INDEPENDENCE POLYNOMIALS OF CIRCULANT GRAPHS

by

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This is the true joy in life, the being used for a purpose recognized by yourself as a mighty one, the being a force of nature, instead of a selfish, feverish little clod of ailments and grievances complaining that the world will not devote itself to making you happy. I am of the opinion that my life belongs to the whole community, and it is my privilege to do for it whatever I can.

Life is no brief candle to me, it is a sort of splendid torch which I've got a hold of for the moment, and I want to make it burn as brightly as possible before handing it on to future generations.

– George Bernard Shaw

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Abstract

The *circulant graph* $C_{n,S}$ is the graph on n vertices (with labels $0, 1, 2, \ldots, n-1$), spread around a circle, where two vertices u and v are adjacent iff their (minimum) distance $|u-v|$ appears in set S. In this thesis, we provide a comprehensive analysis of the *independence polynomial* $I(G, x)$, when $G = C_{n,S}$ is a circulant. The independence polynomial is the generating function of the number of independent sets of G with k vertices, for $k \geq 0$.

While it is NP-hard to determine the independence polynomial $I(G, x)$ of an arbitrary graph G, we are able to determine explicit formulas for $I(G, x)$ for several families of circulants, using techniques from combinatorial enumeration. We then describe a recursive construction for an infinite family of circulants, and determine the independence number of each graph in this family. We use these results to provide four applications, encompassing diverse areas of discrete mathematics. First, we determine a new (infinite) family of star extremal graphs. Secondly, we obtain a formula for the chromatic number of infinitely many integer distance graphs. Thirdly, we prove an explicit formula for the generalized fractional Ramsey function. Finally, we determine the optimal Nordhaus-Gaddum inequalities for the fractional chromatic and circular chromatic numbers. These new theorems significantly extend what is currently known.

Building on these results, we develop additional properties and applications of circulant graphs. We determine a full characterization of all graphs G for which its line graph $L(G)$ is a circulant, and apply our previous theorems to calculate the list colouring number of a specific family of circulants. We then characterize well-covered circulant graphs, and examine the shellability of their independence complexes. We conclude the thesis with a detailed analysis of the roots of $I(C_{n,S}, x)$. Among many other results, we solve several open problems by calculating the density of the roots of these independence polynomials, leading to new theorems on the roots of matching polynomials and rook polynomials.

Abstract

$C_{n,S}$	The circulant graph on n vertices with generating set S
$I(G,x)$	The independence polynomial of graph G
P_n	The path on n vertices
C_n	The cycle on n vertices
K_n	The complete graph on n vertices
$\|G\|$	The order of a graph G, i.e., the number of vertices in G
$\|u-v\|_n$	The circular distance of two vertices u and v in $C_{n,S}$
$\deg(v)$	The degree of a vertex v
$\alpha(G)$	The independence number of G
$\omega(G)$	The clique number of a G
$\chi(G)$	The chromatic number of G
$\overline{G}$	The complement of G
$L(G)$	The line graph of G
$[x^k]P(x)$	The coefficient of the x^k term of $P(x)$
A_n	The circulant $C_{n,\{1,2,\ldots,d\}}$, where $d \geq 1$ is fixed
B_n	The circulant $C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$, where $d \geq 0$ is fixed
$G[H]$	The lexicographic graph product of G with H
$\chi_f(G)$	The fractional chromatic number of G
$\chi_c(G)$	The circular chromatic number of G
$\omega_f(G)$	The fractional clique number of G
$\chi_l(G)$	The list colouring number of G
$G(\mathbb{Z},S)$	The integer distance graph generated by set S
$\rho(G)$	The vertex arboricity number of G
$r(a_1,a_2,\ldots,a_k)$	The Ramsey function of the k-tuple $(a_1,a_2,\ldots,a_k)$
$r_{\omega_f}(a_1,a_2,\ldots,a_k)$	The fractional Ramsey function of the k-tuple $(a_1,a_2,\ldots,a_k)$
$\Delta(G)$	The independence complex of G

Acknowledgements

First and foremost, I'd like to thank my supervisor Jason Brown, for his incredible support and patience during the completion of this thesis. Too often during my graduate career, I would get sidetracked with my numerous extracurricular activities; while all of this was important, Jason inspired in me a desire to focus more on mathematical research, and helped me enjoy the process of writing this thesis. I am extremely thankful to have had him as my supervisor and mentor.

As I reflect back on my four years in Halifax, I am grateful for the many experiences I have had to serve and inspire others. I feel so privileged to have had the opportunity to share my passion for mathematics with thousands of students from both high school and university, and run professional development programs for hundreds of high school teachers and university faculty. While these past four years have certainly been challenging, every day has presented a new opportunity to grow, both mathematically and otherwise. I am so thankful to have a wonderful group of family and friends, who have helped me grow, both personally and professionally. I'd especially like to thank my wife and soulmate Karen, for all of her love, support, and patience.

During periods of stress and overwork, my faith in God has taught me that my life is more than just mathematics, and that my identity is found in things other than work. While I will always struggle with finding the proper balance between my numerous commitments and responsibilities, I am so thankful to be growing in faith and learning to use my gifts to serve God to the best of my ability. I hope that the confidence I have gained in inspiring change over the past four years will motivate me to reach even greater heights in my new life in Ottawa – not by my own ability, but through the grace of my God who teaches me every day that "I can do all things through Christ who strengthens me".

Chapter 1

Introduction

1.1 Basic Terminology

In this thesis, we will use notation from Diestel's textbook on graph theory [58]. Since much of the standard terminology will be familiar, we just cite several definitions that will be used repeatedly.

We will assume that all graphs are simple, i.e., no loops or multiple edges. The graph P_n is the *path* on n vertices, C_n is the *cycle* on n vertices, and K_n is the *complete graph* on n vertices. The number of vertices in a graph $G = (V, E)$ is its *order*, denoted by $|G|$. The *degree* of a vertex v, denoted by $\deg(v)$, is the cardinality of the set $\{u \in V : uv \in E\}$.

An *independent set* of G is a set S with the property that $u, v \in S \rightarrow uv \notin E$. In other words, no pair of vertices in S is adjacent in G. Trivially, any single vertex of G is an independent set. The largest order of an independent set in G is the *independence number* $\alpha(G)$.

