A CHARACTERIZATION OF GRAPHS WITH 3-PATH COVERINGS AND THE EVALUATION OF THE MINIMUM 3-COVERING ENERGY OF A STAR GRAPH WITH M RAYS OF LENGTH 2

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ABSTRACT: The smallest set Q of vertices of a graph G, such that every path on 3 vertices, has at least one vertex in Q, is a minimum 3-covering of G. By attaching loops of weight 1 to the vertices of G we can find the eigenvalues associated with G, and hence the minimum 3-covering energy of G. In this paper we characterize graphs with 3-coverings in terms of non-Q-covered edges, and we determine the minimum 3-covering energy of a star graph with m rays each of length 2.

1. INTRODUCTION

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 (see [1]). This resulted in the idea of the minimum 2-covering energy of a graph in [1] and the minimum 2-covering energy of star graphs with m rays of length 1 were found. This idea was generalized in [2] and the minimum 3-covering energy of complete graphs were determined. In this paper we determine the minimum 3-covering energy of star graphs with m rays of length 2.
2. RESULTS OF MINIMUM 3-COVERINGS OF GRAPHS

All graphs which we shall consider will be finite, simple, loopless and undirected. Let $G$ be such a graph of order $n$ with vertex set $\{v_1, v_2, ..., v_n\}$. A covering (2-covering) of a connected graph $G$ is a set $S$ of vertices of $G$ of such that every edge of $G$ has at least one vertex in $S$. Since an edge is a path length 1 on 2 vertices (a 2-path) we generalize this in [2], in terms of energy, by introducing a 3-covering (or 3-path covering) of a graph $G$ as being a set $Q$ of vertices of $G$ such that every path of $G$ of length 2 (or 3-path) has at least one vertex in $Q$. Any 3-covering set of $G$ of minimum cardinality is called a minimum 3-covering of $G$.

In the following theorems, $Q$ is a 3-covering of $G$, and if the vertex $x$ of $G$, which is not in $Q$, is a pendant vertex (vertex of degree 1) of $G$, that belongs to a path $P = u, v, w, ..., y, x$ of length $s$ from $Q$, where $u$ is the only vertex in $Q$, we say that $P$ is (with respect to $Q$) a $s$-pendant path of $G$ and the edge $yx$ is (with respect to $Q$) the $s$-pendant edge of $P$, and $y$ the middle vertex of a 3-pendant path of $G$. If a vertex $u$ is in $Q$, then the distance of $u$ from $Q$ is taken as 0.

THEOREM 1

No vertex of $G$ can be a distance of more than 2 from $Q$.

Proof

Suppose the vertex $u$ of $G$, that is not in $Q$, is a distance 3 from $Q$. Then there exists a path $uvwx$ of length 3 on 4 vertices such that vertices $u, v, w$ are not in $Q$, but $x$ is in $Q$. We therefore have a path $uvw$ of length 3 with $u, v$ and $w$ not in $Q$, which is a contradiction.
THEOREM 2

If u is a vertex that is a distance 2 from Q, then u is a pendant vertex.

Proof

Suppose u is on the path uvw of length 2, where vertices u,v are not in Q and w is, and no shorter path exist from u to Q. If u is not a pendant vertex, then it must be connected to a vertex y, where y is not in Q. But then it follows that we have a path vuy on 3 vertices u,v and w which does not have any vertex in Q, a contradiction.

THEOREM 3

If uv is an edge of G where u and v do not belong to Q, and neither are pendant vertices, then uv is the middle of a path xuvw P, of length 3 on 4 vertices, such that the ends x and w of the path are both in Q, and/or uv is the edge of the triangle xuv where x is in Q. These edges are disjoint or overlap in both vertices.

Proof

Let uv be an edge of G, neither of which belong to Q or are pendant vertices. Then there must exist vertices w and y such that wuvy is a path on 4 vertices in G. If w is not in Q, then we have a path wuv on 3 vertices with no vertex in Q, a contradiction. Similarly if y is not in Q we get a path uvw on 3 vertices with no vertex in Q. Thus w and y must belong to Q. If w and y are distinct, then we get the 4-path case, otherwise we get the triangle case. Suppose two such edges uv and u’v’ have exactly 1 vertex in common, say v’=u’. Then we have a path uv’u’ where neither u,v’ or u’ are in Q, a contradiction. Thus the edges can overlap in both vertices or they must be disjoint.
The path on 4 vertices in theorem 3 is defined as a 3-covering handle-path of G and the (non-covered) edge uv the middle edge of this handle-path. The triangle in theorem 3 is a 3-covering triangle of G, and the (non-covered) edge, uv, the triangle edge of G. The edge uv in each case is a non-covered edge (with respect to Q) of G.

