The Eigen-3-Cover Ratio of Graphs: Asymptotes, Domination and Areas

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Abstract

The separate study of the two concepts of energy and vertex coverings of graphs has opened many avenues of research. In this paper we combine these two concepts in a ratio, called the *eigen-3-cover ratio*, to investigate the domination effect of the subgraph induced by a vertex 3-covering of a graph G (called the 3-*cover graph* of G), on the original energy of G, where large number of vertices are involved. This is referred to as the *eigen-3-cover domination* and has relevance, in terms of conservation of energy, when a molecule's atoms and bonds are mapped onto a graph with vertices and edges, respectively. If this energy-3-cover ratio is a function of n, the order of graphs belonging to a class of graph, then we discuss its horizontal *asymptotic* behavior and attach the graphs average degree to the Riemann integral of this ratio, thus associating *eigen-3-cover area* with classes of graphs. We found that the eigen-3-cover domination had a strongest effect on the complete graph, while this eigen-3-cover domination had zero effect on star graphs. We show that the eigen-3-cover asymptote of discussed classes of graphs belong to the interval [0,1], and conjecture that the class of complete graphs has the largest eigen-3-cover area of all classes of graphs.

Indexing terms/Keywords

Energy of graphs, eigenvalues, vertex 3-cover, domination, ratios, asymptotes, areas.

Academic Discipline and Sub-Disciplines

Graph theory, combinatorics, algebraic graph theory

SUBJECT CLASSIFICATION

AMS classification 05C99

1. INTRODUCTION

All graphs in this paper are simple and loopless and on n vertices and m edges. We shall use the graph-theoretical notation of Harris, Hirst and Mossinghoff [8].

1.1 Energy, vertex covers and ratios of graphs

Much research has been done involving the energy of a graph (see Adiga, Bayad, Gutman and Srinivas [1] and Coulson, O'Leary and Mallion [4]) and (minimum) vertex coverings of graph (see Adiga, Bayad, Gutman and Srinivas [1]). Ratios have been an important aspect of graph theoretical definitions. Examples of ratios are: expanders (see Alon and Spencer [2]), the central ratio of a graph (see Buckley [3]), eigen-pair ratio of classes of graphs (see Winter and Jessop [14]), Independence and Hall ratios (see Gábor [4]), tree-cover ratio of graphs (see Winter and Adewusi [13]), the eigen-energy formation ratio of graphs (see Winter and Sarvate [18]), the t-complete eigen ratio of graphs (see Winter, Jessop and Adewusi [16]), the chromatic-cover ratio of graphs (see Winter [10]), the chromatic-complete difference ratio of graphs (see Winter [11]), the tree-3-cover ratio of graphs (see Winter [12]) and the eigen-complete difference ratio (see Winter and Ojako [17]) .

In this paper we combine the two concepts of energy and vertex 3-covering of graphs to form a ratio, the eigen-3-cover ratio, associated with a connected graph $G,$ involving the energy of the subgraph $H(S_3)$ of G induced by a 3-vertex cover S_3 (a minimum set of vertices S_3 of $G,$ such that every path on 3 vertices in $G,$ has at least on vertex in S_3 - see Winter [12]) of $G,$ called the *3-cover graph of* $G,$ and the energy of $G.$ This eigen-3-cover ratio allows for the investigation of the domination effect of the energy of the 3-cover graph on the original energy of G, where a large number of vertices are involved – referred to as the *eigen-3-cover domination*. This eigen-3-cover ratio has relevance when molecules with atoms and bonds are mapped onto a graph with vertices and edges, respectively. In terms of conservation of energy, one requires the smallest set S_3 of atoms whose excitation would affect all atoms which can be reached from S_3 by a path of length at most 2, and where a large amount of atoms are involved, the eigen-3-domination effect becomes relevant. If the eigen-3-cover ratio is a function of n, the order of graphs belonging to a particular class of graphs, then we investigated its asymptotic behavior (see Winter and Adewusi [13] , Winter and Jessop [14], Winter, Jessop and Adewusi [16], Winter and Sarvate [18],Winter and Ojako [17], Winter [10], [11], and [12],). The eigen-3-cover domination was determined for known classes of graph. We found that, for the complete graph, the eigen-3-cover domination was the strongest for complete graphs, and for star graphs with rays of length one, no effect at all. By introducing the average degree of a graph together with the Riemann integral of the eigen-3-cover ratio we associated eigen-3-cover area with classes of graphs (see Winter and Adewusi [13] , Winter and Jessop [14], Winter and Sarvate [18], Winter, Jessop and Adewusi [16],Winter and Ojako [17], Winter [10], [11], and [12]).

