement of the graph energy [1].

Another active research in graph theory is topological indices which is very important in chemical graph theory. Morever, Wiener index is has been studied in algebraic combinatorics [6]. The Harary and Wiener indices of graphs are distance-based topological indices, has been introduced by works in [5, 7] and [8], respectively. The Harary index of a graph is defined as,

$$\mathrm{H}(G) = \sum_{x,y \in V} \frac{1}{\mathrm{dist}(x, y)},$$

and the Wiener index of a graph is defined as,

$$\mathrm{W}(G) = \sum_{x,y \in V} \mathrm{dist}(x, y),$$

where V is the set of vertices of G and $\mathrm{dist}(x, y)$ is the distance between the vertices x and y.

In the present paper, we study the relations between the graph energy and its Harary and Wiener index. In Section 2, we give definitions and results for using rest of the paper. In Section 3, we give the results related to the energy and Harary and Wiener index of graphs in terms of graph parameters such as independence number and vertex covering number. In Section 4, we study relations graph energy, Harary index and Wiener index using dominating sets of graphs.

2. Preliminaries

The distance of vertices x,$y \in V$ is the length of the shortest path between x and y and denoted by $\mathrm{dist}(x, y)$. The degree of a vertex x is the number of vertices adjacent to x, denoted by d_x. Given a graph $G = (V, E)$, a *vertex cover* C of G is the subset of V such that every edge of G incident to at least one vertex of C. The minimum cardinality of a vertex cover set of G is called *vertex covering number* and denoted by $\beta(G)$. If any two vertices of a subset $S \subseteq V$ are non-adjacent, then S is said to be an independent set. The cardinality of a maximal independent set of G is called independence number and denoted by $\alpha(G)$. A subset $D \subseteq V$ is called *dominating set* if any vertex in $V \backslash D$ is adjacent to at least one vertex of D. The minimum number of vertices in a dominating set is called *domination number* $\gamma(G)$ of G. The minimum cardinality of an independent and dominating set in a graph G is called *independence domination number* and denoted by $i(G)$. A graph is said to be *well-covered* if every covering sets have the same cardinality, in other words, if $i(G) = \alpha(G)$ for a

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graph G, then G is called well-covered graph. A graph is called *very well-covered*, if it is well-covered and every maximal independent sets of G has $\frac{n}{2}$ vertices with n is even. The join of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph union along with all edges joining $V(G)$ and $V(H)$, the join of graphs G and H is denoted by $G * H$.

Lemma 2.1. *Let $G = (V, E)$ be a graph and C be a minimal vertex covering set. Then $V \backslash C$ is a maximal independent set.*

Next, we give a lemma which will be useful for most of our proofs.

Lemma 2.2. [1, Proposition 3.2] *Let G be a graph and $x \in G$ be a vertex. Then $\varepsilon_G(x) \leq \sqrt{d_x}$, with equality if and only if the connected component containing x is isomorphic to S_n and x is its center vertex.*

Theorem 2.3. [3, Theorem 9] *Let G be a graph with vertex covering set C, Then*

$$\varepsilon(G) \leq 2 \sum_{i \in C} \varepsilon_G(v_i).$$

Theorem 2.4. [1, Theorem 3.3] *Let $G = (V, E)$ be a non-empty connected graph. Then for all $u \in V$,*

$$\varepsilon_G(u) \geq \tfrac{d_u}{\Delta}.$$

The equality holds if and only if G is isomorphic to complete bipartite graph $K_{d,d}$.

3. Harary index, Wiener index and Energy

In this section, we study the energy of graphs in terms of Harary and Wiener indices. For the completeness of the article, we the give proofs of the following lemmas.

