



Realizable degree sequences of inner dual graphs of benzenoid systems

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Abstract

An inner dual graph of a planar rigid benzenoid (hexagonal) system is a subgraph of the triangular lattice with the constraint that any two adjacent faces in the corresponding hexagonal system must be connected via an edge in the inner dual. The maximum degree of any vertex in an inner dual graph of a hexagonal system is 6. In contrast with the already existing algorithms in the literature that are used to check a given degree sequence to be graphically realizable, in this paper, we use a simple technique to check the realizable degree sequences of inner dual graphs of benzenoid systems that form a rich class of molecular graphs in theoretical chemistry. We restrict the maximum degree to 3 and identify, by providing necessary and sufficient conditions on the values of α, β and γ , all the degree sequences of the form $d = (3^\alpha, 2^\beta, 1^\gamma)$ that are graphically (inner dual of planar rigid hexagonal system) realizable. That is, we provide general constructions of the graphs (inner dual of planar rigid hexagonal system) realizing the degree sequences of the form $d = (3^\alpha, 2^\beta, 1^\gamma)$.

Keywords: Hexagonal system, Inner dual graph, Matchstick graph, Degree sequence, Graphical realization, Graphical sequence.

2010 MSC: 05C30, 05C92.

1. Introduction

Let $\pi = (d_1, d_2, \dots, d_n)$ be a non-increasing sequence of non-negative integers. Then π is said to be *graphical*, or a *graphical sequence*, if there exists a simple graph G with n vertices having π as its degree sequence. If such a graph exists, then we say that G is a *graphical realization* of π , or that G realizes the degree sequence π . And π is said to be *planar graphical*, if there exists a planar graph G realizing π . Of the

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Received : 3 November 2022; *Accepted:* 13 December 2022; *Published Online:* 22 December 2022.

many results [1, 7, 8] discussing the graphical degree sequences, the most well-known is a result by Erdős and Gallai [7], stating that π is graphical if and only if

$$\sum_{i=1}^n d_i \equiv 0 \pmod{2}$$

and

$$\sum_{i=1}^r d_i - \sum_{i=r+1}^n \min\{r, d_i\} \leq r(r-1), 1 \leq r \leq n-1$$

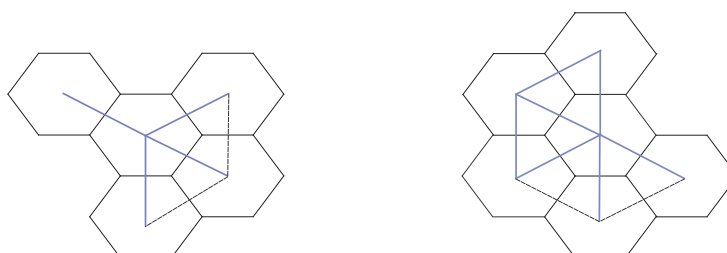
Using Euler’s formula (for polyhedra), a necessary (but not sufficient) condition for π to be *planar graphical* is that

$$\sum_{i=1}^n d_i \leq 6(n-2) \quad , n \geq 3$$

A hexagonal system H , is a connected planar matchstick graph with no cut vertices and whose each face is a hexagon. The faces (hexagons) of H are also called *cells*. An inner dual graph, G , of a hexagonal system H is obtained by placing a vertex in the centre of each regular hexagonal face of H and connecting, by single edges, the vertices of adjacent hexagons. Since, the inner dual graph of a hexagonal system is a subgraph of a triangular lattice, its maximum degree is equal to 6. A degree sequence d is said to be *inner dual hexagonal graphical*, if there exists a hexagonal system, whose corresponding inner dual graph realizes d . In this paper, we study various properties of such degree sequences. A pendent vertex is a vertex that is adjacent with exactly one vertex. Let K_n, C_n, P_n and S_n respectively denote the complete graph, cycle, path and star graph on n vertices.

In [2] spectral properties of He matrices of rigid hexagonal systems (*RHS*) have been studied, where the zero eigenvalues of the He matrices of *RHS* and also the relationship between the number of triangles in the inner dual of *RHS* with the eigenvalues of the He matrices of *RHS* have been investigated, whereby obtaining some upper bound on the He energy of *RHS*.

The motivation for studying hexagonal systems from applications in communication systems, in modern organic chemistry [6], and in mineralogy and crystallography [9] is significant. For references to He matrices, their spectra and He energy, the reader is referred to the literature cited in [2, 4, 5, 6]. The degree sequences of the inner duals of hexagonal systems have been studied for the first time in this paper. These inner dual graphs form a subclass of triangular lattice. But it is interesting to note that not all subgraphs of the triangular lattice are inner dual graphs of hexagonal systems. For example, the graphs shown in Figure 1 with bold edges are subgraphs of triangular lattice but cannot be inner dual graphs of any hexagonal system.



(a) The star graph S_5 is not an inner dual graph of a hexagonal system.

(b) The cycle C_4 with a chord and two pendent at a single vertex is also not inner dual of any hexagonal system.

Figure 1: Examples of graphs that are not inner duals of hexagonal systems.

A characterization of these degree sequences, graph theoretic or not, would be interesting from both

theoretical and application point of view. This is the motivation of our study in this paper. Thus, our main aim is to determine the structure of family of inner duals of hexagonal systems, and their degree sequences.

2. Preliminaries

Let G be the inner dual of a planar rigid hexagonal system, H . Let $|G| = n$ and $\|G\| = m$ be the number of vertices and edges of G , respectively. For $1 \leq i \leq 6$, let k_i be the number of vertices, of G , of degree i . Let f be the number of faces of G and define $f_i = f - 1$ to be the number of bounded faces of G . Then the degree sequence of G is given as

$$d(G) = (6^{k_6}, 5^{k_5}, 4^{k_4}, 3^{k_3}, 2^{k_2}, 1^{k_1})$$

where,

$$\sum_{i=1}^6 k_i = n \quad \text{and} \quad \sum_{i=1}^6 ik_i = 2m$$

In this paper, we restrict the maximum degree of G to 3. That is, we consider the degree sequence of G of the form

$$d(G) = (6^0, 5^0, 4^0, 3^{k_3}, 2^{k_2}, 1^{k_1}) \equiv (3^\alpha, 2^\beta, 1^\gamma)$$

In this case, we have

$$\alpha + \beta + \gamma = n \tag{2.1}$$

$$3\alpha + 2\beta + \gamma = 2m \tag{2.2}$$

Also, by Euler’s formula, we have

$$f_i = m - n + 1 \tag{2.3}$$

Throughout this paper, we write $d(G)$ as simply d . Also, if either α, β or γ is zero, say $\beta = 0$, we write $d = (3^\alpha, 2^0, 1^\gamma)$ as simply $d = (3^\alpha, 1^\gamma)$. Henceforth, for the sake of brevity, by the term *inner dual*, we mean *inner dual graph of a planar rigid hexagonal system*, and we may use the terms *hexagonal inner dual graphical* and *graphical* interchangeably, unless mentioned explicitly.

Due to the geometry of the triangular lattice, the inner dual could either be acyclic or cyclic. An acyclic inner dual is also called *catacondensed* (tree). It should be noted that acyclic inner dual has a special structure: every edge forms either an angle of 120° or 180° with an adjacent edge. Due to this structure, the maximum degree of an acyclic inner dual is 3. On the other hand, a cyclic inner dual is a subgraph of the triangular lattice. Thus, the girth of a cyclic inner dual is either equal to 3 or greater than 7 (see Theorem 3.1 for further discussion). In other words, the degree of each bounded face of a cyclic inner dual has either degree equal to 3 or greater than 7. See Figure 2 for examples of cyclic and acyclic inner dual graphs. This leads us to the following definition of a *hole* of a cyclic inner dual.

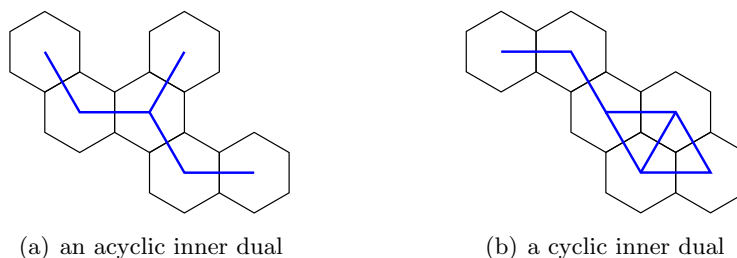


Figure 2: Examples of hexagonal systems along with their inner duals.