2. EIGEN-3-COVER RATIO, ASYMPTOTES, DOMINATION AND AREA

We combine the idea of energy (defined below) and 3-vertex cover (formally defined below) of graphs in the following definitions, to allow for the measure of the domination of the energy of a 3-cover graph over the energy of original graph for large values of n. If one considers a molecule in a graph-theoretical way, where the atoms are the vertices and the edges the bonds between the atoms, then the idea of *energizing* the whole molecule is relevant. Conserving energy will involve the *smallest* set S of atoms which can be energized so that all atoms outside S_3, and connected to S_3 by a path of length at most two, will also be energized. This is equivalent, graphically, to finding a minimum vertex 3-covering of a graph, i.e. every path of length 2 has at least one end in S_3 (see Adiga, Bayad, Gutman and Srinivas [1]). When a large number of atoms are involved, the asymptotic behavior of this eigen-3-cover ratio becomes significant.

Definition 2.1

A minimum vertex cover S (or a 2-vertex cover) of a graph $G,$ is a minimum set of vertices of $G,$ such that every edge (i.e. path of length 2) in $G,$ has at least on vertex in $S.$ This provides the motivation for the following definition.

Definition 2.2

A minimum 3-vertex cover S_3 of a graph $G,$ is a minimum set of vertices of $G,$ such that every path of length 3 in $G,$ has at least on vertex in $S_3.$ See Winter [12].

Definition 2.3

The Huckel Molecular Orbital theory provided the motivation for the idea of the *energy* of a graph - the sum of the absolute values of the eigenvalues associated with the graph (Adiga, Bayad, Gutman and Srinivas [1] and Coulson, O'Leary and Mallion [4]):

$E(G) = \sum_{1}^{n} |\lambda_i|,$ where $\lambda_i,\ 1 \le i \le n$ are eigenvalues of adjacency matrix of graph G .

The definitions below allows for the investigation of the energy-domination of, and the eigen-3-cover areas, of classes of graphs (see Winter and Adewusi [13] , Winter and Jessop [14] and [15], Winter and Sarvate [18] , Winter, Jessop and Adewusi [16], Winter and Ojako[17], Winter[10], [11], and [12] for similar definitions).

Definition 2.4

Let G be a connected graph with minimum 3-covering S_3 of vertices. Let $H(S_3)$, the subgraph of G induced by S_3, be the *3-cover graph* of G.

The *eigen-3-cover ratio* of a graph G of order n, with respect to S_3, is defined as:

$$\text{cov}\{E^{S_3}(G)\} = \frac{|S_3| E(H(S_3))}{nE(G)}$$

where $E(G)$ is the energy of G defined above. If $H(S_3)$ consists of isolated vertices only then we define $E(H(S_3))$ as 1.

Definition 2.5

If $\text{cov}\{E^{S_3}(G)\} = f(n)$ for every $G \in \Im$, where $\Im$ is a class of graphs, then the asymptotic behavior of $f(n)$ is called the *eigen-3-cover asymptote of* $\Im$ and denoted by:

$$as\,\text{cov}\{E^{S_3}(\Im)\}.$$

Eigen-3-cover domination

This asymptote gives a measure of the *domination effect* of the energy of the cover graph on the energy of the original graph, for large values of n, referred to as the *eigen-3-cover domination.*

Definition 2.6

If $\text{cov}\{E^{S_3}(G)\} = f(n)$ for every $G \in \Im$, where $\Im$ is a class of graphs, then the *eigen-3-cover area* is defined as :

$$A_{\Im(n)}^{E^{S_3}} = \frac{2m}{n} \int f(n)dn$$

with $A_{\Im(k)}^{E^{S_3}} = 0$ where k is the smallest number of vertices for which $\text{cov}\{E^{S_3}(G)\} = f(n)$ is defined, and $\frac{2m}{n}$ is the average degree of $G \in \Im$, referred to as the *length* of G while the integral part is its *height* which we always make positive.