A *clique* of G is a set S with the property that $(u \neq v \text{ and } u, v \in S) \rightarrow uv \in E$. In other words, every pair of vertices in S is adjacent in G. The largest order of a clique in G is the *clique number* $\omega(G)$. We note that $\omega(G) = \alpha(\overline{G})$, for all G, where $\overline{G}$ denotes the *complement* of G.

Let Γ be a set of colours. A colouring $\pi : V \rightarrow \Gamma$ of a graph G is *proper* if no two adjacent vertices receive the same colour. The *chromatic number* $\chi(G)$ is the smallest number of colours in a proper colouring of G.

Let $G = (V, E)$ and $G' = (V', E')$ be two graphs. We say that G and G' are *isomorphic* if there exists a bijection $\varphi : V \rightarrow V'$ with $xy \in E$ iff $\varphi(x)\varphi(y) \in E'$, for all $x, y \in V$. We write this as $G \simeq G'$. Such a map φ is an *isomorphism*. If $G = G'$, then φ is an *automorphism*. We will not distinguish between isomorphic graphs: thus, we will always speak of *the* complete graph on n vertices, and so on. A function taking graphs as arguments is a *graph invariant* if it assigns equal values to isomorphic graphs. For example, $\alpha(G)$, $\omega(G)$, and $\chi(G)$ are all graph invariants.

We set $G \cup G' = (V \cup V', E \cup E')$ and $G \cap G' = (V \cap V', E \cap E')$. If $V \cap V' = \emptyset$, then graphs G and G' are *disjoint*. If $V' \subseteq V$ and $E' \subseteq E$, then G' is a *subgraph* of G. We write this as $G' \subseteq G$. If $G' \subseteq G$ and G' contains all the edges $xy \in E$ with $x, y \in V'$, then G' is an *induced subgraph* of G, and we say that V' *induces* G'. If U is a subset of the vertices of G, the graph $G - U$ is formed by deleting all of the vertices in U from G, and deleting all of their incident edges as well. In the case that $U = \{u\}$ for a single vertex u, we just write $G - u$.

A set of edges is *independent* if no two edges share a common vertex, and a set of independent edges is a *matching*. A *perfect matching* is a matching that includes each of the vertices.

In the *line graph* $L(G)$ of graph G, the vertex set is $E(G)$, the edge set of G, and vertices x and y are adjacent in $L(G)$ iff x and y are adjacent as edges in G. For example, $L(K_4)$ is isomorphic to K_6 minus a perfect matching, and $L(C_n) \simeq C_n$ for all $n \geq 3$. Note that a matching of k edges in G corresponds to a set of k independent vertices in $L(G)$, and conversely.

Other definitions will be introduced in the appropriate context. In the next two sections, we define the two most important terms in the thesis, as they will form the basis for everything that follows.

1.2 Circulant Graphs

Definition 1.1 *A* **circulant graph** *of order n has vertex set $V(G) = \mathbb{Z}_n$ and edge set $E(G) = \{uv : u - v \in S\}$, for some* **generating set** *$S \subseteq V(G)$. This set S must not contain the identity element 0, and must be closed under additive inverses. We say that $C_{n,S}$ is the circulant graph of order n with generating set S.*

We note that $C_{n,S}$ is an undirected Cayley graph [81] for the group $G = (\mathbb{Z}_n, +)$. Thus, circulant graphs are a special case of the more general family of Cayley graphs. Since our generating set S must be closed under additive inverses and not contain the identity element, the following is an equivalent definition of $C_{n,S}$.

Definition 1.2 *Given a set* $S \subseteq \{1, 2, 3, \ldots, \lfloor \frac{n}{2} \rfloor\}$*, the* **circulant graph** $C_{n,S}$ *is the graph with vertex set* $V(G) = \mathbb{Z}_n$*, and edge set* $E(G) = \{uv : |u - v|_n \in S\}$*, where* $|x|_n = \min\{|x|, n - |x|\}$ *is the* **circular distance** *modulo* n*.*

We will use this latter definition of $C_{n,S}$ throughout the thesis. Thus, the generating set S will always refer to a subset of $\{1, 2, 3, \ldots, \lfloor \frac{n}{2} \rfloor\}$. In the literature, S is also referred to as the *connection set* [5, 59].

For example, here are the circulants $C_{9,\{1,2\}}$ and $C_{9,\{3,4\}}$.

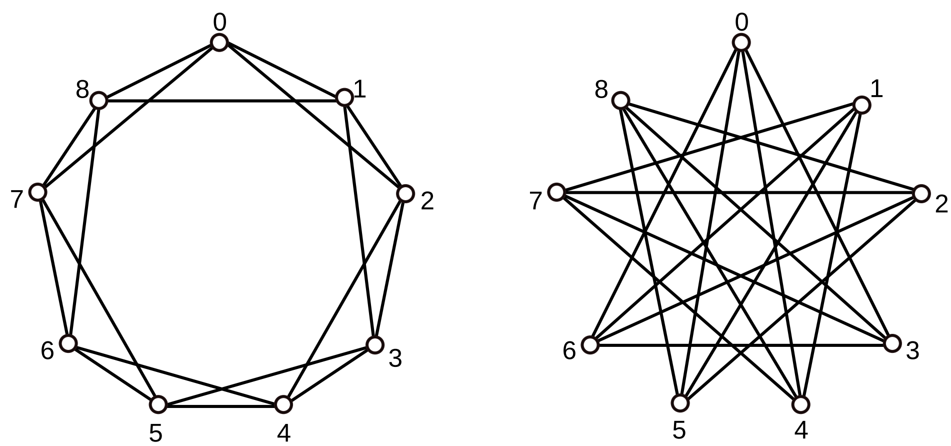

Figure 1.1: The circulant graphs $C_{9,\{1,2\}}$ and $C_{9,\{3,4\}}$.

Note that the circulant $C_{n,\{1,2,3,\ldots,\lfloor \frac{n}{2} \rfloor\}}$ is simply the complete graph K_n. Also, $C_{n,\{1\}}$ is just the cycle C_n. We remark that $C_{n,\{d\}} \simeq C_n$ for any d with $\gcd(d, n) = 1$.