Lemma 3.1. *Let G be a graph and C be its vertex covering set. Then $\varepsilon(G) \leq 2\sqrt{\Delta}|C|$ with equality if and only if G is isomorphic to K_2.*

Proof. By Theorem 2.3, we have $\frac{1}{2}\varepsilon(G) \leq \sum_{x \in C} \varepsilon_G(x)$. Since $\varepsilon_G(x) \leq \sqrt{d_x}$, then we get $\varepsilon(G) \leq 2 \sum_{x \in C} \sqrt{d_x}$. This implies that,

$$\varepsilon(G) \leq 2\sqrt{\Delta}|C|.$$

Assume that the equality holds, then by Lemma 2.2 G is both star graph and well-covered bipartite graph. These imply that $G \cong K_2$. □

Lemma 3.2. *Let G be a graph and α be its independence number. Then $\varepsilon(G) \geq \frac{2\delta\alpha}{\Delta}$. Equality holds if and only if G is isomorphic to complete bipartite graph $K_{\alpha,\alpha}$.*

Proof. Assume that I is a maximum independent set. Then $V\backslash I$ is a vertex covering set. By Theorem 2.3, we have that $\varepsilon(G) \geq 2\sum_{i\in I}\varepsilon_G(u_i)$. Since $\varepsilon_G(u_i) \geq \frac{d_{u_i}}{\Delta}$ for every u_i, it follows that $\varepsilon(G) \geq 2\frac{d_{u_i}|I|}{\Delta}$ for every maximal independent set. Therefore we have, $\varepsilon(G) \geq 2\frac{\delta\alpha}{\Delta}$. If equality holds, then G is isomorphic to complete bipartite graph by Theorem 2.4 with bipartite sets have the cardinality α. □

Theorem 3.3. *Let G be a connected graph on $n \geq 2$ with covering number $\beta \geq 2$ and independence number $\alpha \geq 2$. Then,*

$$\mathrm{H}(G)\frac{2\delta}{\Delta} \leq \varepsilon(G)(\frac{2}{\alpha\beta} + \frac{1}{\alpha^2} + \frac{1}{\alpha^2\beta})$$

Moreover, $\mathrm{H}(G)\frac{2\delta}{\Delta} = \varepsilon(G)$ *holds if and only if* $G \cong K_2$.

Proof. Let I be a maximum independent set. Then I is a dominating set. Now observe that,

$$\mathrm{H}(G) = \sum_{x,y\in V(G)\backslash I}\frac{1}{\mathrm{dist}(x,y)} + \sum_{x,y\in I}\frac{1}{\mathrm{dist}(x,y)} + \sum_{x\in V(G)\backslash I, y\in I}\frac{1}{\mathrm{dist}(x,y)} \tag{3.1}$$

$$\leq \frac{1}{\binom{n-\alpha}{2}} + \frac{1}{2\binom{\alpha}{2}} + \frac{1}{\alpha(n-\alpha)} \tag{3.2}$$

$$= \frac{2}{(n-\alpha)(n-\alpha-1)} + \frac{1}{\alpha(\alpha-1)} + \frac{1}{\alpha(n-\alpha)} = \frac{2}{\beta(\beta-1)} + \frac{1}{\alpha(\alpha-1)} + \frac{1}{\alpha\beta} \tag{3.3}$$

If $\alpha \geq 2$ and $\beta \geq 2$, then we get

$$\mathrm{H}(G) \leq \frac{2}{\beta} + \frac{1}{\alpha} + \frac{1}{\alpha\beta} \leq \alpha(\frac{2}{\alpha\beta} + \frac{1}{\alpha^2} + \frac{1}{\alpha^2\beta}). \tag{3.4}$$

Since $\frac{\varepsilon(G)\Delta}{2\delta} \geq \alpha$, then we get

$$\mathrm{H}(G) \leq \varepsilon(G)\frac{\Delta}{2\delta}(\frac{2}{\alpha\beta} + \frac{1}{\alpha^2} + \frac{1}{\alpha^2\beta}) \tag{3.5}$$

Rearranging the inequality in (3.5), therefore we get

$$\mathrm{H}(G)\frac{2\delta}{\Delta} \leq \varepsilon(G)(\frac{2}{\alpha\beta} + \frac{1}{\alpha^2} + \frac{1}{\alpha^2\beta}) \tag{3.6}$$

If we assume $\mathrm{H}(G)\frac{2\delta}{\Delta} = \varepsilon(G)$ holds, by using the equality condition in Theorem 2.4 it follows that G is a bipartite graph with $\alpha = 1$ and $\beta = 1$. Therefore, $G \cong K_2$. □

Theorem 3.4. *Let G be a graph with covering number β and independence number α. Then,*

$$2\sqrt{\Delta}\mathrm{W}(G) \geq \varepsilon(G)\left((\beta-1)+\frac{\alpha(\alpha-1)}{\beta}+\alpha\right).$$

Equality holds if and only if $G \cong K_2$.