Examples:

2.1 The complete graph K_n

Let G be the compete graph K_n on n vertices.

Then a minimum 3-covering set of K_n is any subset of $n-2$ vertices of K_n. Therefore, for the complete graph K_n, the 3-cover graph $H(S_3)=K_{n-2}$. The eigenvalues of the complete graph on n vertices are 1 (with multiplicity $(n-1)$), and $(n-1)$ with multiplicity 1 (see Jessop [9]), so the energy of the complete graph is

$$E(K_n)=\sum_{i=1}^{n}|\lambda_i|=[(n-1)+(n-1)(1)]=2n-2$$

and therefore the energy of its 3-cover graph is

$$E(H(S_3))=E(K_{n-2})=2(n-2)-2=2n-6.$$

Hence,

$$\operatorname{cov}\{E^{S_3}(K_n)\}=\tfrac{|S_3|E(H(S_3))}{nE(G)}=\frac{(n-2)(2n-6)}{n(2n-2)}=\frac{2(n-2)(n-3)}{2n(n-1)}=\frac{(n-2)(n-3)}{n(n-1)}$$ and

$$as\operatorname{cov}\{E^{S_3}(K_n)\}=1.$$

Then $A_{K_n}^{E^{S_3}}=\dfrac{2m}{n}\int f(n)dn$

$$=(n-1)\int\frac{(n-2)(n-3)}{n(n-1)}dn$$

$$=\int\frac{(n-2)(n-3)}{n}dn$$

$$=\int n-5+\frac{6}{n}dn$$

$$=\frac{n^2}{2}-5n+6\ln n+c.$$

Now, $A_{K_2}^{E^{S_3}} = 0 \Rightarrow c = -6,$ so

$$A_{K_n}^{E^{S}} = \frac{n^2}{2} - 5n + 6\ln n - 6.$$

2.2 The complete split-bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$

Let G be the complete split-bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$. Then we have S_3 consisting of one of the partite sets on $\frac{n}{2}$ vertices, and its 3-cover graph the set of $\frac{n}{2}$ isolated vertices and therefore $E(H(S_3))=1$.

The eigenvalues of the complete split-bipartite graph graph $K_{\frac{n}{2},\frac{n}{2}}$ are 0 (with multiplicity $n-2$), $+\frac{n}{2}$ (with multiplicity 1), and $-\frac{n}{2}$ (with multiplicity 1) (see Jessop [9]), so $E(G)=n.$ Therefore,

$$\operatorname{cov}\{E^{S_3}(K_{\frac{n}{2},\frac{n}{2}})\}=\frac{|S_3|E(H(S_3))}{nE(G)}=\frac{\frac{n}{2}.1}{nE(G)}=\frac{n}{n.n}=\frac{1}{n} \text{ and}$$

$$as\operatorname{cov}\{E^{S_3}(K_{\frac{n}{2},\frac{n}{2}})\}=0.$$

Therefore, $A_{K_{\frac{n}{2},\frac{n}{2}}}^{E^{S_3}}=\frac{2m}{n}[\int\frac{1}{n}dn]=\frac{n}{2}(\ln n+c)$ and

$$A_{K_{1,1}}^{E^{S_3}}=0\Rightarrow c=-\ln 2.$$

Hence the eigen-3-cover area of the complete-split bipartite graph is

$$A_{K_{\frac{n}{2},\frac{n}{2}}}^{E^{S_3}}=\frac{n}{2}(\ln n-\ln 2).$$

2.3 The cycle graph C_n on $n = 3k$ vertices

Let G be the cycle graph C_n on $n = 3k$ vertices. Then a minimum 3-vertex cover will be the $\frac{n}{3}$ vertices of the disconnected graph induced by every third vertex of the cycle, so that $|S_3| = \frac{n}{3}$ and $E(H(S_3)) = 1$.

