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The energy of the Mycielskian of a regular graph

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Abstract

Let G be a finite connected simple graph and $\mu(G)$ be the Mycielskian of G. We show that for connected graphs G and H, $\mu(G)$ is isomorphic to $\mu(H)$ if and only if G is isomorphic to H. Furthermore, we determine the energy of the Mycielskian of a connected regular graph G in terms of the energy $\mathcal{E}(G)$ of G, where the energy of G is the sum of the absolute values of the eigenvalues of G. The energy of a graph has its origin in chemistry in that the energy of a conjugated hydrocarbon molecule computed using the Hückel theory in quantum chemistry coincides with the graph energy of the corresponding molecular graph. We show that if G is a regular graph of order n with $\mathcal{E}(G) > 3n$, then $\mu(G)$ is hyperenergetic.

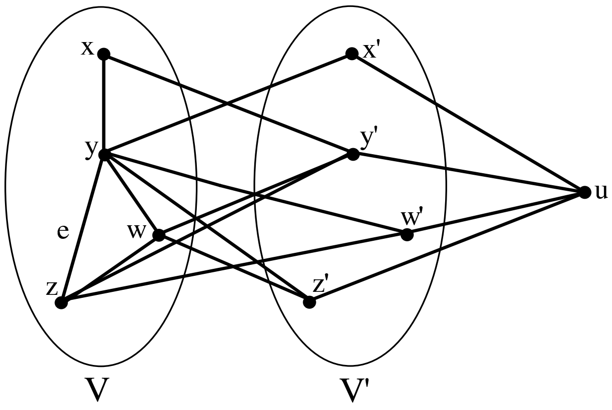

Figure 1: $\mu(K_{1,3}+e)$

1 Introduction

We consider only finite simple connected graphs. The construction of triangle-free k-chromatic graphs, where $k \geq 3$, was raised in the middle of the 20th century. In answer to this question, Mycielski [21] developed an interesting graph transformation known as the *Mycielskian* as follows: For a graph $G = (V, E)$, the Mycielskian of G is the graph $\mu(G)$ with vertex set consisting of the disjoint union $V \cup V' \cup \{u\}$, where $V' = \{x' : x \in V\}$, and edge set $E \cup \{x'y : xy \in E\} \cup \{x'u : x' \in V'\}$. We denote $V(\mu(G))$ by the triad (V, V', u). We call x' the twin of x in $\mu(G)$ and vice versa, and call u the root of $\mu(G)$. Figure 1 displays the Mycielskian of the graph $K_{1,3} + e$. It is well-known [21] that if G is triangle free, then so is $\mu(G)$, and that the chromatic number $\chi(\mu(G)) = \chi(G) + 1$. The generalized Mycielskian $\mu_m(G)$ of G is obtained by iterating the construction of V', m times. For the precise definition and a study of generalized Mycielskians, see [4, 20].

For a vertex v of G, $N_G(v)$ stands for the set of neighbors of v in G, the open neighborhood of v in G, and $N_G[v] = N(v) \cup \{v\}$ denotes the closed neighborhood of v in G. We recall that two simple graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if and only if there exists a bijection $\phi : V_1 \to V_2$ such that $uv \in E_1$ if and only if $\phi(u)\phi(v) \in E_2$. Moreover, graph isomorphism defines an equivalence relation on the class of all simple graphs.

Lemma 1.1. *Let $f : G \to H$ be a graph isomorphism of G onto H. Then $f(N_G(x)) = N_H(f(x))$. Furthermore, $G - x \cong H - f(x)$, and $G - N_G[x] \cong H - N_H[f(x)]$ under the restriction maps of f to the respective domains.*

Proof. The proof follows from the definition of graph isomorphism. □

2 Isomorphism of Mycielskians

For a vertex v of a graph G, let $d_G(v)$ denote the degree of v in G. We first prove that the Mycielskian of a graph determines the graph uniquely up to isomorphism.