Circulant graphs have been investigated in fields outside of graph theory. For example, for geometers, circulant graphs are known as *star polygons* [52]. Circulants have been used to solve problems in group theory, as shown in [5], as well as number theory and analysis [55]. They are well-studied in network theory, as they model practical data connection networks [11, 100]. Circulant graphs (and circulant matrices) have important applications to the theory of designs and error-correcting codes [156]. Various papers have been written on the theory of circulant graphs [1, 5, 46, 48, 55, 56, 59, 68, 78, 82, 121, 123, 140, 141, 181], but no paper has yet explored the properties of independence in circulant graphs.

1.3 The Independence Polynomial

Definition 1.3 *The* **independence polynomial** $I(G,x)$ *is* $\sum_{k=0}^{n} i_k x^k$*, where* i_k *is the number of independent sets of cardinality* k *in* G*.*

In other words, $I(G,x)$ is the generating function of the number of independent sets of G, where the coefficients represent the number of independent sets of each cardinality. In this thesis, we will derive many properties of the independence polynomial $I(G,x)$, primarily when G belongs to the family of circulant graphs.

Since the independence polynomial was first introduced [87], it has proven to be a fruitful area of combinatorial research [22, 23, 25, 26, 42, 74, 97, 98, 118, 119, 120, 130, 133, 165]. Also, independence polynomials are known to have important applications to combinatorial chemistry and statistical physics [120, 159].

We will develop new formulas and properties of independence polynomials, and apply these theorems to solve problems from other areas of discrete mathematics.

To illustrate, we calculate the independence polynomial of the 6-cycle C_6. We have $i_0 = 1$ (the empty set) and $i_1 = 6$, since we can select any of the six vertices. The coefficient i_2 is simply the number of non-edges of G, which equals $\binom{n}{2} - |E(G)| = 9$. It is clear that $i_k = 0$ for $k \geq 4$. Finally, there are only two independent sets for $k = 3$, namely $\{0, 2, 4\}$ and $\{1, 3, 5\}$.

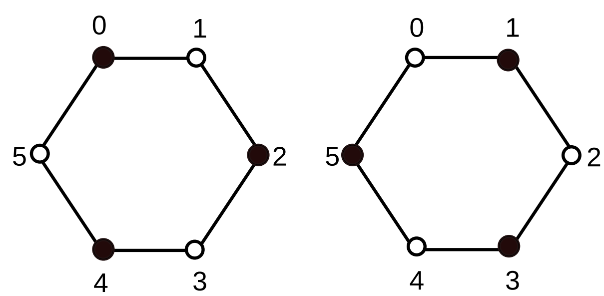

Figure 1.2: Two independent sets of size 3 in C_6.

Therefore, the independence polynomial of C_6 is $I(C_6, x) = 1 + 6x + 9x^2 + 2x^3$. By definition, it follows that for all graphs G, the independence number $\alpha(G)$ is equal to $\deg(I(G,x))$, the *degree* of the independence polynomial $I(G,x)$.

Definition 1.4 *For any polynomial $P(x)$, $[\boldsymbol{x^k}]\boldsymbol{P(x)}$ is the coefficient of the x^k term in $P(x)$.*

For example, we have $[x^2]I(C_6, x) = 9$ and $[x^4]I(C_6, x) = 0$. Note that for any G, $[x^0]I(G, x) = 1$ and $[x^1]I(G, x) = |G|$.

Using various techniques in combinatorial enumeration, we will derive explicit formulas for $I(G, x)$ for several families of circulant graphs. In the process, we will find out much information about the independent sets of G. Not only will we have an immediate formula for $\alpha(G)$, we will also acquire other information at no cost, such as showing that G contains more independent sets of one cardinality than another (equivalent to verifying that $i_p > i_q$ for some p and q), or determining the total number of independent sets in G (equivalent to evaluating $I(G, x)$ at $x = 1$).

We will develop several applications of independence polynomials in this thesis. Here we describe one such application. In Chapter 4, we will examine *well-covered graphs*, which are graphs for which every independent set can be extended to a maximum independent set. In a well-covered graph, a maximum independent set can be found by applying the greedy algorithm. However, it is not clear how to enumerate *all* maximum independent sets. By obtaining a formula for $[x^{\alpha(G)}]I(G, x)$, we will know exactly how many maximum independent sets must appear in G. Thus, once our enumeration technique has found $[x^{\alpha(G)}]I(G, x)$ independent sets of maximum cardinality, we can immediately stop, because we know that there cannot be any more. Once we have found all of the maximum independent sets, we can prove that a circulant is not well covered by finding an independent set that cannot be extended to any of these $[x^{\alpha(G)}]I(G, x)$ maximum independent sets. This will enable us to derive classification theorems of well-covered circulant graphs, and formally prove that certain circulants are not well-covered.

For some graphs G, it is very easy to compute the independence polynomial $I(G, x)$. As an example, if $G = K_n$, then clearly $I(K_n, x) = 1 + nx$, since there are no independent sets of cardinality 2 or more. But computing $I(G, x)$ for an arbitrary graph G is NP-hard [79], even when G is restricted to the family of circulant graphs [46]. Note that there is a simple reduction formula [87] which calculates any independence polynomial $I(G, x)$ in exponential time.

Theorem 1.5 ([87]) *For any vertex v,*

$$I(G,x) = I(G-v,x) + x \cdot I(G-N[v],x),$$

where the closed neighbourhood $N[v]$ is the set $\{u : \ u = v \text{ or } uv \in E\}$.

We also mention the following theorem, which deals with unions of disjoint graphs.

Theorem 1.6 ([87]) *Let G and H be disjoint graphs. Then*

$$I(G \cup H, x) = I(G,x) \cdot I(H,x).$$

Let us briefly discuss the *dependence polynomial* $D(G,x)$, which is introduced in [74]. The polynomial $D(G,x)$ is equal to $\sum c_k x^k$, where c_k represents the number of cliques (i.e., dependent sets) of cardinality k in G. By this definition, it is clear that $D(G,x) = I(\overline{G},x)$, for all graphs G. Thus, we will not consider dependence polynomials in this thesis, as $D(G,x)$ is simply the independence polynomial of $\overline{G}$.