The eigenvalues of the cycle graph C_n are $2\cos\left(\frac{2\pi j}{n}\right); j = 0,\ldots,n-1$ for $n \geq 3$, (see Jessop [9]), so the energy of the cycle graph is

$$E(C_n) = 2\sum_{j=0}^{n-1}\left|\cos\left(\frac{2\pi j}{n}\right)\right| \leq 2n.$$

Then

$$\operatorname{cov}\{E^{S_3}(C_n)\} = \frac{|S_s|E(H(S_s))}{nE(G)} = \frac{\frac{n}{3}.1}{n2\sum_{j=0}^{n-1}\left|\cos(\frac{2\pi j}{n})\right|} = \frac{1}{6\sum_{j=0}^{n-1}\left|\cos\left(\frac{2\pi j}{n}\right)\right|} \geq \frac{1}{6n}.$$

Then, $A_{C_n}^{E^{S_3}} = 2\int \frac{n}{3n2\sum_{0}^{n-1}\left|\cos(\frac{2\pi j}{n})\right|}dn \geq 2\int \frac{1}{6n}dn \geq 2(\ln 6n + c).$

2.4 The path graph P_n on $n = 3k$ vertices

Let G be the path graph P_n on $n = 3k$ vertices. Then a minimum 3-vertex cover will consist of every third vertex of P_n by considering the first vertex of the path and then skipping 2 vertices so that the cover graph consists of $\frac{n}{3}$ isolated vertices.

The eigenvalues of the path graph P_n are $2\cos\left(\frac{\pi j}{n+1}\right)$; $j = 1,\ldots,n$ for $n \geq 3$, (see Jessop [9]), so the energy of the path graph is:

$$E(P_n) = 2\sum_{j=1}^{n}\left|\cos\left(\frac{\pi j}{n+1}\right)\right| \leq 2n.$$

Then,

$$\operatorname{cov}\{E^{S_3}(P_n)\} = \frac{|S_3|E(H(S))}{nE(P_n)} = \frac{\frac{n}{3}.1}{n2\sum_{j=1}^{n}\left|\cos\left(\frac{\pi j}{n+1}\right)\right|} = \frac{1}{6\sum_{j=1}^{n}\left|\frac{\cos \pi j}{n+1}\right|} \geq \frac{1}{6n}.$$

Then, $A_{P_n}^{E^{S_3}} \geq \frac{2m}{n}\int\frac{1}{6n}dn = \frac{2(n-1)}{n}\int\frac{1}{6n}dn = \frac{2(n-1)}{n}(\ln(6n)+c).$

2.5 The wheel W_n with $n-1$ spokes, and with $n=3k+1$

Let G be the wheel graph W_n, with $n-1$ spokes and where $n=3k+1$. Then the 3-vertex covering of W_n consists of the central vertex and every third vertex of the cycle, so the 3-cover graph is the star graph with $\frac{n-1}{3}$ rays of length 1.

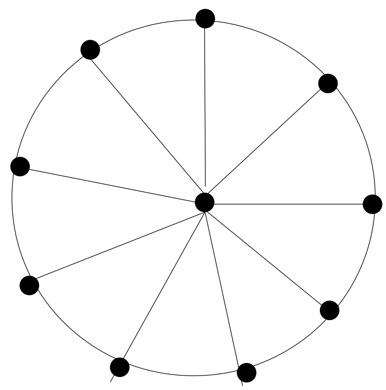

Figure 2.5.1: Wheel graph W_{10}

The eigenvalues of the star graph on m rays of length 1, are 0 (with multiplicity $n-2$), and $\pm\sqrt{m}$ (each with multiplicy 1) (see Jessop [9]). Then $|S_3| = \frac{n-1}{3}+1=\frac{n+2}{3}$ and the energy of the 3-cover graph $H(S_3)$ is

$$E(H(S_3))=\sum_{i=1}^{\frac{n+2}{3}}|\lambda_i| = \left(\frac{n+2}{3}-2\right)(0)+\left|\sqrt{\frac{n-1}{3}}\right|+\left|-\sqrt{\frac{n-1}{3}}\right| = 2\sqrt{\frac{n-1}{3}} .$$