Definition 2.1. (*Hole*) A bounded face of a cyclic inner dual with degree greater than 7 is defined as a *hole* of the inner dual. We represent by R the set of all holes of a cyclic inner dual. If we let F_3 to be the set of faces with degree equal to 3, and define $f_3 = |F_3|$ and $\rho = |R|$, then we have

$$f_i = f_3 + \rho \tag{2.4}$$

Figure 3 shows an example of a cyclic inner dual and its holes. Here $R = \{R_1, R_2\}$, $deg(R_1) = 11$, $deg(R_2) = 14$, $\rho = 2$, $F_3 = \{F'_1, F'_2, F'_3, F'_4\}$, $f_3 = 4$ and $f_i = 6$

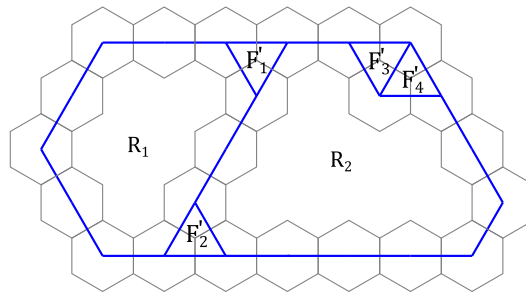


Figure 3: A cyclic inner dual and its *holes*

Definition 2.2. (*Gadgets*) There are three possible configurations (subgraphs) when only vertices of degree 3 are added (see Figure 4). We call these configurations *gadgets* and represent by D' , T' and C' the gadgets *diamond*, *triangle* and *claw*, respectively. We also define D , T , and C to be the number of gadgets D' , T' and C' in G , respectively.

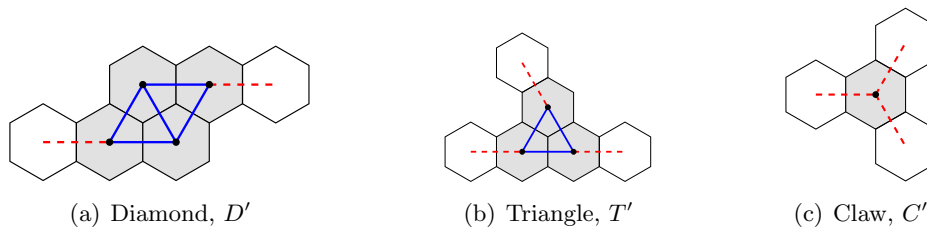


Figure 4: *Gadgets*: Three possible configurations when only vertices of degree 3 are added.

3. Degree Sequences of Inner Duals with Maximum Degree 3

In this section, we find necessary and sufficient condition(s) for a given degree sequence with maximum degree 3 to be inner dual hexagonal graphical. We also present inner dual constructions if the given degree sequence is inner dual graphical. In the context of each figure that shows a construction for a degree sequence, the edges shown in bold represent the base case, whereas the edges shown as dotted lines represent induction (induction on the number of copies of inductive subgraph). There are $\binom{3}{1} + \binom{3}{2} + \binom{3}{3} = 7$ cases to be discussed for different values of α, β and γ .

Three cases when $\alpha = 0$ are discussed in the following theorem.

Theorem 3.1.

- (a) $d = (3^0, 2^0, 1^\gamma)$ is graphical iff $\gamma = 2$.
- (b) $d = (3^0, 2^\beta, 1^\gamma)$ is graphical iff $\gamma = 2$.
- (c) $d = (3^0, 2^\beta, 1^0)$ is graphical iff $\beta \in \{3, 8, 9, 10, \dots\}$.

Proof.

(i) Setting $\alpha, \beta = 0$ in (2.1) and (2.2) and then simplifying gives $n = 2m$. Substituting this in (2.3) and using the fact that $f_i \geq 0$ yields $m = 1$ and $n = \gamma = 2$. This implies that $d = (3^0, 2^0, 1^\gamma)$ is graphical if and only if $\gamma = 2$. This degree sequence is that of an inner dual with just one edge.

(ii) Setting $\alpha = 0$ in (2.1) and (2.2) and solving for m and n gives $n = \beta + \gamma$ and $m = \beta + \frac{\gamma}{2}$. Substituting these values of n and m in (2.3) and using the fact that $f_i \geq 0$ yields $\gamma = 2$. This implies $d = (3^0, 2^\beta, 1^\gamma)$ is graphical if and only if $\gamma = 2$ and $\beta = n - 2$. This degree sequence is that of an inner dual that is a path (see Figure 5 (a)).

(iii) Setting $\alpha, \gamma = 0$ in (2.1) and (2.2) and simplifying gives $n = m$. Substituting this in (2.3) gives $f_i = 1$. Note that a graph with exactly one interior face $f_i = 1$ is a circular graph. We now find the values of β that makes $d = (3^0, 2^\beta, 1^0)$ a graphical degree sequence. By definition of hexagonal system, an empty cell (not represented by a vertex in the inner dual) cannot have all its adjacent cells included in the inner dual (see Figure 5 (b)). This implies that $n = \beta \neq 4, 5, 6, 7$. Clearly, $d = (3^0, 2^\beta, 1^0)$ is graphical if $\beta \in \{3, 8, 9, 10, \dots\} = \{3\} \cup \{8 + 2k : k \in \mathbb{N} \cup \{0\}\} \cup \{9 + 2k : k \in \mathbb{N} \cup \{0\}\}$ (see Figure 5 (c), (d) and (e)). □

After proving the following lemmas, we will then discuss the case $\beta = 0, \alpha, \gamma \neq 0$ in Theorem 3.4.

Lemma 3.2. *Let $\alpha \neq 0$. Then $d = (3^\alpha, 2^\beta, 1^\gamma)$ has an acyclic graphical realization iff $\alpha = i, \beta = n - 2i - 2$ and $\gamma = i + 2$ for $i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1$.*

Proof. Clearly if $n < 4$ then $\alpha = 0$, so let $n \geq 4$ and $\alpha = i$. Multiplying equation (2.1) by 2 and subtracting it from (2.2) and then simplifying for γ gives $\gamma = \alpha - 2(m - n)$. In this equation, substituting $m = n - 1$ (a necessary and sufficient condition for a tree) gives $\gamma = \alpha + 2 = i + 2$ and then from (2.1) we have $\beta = n - 2i - 2$. Note that since $\gamma = i + 2$ we have $i \leq \lfloor \frac{n}{2} \rfloor - 1$. The construction of the inner dual realizing the degree sequence $d = (3^i, 2^{n-2i-2}, 1^{i+2})$ for $i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1$ is shown in Figure 6. □

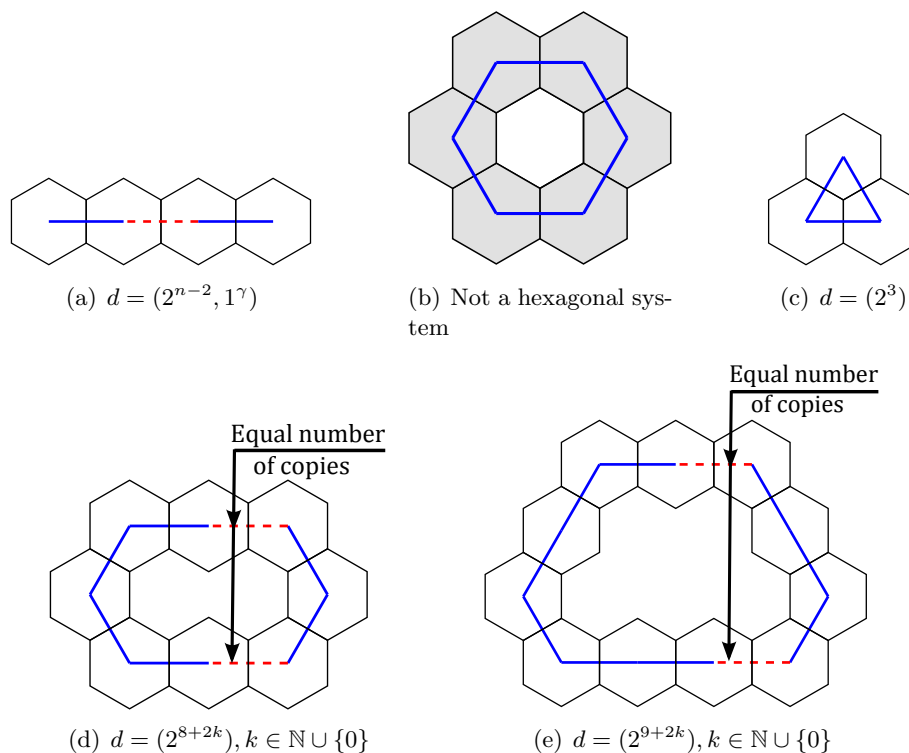


Figure 5: Theorem 1 figures.