We conclude this chapter by introducing two more graph polynomials, which we will refer to several times in the following chapters.

Definition 1.7 *For any graph G, the* **chromatic polynomial** $\pi(G,x)$ *is the function that gives the number of proper colourings of the vertices of G using x colours.*

As a trivial example, $\pi(K_3,x) = x(x-1)(x-2) = x^3 - 3x^2 + 2x$. Much work has been done in the study and analysis of chromatic polynomials [20, 24, 38, 61, 68, 97, 101, 112, 126, 153, 162, 166].

Definition 1.8 *For any graph G, the* **matching polynomial** $M(G,x)$ *is*

$$M(G,x) = \sum_{k \geq 0} (-1)^k m_k x^{n-2k},$$

where m_k is the number of matchings in G with exactly k edges.

For example, $M(C_6,x) = x^6 - 6x^4 + 9x^2 - 2$. Since a matching of k edges in G corresponds to a set of k independent vertices in the line graph $L(G)$, it follows that the i_k coefficient of $I(L(G),x)$ is equal to the m_k coefficient in $M(G,x)$. In other words, $I(L(G),x) = \sum_{k \geq 0} m_k x^k$. Therefore, the following result holds.

Proposition 1.9 ([87]) *For all graphs G, $M(G,x) = x^n \cdot I(L(G), -\frac{1}{x^2})$.*

Therefore, we may regard the independence polynomial as a generalization of the matching polynomial. Like the independence polynomial, $M(G,x)$ is a graph polynomial that has been studied by combinatorialists [68, 81, 87]. Matching polynomials have important applications to statistical physics, and arise in the theory of monomer-dimer systems [96].

1.4 Overview of the Thesis

In Chapter 2, we investigate the independence polynomial of a general circulant graph $G = C_{n,S}$, and attempt to find formulas for $I(G,x)$. Since it is NP-hard [46] to determine $I(G,x)$ for an arbitrary circulant graph $G = C_{n,S}$, we know that it is highly improbable that an explicit formula for $I(C_{n,S},x)$ can be developed. Nevertheless, we find a formula for $I(C_{n,S},x)$ for three general families of circulants: when S is of the form $\{1,2,\ldots,d\}$, when S is of the form $\{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$, and when G is any circulant of degree at most three. We then discuss graph products, and show that the lexicographic product of any two circulants is also a circulant, which enables us to derive additional explicit formulas for $I(C_{n,S},x)$. We discuss the computational complexity of evaluating independence polynomials, and show that evaluating $I(G,x)$ at $x = t$ is $\#P$-hard for every non-zero value of t. We conclude the chapter by determining all circulant graphs that are uniquely characterized by its independence polynomial, and discuss instances when two non-isomorphic circulants have the same independence polynomial.

In Chapter 3, we describe a construction for an infinite family of circulants, and determine a recursive formula for $\deg(I(G,x)) = \alpha(G)$, for every graph in this infinite family. We provide four applications of this result, encompassing diverse areas of discrete mathematics. First, we determine a new (infinite) family of star extremal graphs. Secondly, we obtain a formula for the chromatic number of infinitely many integer distance graphs. Thirdly, we prove an explicit formula for the generalized fractional Ramsey function, solving an open problem from [102, 117]. Finally, we determine the optimal Nordhaus-Gaddum inequalities for the fractional chromatic and circular chromatic numbers. These new results significantly extend (or completely solve) much of what is currently known.

In Chapter 4, we investigate additional properties of circulant graphs, and use our results from the previous two chapters to develop various applications. First, we provide a full characterization of all graphs G for which its line graph $L(G)$ is a circulant. Then we examine list colourings, and provide a clever application of independence polynomials to determine the list colouring number of a particular family of circulant graphs. We then investigate well-covered circulants, and give a partial characterization of circulant graphs that are well-covered. We show that the general problem is intractable, by proving that it is co-NP complete to determine if an arbitrary circulant is well-covered. To conclude the chapter, we examine independence complexes of circulants, and classify circulants for which their independence complexes are pure and shellable.

In Chapter 5, we investigate the roots of the independence polynomial $I(C_{n,S}, x)$. We prove that the roots of $I(G, x)$ are dense in the complex plane $\mathbb{C}$, even when G is restricted to one particular family of circulants. We investigate the roots of $I(C_{n,S}, x)$, where S is an arbitrary subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. We provide best bounds for the roots of maximum and minimum moduli, and determine conditions for when the roots of $I(C_{n,S}, x)$ are rational. To conclude the chapter, we examine the closures of the roots of independence polynomials, answering an open problem in [23, 97]. We prove that this theorem on the roots of independence polynomials implies new results on the closures of roots of matching polynomials and rook polynomials.

Chapter 2

Formulas for Independence Polynomials

In this chapter, we investigate the independence polynomials of circulant graphs. As we will see, calculating formulas for $I(G, x)$ is an extremely difficult task. Nevertheless, we will find an explicit formula for several families of circulants $C_{n,S}$, where S is some particular subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$.

First, we will investigate the families with generating set $S = \{1, 2, \ldots, d\}$ and then examine its complement set $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. We will use these results to determine explicit formulas for $I(C_{n,S}, x)$ for all circulants of degree at most 3. We discuss graph products to generate even more formulas for $I(C_{n,S}, x)$, and then apply the lexicographic product to prove that there is no polynomial-time algorithm to evaluate the value of $I(G, t)$ for any $t \neq 0$. We conclude the chapter by determining all circulant graphs that are uniquely characterized by its independence polynomial, and discuss instances when two non-isomorphic circulants have the same independence polynomial.

2.1 The Family $S = \{1, 2, \ldots, d\}$

Consider the generating set $S = \{1, 2, \ldots, d\}$, where $1 \leq d \leq \lfloor \frac{n}{2} \rfloor$ is a given integer. The circulant $C_{n,S}$ is then equivalent to the d^{th} *power* of C_n [58], where two vertices are adjacent iff their distance is at most d. Powers of cycles have been a rich study of investigation [10, 18, 114, 122, 127], with important connections to the analysis of perfect graphs [9, 41, 43, 128].