The eigenvalues of the wheel graph on n vertices are $1\pm\sqrt{n}$; $2\cos\frac{2\pi j}{n-1}$; $j=1,\ldots,n-2$ (see Jessop [9]). Therefore, the energy of the wheel graph is

$$E(W_n) = |1+\sqrt{n}|+|1-\sqrt{n}|+\sum_{j=1}^{n-2}2\left|\cos\frac{2\pi j}{n-1}\right|$$

$$=1+\sqrt{n}-1+\sqrt{n}+\sum_{j=1}^{n-2}\left|2\cos\frac{2\pi j}{n-1}\right|$$

$$=2\sqrt{n}+\sum_{j=1}^{n-2}\left|2\cos\frac{2\pi j}{n-1}\right|$$

$$\leq 2\sqrt{n}+2(n-2).$$

Then, $\operatorname{cov}\{E^{S_3}(W_n)\} = \frac{|S_3|E(H(S_3))}{nE(W_n)}$

$$=\frac{\left(\frac{n+2}{3}\right)2\sqrt{\frac{n-1}{3}}}{nE(W_n)}$$

$$=\frac{2\sqrt{\frac{n-1}{3}}(n+2)}{3n(2\sqrt{n}+\sum_{j=1}^{n-2}\left|2\cos\frac{2\pi j}{n-1}\right|)}$$

$$\geq\frac{\sqrt{n-1}(n+2)}{3\sqrt{3n}(\sqrt{n}+(n-2))}$$

and $as\operatorname{cov}\{E^{S_3}(W_n)\}=0.$

Then,

$$A_{W_n}^{E^S}=\frac{2m}{n}\int f(n)dn \quad =\frac{2.2(n-1)}{n}\int\frac{\sqrt{n-1}(n+2)}{3\sqrt{3n}\left(\sqrt{n}+\sum_{k=1}^{n-2}\left|\cos\frac{2\pi k}{n-1}\right|\right)}dn$$

$$\geq\frac{4(n-1)}{3\sqrt{3}}\int\frac{\sqrt{n-1}(n+2)}{\sqrt{n}(\sqrt{n}+(n-2))}dn.$$

2.6 Star graphs $S_{r,1}$ on n vertices with r rays of length 1

Let G be the star graph $S_{r,1}$ with r rays of length 1. Then vertex 3-cover S_3 comprises of the center vertex only with $|S_3| = 1$ and $E(H(S_3)) = 1$.

Then

$$\operatorname{cov}\{E^{S_3}(S_{r,1})\} = \frac{|S_3|E(H(S_3))}{nE(S_{r,1})} = \frac{1}{n2\sqrt{n-1}} = \frac{1}{2n\sqrt{n-1}},\ \text{and}\ as\operatorname{cov}\{E^{S_3}(S_{r,1})\} = 0.$$

Then, $A_{S_{r,1}}^{E^{S_3}} = \dfrac{2m}{n}\displaystyle\int f(n)dn = \dfrac{2(n-1)}{n}\displaystyle\int \dfrac{1}{2n\sqrt{n-1}}dn = \dfrac{(n-1)}{n}\displaystyle\int \dfrac{1}{n\sqrt{n-1}}dn.$

Let $n = \sec^2 x$, then $dn = 2\sec^2 x \tan x dx$, so

$$A_{S_{r,1}}^{E^{S_3}} = \frac{(n-1)}{n}\int 2dx = \frac{(n-1)}{n}(2arc\sec\sqrt{n} + c)\ .$$

With $A_{S_{1,1}}^{E^S} = 0$, then $c = -2arc\sec\sqrt{2}.$

So $A_{S_{r,1}}^{E^{S_3}} = \dfrac{(n-1)}{n}(2arc\sec\sqrt{n} + -2arc\sqrt{2}).$

2.7 Star graph $S_{r,2}$ with r rays of length 2

Let G be the star graph $S_{r,2}$ with r rays of length 2. Then vertex 3-cover S_3 of G comprises of the center vertex only, with $|S_3| = 1$ and $E(H(S_3)) = 1$.

The eigenvalues of $S_{r,2}$ are 1 and -1, each with multiplicity $r-1 = \frac{n-3}{2}$, one eigenvalue 0, and two eigenvalues $\lambda = \pm\sqrt{r+1} = \pm\sqrt{\frac{n+1}{2}}$.