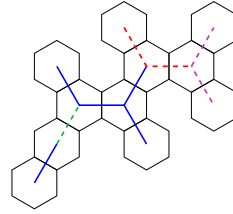


Figure 6: An inner dual tree for $d = (3^i, 2^{n-2i-2}, 1^{i+2})$.

When $\beta = 0$ then degree of any vertex is either 3 or 1, thus n is even. We have the following lemma.

Lemma 3.3. *The degree sequences with $\beta = 0$ are characterized as follows.*

- (a) *Let $n \equiv 0 \pmod{4}$. Then $d = (3^{n-2}, 1^2)$ is graphical iff $n \geq 20$.*
- (b) *Let $n \equiv 2 \pmod{4}$. Then $d = (3^{n-1}, 1^1)$ is graphical iff $n \geq 30$.*
- (c) *Let $n \equiv 0 \pmod{4}$. Then $d = (3^{n-1}, 1^1)$ is graphical iff $n \geq 32$.*

Proof. We leave the proofs of statements (b) and (c) as these statements could be proved using the similar technique used below to prove statement (a) of the lemma.

Note that if $d = (3^{n-2}, 1^2)$ is graphical for $n = 4, 8$ or 12 , then it must also be graphical for $n = 16$ (by concatenating a diamond to a pendant edge). So, we now show that $d = (3^{n-2}, 1^2)$ is not graphical for $n = 16$.

From equations (2.1), (2.2) and (2.3), we have $f_i = 1 - n + m = 1 - (\alpha + \beta + \gamma) + \frac{3\alpha + 2\beta + \gamma}{2}$, that is,

$$f_i = \frac{\alpha}{2} - \frac{\gamma}{2} + 1 \tag{3.1}$$

It is worth mentioning that f_i is independent of the value of β . The gadgets (shown as bold edges in Figure 4) contribute to the vertices of degree 3. Since a diamond (D') and a triangle (T') contribute to 4 and 3 vertices, respectively, it follows that $4D + 3T \leq \alpha$. Also, since D' and T' contribute to 2 and 1 interior faces, respectively, we have $f_3 = 2D + T$. So, from the last two equations and equation (2.4), we have

$$\begin{aligned} 4D + 3T \leq \alpha &\Rightarrow 2(2D + T) + T \leq \alpha \Rightarrow T \leq \alpha - 2f_3 \Rightarrow T \leq \alpha - 2(f_i - \rho) \\ &\Rightarrow T \leq 2\rho \end{aligned} \tag{3.2}$$

For $n = 16$ ($\alpha = 14, \gamma = 2$), $f_i = 7$ from equation (3.1). Now, note that $\rho \leq 1$, for if $\rho \geq 2$ then apart from the two pendant vertices, we have 14 remaining vertices, all of which cannot be of degree 3. So, subject to the constraints $f_i = 7, \rho = 0$ or 1 , the set of tuples (D, T) that satisfies the equation $f_i - \rho = f_3 = 2D + T$ is $\{(3, 0), (2, 2)\}$. All non-isomorphic simple planar graphs with $n = 16, \alpha = 14$ and $\gamma = 2$ for $\{(D, T)\} = \{(3, 0), (2, 2)\}$ are shown in the Figure 7, none of which is embeddable in the triangular lattice. Hence, we deduce that for $n \equiv 0 \pmod{4}$, if $d = (3^{n-2}, 1^2)$ is graphical then $n > 16$.

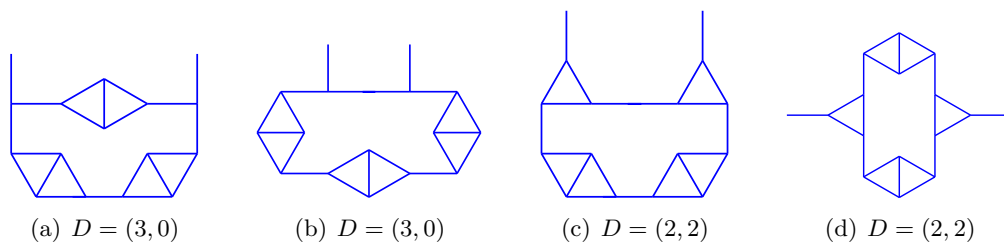


Figure 7: Non-isomorphic graphs for $n = 16$ ($\alpha = 14, \gamma = 2$)

The inner dual for $d = (3^{n-2}, 1^2)$ with $n = 20$ is shown in Figure 8 (a), whereas Figure 8 (b) shows that

$d = (3^{n-2}, 1^2)$ is graphical for all $n \geq 20$ with $n \equiv 0 \pmod{4}$. The inner duals for the degree sequences of statements (b) and (c) of the lemma are shown in Figure 8 (c) and (d), respectively.

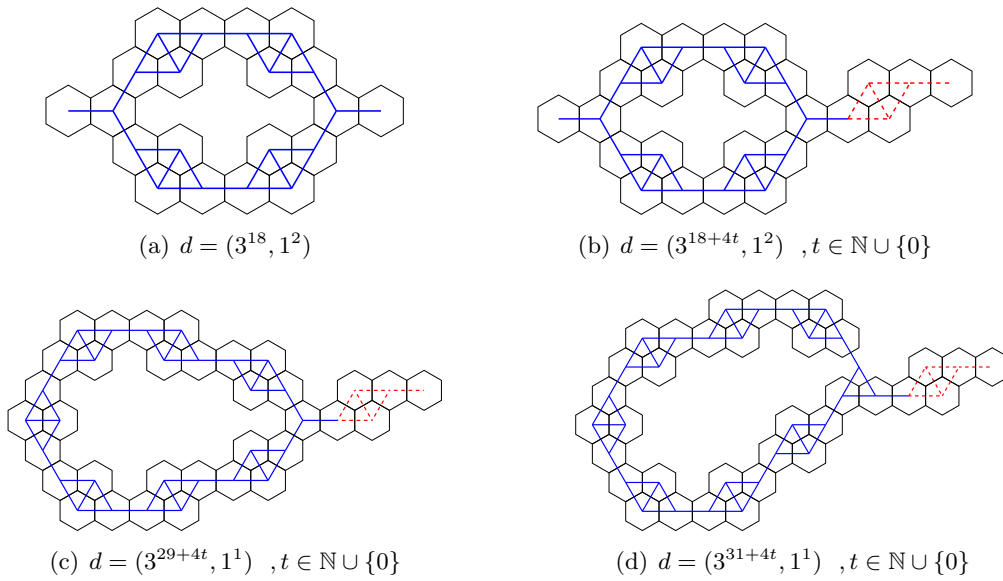


Figure 8: Graphs with degree sequences of special forms

□

Theorem 3.4. $d = (3^\alpha, 2^0, 1^\gamma)$ is graphical iff one of the following two conditions is satisfied (depending upon the cyclic nature of the inner dual graph):

- (a) *Acyclic (inner dual is a tree) :*
 $\alpha = i, \gamma = i + 2 \quad ; \quad i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor - 1, \quad n \geq 4$
- (b) *Cyclic :*
 n is even ($n = 2k$) : $\alpha = k + i, \quad \gamma = k - i,$
 $\begin{cases} i = 0, 1, \dots, k - 2 & ; \quad n \equiv 2 \pmod{4}, \quad n \geq 6 \\ i = 0, 1, \dots, k - 3 & ; \quad n \equiv 0 \pmod{4}, \quad n \geq 6 \\ i = k - 2 & ; \quad n \equiv 0 \pmod{4}, \quad n \geq 20 \\ i = k - 1 & ; \quad n \equiv 0 \pmod{4}, \quad n \geq 32 \\ i = k - 1 & ; \quad n \equiv 2 \pmod{4}, \quad n \geq 30 \end{cases}$

Proof. The degree sequence $d = (3^\alpha, 2^0, 1^\gamma)$ may either have an acyclic or a cyclic inner dual graphical realization. If $d = (3^\alpha, 2^0, 1^\gamma)$ has an acyclic graphical realization then the condition (a) follows from Lemma 3.2.

We now consider the case when $d = (3^\alpha, 2^0, 1^\gamma)$ has cyclic inner dual realization. Since only three configurations are possible (see the definition of *gadgets*) when a vertex of 3 is added, it is clear that $n \geq 6$. Also since $\beta = 0$ and $\alpha, \gamma \neq 0$, from equation (2.2) it follows that the number of vertices of odd degree(s) must be even, that is $n = 2k$. By setting $f_i \geq 1$ in (2.3), we get $m \geq n$. So, from this inequality and equations (2.1) and (2.2), we have

$$m \geq n \Rightarrow \frac{3\alpha + 2\beta + \gamma}{2} \geq \alpha + \beta + \gamma \Rightarrow \alpha \geq \gamma \tag{3.3}$$

Note that equation (3.3) is independent of the value of β . Since $n = 2k$, it follows from (3.3) that $\alpha \geq k$. We claim that for $n \geq 6$, $d = (3^\alpha, 2^0, 1^\gamma)$ has a cyclic graphical inner dual realization iff $\alpha = k + i$,

$\gamma = k - i$ ($\because \alpha + \gamma = n \Rightarrow \gamma = n - \alpha = 2k - (k + i) = k - i$) where $i = 0, 1, \dots, k - 2$ if $n \equiv 2 \pmod{4}$ and $i = 0, 1, \dots, k - 3$ if $n \equiv 0 \pmod{4}$.