In this section, we derive a formula for $I(C_{n,S}, x)$, where $S = \{1, 2, \ldots, d\}$ for some fixed integer $1 \leq d \leq \lfloor \frac{n}{2} \rfloor$. As a corollary, this gives us a formula for $I(C_n, x)$, by setting $d = 1$. First, we need a definition and a lemma.

Definition 2.1 *Let $d \geq 1$ be a fixed integer. For each n, set $\boldsymbol{A_n} := C_{n,\{1,2,\ldots,d\}}$.*

By this definition, note that $A_n = K_n$ for $n \leq 2d+1$. Thus, we may assume that $1 \leq d \leq \lfloor \frac{n}{2} \rfloor$. For this fixed d, we now determine a recursive formula for $I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$.

Lemma 2.2 *$I(A_n, x) = I(A_{n-1}, x) + x \cdot I(A_{n-d-1}, x)$, for all $n \geq 2d+2$.*

Proof: Since $n \geq 2d+2$, we have $\alpha(A_n) \geq 2$. We see trivially that the x^0 and x^1 coefficients are equal in the given identity. So fix $k \geq 2$. We will show that the x^k coefficients are equal as well.

Let $\{v_1, v_2, \ldots, v_k\}$ be an independent set of cardinality $k \geq 2$ in A_n, with $0 \leq v_1 < v_2 < \ldots < v_k \leq n-1$. Since the circular distance satisfies the inequality $|u-v|_n > d$ for all non-adjacent vertices u and v in A_n, we have $v_{i+1} - v_i > d$ for all $1 \leq i \leq k-1$, and $n + (v_1 - v_k) > d$. This can be seen by placing n points equally around a circle, and noticing that each (adjacent) pair of chosen vertices is separated by distance greater than d. We will expand on this idea in the following section when we formally define *difference sequences*.

We classify our independent sets $\{v_1, v_2, \ldots, v_k\}$ of A_n into two families:

(a) $S_1 = \{\{v_1, v_2, \ldots, v_k\}$ independent in $A_n :\ v_k - v_{k-1} = d+1\}$.

(b) $S_2 = \{\{v_1, v_2, \ldots, v_k\}$ independent in $A_n :\ v_k - v_{k-1} > d+1\}$.

Since $S_1 \cap S_2 = \emptyset$, it follows that $[x^k]A_n = |S_1| + |S_2|$. We will show that $|S_1| = [x^{k-1}]A_{n-d-1}$ and $|S_2| = [x^k]A_{n-1}$.

Case 1: Proving $|S_1| = [x^{k-1}]A_{n-d-1}$.

We establish a bijection ϕ between S_1 and the set of $(k-1)$-tuples that are independent in A_{n-d-1}. This will prove that $|S_1| = [x^{k-1}]A_{n-d-1}$.

For each element in S_1, define

$$\phi(v_1, v_2, \ldots, v_k) = \{v_1, v_2, \ldots, v_{k-1}\}.$$

Since $v_k = v_{k-1} + (d+1)$, ϕ is one-to-one. Construct the graph A'_n by contracting all of the vertices from the set $\{v_{k-1}+1, v_{k-1}+2, \ldots, v_k\}$ to v_{k-1}. Then $A'_n \simeq A_{n-d-1}$.

We claim that $\phi(v_1, v_2, \ldots, v_k)$ is an independent set of A'_n iff $\{v_1, v_2, \ldots, v_k\}$ is an element of S_1. To prove this claim, we list the necessary and sufficient conditions, and show that they are equivalent.

Note that $\phi(v_1, v_2, \ldots, v_k)$ is an independent set of A'_n iff

(a) $v_{i+1} - v_i > d$ for $1 \leq i \leq k-2$.

(b) $(n-d-1) + v_1 - v_{k-1} > d$.

Also, $\{v_1, v_2, \ldots, v_k\}$ is an element of S_1 iff

(a) $v_{i+1} - v_i > d$ for $1 \leq i \leq k-2$.

(b) $v_k - v_{k-1} = d + 1$.

(c) $n + v_1 - v_k > d$.

We now show that these two sets of conditions are equivalent.

Note that the condition $v_{i+1} - v_i > d$ for $1 \leq i \leq k-2$ is true in both cases. If $\phi(v_1, v_2, \ldots, v_k) = \{v_1, v_2, \ldots, v_{k-1}\}$ is an independent set of A'_n, then $(n-d-1) + v_1 - v_{k-1} > d$. Let $v_k = v_{k-1} + (d+1)$. Then, $\{v_1, v_2, \ldots, v_{k-1}, v_k\}$ is an independent set of A_n, since $(n-d-1) + v_1 - (v_k - (d+1)) > d$, or $n + v_1 - v_k > d$. Therefore, $\{v_1, v_2, \ldots, v_k\}$ is an element of S_1.

Now we prove the converse. If $\{v_1, v_2, \ldots, v_k\}$ is an element of S_1, then $v_k - v_{k-1} = d+1$ and $n + v_1 - v_k > d$. Adding, this implies that $(v_k - v_{k-1}) + (n + v_1 - v_k) > 2d+1$, or $(n-d-1) + v_1 - v_{k-1} > d$. Hence, $\phi(v_1, v_2, \ldots, v_k)$ is an independent set of A'_n.

Therefore, we have established that ϕ is a bijection between the sets in S_1 and the independent sets of cardinality $k-1$ in $A'_n \simeq A_{n-d-1}$. We conclude that $|S_1| = [x^{k-1}]A_{n-d-1}$.

<u>*Case 2:*</u> Proving $|S_2| = [x^k]A_{n-1}$.

We now establish a bijection φ between S_2 and the set of independent k-tuples in A_{n-1}. For each element $(v_1, v_2, \ldots, v_{k-1}, v_k)$ of S_2, define

$$\varphi(v_1, v_2, \ldots, v_{k-1}, v_k) = \{v_1, v_2, \ldots, v_{k-1}, v_k - 1\}.$$

Observe that φ is one-to-one. Construct the graph A''_n by contracting v_k to $v_k - 1$. Then, $A''_n \simeq A_{n-1}$. We claim that $\varphi(v_1, v_2, \ldots, v_k)$ is an independent set of A''_n iff $\{v_1, v_2, \ldots, v_k\}$ is an element of S_2. As we did in the previous case, we establish this claim by listing the necessary and sufficient conditions, and showing that they are equivalent.