**THEOREM 4**

If u is a vertex of G then either: (1) u is in Q, or (2) if u is not in Q then (2.1) u is a pendant vertex of a 2-pendant path or a 1-pendant path or (2.2) if u is not a pendant vertex, then (2.2.1) u is the middle vertex of a 2-pendant path uvw where v is in Q and w is a pendant vertex and/or (2.2.2) u belongs to the path xuv on 3 vertices where x and v are in Q (defined as a 3-covering V path of G) and/or (2.2.3) u belongs to the middle edge of a 3-covering handle-path of G and/or u belongs to the triangle edge of a 3-covering triangle of G.

**THEOREM 5**

If u is a vertex of G that is not in Q and is a pendant vertex, then u is a pendant vertex of either a 2-pendant path or a 1-pendant path of G. Thus no s-pendant paths exist of length greater than 2.

**THEOREM 6**

If uv is an edge of G, where neither u nor v belongs to Q (i.e. a non-covered edge of G, then either uv is a pendant edge of a 2-pendant path of G, or uv is the middle edge of a 3-covering handle-path of G, or uv is the triangle edge of a 3-covering triangle of G; the edges must be disjoint, or overlap in both vertices in the case of the non-pendant edges.

Thus there are only 3 types of non-Q-covered edges of a graph G with a 3-covering set Q- a 2-pendant edge, a middle edge of a handle path, and a triangle
edge – referred to as a 2-pendant, handle or triangle edge. These edges are disjoint except for the edges of the non-pendant kind which can overlap in both vertices. (If a 2-pendant edge uv has v in common with a handle or triangle edge vw, then we will have a path uvw with no vertex in Q.)

THEOREM 7

A graph G has a 3-covering Q if and only if the non-Q-covered edges of G are either 2-pendant, handle or triangle edges which are disjoint except for non-pendant edges which can overlap in both vertices.

3. MOLECULAR STRUCTURES AND ENERGY

The minimum 2-covering energy of molecular structures given in [1] involves the smallest set of atoms, such that every atom of the structure, is either in the set, or is connected (via bonds) directly to at least one vertex of the set. This is generalized to a minimum 3-covering energy of molecular structures, where the smallest set Q of atoms is considered, such that every atom, is either in the set, or connected by a path (of bonded atoms) of length at most 2, to at least one atom in the set.

If two atoms u and v are bonded by the edge uv, and neither u and v are in Q, then we say the pair of bonded atoms are non-Q-covered. In terms of energy of a structure, in order, say, to prevent destabilization, we may seek the smallest set Q of atoms to be energized, such that all non-Q-covered bonded atoms are either, as edges, 2-pendant, handle or triangle edges of the structure (where the edges are disjoint and the non-pendant edges may overlap in both vertices).
4. THE MINIMUM-3-COVERING ENERGY OF A GRAPH

A minimum 3-covering matrix of G with a minimum 3-covering set Q of vertices is a matrix:

$$A^3_Q(G) = (a_{i,j})$$

where

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G) \\ 1 & \text{if } i = j \text{ and } v_i \in Q \\ 0 & \text{otherwise} \end{cases}$$

The middle condition (*) is equivalent to loops of weight 1 being attached to the vertices of Q.

The characteristic polynomial of $A^3_Q(G)$ is then denoted by

$$f_n(G, \lambda) := \det(\lambda I - A^3_Q(G))$$

The minimum 3-covering energy (See [1]) is then defined as:

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

Where $\lambda_i$ (the minimum 3-covering eigenvalues) are the n real roots of the characteristic polynomial.

5. THE GENERALIZED STAR GRAPH

The star graph on m+1 vertices with m rays of length 1, can be generalized to a star graph with m rays of length n-1:
Take \( m \) copies of the path \( P_n \), join the paths at their end vertices, in the centre vertex \( u \); denote the graph on \( n + (n - 1)(m - 1) = mn - m + 1 \) vertices by \( S_{1,mP_n} \); \( m \geq 2, n \geq 2 \)

If \( n = 2 \) and \( m \geq 3 \), then we get the star graph \( K_{1,m} \) with \( m \) rays of length 1 which has a minimum 3-covering eigenvalues the same as the minimum 2-covering eigenvalues of \( K_{1,m} \); the two non-zero eigenvalues are given in [1]:

\[
\frac{1 + \sqrt{4m + 1}}{2}, \frac{1 - \sqrt{4m + 1}}{2}
\]

which implies that the minimum 3-covering energy of \( K_{1,m} \) is \( \sqrt{4m + 1} \).