It has already been noted that (3.1) is independent of the value of β . So, setting $\alpha = k + i$ and $\gamma = k - i$ in (3.1) gives $f_i = 1 + i$. We now present general cyclic construction realizing the degree sequence $d = (3^\alpha, 2^0, 1^\gamma)$ for $n \geq 6$, satisfying the conditions claimed in the preceding paragraph.

We can see the construction of G (see Figure 9) as union of a cyclic graph \tilde{C} and a tree \tilde{T} . Let $n, n_{\tilde{C}}$ and $n_{\tilde{T}}$ be the cardinality of the vertex sets of G, \tilde{C} and \tilde{T} respectively (with slight abuse of notations). Also, let $d = (3^\alpha, 1^\gamma), d_{\tilde{C}} = (3^{\alpha_{\tilde{C}}}, 1^{\gamma_{\tilde{C}}})$ and $d_{\tilde{T}} = (3^{\alpha_{\tilde{T}}}, 1^{\gamma_{\tilde{T}}})$ be the degree sequences of G, \tilde{C} and \tilde{T} respectively. We now present two cases based on the parity of f_i .

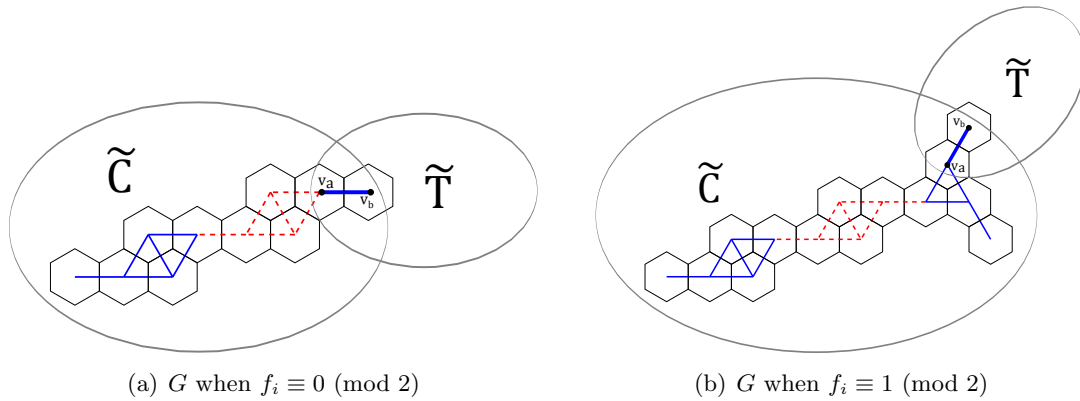


Figure 9: Construction of G as a union of \tilde{C} and \tilde{T}

Case 1: $f_i \equiv 0 \pmod{2}$ (see Figure 9 (a))

By construction of \tilde{C} , $\alpha_{\tilde{C}} = 2f_i$ and $\gamma_{\tilde{C}} = 1$. So,

$$\begin{aligned} \alpha &= \alpha_{\tilde{C}} + \alpha_{\tilde{T}} \Rightarrow \alpha_{\tilde{T}} = \alpha - \alpha_{\tilde{C}} = (k + i) - 2f_i = (k + i) - 2(1 + i) = k - 2 - i, \text{ and} \\ \gamma &= \gamma_{\tilde{C}} + \gamma_{\tilde{T}} - 1 \Rightarrow \gamma_{\tilde{T}} = \gamma - \gamma_{\tilde{C}} + 1 = (k - i) - 1 + 1 = k - i \\ &\Rightarrow \gamma_{\tilde{T}} = \alpha_{\tilde{C}} + 2 \end{aligned}$$

From Lemma 3.2, we know that $d_{\tilde{T}} = (3^{\alpha_{\tilde{T}}}, 1^{\gamma_{\tilde{T}}}) = (3^{\alpha_{\tilde{T}}}, 1^{\alpha_{\tilde{T}}+2})$ is graphical (ignoring trivial cases of i).

Case 2: $f_i \equiv 1 \pmod{2}$ (see Figure 9 (b))

By construction of \tilde{C} , $\alpha_{\tilde{C}} = 2(f_i - 1) + 3 = 2f_i + 1$ and $\gamma_{\tilde{C}} = 2$. So,

$$\begin{aligned} \alpha &= \alpha_{\tilde{C}} + \alpha_{\tilde{T}} \Rightarrow \alpha_{\tilde{T}} = \alpha - \alpha_{\tilde{C}} = (k + i) - 2f_i - 1 = (k + i) - 2(1 + i) - 1 = k - 3 - i, \text{ and} \\ \gamma &= \gamma_{\tilde{C}} + \gamma_{\tilde{T}} - 1 \Rightarrow \gamma_{\tilde{T}} = \gamma - \gamma_{\tilde{C}} + 1 = (k - i) - 2 + 1 = k - 1 - i \\ &\Rightarrow \gamma_{\tilde{T}} = \alpha_{\tilde{T}} + 2 \end{aligned}$$

From Lemma 3.2, we know that $d_{\tilde{T}} = (3^{\alpha_{\tilde{T}}}, 1^{\gamma_{\tilde{T}}}) = (3^{\alpha_{\tilde{T}}}, 1^{\alpha_{\tilde{T}}+2})$ is graphical (ignoring trivial cases of i).

The conditions $n \geq 20$ for $i = k - 2$ and $n \equiv 0 \pmod{4}$, $n \geq 32$ for $i = k - 1$ and $n \equiv 0 \pmod{4}$, and $n \geq 30$ for $i = k - 1$ and $n \equiv 2 \pmod{4}$ follow from Lemma 3.3. \square

Now, we discuss the case $\gamma = 0$ and $\alpha, \beta \neq 0$ in Theorem 3.5 and Corollary 3.6.

Theorem 3.5. For $n \geq 4$ ($n \neq 5$), let $n = 2k$ or $2k + 1$ and $\gamma = 0$, then

$$\alpha = 2i, \quad i = 1, 2, \dots, k - 2 \text{ or } k - 1 \text{ depending upon whether } n \equiv 2 \pmod{4}$$

$$\text{or } n \equiv 0 \pmod{4} \text{ and } n \equiv 1 \pmod{2}$$

$$\text{then } \beta = 2k - 2i \text{ for } n \equiv 0 \pmod{2}$$

$$\text{and } \beta = 2k - 2i + 1 \text{ for } n \equiv 1 \pmod{2}$$

Proof. Let v_1, v_2, \dots, v_n be the vertices of inner dual of hexagonal system. For $\gamma = 0$, α must be even that is $\alpha \equiv 0 \pmod{2}$ (by handshaking lemma). Note that graph cannot end on a pendant vertex as $\gamma = 0$. Thus the end points of the inner dual graph are shown in the following figure 10.

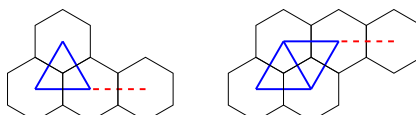


Figure 10: End points of graph where $\gamma = 0$

For $n = 4$ we have only a diamond shape inner dual graph.

Now we consider the cases when $n \geq 6$ for different values of i :

With $i = 1$ and $\alpha = 2$, the graph can be constructed as shown in Figure 11.

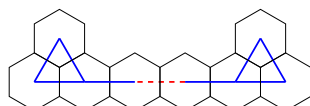


Figure 11: An inner dual for $\gamma = 0$ and $\alpha = 2$

For $i \geq 2$ any three vertices with degree 2 can be joined in such a way that they will result in two vertices of degree 3 and one vertex of degree 2 to convert a graph from $\alpha = 2i$ to $\alpha = 2(i + 1)$ (See Figure 12).