Note that $\varphi(v_1, v_2, \ldots, v_k)$ is an independent set of A''_n iff

(a) $v_{i+1} - v_i > d$ for $1 \leq i \leq k-2$.

(b) $(v_k - 1) - v_{k-1} > d$.

(c) $(n-1) + v_1 - (v_k - 1) > d$.

Also, $\{v_1, v_2, \ldots, v_k\}$ is an element of S_2 iff

(a) $v_{i+1} - v_i > d$ for $1 \leq i \leq k-2$.

(b) $v_k - v_{k-1} > d + 1$.

(c) $n + v_1 - v_k > d$.

Clearly, these sets of conditions are equivalent. Therefore, we have established that φ is a bijection between the sets in S_2 and the independent sets of cardinality k in $A''_n \simeq A_{n-1}$. We conclude that $|S_2| = [x^k]A_{n-1}$.

Therefore, we have shown that $[x^k]A_n = [x^{k-1}]A_{n-d-1} + [x^k]A_{n-1}$ for all $n \geq 2d+2$, which implies that $I(A_n, x) = I(A_{n-1}, x) + x \cdot I(A_{n-d-1}, x)$. ∎

Now we find an explicit formula for $I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$, where $d \geq 1$ is a fixed integer.

Theorem 2.3 *Let $n \geq d+1$. Then $\deg(I(A_n, x)) = \lfloor \frac{n}{d+1} \rfloor$ and*

$$I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x) = \sum_{k=0}^{\lfloor \frac{n}{d+1} \rfloor} \frac{n}{n-dk} \binom{n-dk}{k} x^k.$$

Proof: By Lemma 2.2, $I(A_n, x) = I(A_{n-1}, x) + x \cdot I(A_{n-d-1}, x)$, for $n \geq 2d+2$. We will prove the theorem using generating functions.

$$\text{Let } f_n = \begin{cases} I(A_n, x) & \text{for } n \geq d+1 \\ 1 & \text{for } 1 \leq n \leq d \\ d+1 & \text{for } n = 0 \end{cases}$$

Each f_n is a polynomial in x. First, we verify that $f_n = f_{n-1} + xf_{n-d-1}$, for all $n \geq d+1$. This recurrence is true for $n \geq 2d+2$, by Lemma 2.2. For $d+2 \leq n \leq 2d+1$, we have $f_n = 1 + nx = (1 + (n-1)x) + x \cdot 1 = f_{n-1} + xf_{n-d-1}$. Finally, for $n = d+1$, we have $f_{d+1} = 1 + (d+1)x = f_d + xf_0$. Thus, $f_n = f_{n-1} + xf_{n-d-1}$, for all $n \geq d+1$.

Let $F(x, y) = \sum_{p=0}^{\infty} f_p y^p$. For each $n \geq d+1$, we will show that

$$[x^k y^n]F(x, y) = \frac{n}{n-dk}\binom{n-dk}{k}.$$

Since $f_n = f_{n-1} + xf_{n-d-1}$, for all $n \geq d+1$, we have

$$\begin{aligned}
\sum_{n=d+1}^{\infty} f_n y^n &= \sum_{n=d+1}^{\infty} f_{n-1} y^n + \sum_{n=d+1}^{\infty} f_{n-d-1} x y^n \\
F(x, y) - \sum_{n=0}^{d} f_n y^n &= y\left(F(x, y) - \sum_{n=0}^{d-1} f_n y^n\right) + xy^{d+1}F(x, y) \\
F(x, y)(1 - y - xy^{d+1}) &= f_0 + f_1 y + \sum_{n=2}^{d} f_n y^n - f_0 y - \sum_{n=1}^{d-1} f_n y^{n+1} \\
F(x, y)(1 - y - xy^{d+1}) &= f_0 + f_1 y + \sum_{n=2}^{d} y^n - f_0 y - \sum_{n=2}^{d} y^n \\
F(x, y)(1 - y - xy^{d+1}) &= (d+1) + y - (d+1)y \\
F(x, y) &= (d+1-dy)(1 - y - xy^{d+1})^{-1}
\end{aligned}$$

$$
\begin{aligned}
&= (d+1-dy)\sum_{t=0}^{\infty}(y+xy^{d+1})^t \\
&= (d+1-dy)\sum_{t=0}^{\infty} y^t(1+xy^d)^t \\
&= (d+1-dy)\sum_{t=0}^{\infty}\sum_{u=0}^{\infty}\binom{t}{u}x^u y^{t+du} \\
&= (d+1)\sum_{t,u=0}^{\infty}\binom{t}{u}x^u y^{t+du} - d\sum_{t,u=0}^{\infty}\binom{t}{u}x^u y^{t+du+1}.
\end{aligned}
$$

Now we extract the $x^k y^n$ coefficient of $F(x,y)$.

$$
\begin{aligned}
[x^k y^n]F(x,y) &= [x^k y^n](d+1)\sum_{t,u=0}^{\infty}\binom{t}{u}x^u y^{t+du} - [x^k y^n]d\sum_{t,u=0}^{\infty}\binom{t}{u}x^u y^{t+du+1} \\
&= (d+1)\binom{n-dk}{k} - d\binom{n-dk-1}{k} \\
&= \binom{n-dk}{k} + d\left[\binom{n-dk}{k} - \binom{n-dk-1}{k}\right] \\
&= \binom{n-dk}{k} + d\binom{n-dk-1}{k-1} \\
&= \binom{n-dk}{k} + \frac{dk}{n-dk}\binom{n-dk}{k} \\
&= \frac{n}{n-dk}\binom{n-dk}{k}.
\end{aligned}
$$

Therefore, we have proven that $[x^k]I(A_n,x) = [x^k y^n]F(x,y) = \frac{n}{n-dk}\binom{n-dk}{k}$. We note that this coefficient is non-zero precisely when $n-dk \geq k$, which is equivalent to the inequality $k \leq \frac{n}{d+1}$. Hence, $\deg(I(A_n,x)) = \lfloor \frac{n}{d+1} \rfloor$.