Theorem 2.1. *For connected graphs G and H, $\mu(G) \cong \mu(H)$ if and only if $G \cong H$.*

Proof. If $G \cong H$, then trivially $\mu(G) \cong \mu(H)$. So assume that G and H are connected and that $\mu(G) \cong \mu(H)$. When $n = 2$ or 3, the result is trivial. So assume that $n \geq 4$. If G is of order n, then $\mu(G)$ and $\mu(H)$ are both of order $2n+1$, and so H is also of order n. Let $f : \mu(G) \to \mu(H)$ be the given isomorphism, where $V(\mu(G))$ and $V(\mu(H))$ are given by the triads (V_1, V_1', u_1) and (V_2, V_2', u_2) respectively.

We look at the possible images of the root u_1 of $\mu(G)$ under f. Both u_1 and u_2 are vertices of degree n. If $f(u_1) = u_2$, then, by Lemma 1.1, $G = \mu(G) - N[u_1] \cong \mu(H) - N[u_2] = H$.

Next, we claim that $f(u_1) \notin V_2$. Suppose $f(u_1) \in V_2$. Since $d_{\mu(H)}(f(u_1)) = d_{\mu(G)}(u_1) = n$, it follows from the definition of the Mycielskian, that in $\mu(H)$, $\frac{n}{2}$ neighbors of $f(u_1)$ belong to V_2 while another $\frac{n}{2}$ neighbors (the twins) belong to V_2'. (This forces n to be even). These n neighbors of $f(u_1)$ form an independent subset of $\mu(H)$. Then $H' = \mu(H) - N_{\mu(H)}[f(u_1)] \cong \mu(G) - N_{\mu(G)}[u_1] = G$. Now if $x \in V_2$ is adjacent to $f(u_1)$ in $\mu(H)$, then x is adjacent to $f(u_1)'$, the twin of $f(u_1)$ belonging to V_2' in $\mu(H)$. Further $d_{H'}(f(u_1)') = 1 = d_G(v)$, where $v \in V_1$ (the vertex set of G) corresponds to $f(u_1)'$ in $\mu(H)$. But then $d_{\mu(G)}(v)$=2, while $d_{\mu(H)}(f(u)') = \frac{n}{2} + 1 > 2$, as $n \geq 4$. Hence this case cannot arise.

Finally, suppose that $f(u_1) \in V_2'$. Set $f(u_1) = y'$. Then y, the twin of y' in $\mu(H)$, belongs to V_2. As $d_{\mu(G)}(u_1) = n$, $d_{\mu(H)}(y') = n$. The vertex y' has $n-1$ neighbors in V_2, say, $x_1, x_2, \ldots, x_{n-1}$. Then $N_H(y) = \{x_1, x_2, \ldots, x_{n-1}\}$, and hence y is also adjacent to $x_1', x_2', \ldots, x_{n-1}'$ in V_2'. Further, as $N_{\mu(G)}(u_1)$ is independent, $N_{\mu(H)}(y')$ is also independent. Therefore $H =$ star $K_{1,n-1}$ consisting of the edges $yx_1, yx_2, \ldots, yx_{n-1}$. Moreover, $G = \mu(G) - N[u_1] \cong \mu(H) - N[y']$= star $K_{1,n-1}$ consisting of the edges $yx_1', yx_2', \ldots, yx_{n-1}'$. Thus $G \cong K_{1,n-1} \cong H$. □

We note that the Mycielskian of a simple disconnected graph can be defined in an analogous way and that Theorem 2.1 has a natural extension to the case of disconnected graphs.

A connected graph G is fall colorable [6] using k colors if G has a proper k-vertex coloring $\{V_1, V_2, \ldots, V_k\}$ such that each vertex of G is a color dominating vertex, that is, if $v \in V_i$, then v has a neighbor in each V_j, $1 \leq j \leq k$, $i \neq j$.

For any graph G, define G^* as follows [3]: If G is of order n and has vertex set $V = \{v_1, v_2, \ldots, v_n\}$, G^* is the supergraph of G of order $2n$ got by choosing a new vertex v_i' for each vertex v_i of G and making v_i' adjacent in G^* to all the vertices in $V - \{v_i\}$. Let $V' = \{v_1', v_2', \ldots, v_n'\}$. We call V' the set of external vertices of G^* and V, the set of internal vertices.

Let $V_i = \{v_i, v_i'\}$, $1 \leq i \leq n$. Then $\{V_1, V_2, \ldots, V_n\}$ is a fall color partition of G^* so that G^* is fall colorable.