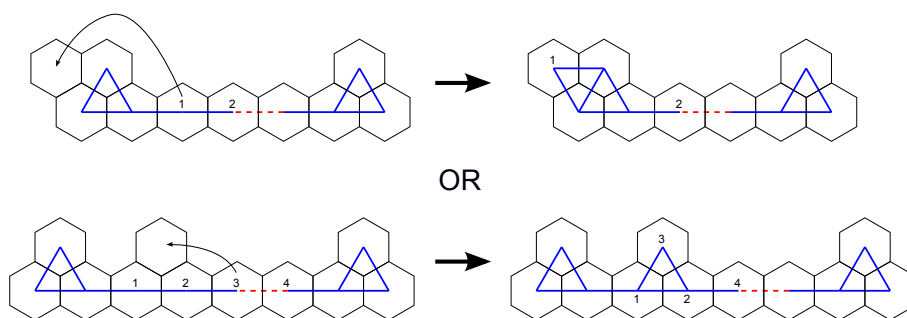


Figure 12: An inner dual for transition from i to $i + 1$

When there are three or more triangles in an inner dual they can be changed into diamonds to convert a graph from $\alpha = 2i$ to $\alpha = 2(i + 1)$ as shown in Figure 13.

For $n \equiv 0 \pmod{4}$, maximum value of $i = k - 1$ can be achieved with the construction shown in Figure 14.

For $n \equiv 1 \pmod{4}$ maximum value of $i = k - 1$ can be achieved with the construction shown in Figure 15, whereas, for $n \equiv 3 \pmod{4}$ maximum value of $i = k - 1$ can be achieved with the construction shown in Figure 16.

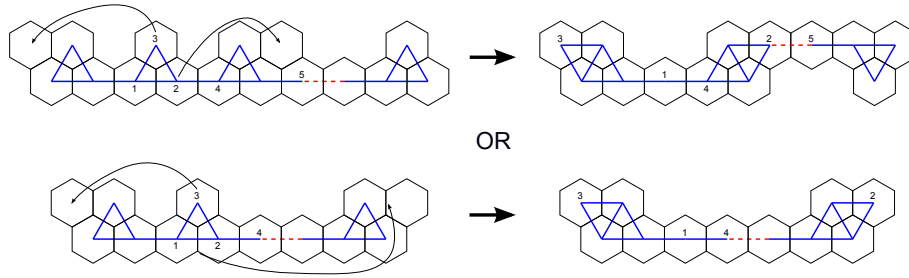


Figure 13: An inner dual showing triangle to diamond construction to go from i to $i + 1$

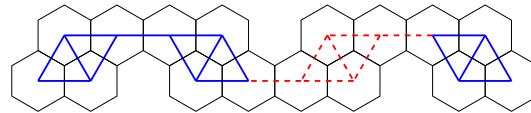


Figure 14: An inner dual showing maximum value of α when $n \equiv 0 \pmod{4}$

For $n \equiv 2 \pmod{4}$, graph at $i = k - 1$ does not exist with just cycles of 3 as when $i = k - 1$, $\beta = 2$ which is possible only with composition of diamonds, but 4 does not divide n . Thus maximum $i = k - 2$ (see Figure 17)

□

Note that the only cases left in Theorem 3.5 are when $\alpha = n - 2$, $\beta = 2$ for $n \equiv 2 \pmod{4}$ and $\alpha = n - 1$, $\beta = 1$ for $n \equiv 1 \pmod{2}$. These cases are discussed in the following corollary.

Corollary 3.6.

1. Let $n \equiv 2 \pmod{4}$. Then $d = (3^{n-2}, 2^2)$ is graphical if and only if $n \geq 18$.
2. Let $n \equiv 1 \pmod{2}$. Then $d = (3^{n-1}, 2^1)$ is graphical if and only if $n \geq 29$.

Proof. Note that $\alpha = n - 2$, $\beta = 2$ is not possible with only cycles of 3 as $\beta = 2$ implies that there are only diamonds in the graph. That would mean $n \equiv 0 \pmod{4}$, a contradiction! Thus there needs to be at least one face $\in R$ for $\alpha = n - 2$, $\beta = 2$ where R is the family of holes.

It follows from lemma 3.3 that the least value of n for which $\alpha = n - 2$, $\beta = 2$ is 18 and similarly the least value of n for which $\alpha = n - 1$, $\beta = 1$ is 29.

Induction on diamonds imply that hexagonal inner dual graph exists for all $n \geq 18$ ($n \equiv 2 \pmod{4}$) and $n \geq 29$ ($n \equiv 1 \pmod{2}$) as shown in Figure 18.

□

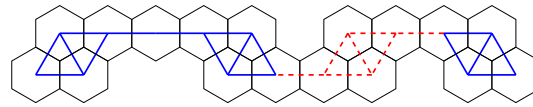


Figure 15: An inner dual showing maximum value of α when $n \equiv 1 \pmod{4}$

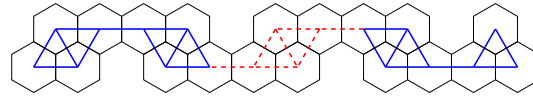


Figure 16: An inner dual showing maximum value of α when $n \equiv 3 \pmod{4}$

In the following results, we discuss the case when $\alpha, \beta, \gamma \neq 0$.

Theorem 3.7. *When $\alpha, \beta, \gamma \neq 0$ then the multiplicities of the degrees of inner dual of hexagonal system is the rearrangement of the elements of integer partition of n with the following conditions:*

1. $\alpha \geq \gamma$ for all $n \geq 4$.
2. α and γ are of same parity.
3. $1 \leq \alpha \leq n - 2$ for $n \equiv 1 \pmod{4}$
 $1 \leq \alpha \leq n - 3$ otherwise,

where α, β and γ are the multiplicities of the vertices of degree 3, 2 and 1 respectively.

Proof. In standard representation, a partition of n is given by a sequence $x_1 \dots x_m$, where $x_1 \geq x_2 \geq \dots \geq x_m$ and $x_1 + x_2 + \dots + x_m = n$ [3].

The value of α cannot be less than γ as for the minimum value of n with at least one triangle we have $\alpha = \gamma$ and with two triangles $\alpha > \gamma$. Thus $\alpha \geq \gamma$.

To show that for α even γ is also even and for α odd γ is also odd it is enough to recall that number of odd degree vertices in a graph should be even by well known handshaking lemma.

The upper bound for α when $n \equiv 0 \pmod{2}$ is $n - 3$ as least value of β, γ can be 1(odd) which implies that α is even. This violates handshaking lemma thus both β and γ cannot be odd at the same time. Therefore, least value of $\beta + \gamma = 3$ and maximum $\alpha = n - 3$ when $n \equiv 0 \pmod{2}$.

We can remove one pendent vertex (see fig. 19) to get $d = (3^{n-2}, 2^1, 1^1)$ from the construction of inner dual given in theorem 3.5 for $d = (3^{n-2}, 1^2)$, $n \equiv 2 \pmod{4}$, thus upper bound for α when $n \equiv 1 \pmod{4}$ is $n - 2$.

Likewise, we can add a vertex adjacent to a pendent (see fig. 20) to get $d = (3^{n-3}, 2^1, 1^2)$, thus upper bound for α when $n \equiv 3 \pmod{4}$ is $n - 3$, with just cycles of three.

It can be proved through slight adjustments to the construction given in theorem 3 that all degree sequences subject to the above constraints are hexagonal inner dual graphical. For example to achieve $d = (3^4, 2^4, 1^2)$, we need to add 2 vertices to $d = (3^2, 2^6)$. (Figure. 21)

□

Corollary 3.8. *In theorem 3.7, for $n \equiv 3 \pmod{4}$, $\alpha = n - 2, \beta = 1, \gamma = 1$ is hexagonal inner dual graph if and only if $n \geq 19$.*

Proof. Removing one pendent from construction for $\alpha = n - 2, \gamma = 2$ for $n = 20$ in lemma 3.3 gives desired degree sequence at $n = 19$.