The energy of this graph is therefore

$$E(S_{r,2}) = \left(\frac{n-3}{2}\right) + \left(\frac{n-3}{2}\right) + \left(2\sqrt{\frac{n+1}{2}}\right) = (n-3) + \sqrt{2}\sqrt{n+1}.$$

Then

$$\operatorname{cov}\{E^{S_3}(S_{r,1})\} = \frac{|S_3| E(H(S_3))}{nE(S_{r,2})} = \frac{1}{n\left((n-3)+\sqrt{2}\sqrt{n+1}\right)},$$

and $as\operatorname{cov}\{E^{S_3}(S_{r,2})\} = 0.$

Then $A_{S_{r,2}}^{E^{S_2}} = \frac{2m}{n}\int f(n)dn = \frac{2(n-1)}{n}\int \frac{1}{n\left((n-3)+\sqrt{2}\sqrt{n+1}\right)}dn$.

2.8 Lollipop graph

Lemma 1

Let G be a graph with an end vertex x_1 adjacent to vertex x_2, and let G' be the subgraph of G induced by removing the vertex x_1. and let G'' be the subgraph of G induced by removing the vertex x_2. Then (see Haemers [7]):

$$P_{A(G)}(\lambda) = \lambda P_{A(G')}(\lambda) - P_{A(G'')}(\lambda)$$

where $P_{A(G)}(\lambda)$ is the characteristic polynomial $\det(A(G) - \lambda I)$.

Example with complete graph joined to end vertex

Let $G = LP_n$ be the complete graph K_{n-1} on $n-1$ vertices, joined to a single end vertex x_2 by an edge $x_1 x_2$.

Then we have

$$\begin{aligned}
P_{A(G)}(\lambda) &= \lambda P_{A(G')}(\lambda) - P_{A(G'')}(\lambda) \\
&= \lambda(\lambda+1)^{n-2}(\lambda-(n-2)) - \lambda(\lambda+1)^{n-3}(\lambda-(n-3)) \\
&= \lambda(\lambda+1)^{n-3}[(\lambda+1)(\lambda-(n-2)-(\lambda-(n-3))] \\
&= \lambda(\lambda+1)^{n-3}[(\lambda^2-\lambda(n-2)+\lambda-(n-2)-\lambda+(n-3)] \\
&= \lambda(\lambda+1)^{n-3}[(\lambda^2-\lambda(n-2)-1].
\end{aligned}$$

The roots of the quadratic are $\lambda = \dfrac{(n-2) \pm \sqrt{n^2 - 4n + 4 + 4}}{2}$, so we have eigenvalues of LP_n as

$\lambda = 0$, $\lambda = -1$ (with multiplicity $n-3$), $\lambda = \dfrac{(n-2)+\sqrt{n^2-4n+8}}{2}$, and $\lambda = \dfrac{(n-2)-\sqrt{n^2-4n+8}}{2}$.

The energy of this graph is therefore

$$E(LP_n) = 0 + 1(n-3) + \frac{(n-2)+\sqrt{n^2-4n+8}}{2} + \frac{\sqrt{n^2-4n+8}-(n-2)}{2}$$

$$=(n-3)+\sqrt{n^2-4n+8}, \quad \text{for } n \geq 4 \ .$$

A 3-cover graph is the subgraph induced by $n-3$ vertices of the complete graph K_{n-1} including x_1 so that its energy is

$$E(H(S_3)) = E(K_{n-3}) = 2(n-3)-2 = 2n-8$$

Hence

$$\operatorname{cov}\{E^{S_3}(LP_n)\} = \frac{|S_3|E(H(S_3))}{nE(LP_n)} = \frac{(n-3)(2n-8)}{n\left((n-3)+\sqrt{n^2-4n+8}\right)}.$$

For large n this behaves like

$$\frac{2n^2}{n(n+n)} = \frac{2n^2}{2n^2} = 1, \quad \text{so that } as\operatorname{cov}\{E^{S_3}(LP_n)\} = 1.$$

Then $A_{LP_n}^{E^{S_3}} = \frac{2m}{n}\int f(n)dn$

$$= \frac{((n-1)(n-2)+2)}{n}\int \frac{(n-3)(2n-8)}{n\left((n-3)+\sqrt{n^2-4n+8}\right)}dn$$

$$= \frac{\left(n^2-3n+4\right)}{n}\int \frac{(n-3)(2n-8)}{n\left((n-3)+\sqrt{n^2-4n+8}\right)}dn \ .$$

2.9 Dual star graph DuS_n

A dual star DuS_n is defined as two star graphs with m rays of length 1 (each on $\frac{n}{2}$ vertices) joined by an edge (its center edge) connecting their centers.