6. THE STAR GRAPH WITH \( m \) RAYS OF LENGTH 2

If \( n = 3 \) and \( m \geq 2 \), then we label the vertices of the star graph \( S_{1,mP_3} \) with \( m \) rays of length 2 on \( 2m + 1 \) vertices as follows:

Centre vertex is \( u \), the set of \( m \) vertices a distance 1,2 respectively, from \( u \) is labeled:

\( V_1 = \{v_1^1, v_2^1, ..., v_m^1\}, \quad V_2 = \{v_1^2, v_2^2, ..., v_m^2\} \)

The possible 3-covering sets are \( \{u\}; V_1 \); \( V_2 \) but the minimum 3-covering is the former set.

For constructing the adjacency matrix \( A \) of the \( S_{1,mP_3} \) we label the center \( u \) as \( v_1 \), the vertices of \( V_1, V_2 \) as \( V_1 = \{v_2, v_3, ..., v_{m+1}\}, \quad V_2 = \{v_{m+2}, v_{m+3}, ..., v_{2m+1}\} \) respectively.
For \( n = 3, m = 2 \) we have the path \( P_2 \) with minimum 3-covering \( Q = \{ v_1 \} \) with
minimum 3-covering adjacency matrix:

\[
A_Q^3(S_{1,2P_3}) = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
\end{bmatrix}
\]

so that the characteristic equation is:

\[
\det(\lambda I - A_Q^3(S_{1,2P_3})) = \det\begin{bmatrix}
\lambda -1 & -1 & -1 & 0 & 0 \\
-1 & \lambda & 0 & -1 & 0 \\
0 & -1 & \lambda & 0 & -1 \\
0 & 0 & -1 & 0 & \lambda \\
\end{bmatrix}_{5 \times 5}
\]

and expanding using first row:

\[
\begin{array}{c}
| \lambda & 0 & -1 & 0 | + | -1 & 0 & -1 & 0 | + | -1 & \lambda & -1 & 0 | \\
0 & \lambda & 0 & -1 \\
-1 & 0 & \lambda & 0 \\
0 & -1 & 0 & \lambda \\
\end{array}
\]

Expanding the last 2 matrix determinants about the 3\(^{rd}\) and 4\(^{th}\) rows:

\[
\begin{array}{c}
| \lambda & 0 & -1 & 0 | + | -1 & 0 & -1 | + | -1 & \lambda & -1 | \\
0 & \lambda & 0 & -1 \\
-1 & 0 & \lambda & 0 \\
0 & -1 & 0 & \lambda \\
\end{array}
\]

Expanding the last two matrix determinants about the 1\(^{st}\) and 2\(^{nd}\) rows respectively:
The first determinant involves the circulant matrix with solutions:

\[ \exp \left( \frac{2\pi ij}{4} \right)^2 = \exp (\pi ij); \quad n = 0, 1, 2, 3. \]

The second determinant involves the circulant matrix with solutions:

\[ \exp \left( \frac{2\pi ij}{2} \right)^1 = \exp (\pi ij); \quad n = 0, 1. \]

Thus the characteristic equation is:

\[
(\lambda - 1)^3(\lambda + 1)^2 - 2\lambda(\lambda - 1)(\lambda + 1) = (\lambda - 1)(\lambda + 1)[(\lambda - 1)^2(\lambda + 1) - 2\lambda]
\]

\[
= (\lambda - 1)(\lambda + 1)[(\lambda^2 - 1)(\lambda - 1) - 2\lambda] = (\lambda - 1)(\lambda + 1)[(\lambda^3 - \lambda^2 - \lambda + 1) - 2\lambda]
\]

\[
= (\lambda - 1)(\lambda + 1)[(\lambda^3 - \lambda^2 - 3\lambda + 1)]
\]

We generalize this to finding the characteristic equation of a star graph on 2m +1 vertices with m rays of length 2:

For \( m \geq 2 \) and n=3 we have 2m +1 vertices:

\( u, v_1^1, v_2^1, \ldots, v_m^1, v_1^2, v_2^2, \ldots, v_m^2 \)
\[
A(S_{1,mP_3}) = \begin{bmatrix}
1 & 1 & 1 & : & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 \\
: & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & : & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
: & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
\end{bmatrix}_{(2m+1) \times (2m+1)}
\]
so that the characteristic equation:

\[
\det(\lambda I - A(S_{1,mP_3})) = \det \begin{bmatrix}
\lambda & -1 & -1 & : & -1 & 0 & 0 \\
-1 & \lambda & 0 & 0 & -1 & 0 & 0 \\
: & 0 & : & 0 & 0 & -1 & 0 \\
-1 & 0 & 0 & \lambda & 0 & 0 & -1 \\
0 & -1 & 0 & 0 & \lambda & 0 & 0 \\
: & 0 & -1 & 0 & 0 & \lambda & 0 \\
0 & 0 & : & -1 & 0 & 0 & \lambda \\
\end{bmatrix}_{(2m+1)(2m+1)}
\]