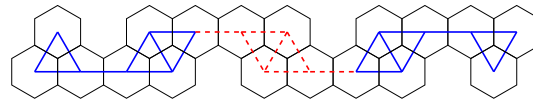


Figure 17: An inner dual showing maximum value of α when $n \equiv 2 \pmod{4}$

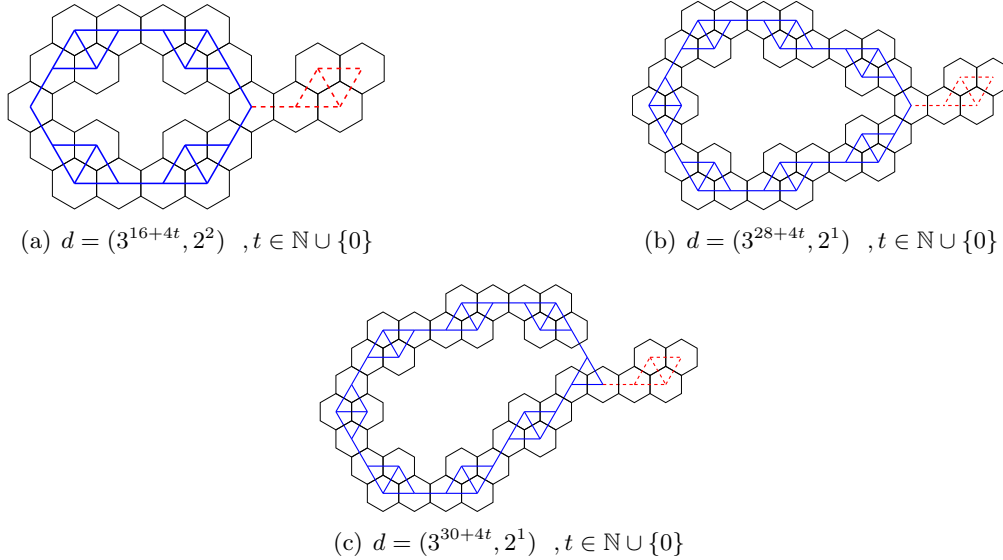


Figure 18: Graphs with degree sequences of special forms

Similar argument as was given in lemma 3.3 shows that $\alpha = n - 2, \beta = 1, \gamma = 1$ does not exist for $n < 19, n \equiv 3 \pmod{4}$.

All $n > 19, n \equiv 3 \pmod{4}$ with $\alpha = n - 2, \beta = 1, \gamma = 1$ are hexagonal inner dual graphical as can be shown by addition of diamonds to the pendent vertex. (figure 22)

□

Now, we discuss the final case when $\beta, \gamma = 0$ and $\alpha \neq 0$.

Theorem 3.9. *The degree sequence $d = (3^\alpha, 2^0, 1^0)$ is graphical iff $\alpha \in \mathbb{N} \setminus A$, where $A = \{x \in \mathbb{N} : x \text{ is odd or } x = 2, 4, 6, \dots, 22, 26, 28, 30, 38\}$.*

Proof. (if)

From equation (2.2), we know that the number of vertices of odd degree(s) must be even, so clearly $\alpha \equiv 1 \pmod{2}$. The smallest 3-regular planar matchstick graph has 8 vertices, so $\alpha \neq 2, 4, 6$. And for $n = 8$, the only 3-regular matchstick graph is as shown in Figure 23 (a), which is not embeddable in the triangular lattice since it contains a cycle of length 6.

We now show that $\alpha \neq 10, 12, 14, 16, 26$. Using similar arguments, it could be shown that $\alpha \neq 18, 20, 22, 28, 30, 38$. By setting $n = \alpha$ and $2m = 3\alpha$ in (2.3), we have

$$f_i = 1 + \frac{\alpha}{2} \tag{3.4}$$

As noted earlier, only three configurations, that we call gadgets (shown as bold edges in Figure 4), are possible when a vertex of degree 3 is added. So a 3-regular inner dual must be made up of these three gadgets with each gadget connected by a straight edge (shown as dotted edges in Figure 4). Since a diamond (D'), a

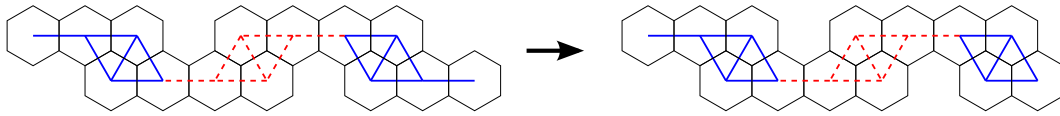


Figure 19: Upper bound for $n \equiv 1 \pmod{4}$

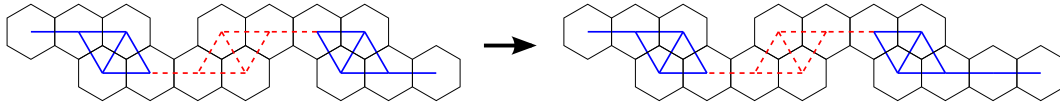


Figure 20: Upper bound for $n \equiv 3 \pmod{4}$

triangle (T') and a claw (C') contribute to 4, 3, and 1 vertices, respectively, we have

$$4D + 3T + C = n = \alpha \tag{3.5}$$

Also, since D' and T' contribute to 2 and 1 interior faces, respectively, substituting $f_3 = 2D + T$ in equation (2.4) yields

$$f_i = \rho + 2D + T \tag{3.6}$$

So, using equations (3.4), (3.5) and (3.6), we have

$$\begin{aligned} 2(2D + T) + T + C = \alpha &\Rightarrow 2(f_i - \rho) + T + C = \alpha \Rightarrow T + C = \alpha - 2(1 + \frac{\alpha}{2} - \rho) \\ T + C &= 2(\rho - 1) \end{aligned} \tag{3.7}$$

We now find the tuples (D, T, C) , for $n = 10, 12, 14, 26$, with $D, T, C \in \mathbb{N} \cup \{0\}$, subject to constraint equations (3.5) and (3.7).

- $n = 10 \Rightarrow \rho = 0 \text{ or } 1 \Rightarrow T + C = 0 \Rightarrow \text{no solutions}$
- $n = 12 \Rightarrow \rho = 0 \text{ or } 1 \Rightarrow T + C = 0 \Rightarrow \{(D, T, C)\} \equiv \{(3, 0, 0)\}$
- $n = 14 \Rightarrow \rho = 0 \text{ or } 1 \Rightarrow T + C = 0 \Rightarrow \text{no solutions}$
- $n = 16 \Rightarrow \rho = 0 \text{ or } 1 \Rightarrow T + C = 0 \Rightarrow \{(D, T, C)\} \equiv \{(4, 0, 0)\}$

$$\begin{aligned} n = 26 &\Rightarrow \rho = 0, 1, 2 \text{ or } 3 \\ \Rightarrow T + C &= \begin{cases} 0 & ; \rho = 0, 1 \\ 2 & ; \rho = 2 \\ 4 & ; \rho = 3 \end{cases} \Rightarrow \{(D, T, C)\} \equiv \left\{ \underbrace{\begin{matrix} \rho=2 \\ (5, 2, 0), (6, 0, 2) \end{matrix}}_{\rho=3}, \underbrace{\begin{matrix} (4, 3, 1), (5, 1, 3) \end{matrix}}_{\rho=3} \right\}. \end{aligned}$$

For $n = 12$ (with $(D, T, C) = (3, 0, 0)$) and $n = 16$ (with $(D, T, C) = (4, 0, 0)$), the only possible 3-regular non-isomorphic graphs are as shown in Figure 23 (b) and (c), respectively, which are not embeddable in the triangular lattice. For $n = 26$, we show that a 3-regular planar graph subject to $(D, T, C) = (5, 2, 0)$ is not embeddable in the triangular lattice. Similar arguments could be used to show that a planar graph subject to $(D, T, C) = (6, 0, 2), (4, 3, 1)$ or $(5, 1, 3)$ is not embeddable in the triangular lattice.

First, note that a simple planar 3-regular graph with $(D, T, C) = (5, 2, 0)$ is of the form shown in Figure 24. Now, consider the subgraph shown as shaded in this figure. Since this subgraph has two pendant vertices, from Lemma 3.3 it follows that the number of vertices of the subgraph of Figure 24 in consideration must have at least 20 vertices, if it is to be embeddable in the triangular lattice. This implies that $4(p + q) + 8 \geq 20$, that is, $p + q \geq 3$. Similarly, $4(q + r) + 8 \geq 20$, that is, $q + r \geq 3$. So, the solution

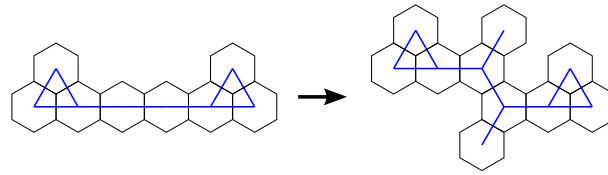


Figure 21: $d = (3^2, 2^6) \rightarrow d = (3^4, 2^4, 1^2)$

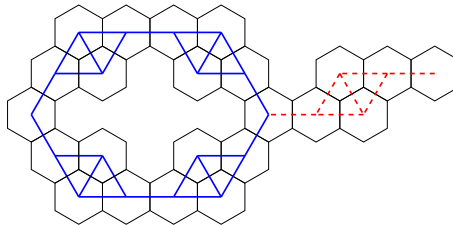


Figure 22: $d = (3^{n-2}, 2^1, 1^1)$ for $n \geq 19$ and $n \equiv 3 \pmod{4}$

set of the tuples (p, q, r) subject to constraints $p + q \geq 3, q + r \geq 3, p + q + r = D = 5$ and $p, q, r \geq 0$ is $\{(0, 3, 2), (0, 4, 1), (0, 5, 0), (1, 2, 2), (1, 3, 1), (1, 4, 0), (2, 1, 2), (2, 2, 1), (2, 3, 0)\}$. For any tuple (p, q, r) belonging to this set, Figure 24 is not embeddable in the triangular lattice.