We conclude that $I(C_{n,\{1,2,\ldots,d\}},x) = \displaystyle\sum_{k=0}^{\lfloor \frac{n}{d+1} \rfloor} \frac{n}{n-dk}\binom{n-dk}{k}x^k.$ ∎

As a corollary, we have a formula for $I(C_n,x)$ by setting $d=1$. This formula has previously appeared in the literature, via alternate methods of proof.

Corollary 2.4 ([81, 87]) $I(C_n,x) = \displaystyle\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n}{n-k}\binom{n-k}{k}x^k.$

It would be ideal if similar recurrence relations could be found for other sets S. This would enable us to find explicit formulas for $I(G, x)$ for many other families of circulant graphs. However, no simple recurrence relation appears to exist for any other set (or family) S, even for the two-element set $S = \{1, \lfloor \frac{n}{2} \rfloor\}$. Thus, we will need to develop more sophisticated techniques to compute our independence polynomials.

We now develop a sophisticated combinatorial technique to compute the dependence polynomial of the d^{th} power of C_n, i.e., the independence polynomial of $C_{n,S}$, where $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$.

2.2 The Family $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$

Definition 2.5 *Let $d \geq 0$ be a fixed integer. For each $n \geq 2d+2$, define the graph* $\boldsymbol{B_n}$ *as the complement of A_n. Specifically,*

$$B_n := \overline{A_n} = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}.$$

Note that if $n = 2d+2$, then B_n is the disjoint union of $d+1$ copies of K_2, so $I(B_n, x) = [I(K_2, x)]^{d+1} = (1+2x)^{d+1}$, by Theorem 1.6. We will find an explicit formula for $I(B_n, x) = I(\overline{A_n}, x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}, x)$, for all $n \geq 2d+2$. Our formula will be extremely complicated, and the proof will require many technical lemmas.

First, we introduce the following definition, which will be used frequently throughout the thesis.

Definition 2.6 *For each k-tuple $\{v_1, v_2, \ldots, v_k\}$ of the vertices of a graph G on n vertices, with $0 \leq v_1 < v_2 < \ldots < v_k \leq n-1$, the* **difference sequence** *is*

$$(d_1, d_2, \ldots, d_k) = (v_2 - v_1, v_3 - v_2, \ldots, v_k - v_{k-1}, n + v_1 - v_k).$$

As we did in the proof of Lemma 2.2, we can visualize difference sequences as follows: spread n vertices around a circle, and highlight the k chosen vertices $v_1, v_2, \ldots, v_k$. Now let d_i be the distance between v_i and v_{i+1}, for each $1 \leq i \leq k$ (note: $v_{k+1} := v_1$).

In other words, the d_i's just represent the distances between each pair of highlighted vertices. By this reasoning, it is clear that $\sum_{i=1}^{k} d_i = n$ and that $v_j = v_1 + \sum_{i=1}^{j-1} d_i$ for each $1 \leq j \leq k$.

Difference sequences will be of tremendous help in counting the number of independent sets. We will carefully study the structure of these difference sequences, and determine a direct correlation to independent sets.

To illustrate with an example, suppose we have $n = 14$ and $d = 4$. Then $\{0, 1, 11, 12\}$ is an independent set of cardinality 4 in $B_{14} = C_{14,\{5,6,7\}}$. The corresponding difference sequence is $(1, 10, 1, 2)$. For each $0 \leq j \leq 13$, consider the set $I_j = \{j, j+1, j+11, j+12\}$, where the elements are reduced modulo 14 and sorted in increasing order. For example, $I_7 = \{4, 5, 7, 8\}$, which has a difference sequence of $(1, 2, 1, 10)$. Note that each I_j is an independent set, and that its difference sequence must be a cyclic permutation of $D = (1, 10, 1, 2)$. Furthermore it is apparent that the I_j's are the only (independent) sets with a difference sequence that is a cyclic permutation of D.

Instead of directly enumerating the independent sets I of B_n, it will be easier to determine all possible difference sequences D that correspond to an independent set of B_n, and then enumerate the number of independent sets corresponding to these difference sequences. For notational convenience, we introduce the following definition.

Definition 2.7 *A difference sequence $D = (d_1, d_2, \ldots, d_k)$ of the circulant $C_{n,S}$ is* $\boldsymbol{(n,S)}$**−valid** *if no cyclic subsequence of consecutive d_i's sum to an element in S.*

By a *cyclic* subsequence of consecutive terms, we refer to subsequences such as $(d_{k-2}, d_{k-1}, d_k, d_1, d_2, d_3, d_4)$. From now on, when we refer to subsequences of D, this will automatically include all cyclic subsequences.

For further notational convenience, we will just say that D is *valid*, since the pair (n, S) will be clear in all situations.

We note that each independent set I of B_n maps to a valid difference sequence D. The following lemma is immediate from the definitions, and so we omit the proof.

Lemma 2.8 *Let* $I = \{v_1, v_2, \ldots, v_k\}$ *have difference sequence* $D = (d_1, d_2, \ldots, d_k)$. *Then,* I *is independent in* $C_{n,S}$ *iff* D *is valid.*

We will now describe an explicit construction of all valid difference sequences with k elements, and this will yield the total number of independent sets with cardinality k. We will find a formula for $I(B_n, x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}}, x)$, for all $n \geq 2d+2$. As a preliminary result, we cite the following result by Michael and Traves, which is straightforward to prove.

Proposition 2.9 ([133]) *Let* $n \geq 3d+1$. *Then,* $I(B_n, x) = 1 + nx(1+x)^d$.

However, it is a difficult matter to compute $I(B_n, x)$ for $2d+2 < n \leq 3d$. In this case, there is no known combinatorial technique to determine the number of independent sets of cardinality k. Much more sophisticated methods are required to develop an explicit formula for $I(B_n, x)$, as evidenced by the statement of the following theorem, which is the main result in this section.

Theorem 2.10 *Let* $r = n - 2d - 2 \geq 0$. *Then,*

$$I(B_n, x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}}, x) = 1 + \sum_{l=0}^{\lfloor\frac{d}{r+2}\rfloor} \frac{n}{2l+1}\binom{d-lr}{2l} x^{2l+1}(1+x)^{d-l(r+2)}.$$

From this theorem, we can deduce corollaries such as the following. The first identity is simply Proposition 2.9.

Corollary 2.11 *Let* (n, d) *be an ordered pair of positive integers satisfying* $n \geq 2d+2$.