Theorem 2.2. *For (connected) graphs G and H, $G \cong H$ if and only if $G^* \cong H^*$.*

Proof. Suppose $G^* \cong H^*$. If G is of order n, G^* and H^* are both of order $2n$, and hence H is also of order n. Let A denote the set of external vertices of G^* and B, the set of external vertices of H^*. Then in G^*, each vertex of A has degree $n-1$ and each vertex of $V(G^*) \setminus A$ has degree at least n, while in H^*, each vertex of B has degree $n-1$ and each vertex of $V(H^*) \setminus B$ has degree at least n. Hence the isomorphism f maps A onto B. Further, by Lemma 1.1, $G^* - A \cong H^* - B$ and hence $G \cong H$. □

Theorem 2.3 ([4])**.** *For any (connected) graph G, $\mu(G)$ is non-fall colorable.*

Theorems 2.1 and 2.2 show that for any graph G both the derived graphs $\mu(G)$ and G^* determine G uniquely upto isomorphism. However, with regard to fall coloring, they behave in exactly the opposite ways in that for any graph G, $\mu(G)$ is non-fall colorable while G^* is fall colorable. Moreover, Theorems 2.1 and 2.2 show that the cardinalities of the set of all Mycielskians and the set of all graphs G^* are at least as large as the set of all connected graphs. Since the set of all connected graphs is countably infinite, we have the following result:

Corollary 2.4. *The cardinalities of the set of all (connected) fall colorable graphs and the set of all (connected) non-fall colorable graphs are both countably infinite.* □

We remark that Corollary 2.4 can be inferred by other means as well.

3 Energy of the Mycielskian of a regular graph

Let $G = (V, E)$ be a simple graph of order n with vertex set $V = \{v_1, \ldots, v_n\}$. The adjacency matrix of G is the $n \times n$ matrix $A = (a_{ij})$, where $a_{ij} = 1$ or 0 according as $v_i v_j \in E$ or not. A is a real symmetric matrix and hence its spectrum, namely, the set of its eigenvalues, is real. Let the spectrum of G (= the spectrum of A) be $\{\lambda_1 \geq \cdots \geq \lambda_n\}$. Then the energy $\mathcal{E}(G)$ of G is defined as $\sum_{i=1}^{n} |\lambda_i|$. The concept of graph energy arose in quantum chemistry where certain numerical quantities, such as the heat conduction of hydrocarbon molecules, are related to the total π-electron energy of conjugated hydrocarbon molecules. Indeed, the π-electron energy of any conjugated hydrocarbon molecule coincides with the energy of the corresponding molecular graph [5, 9, 10].

We now determine the energy of the Mycielskian of a k-regular graph G in terms of the energy of G. Some recent papers that deal with the energy of regular graphs are [1, 11, 14, 15, 19].

Theorem 3.1. *Let G be a k-regular graph on n vertices. Then the energy $\mathcal{E}(\mu(G))$ of $\mu(G)$ is given by:*

$$\mathcal{E}(\mu(G)) = \sqrt{5}\mathcal{E}(G) - (\sqrt{5}-1)k + 2|t_3|, \tag{3.1}$$

where $\mathcal{E}(G)$ is the energy of G and t_3 is the unique negative root of the cubic

$$t^3 - kt^2 - (n+k^2)t + kn. \tag{3.2}$$

Proof. Denote by A the adjacency matrix of G. As A is real symmetric, $A = PDP^T$, where D is the diagonal matrix $\mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, and P is an orthogonal matrix with orthonormal eigenvectors p_i's, that is, $Ap_i = \lambda_i p_i$ for each i. In particular, if e denotes the n-vector with all entries equal 1, then $p_1 = \frac{e}{\sqrt{n}}$ (G being regular). Hence $e^T p_i$=0 for $i = 2, \ldots, n$, and consequently $e^T P = [\sqrt{n}, 0, \ldots, 0]$.