This completes *if* part of the proof.

(only if)

Note that,

$$\begin{aligned}
 A' = \mathbb{N} \setminus A &= \{24, 32, 34, 36, 40, 42, 44, 46, 48, 50, 52, 54, \dots\} \\
 &= \underbrace{\{24 + 8k : k \in \mathbb{N} \cup \{0\}\}}_{A'_1} \cup \underbrace{\{32 + 8k : k \in \mathbb{N} \cup \{0\}\}}_{A'_2} \cup \underbrace{\{36 + 8k : k \in \mathbb{N} \cup \{0\}\}}_{A'_3} \cup \underbrace{\{46\}}_{A'_4} \\
 &\quad \cup \underbrace{\{54 + 8k : k \in \mathbb{N} \cup \{0\}\}}_{A'_5}
 \end{aligned}$$

The inner dual graphs that realizes the degree sequence $d = (3^\alpha, 2^0, 1^0)$ for $\alpha \in A'_i, (1 \leq i \leq 5)$ are shown in Figure 25.

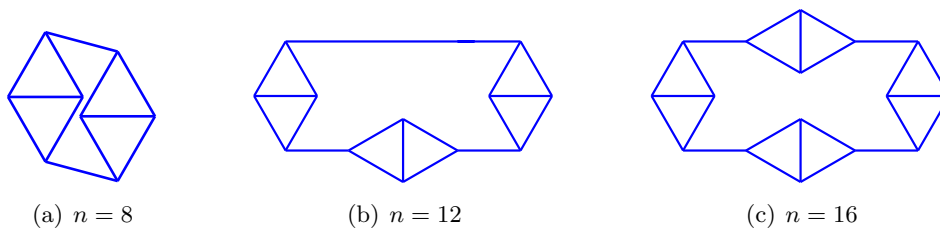


Figure 23: 3-regular simple planar graphs on n vertices.

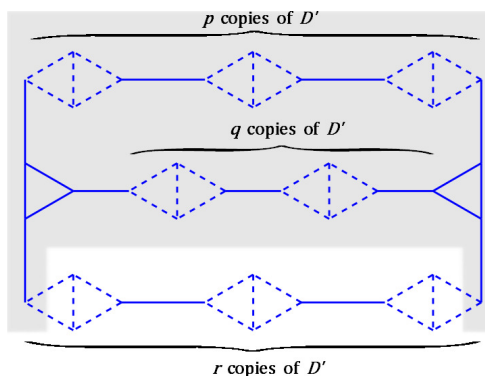


Figure 24: 3-regular planar graph with $(D, T, C) = (5, 2, 0)$

□

4. Generating function for the degree sequence of inner dual graph with maximum degree 3

There is also a scope for finding appropriate generating function for the degree sequence, for further details we refer [10].

We present here a few results in the form of corollaries. In fact they are coming out from the above theorem, which establishes exact relationship between α, β , and γ . The first corollary is a result based on the degree sequence of inner dual graph. All other results in the following are based on the multiplicities α, β and γ .

Corollary 4.1. *If $\alpha = \gamma$ and $\beta = \alpha + \gamma$ then the degree sequence $3^\alpha, 2^{\alpha+\gamma}, 1^\gamma$ will hold for inner dual graph and these terms (multiplicities of the degree sequence of inner dual) are the coefficients of the generating function*

$$C(n) = 1 + 2 \times [3|n] = 1 + 2 \left(\frac{1 + 2 \cos(\frac{2n\pi}{3})}{3} \right),$$

where $[x|y] = 1$ when x divides y and 0 otherwise.

Proof. Let $\alpha = \gamma$ and $\beta = \alpha + \gamma$, we will show that these values come from theorem 4. According to the theorem 4 we have

$$1 \leq \alpha \leq n - 2 \text{ for } n \equiv 1(\text{mod } 4)$$

and

$$1 \leq \alpha \leq n - 3 \text{ otherwise}$$

and

$$1 \leq \gamma \leq \alpha - 2 \text{ for each } \alpha$$

We are considering the case for $\alpha = \gamma$ then $\beta = n - (\alpha + \gamma)$ Putting $\beta = \alpha + \gamma$, we have $\alpha + \gamma = n - (\alpha + \gamma)$ this gives $\alpha + \gamma = \frac{n}{2} \Rightarrow n$ must be even and it is a multiple of 4 as $\alpha = \gamma \neq 0$.

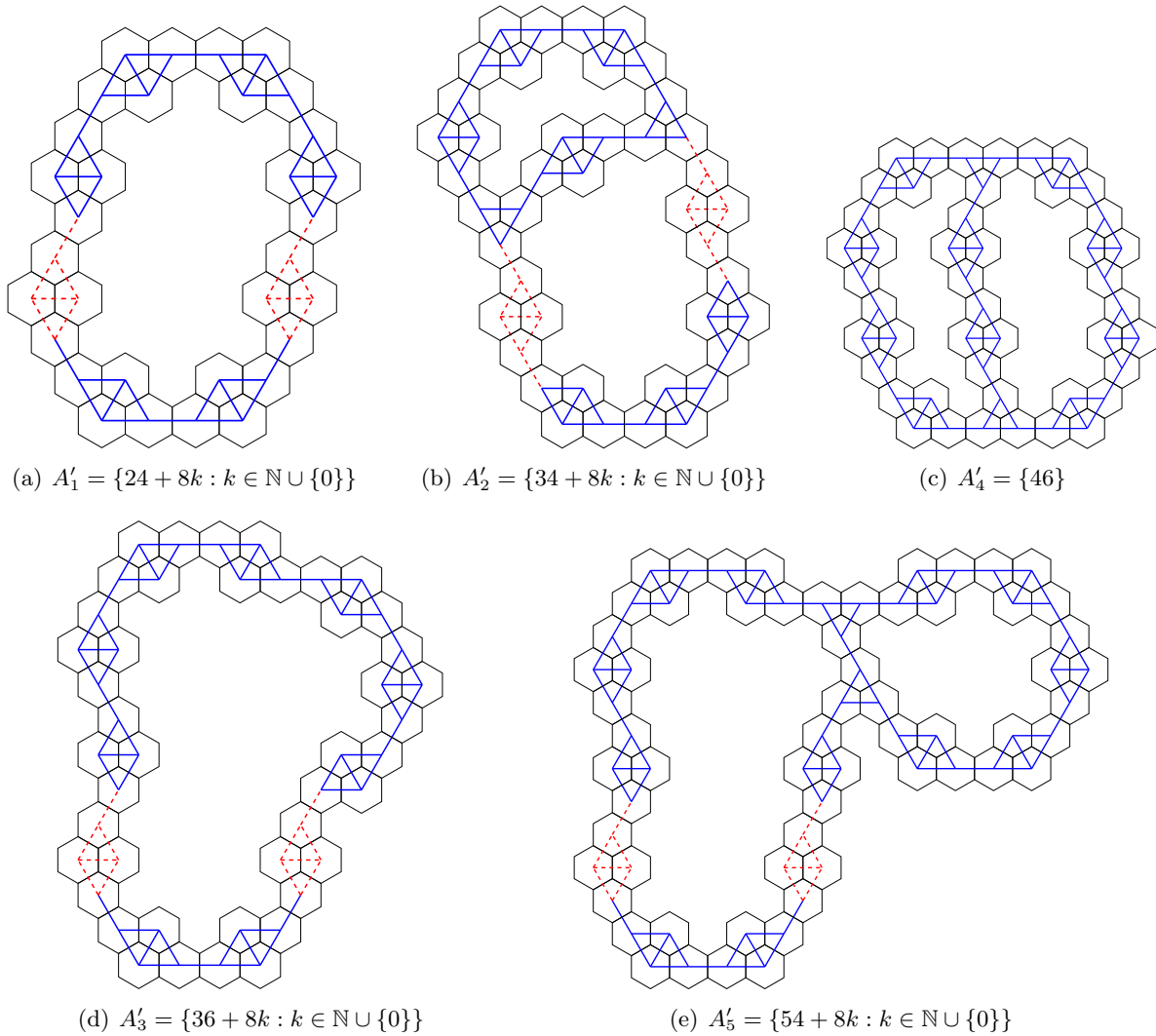


Figure 25: 3-regular inner dual hexagonal graphs

It can also be justified as α and γ are the multiplicities of odd degree vertices. Since $\alpha = \gamma$ therefore, $\alpha + \gamma$ must be even. Furthermore, increasing the multiplicities $\alpha, \alpha + \gamma$ and γ will increase the quantities 4 times the previous one. Thus it represents the case when $n \equiv 0 \pmod{4}$.

$$\Rightarrow 1 \leq \alpha, \gamma \leq n - 3 \text{ and } \alpha = \gamma$$

and

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

Hence $\beta = \alpha + \gamma$. Hence $(3^\alpha, 2^{\alpha+\gamma}, 1^\gamma)$ forms an inner dual degree sequence. The multiplicities $\alpha, \alpha + \gamma$ and γ gives the following terms

$$1, 2, 1, 1, 2, 1, 1, 2, 1, 1, 2, 1, 1, 2, 1, 1, 2, 1, 1, 2, 1, 1, 2, 1, 1, \dots$$

the terms in the above sequence in fact are the coefficients of generating function $f(n)$, where $f(n) = 1 + 2 \times [3|n] = 1 + 2(1 + 2 \times \cos(2 \times n \times \pi/3)/3)$, where $[x|y] = 1$ when x divides y , 0 otherwise.