Expanding the determinant using the first row:

\[
= (\lambda - 1) \begin{bmatrix}
\lambda & 0 & 0 & -1 & 0 & 0 \\
0 & \lambda & 0 & 0 & -1 & 0 \\
0 & 0 & \lambda & 0 & 0 & -1 \\
-1 & 0 & 0 & \lambda & 0 & 0 \\
0 & -1 & 0 & 0 & \lambda & 0 \\
0 & 0 & -1 & 0 & 0 & \lambda \\
\end{bmatrix}_{(2m) \times (2m)}
\]
Followed by $m$ determinants:

$$\begin{vmatrix}
-1 & 0 & 0 & -1 & 0 & 0 \\
-1 & \lambda & 0 & 0 & -1 & 0 \\
-1 & 0 & \lambda & 0 & 0 & -1 \\
0 & 0 & 0 & \lambda & 0 & 0 \\
0 & -1 & 0 & 0 & \lambda & 0 \\
0 & 0 & -1 & 0 & 0 & \lambda \\
\end{vmatrix}_{2m \times 2m}$$

Expanding the last $m$ matrix determinants about the $(m+1)^{th}$, $(m+2)^{th}$, ..., $2m^{th}$ rows respectively:
\[
\begin{vmatrix}
\lambda & 0 & 0 & -1 & 0 & 0 \\
0 & \lambda & 0 & 0 & -1 & 0 \\
0 & 0 & \lambda & 0 & 0 & -1 \\
-1 & 0 & 0 & \lambda & 0 & 0 \\
0 & -1 & 0 & 0 & \lambda & 0 \\
0 & 0 & -1 & 0 & 0 & \lambda \\
\end{vmatrix}
\]

\[
(\lambda - 1) + \lambda
\]

\[
\begin{vmatrix}
-1 & \lambda & 0 & -1 & 0 \\
-1 & 0 & 0 & 0 & 0 \\
-\lambda & -1 & 0 & \lambda & 0 \\
0 & -1 & 0 & \lambda & 0 \\
0 & 0 & -1 & 0 & \lambda \\
\end{vmatrix}
\]

Last \( m \) determinants expanding using row 1, 2, \ldots, \( m \) respectively:

\[
\begin{vmatrix}
\lambda & 0 & 0 & -1 & 0 & 0 \\
0 & \lambda & 0 & 0 & -1 & 0 \\
0 & 0 & \lambda & 0 & 0 & -1 \\
-1 & 0 & 0 & \lambda & 0 & 0 \\
0 & -1 & 0 & 0 & \lambda & 0 \\
0 & 0 & -1 & 0 & 0 & \lambda \\
\end{vmatrix}_{2m \times 2m}
\]

\[
\begin{vmatrix}
\lambda & 0 & -1 & 0 \\
0 & \lambda & 0 & -1 \\
-1 & 0 & \lambda & 0 \\
0 & -1 & 0 & \lambda \\
\end{vmatrix}_{(2m-2) \times (2m-2)}
\]

The first matrix comes from the circulant matrix with eigenvalues

\[
[\exp\left(\frac{2\pi j i}{2m}\right)]^m; \quad j = 0, 1, 2, \ldots, 2m - 1, = (-1); \text{m times}; (1); \text{m times}
\]
The second matrix comes from the circulant matrix with eigenvalues:

\[
[\exp\left(\frac{2\pi ij}{2m-2}\right)]^{m-1}; \quad j = 0,1,2,\ldots,2m-2, = (-1); m - 1 \text{ times}; (1); m - 1 \text{ times}
\]

Which yields the characteristic equation:

\[
(\lambda - 1)^{m+1}(\lambda + 1)^m - m\lambda(\lambda - 1)^{m-1}(\lambda + 1)^{m-1}
\]

\[
= (\lambda - 1)^{m-1}(\lambda + 1)^{m-1}[(\lambda - 1)^2(\lambda + 1) - m\lambda]
\]

\[
= (\lambda - 1)^{m-1}(\lambda + 1)^{m-1}[(\lambda^2 - 1)(\lambda - 1) - m\lambda]
\]

\[
= (\lambda - 1)^{m-1}(\lambda + 1)^{m-1}[(\lambda^3 - \lambda^2 - (m+1)\lambda + 1]
\]