Now, by the definition of $\mu(G)$, the adjacency matrix of $\mu(G)$ is the matrix of order $(2n+1)$ given by

$$\mu(A) = \begin{bmatrix} A & A & 0 \\ A & 0 & e \\ 0 & e^T & 0 \end{bmatrix}.$$

Since $A = PDP^T$, we have

$$\begin{aligned} \mu(A) &= \begin{bmatrix} PDP^T & PDP^T & 0 \\ PDP^T & 0 & e \\ 0 & e^T & 0 \end{bmatrix} \\ &= \begin{bmatrix} P & 0 & 0 \\ 0 & P & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} D & D & 0 \\ D & 0 & P^T e \\ 0 & e^T P & 0 \end{bmatrix} \begin{bmatrix} P^T & 0 & 0 \\ 0 & P^T & 0 \\ 0 & 0 & 1 \end{bmatrix}. \end{aligned}$$

Since P is an orthogonal matrix, the spectrum of $\mu(A)$ is the same as the spectrum of

$$B = \begin{bmatrix} D & D & 0 \\ D & 0 & [\sqrt{n}, 0, \ldots, 0]^T \\ 0 & [\sqrt{n}, 0, \ldots, 0] & 0 \end{bmatrix}.$$

The determinant of the characteristic matrix of B is given by

$$\left| \begin{array}{cccc:cccc:c} t-\lambda_1 & & & 0 & -\lambda_1 & & & 0 & 0 \\ & t-\lambda_2 & & & & -\lambda_2 & & & 0 \\ & & \ddots & & & & \ddots & & \vdots \\ 0 & & & t-\lambda_n & 0 & & & -\lambda_n & 0 \\ \hdashline -\lambda_1 & & & 0 & t & & & 0 & -\sqrt{n} \\ & -\lambda_2 & & & & t & & & 0 \\ & & \ddots & & & & \ddots & & \vdots \\ 0 & & & -\lambda_n & 0 & & & t & 0 \\ \hdashline 0 & 0 & \cdots & 0 & -\sqrt{n} & 0 & \cdots & 0 & t \end{array} \right|.$$

We now expand $\det(tI - B)$ along its first, $(n+1)^{\text{st}}$ and $(2n+1)^{\text{st}}$ columns by Laplace's method [7]. In this expansion, only the 3×3 minor which is common to the above three columns and the 1^{st}, $(n+1)^{\text{st}}$ and the $(2n+1)^{\text{st}}$ rows is nonzero. This minor is

$$M_1 = \begin{vmatrix} x - \lambda_1 & -\lambda_1 & 0 \\ -\lambda_1 & 0 & -\sqrt{n} \\ 0 & -\sqrt{n} & 0 \end{vmatrix}.$$

We now expand the complementary minor of M_1 along the 2^{nd} and $(n+2)^{\text{nd}}$ columns, and then the resulting complementary minor by the 3^{rd} and $(n+3)^{\text{rd}}$ columns and so on. These expansions give the spectrum of $\mu(A)$ to be the union of the spectra of the matrices

$$\begin{bmatrix} \lambda_1 & \lambda_1 & 0 \\ \lambda_1 & 0 & \sqrt{n} \\ 0 & \sqrt{n} & 0 \end{bmatrix}, \begin{bmatrix} \lambda_2 & \lambda_2 \\ \lambda_2 & 0 \end{bmatrix}, \ldots, \begin{bmatrix} \lambda_n & \lambda_n \\ \lambda_n & 0 \end{bmatrix}.$$

Another way to see this is to observe that B is orthogonally similar to the direct sum of the above n matrices. Thus the spectrum of $\mu(A)$ is

$$\{t_1, t_2, t_3, \lambda_2(\frac{1 \pm \sqrt{5}}{2}), \ldots, \lambda_n(\frac{1 \pm \sqrt{5}}{2})\}$$

where t_1, t_2, t_3 are the roots of the cubic polynomial $t^3 - kt^2 - (n + k^2)t + kn$, (note that since G is k-regular, $\lambda_1 = k$) which has two positive roots and one negative root, say, $t_1 > t_2 > 0 > t_3$.