Proof. Assume that I is a maximal independent set of G. Then it is clear that I is a dominating set of G. Then we get,

$$\mathrm{W}(G) = \sum_{x,y\in V(G)\setminus I} \mathrm{dist}(x,y) + \sum_{x,y\in I} \mathrm{dist}(x,y) + \sum_{x\in V(G)\setminus I, y\in I} \mathrm{dist}(x,y)$$

$$\geq \binom{n-\alpha}{2} + 2\binom{n}{2} + \alpha(n-\alpha) \tag{3.7}$$

$$= \frac{(n-\alpha)(n-\alpha-1)}{2} + \alpha(\alpha-1) + \alpha(n-\alpha)$$

$$= \beta\left(\frac{\beta-1}{2}+\frac{\alpha(\alpha-1)}{\beta}+\alpha\right). \tag{3.8}$$

By Lemma 3.1, we deduce, $\frac{\varepsilon(G)}{2\sqrt{\Delta}} \leq \beta$. Using this inequality in (3.8), we can conclude that,

$$2\sqrt{\Delta}\mathrm{W}(G) \geq \varepsilon(G)(\frac{\beta-1}{2}+\frac{\alpha(\alpha-1)}{\beta}+\alpha).$$

Now assume that equality holds. If equality holds for 3.7. Then by [**?**, Theorem 4.3], every u and v forms an edge for $u, v \in V(G)\setminus I$ and also every vertex in I is adjacent to vertices of $V(G)\setminus I$. This implies that $G \cong K_n * E_m$. Moreover, by considering Lemma 3.1, we deduce that $G \cong K_2$. Since K_2 is join of two discrete vertices, then equality holds whenever $G \cong K_2$. □

Theorem 3.5. *Let G be a very well-covered graph over n vertices. Then the followings hold,*

(1) *we have, $\frac{\mathrm{H}(G)}{\varepsilon(G)} \geq \frac{\delta}{\Delta}(\frac{12n-8}{n^2-2n})$. Equality holds if and only if $G \cong K_2$.*
(2) *we have, $\frac{\mathrm{W}(G)}{\varepsilon(G)} \geq \frac{3n-4}{4\sqrt{\Delta}}$. Equality holds if and only if $G \cong K_2$.*

Proof. Since G is a very well-covered graph, then by definition and Lemma 2.1, we have $\alpha = \beta = \frac{n}{2}$. Replacing α and β with $\frac{n}{2}$ in Theorem 3.3 and Theorem 3.4 yields to $\frac{\mathrm{H}(G)}{\varepsilon(G)} \geq \frac{\delta}{\Delta}(\frac{12n-8}{n^2-2n})$ and $\frac{\mathrm{W}(G)}{\varepsilon(G)} \geq \frac{3n-4}{4\sqrt{\Delta}}$. □

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4. Dominating sets, Wiener and Harary indices and energy

In this section, we discuss the energy of vertices which belong to the dominating sets.