Thus the graph has minimum 3-covering eigenvalues 1 and -1, each of multiplicity m-1, and 3 eigenvalues from the roots of the cubic equation:

\[
\lambda^3 - \lambda^2 - (m+1)\lambda + 1 = 0
\]

**THEOREM 8**

The minimum 3-covering energy of the star graph with m rays of length 2 is:

\[
2m - 2 + |x_1| + |x_2| + |x_3| \quad \text{where } x_1, x_2, x_3 \text{ are the roots of the cubic equation:}
\]

\[
\lambda^3 - \lambda^2 - (m+1)\lambda + 1 = 0.
\]

The 3 roots can be found in (cubic functions in Wikipedia):

\[
x_1 = -\frac{b}{3}
\]

\[
-\frac{1}{3}\sqrt[3]{\frac{1}{2}\left[2b^3 - 9bc + 27d + \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3}\right]}
\]
\[-\frac{1}{3} \sqrt{\frac{1}{2} \left[ 2b^3 - 9bc + 27d - \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3} \right]} \]

\[ x_2 = -\frac{b}{3} \]
\[ + \frac{1 + \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ 2b^3 - 9bc + 27d + \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3} \right]} \]
\[ + \frac{1 - \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ 2b^3 - 9bc + 27d - \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3} \right]} \]

\[ x_3 = -\frac{b}{3} \]
\[ + \frac{1 - \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ 2b^3 - 9bc + 27d + \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3} \right]} \]
\[ + \frac{1 + \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ 2b^3 - 9bc + 27d - \sqrt{(2b^3 - 9bc + 27d)^2 - 4(b^2 - 3c)^3} \right]} \]

With \( a=1, b=-1, c=-(m+1) \) and \( d=1:\)

\[ x_1 = \frac{1}{3} \]
\[ - \frac{1}{3} \sqrt{\frac{1}{2} \left[ -2 - 9(m+1) + 27 + \sqrt{(-2 - 9(m+1) + 27)^2 - 4(3m+4)^3} \right]} \]
\[ - \frac{1}{3} \sqrt{\frac{1}{2} \left[ -2 - 9(m+1) + 27 - \sqrt{(-2 - 9(m+1) + 27)^2 - 4(3m+4)^3} \right]} \]

\[ x_2 = \frac{1}{3} \]
\[ + \frac{1 + \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ -2 - 9(m+1) + 27 + \sqrt{(-2 - 9(m+1) + 27)^2 - 4(3m+4)^3} \right]} \]
\[ + \frac{1 - \sqrt{3}}{6} \sqrt{\frac{1}{2} \left[ -2 - 9(m+1) + 27 - \sqrt{(-2 - 9(m+1) + 27)^2 - 4(3m+4)^3} \right]} \]
\[ x_3 = \frac{1}{3} \]

\[ + \frac{1-\sqrt{3}}{6} \left( \frac{1}{2} \left[ -2 - 9(m + 1) + 27 + \sqrt{(-2 - 9(m + 1) + 27)^2 - 4(3m + 4)^3} \right] \right) \]

\[ + \frac{1+\sqrt{3}}{6} \left( \frac{1}{2} \left[ -2 - 9(m + 1) + 27 - \sqrt{(-2 - 9(m + 1) + 27)^2 - 4(3m + 4)^3} \right] \right) \]

Simplifying:

\[ x_1 = \frac{1}{3} \]

\[ - \frac{1}{3} \left( \frac{1}{2} \left[ 16 - 9m + \sqrt{27m^3 + 189m^2 - 144m + 308} \right] \right) \]

\[ - \frac{1}{3} \left( \frac{1}{2} \left[ 16 - 9m - \sqrt{27m^3 + 189m^2 - 144m + 308} \right] \right) \]

\[ x_2 = \frac{1}{3} \]

\[ + \frac{1+\sqrt{3}}{6} \left( \frac{1}{2} \left[ 16 - 9m + \sqrt{27m^3 + 189m^2 - 144m + 308} \right] \right) \]

\[ + \frac{1-\sqrt{3}}{6} \left( \frac{1}{2} \left[ 16 - 9m - \sqrt{27m^3 + 189m^2 - 144m + 308} \right] \right) \]

\[ x_3 = \frac{1}{3} \]

\[ + \frac{1-\sqrt{3}}{6} \left( \frac{1}{2} \left[ 16 - 9m + \sqrt{27m^3 + 189m^2 - 144m + 308} \right] \right) \]
\[ + \frac{1 + \sqrt{3}}{6} \sqrt{\frac{1}{2} [16 - 9m - \sqrt{27m^3 + 189m^2 - 144m + 308}]} \]

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