Let $\mathcal{E}(G)$ denote the energy of G. Then $\mathcal{E}(G) = \sum_i |\lambda_i| = k + |\lambda_2| + \cdots + |\lambda_n|$. Hence the energy of the Mycielskian $\mu(G)$ of G, when G is k-regular, is

$$\begin{aligned} \mathcal{E}(\mu(G)) &= |t_1| + |t_2| + |t_3| + \left(\left| \frac{1+\sqrt{5}}{2} \right| + \left| \frac{1-\sqrt{5}}{2} \right| \right) \big(|\lambda_2| + \cdots + |\lambda_n|\big) \\ &= t_1 + t_2 + |t_3| + \sqrt{5}(|\lambda_2| + \cdots + |\lambda_n|) \\ &= k - t_3 + |t_3| + \sqrt{5}(\mathcal{E}(G) - k) \\ &= \sqrt{5}\mathcal{E}(G) - (\sqrt{5} - 1)k + 2|t_3|. \end{aligned}$$

□

An application of Theorem 3.1.

A simple graph G of order n is called hyperenergetic if $\mathcal{E}(G) > 2(n-1) = \mathcal{E}(K_n)$, where K_n is the complete graph on n vertices; otherwise it is called non-hyperenergetic. Hyperenergetic graphs are important because molecular graphs with maximum energy correspond to maximal stable π-electron systems [8, 13, 18, 23]. By definition, K_n is non-hyperenergetic. For K_n, $t_3 \in (-1, 0)$, and substitution of $k = n - 1$ in equation (3.1) shows that $\mu(K_n)$ is non-hyperenergetic.

It is known that the maximum energy that a graph G of order n can have is $\frac{n^{\frac{3}{2}}+n}{2}$ and that G has maximum energy if and only if it is a strongly regular graph with parameters $\left(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4}\right)$ [12, 17]. If $n > 25$, and G has maximum energy, then $\mathcal{E}(G) > 3n > 2(n-1)$ and hence G is hyperenergetic. Also from equation (3.1),

$$\begin{aligned}\mathcal{E}(\mu(G)) > 3n\sqrt{(}5) - (\sqrt{(}5) - 1)k + 2|t_3| &> 3n\sqrt{(}5) - (\sqrt{(}5) - 1)(n-1)\\ &> 2\sqrt{(}5)n + \sqrt{(}5) + 1 > 4n\\ &= 2[(2n+1) - 1].\end{aligned}$$

Hence the Mycielskians of maximal energy graphs of order $n > 25$ are all hyperenergetic. More generally, if G is a regular graph of order n and $\mathcal{E}(G) > 3n$, then $\mu(G)$ is hyperenergetic.

3.2 Examples.

We now present two examples. Consider two familiar regular graphs, namely, the Petersen graph P and a unitary Cayley graph.

1. The Petersen graph P.
For P, $n = 10$, $m = 15$ and $k = 3$. The spectrum of P is $\left(3^{(1)}, 1^{(5)}, -2^{(4)}\right)$, where $a^{(b)}$ means that a is repeated b times. Hence $\mathcal{E}(P) = 16$. Now for P, the polynomial (3.2) is $t^3 - 3t^2 - 19t + 30$, and its unique negative root t_3 is ≈ -3.8829. Thus from equation (3.1), $\mathcal{E}(\mu(P)) \approx 16\sqrt{5} - (\sqrt{5}-1)3 + 2(3.8829) = 39.8347 < 40 = 2(21-1)$, where 21 is the order of $\mu(P)$. Consequently, $\mu(P)$ is non-hyperenergetic.

2. The unitary Cayley graph $G = \mathrm{Cay}(\mathbb{Z}_{210}, U)$ [2, 13, 16, 22].
Here U is the group of multiplicative units of the additive group $(\mathbb{Z}_{210}, +)$. Then $\mathcal{E}(G) = 2^4\phi(210) = 768 > 3 \times 210 = 3n$, where ϕ is the Euler totient function. Since $n = 210$, $k = \phi(210) = 48$, the polynomial (3.2) becomes $t^3 - 48t^2 - 2514t + 10080$ for which the unique negative root t_3 is ≈ -34.18. Now from equation (3.1), $\mathcal{E}(\mu(G)) \approx 768\sqrt{5} - (\sqrt{5}-1)48 + 2(34.18) = 1726.352 > 2((2n+1)-1) = 840$. Thus $\mu(\mathrm{Cay}(\mathbb{Z}_{210}, U))$ is hyperenergetic, as expected.

We conclude with an open problem.

Open Problem:
Does there exist an infinite family of non-hyperenergetic graphs whose Mycielskians are hyperenergetic?

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