This graph has 4 non-zero eigenvalues found as solutions of the following equation (see Haemers [6]):

$$x^4-(2m+1)x^2+m^2=0$$

$$\Rightarrow x^4-(n-1)x^2+\frac{(n-2)^2}{4}$$

$$\Rightarrow x^2=\frac{(n-1)\pm\sqrt{(n-1)^2-(n-2)^2}}{2}=\frac{(n-1)\pm\sqrt{2n-3}}{2}$$

$$\Rightarrow x=\pm\sqrt{\frac{(n-1)+\sqrt{2n-3}}{2}}\ \ or\ \ \pm\sqrt{\frac{(n-1)-\sqrt{2n-3}}{2}}$$

Thus $E(DuS_n)=2\sqrt{\frac{(n-1)+\sqrt{2n-3}}{2}}+2\sqrt{\frac{(n-1)-\sqrt{2n-3}}{2}}$.

A 3-cover set S_3 consists of the vertices of the center edge of the graph.

Hence,

$$\operatorname{cov}\{E^{S_3}(DuS_n)\}=\frac{|S_3|E(H(S_3))}{nE(G)}=\frac{2.2}{nE(G)}=\frac{4}{n\left(2\sqrt{\frac{(n-1)+\sqrt{2n-3}}{2}}+2\sqrt{\frac{(n-1)-\sqrt{2n-3}}{2}}\right)}$$

For large n this ratio behaves like $\frac{4}{n\left(4\frac{\sqrt{n}}{\sqrt{2}}\right)}=\frac{\sqrt{2}}{n^{\frac{3}{2}}}=\sqrt{2}n^{-\frac{3}{2}}$ so that

$$as\operatorname{cov}\{E^{S_3}(DuS_n)\}=0.$$

Then,

$$A_{DuS_n}^{E^{S_3}} = \frac{2(n-1)}{n}\int f(n)dn = \frac{2(n-1)}{n}\int \frac{4}{n\left[2\sqrt{\frac{(n-1)+\sqrt{2n-3}}{2}}+2\sqrt{\frac{(n-1)-\sqrt{2n-3}}{2}}\right]}dn.$$

Thus for large n the area associated with this ratio is:

$$A_{DuS_n}^{E^{S_3}} = \frac{2m}{n}[\int \sqrt{2}n^{-\frac{3}{2}}dn] = \frac{\sqrt{2}(2n-2)}{n}(-2n^{-\frac{1}{2}}+c);. \ n \text{ large.}$$

Making the height aspect positive we have:

$$A_{DuS_n}^{E^{S_3}} = \frac{2\sqrt{2}(n-2)}{n}(2n^{-\frac{1}{2}}+c);$$

$$A_{DuS_4}^{E^{S_3}} = 0 \Rightarrow c = -1$$

Therefore, for large n, $A_{DuS_n}^{E^{S_3}} = \frac{2\sqrt{2}(n-2)}{n}(2n^{-\frac{1}{2}}-1).$

Theorem 2

The eigen-3-cover ratio, asymptote and area respectively for the following classes $\Im$ of graphs are:

Class	Eigen-3-cover	Asymptote	Area
K_n	$\frac{(n-2)(n-3)}{n(n-1)}$	1	$\frac{n^2}{2}-5n+6\ln n-6$
$K_{\frac{n}{2},\frac{n}{2}}$	$\frac{1}{n}$	0	$\frac{n}{2}(\ln n-\ln 2)$
C_n; $n=3k$	$\frac{n}{6n\sum_{j=0}^{n-1}\left\lvert\cos(\frac{2\pi j}{n})\right\rvert}\geq\frac{1}{6n}$		$\geq 2(\ln(6n)+c)$
P_n; $n=3k$	$\frac{1}{6\sum_{j=1}^{n}\left\lvert\frac{\cos\pi j}{n+1}\right\rvert}\geq\frac{1}{6n}$		$\geq\frac{2(n-1)}{n}(\ln(6n)+c)$
W_n $n=3k+1$	$\frac{\sqrt{n-1}(n+2)}{3\sqrt{3n}\left(\sqrt{n}+\sum_{k=1}^{n-2}\left\lvert\cos\frac{2\pi k}{n-1}\right\rvert\right)}\geq\frac{\sqrt{n-1}(n+2)}{3\sqrt{3n}(\sqrt{n}+(n-2))}$	0	$\geq\frac{4(n-1)}{3\sqrt{3}}\int\frac{\sqrt{n-1}(n+2)}{\sqrt{n}(\sqrt{n}+(n-2))}dn.$
$S_{r,1}$	$\frac{1}{2n\sqrt{n-1}}$	0	$\frac{(n-1)}{n}(2arc\sec\sqrt{n}-2arcs\sec\sqrt{2})$
$S_{r,2}$	$\frac{n-1}{n\left(n-3+\sqrt{2}\sqrt{n+1}\right)}$	0	$\frac{2(n-1)}{n}\int\frac{1}{n\left((n-3)+\sqrt{2}\sqrt{n+1}\right)}dn$
LP_n	$\frac{(n-3)(2n-8)}{n\left((n-3)+\sqrt{n^2-4n+8}\right)}$	1	$\frac{\left(n^2-3n+4\right)}{n}\int\frac{(n-3)(2n-8)}{n\left((n-3)+\sqrt{n^2-4n+8}\right)}dn$
DuS_n	$\frac{4}{n\left(2\sqrt{\frac{(n-1)+\sqrt{2n-3}}{2}}+2\sqrt{\frac{(n-1)-\sqrt{2n-3}}{2}}\right)}$	0	$\frac{2\sqrt{2}(n-2)}{n}(2n^{-\frac{1}{2}}-1)$ n large

Corollary 1

If $\operatorname{cov}\{E^{S_3}(G)\}=\frac{\lvert S_3\rvert E(H(S_3))}{nE(G)}=f(n)$ for each $G\in\Im$, then $as\operatorname{cov}\{E^{S_3}(\Im)\}\in[0,1]$ for all classes of graphs examined in the theorem above.

Conjecture 1

The complete graph possesses the largest eigen-3-cover area of all classes of graphs.

3. Conclusion

In this paper we combined the concepts of energy and 3-vertex covering S_3 of G (the 3-covering graph is the subgraph $H(S_3)$ of G induced by S_3) to determine the domination effect of the energy of the 3-covering graph on the main graph G. This involved the eigen-3-cover ratio $\text{cov}\{E^{S_3}(G)\} = \frac{|S_3|E(H(S_3))}{nE(G)}$.

Regarding a molecule in a graph-theoretical way, where the atoms are the vertices and the edges the bonds between the atoms, then the idea of *energizing* the whole molecule is relevant. Conserving energy will involve the *smallest* set S_3 of atoms which can be energized so that all atoms outside S_3, and connected to S_3 by a path of length at most two, also be energized. This is equivalent, graphically, to finding a minimum 3-vertex covering of a graph. When a large number of atoms are involved, the asymptotic behavior of this eigen-3-cover ratio becomes significant as illustrated by complete graphs having the strongest eigen-3-cover domination, implying that activation of its 3-vertex cover will result in *immediate* activation of all atoms when a large number of atoms are involved.

If this eigen-3-cover ratio is a function of n, the order of G belonging to a class of graphs, then we determined the horizontal asymptote of the ratio, and by attaching the average degree of G to the Riemann integral we found the eigen-3-cover area of classes of graphs. We found that the eigen-3-cover asymptote value (the domination effect) for classes of graphs investigated belongs to the interval [0,1] and claim that the eigen-3-cover area of the complete graph, is greatest of all eigen-3-cover areas of classes of graphs.

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