Remark 4.1. *Given a graph $G = (V, E)$ with $V = \{x_1, x_2, \ldots, x_n\}$, by (1.1) it is well-known that $\varepsilon(G) = \varepsilon_G(x_1) + \varepsilon_G(x_2) + \cdots + \varepsilon_G(x_n)$. Let D be a dominating set of G. Then $V \backslash D$ is a dominating set of G as well. Since sets D and $V \backslash D$ are both dominating sets then by the identity (1.1), we can seperate the dominating sets of G into low energy dominating set, denoted by D_L, that is the set $\frac{1}{2}\varepsilon(G) \geq \sum_{i \in D_L} \varepsilon_G(d_i)$ and high energy dominating set, denoted by D_H, that is the set $\frac{1}{2}\varepsilon(G) \leq \sum_{i \in D_H} \varepsilon_G(d_i)$. Note that, if $G = (U, V; E)$ is a bipartite graph, then both sets U and V are dominating sets, hence $\sum_{i \in U} \varepsilon_G(u_i) = \sum_{j \in V} \varepsilon_G(v_j)$ ([2, Proposition 3.9]).*

Next, we can give the relations of energy and Wiener index of a graph in terms of its dominating sets.

Theorem 4.2. *Let G be a graph with dominatig set D. Then followings hold:*

(1) If D is a low energy dominating set, then
$$\varepsilon(G)\mathrm{H}(G) \geq 2\frac{\delta}{\Delta}\left(\frac{2}{|D_L - 1|} + \frac{1}{|n - |D_L|}\right).$$
(2) If D is a high energy dominating set, then
$$2\sqrt{\Delta}\mathrm{W}(G) \geq \varepsilon(G)\left(\frac{2n - |D_H| - 1}{2}\right).$$

Proof. (1) Let $\mathrm{W}(G)$ be Wiener index. Then we have,

$$\mathrm{W}(G) = \sum_{x,y \in D} \frac{1}{\mathrm{dist}(x,y)} + \sum_{x \in D, y \in V \backslash D} \frac{1}{\mathrm{dist}(x,y)}$$
$$\geq \frac{1}{\begin{pmatrix} |D| \\ 2 \end{pmatrix}} + \frac{1}{|D|\left(|n - |D|\right)}$$
$$= \frac{2}{|D||D-1|} + \frac{1}{|D|\left(|n - |D|\right)}. \tag{4.1}$$

On the other hand, from Remark 4.1, we have that

$\frac{1}{2}\varepsilon(G) \geq \sum_{x \in D_L} \varepsilon_G(x)$. This implies that $\frac{1}{2}\varepsilon(G) \geq \sum_{x \in D_L} \frac{d_x}{\Delta}$ by [1, Theorem 3.3]. Hence we get that,

$$\varepsilon(G) \geq 2|D_L|\frac{\delta}{\Delta}.$$

which implies $\frac{1}{|D_L|} \geq \frac{2\delta}{\varepsilon(G)\Delta}$. Combining this inequality with (4.1), we can deduce that,

http://dx.doi.org/10.22108/toc.2023.132397.1955

$$\varepsilon(G)\ \mathrm{H}(G) \geq 2\frac{\delta}{\Delta}\left(\frac{2}{|D_L - 1|} + \frac{1}{|n - |D_L|}\right).$$

(2) Let $\mathrm{W}(G)$ be Wiener index of G. Then we have,

$$\begin{aligned}\mathrm{W}(G) &= \sum_{x,y\in D} \mathrm{dist}(x,y) + \sum_{x\in D, y\in V\setminus D} \mathrm{dist}(x,y) \\ &\geq \binom{D}{2} + |D|\,(n - |D|) \\ &= \frac{|D|\,|D-1|}{2} + |D|\,(n-|D|) \qquad (4.2)\end{aligned}$$

Since $\varepsilon(G) \leq 2\sqrt{\Delta}\,|D_H|$, using this inequality in (4.2) and considering dominating set D as high energy dominating set, therefore we can get

$$2\sqrt{\Delta}\mathrm{W}(G) \geq \varepsilon(G)\left(\frac{2n - |D_H| - 1}{2}\right).$$

□

5. Concluding Remarks

The relations energy of a graph G and distance-based topological indices such as Harary index and Wiener index are given in terms of dominating sets. For future direction we can give the following question,

Question Let D be a dominating set of a graph $G = (V, E)$. Then $\sum_{i\in D} \varepsilon_G(x_i) = \sum_{j\in V\setminus D} \varepsilon_G(x_j)$ if and only if G is a bipartite graph.

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