Corollary 4.2. *If $\alpha = 3\gamma$ and $\beta = \alpha - \gamma$ then the degree sequence $3^\alpha, 2^{\alpha-\gamma}, 1^\gamma$ will hold for inner dual graph and these terms(multiplicities of the degree sequence of inner dual) are the coefficients of the generating function*

$$C(n) = n \bmod 3 + (n + 1) \bmod 3, \text{ with } n \geq 0.$$

Proof. Let $\alpha = 3\gamma$ and $\beta = \alpha - \gamma$, we will show that these values come from theorem 4. Since

$$1 \leq \alpha \leq n - 2 \text{ for } n \equiv 1(\text{mod } 4)$$

and

$$1 \leq \alpha \leq n - 3 \text{ otherwise}$$

and

$$1 \leq \gamma \leq \alpha - 2 \text{ for each } \alpha$$

We are considering the case for $\alpha = 3\gamma$ then $\beta = n - (\alpha + \gamma)$ Putting $\beta = \alpha - \gamma$, we have $\alpha - \gamma = n - (\alpha + \gamma)$ this gives $\alpha = \frac{n}{2} \Rightarrow n$ must be even and it is a multiple of 6 as $\alpha = 3\gamma \neq 0$

It can also be justified as α and γ are the multiplicities of odd degree vertices. Since $\alpha = 3\gamma$ therefore, $\alpha + 3\gamma$ must be even and a multiple of 4. Furthermore, increasing the multiplicities $\alpha, \alpha - \gamma$ and γ will increase the quantities 6 times the previous one. Thus this is the case when $n \equiv 0(\text{mod } 4)$ and $n \equiv 2(\text{mod } 4)$.

$$\Rightarrow 1 \leq \alpha, \gamma \leq n - 2 \text{ and } \alpha = 3\gamma$$

and

$$\beta = n - (\alpha + \gamma) = n - \frac{n}{2} - \frac{n}{6} = \frac{n}{3}$$

Hence $\beta = \alpha - \gamma$. Hence $3^\alpha, 2^{\alpha-\gamma}, 1^\gamma$ forms an inner dual degree sequence. The multiplicities $\alpha, \alpha + \gamma$ and γ gives the following terms

$$3, 2, 1, 3, 2, 1, 3, 2, 1, 3, 2, 1, 3, 2, 1, 3, 2, 1, 3, 2, 1, 3, 2, 1, \dots$$

Terms in the above sequence infact are the coefficients of generating function $f(n)$, where $f(n) = n \text{ mod } 3 + (n + 1) \text{ mod } 3$, with $n \geq 0$. □

Similar arguments can be used to prove other exact relationship between α, β and γ for $3^\alpha, 2^\beta, 1^\gamma$ which form the degree sequence for inner dual graphs. The terms in the degree sequence are exactly the coefficients of the generating functions. In the following we also summarize various degree sequences and their respective generating functions.

Exact Relation	The n-th Coefficient of Generating Function
$\alpha = \beta = \gamma$	$C(n) = \lfloor \frac{n}{3} \rfloor + 1 \quad n > 0$
$\alpha = \gamma$ $\beta = 2\alpha + \gamma$	$C(n) = 1 + 2(\frac{1+2\cos(\frac{2n\pi}{3})}{3}) \quad n \geq 0$
$\alpha = \gamma$ $\beta = \frac{\alpha+\gamma}{4}$	$C(n) = \frac{1}{9}\{8(n \bmod 3) + 5[(n+1) \bmod 3] + 2[(n+2) \bmod 3]\} \quad n > 0$
$\alpha = 3\gamma$ $\beta = \alpha - 2\gamma$	$C(n) = 1 + 2(\frac{1+2\cos(\frac{2n\pi}{3})}{3}), \quad n > 0.$
$\alpha = 3\gamma$ $\beta = \alpha$	$C(n) = \frac{7-4\cos(\frac{2\pi n}{3})}{3} \quad n > 0$
$\alpha = 2\gamma$ $\beta = \frac{\alpha-\gamma}{2}$	$C(n) = 2^{\text{mod}(n,3)} \quad n \geq 2$
$\alpha = \gamma$ $\beta = \frac{\alpha+\gamma}{3}$	$C(n) = f_{n-1} + f_{n-2} - 2[\lfloor \frac{f_{n-1}}{3} \rfloor + \lfloor \frac{f_{n-2}}{3} \rfloor]$
$\alpha = 3\gamma$ $\beta = \alpha + \gamma$	$C(n) = \frac{1}{6}\{3(n \bmod 6) - [(n+1) \bmod 6] - 4[(n+2) \bmod 6] - 3[(n+3) \bmod 6] + [(n+4) \bmod 6] + 4[(n+5) \bmod 6]\}, n \geq 0$
$\alpha = \gamma$ $\beta = 2\alpha + \frac{\gamma}{2}$	$C(n) = (n \bmod 3) + 2[(n+1) \bmod 3] - 2 * [C(2n, n) \bmod 2] - 5C[(n+1)^2, n+3] \bmod 2, \quad n \geq 0$
$\alpha = \gamma$ $\beta = \frac{\alpha+\gamma}{8}$	$C(n) = (x + 4x^2 + x^3)/(1 - x^3)$
$\alpha = 3\gamma$ $\beta = \alpha + 2\gamma$	$C(n) = \frac{1}{3}[7(n \bmod 3) + ((n+1) \bmod 3) + ((n+2) \bmod 3)] \quad n > 0$
$\alpha = 5\gamma$ $\beta = \alpha - \gamma$	$C(n) = \frac{-5}{6}(n \bmod 6) - [(n+1) \bmod 6] + 4[(n+2) \bmod 6] + 5[(n+3) \bmod 6] + [(n+4) \bmod 6] - 4[(n+5) \bmod 6], n \geq 0$
$\alpha = 3\gamma$ $\beta = \frac{\alpha}{2}$	$C(n) = \frac{-9}{6}(n \bmod 6) + 8[(n+1) \bmod 6] - 5[(n+2) \bmod 6] + 9[(n+3) \bmod 6] - 8[(n+4) \bmod 6] + 5[(n+5) \bmod 6], n \geq 0$
$\alpha = 7\gamma$ $\beta = \alpha - 3\gamma$	$C(n) = \frac{1}{3}7(n \bmod 3) + 7[(n+1) \bmod 3] - 2[(n+2) \bmod 3], n \geq 0$
$\alpha = 3\gamma$ $\beta = 2\alpha + 3\gamma$	$C(n) = 3^{n \bmod 13} \quad n > 0$
$\alpha = 7\gamma$ $\beta = \alpha - 2\gamma$	$C(n) = \frac{1}{3}-4(n \bmod 6) - 2[(n+1) \bmod 6] - [(n+2) \bmod 6] + 4[(n+3) \bmod 6] + 2 * [(n+4) \bmod 6] + [(n+5) \bmod 6] \quad n \geq 0$
$\alpha = 2\gamma$ $\beta = \alpha + 2\gamma$	$C(n) = 2^{n \bmod 14} \quad n > 1$

Conclusion

In this paper, all the hexagonal inner dual graphical degree sequences with maximum degree $3k, k$ have been identified and their respective graphical realizations have been presented. All degree sequences which can generate a-cyclic graphs in hexagonal inner dual system have been looked upon, however for graphs containing cycles, there is scope for work with maximum degree 4 or greater. Moreover, we also find relationships between degree sequences and their respective generating functions which are based on some conditions. Further work on higher degree sequences is underway and will be published soon.

Acknowledgements:

Hasan Baloch and Rameez Ragheb wish to thank Lahore University of Management Sciences (LUMS) for the financial support through research assistant ship and financial aid to complete this project.

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