(a) If $\frac{n}{d} > 3$, *then* $I(B_n, x) = 1 + nx(1+x)^d$.

(b) If $\frac{5}{2} < \frac{n}{d} \leq 3$, *then* $I(B_n, x) = 1 + nx(1+x)^d + \frac{n}{3}\binom{3d-n+2}{2}x^3(1+x)^{3d-n}$.

(c) If $\frac{7}{3} < \frac{n}{d} \leq \frac{5}{2}$, *then* $I(B_n, x)$ *equals*

$$1 + nx(1+x)^d + \frac{n}{3}\binom{3d-n+2}{2}x^3(1+x)^{3d-n} + \frac{n}{5}\binom{5d-2n+4}{4}x^5(1+x)^{5d-2n}.$$

<u>Proof:</u> Let n and d be fixed. For each $l \geq 0$, define the polynomial

$$g_l(x) = \frac{n}{2l+1}\binom{d-lr}{2l} x^{2l+1}(1+x)^{d-l(r+2)}.$$

In Theorem 2.10, the expression $g_l(x)$ is summed from $l = 0$ to $l = \lfloor \frac{d}{r+2} \rfloor = \lfloor \frac{d}{n-2d} \rfloor$.

If $n > 3d$, then $\frac{d}{n-2d} < \frac{d}{d} = 1$, and so $\lfloor \frac{d}{n-2d} \rfloor = 0$. It follows that $I(B_n, x) = 1 + g_0(x) = 1 + nx(1+x)^d$.

If $\frac{5}{2} < \frac{n}{d} \leq 3$, then $1 = \frac{d}{d} \leq \frac{d}{n-2d} < \frac{d}{\frac{d}{2}} = 2$, and so $\lfloor \frac{d}{n-2d} \rfloor = 1$. It follows that $I(B_n, x) = 1 + g_0(x) + g_1(x)$. We now compute $g_0(x)$ and $g_1(x)$ to get the desired identity.

If $\frac{7}{3} < \frac{n}{d} \leq \frac{5}{2}$, then $2 = \frac{d}{\frac{d}{2}} \leq \frac{d}{n-2d} < \frac{d}{\frac{d}{3}} = 3$, and so $\lfloor \frac{d}{n-2d} \rfloor = 2$. It follows that $I(B_n, x) = 1 + g_0(x) + g_1(x) + g_2(x)$. We now compute $g_0(x)$, $g_1(x)$, and $g_2(x)$ to get the desired identity. ∎

It appears that these identities cannot be simplified any further, and that Theorem 2.10 is the closed-form identity that we seek. To prove Theorem 2.10, we require several technical combinatorial lemmas. However, the first one is straightforward.

Lemma 2.12 *Let n and k be positive integers, with $n \geq k$. Let $\tau(n,k)$ be the number of ordered k-tuples $(a_1, a_2, \ldots, a_k)$ of positive integers such that $\sum_{i=1}^{k} a_i \leq n$. Then, $\tau(n,k) = \binom{n}{k}$.*

<u>Proof:</u> By a simple and well-known combinatorial argument, there are $\binom{j-1}{k-1}$ ordered k-tuples $(a_1, a_2, \ldots, a_k)$ of positive integers with sum exactly j. Therefore, $\tau(n,k) = \binom{k-1}{k-1} + \binom{k}{k-1} + \binom{k+1}{k-1} + \ldots + \binom{n-1}{k-1} = \binom{n}{k}$, which follows from repeated applications of Pascal's Identity. ∎

We now introduce l-constructible difference sequences. While the definition may appear contrived, it is precisely the insight we need to count the number of valid difference sequences of B_n. We will show that every valid difference sequence is uniquely l-constructible, for exactly one integer $l \geq 0$. Then in our proof of Theorem 2.10, we will enumerate the number of l-constructible difference sequences to determine the number of independent sets of each cardinality.

Definition 2.13 *Let D be a difference sequence of $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$, where $n \geq 2d+2$. Then, for each integer $l \geq 0$, D is* ***l*-constructible** *if D can be expressed in the form*

$$D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}$$

such that the following properties hold.

1. *Each p_i is an integer satisfying $p_i \geq n - 2d$.*
2. *Each Q_i is a sequence of integers, possibly empty.*
3. *Let S be any (cyclic) subsequence of consecutive terms in D with sum $\sum S$. If S contains at most l of the p_i's, then $\sum S \leq d$. Otherwise, $\sum S \geq n - d$.*

We will prove that every valid difference sequence can be expressed uniquely as an l-constructible sequence, for exactly one $l \geq 0$. We will then enumerate the number of l-constructible sequences for each l, which will give us the total number of valid difference sequences.

A difference sequence D of $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$ is valid iff no subsequence of consecutive terms adds up to an element in $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. Since the complement of any consecutive subsequence of D is also a consecutive subsequence of D, there exists a consecutive subsequence with sum t iff there exists a consecutive subsequence with sum $n - t$. In other words, D is valid iff no subsequence of consecutive terms sums to an element in $[d+1, n-d-1]$.

By the third property in the definition of l-constructibility (see above), every l-constructible sequence is necessarily valid because every subsequence of consecutive terms has sum at most d or at least $n-d$, and hence falls outside of the forbidden range $[d+1, n-d-1]$. So every l-constructible sequence is a valid difference sequence. In the next two lemmas, we prove that every valid difference sequence is *uniquely* l-constructible, for exactly one $l \geq 0$. First, we construct an l that satisfies the conditions, and then prove that no other l suffices.

To supplement the technical details of the following proof, let us describe our method by illustrating an example.

Consider the case $n = 89$ and $d = 40$. It is straightforward to show that the difference sequence $D = \{9, 1, 9, 1, 9, 20, 10, 19, 2, 9\}$ is valid, i.e., no subsequence of consecutive elements sums to any $S \in [41, 48]$. We prove that this difference sequence D is uniquely 2-constructible, up to cyclic permutation.

Lemma 2.14 *Let D be a valid difference sequence of B_n. Then there exists an integer $l \geq 0$ such that D is l-constructible. For this integer l, D is l-constructible in a unique way up to cyclic permutation, i.e., there is only one way to select the Q_i's and p_i's so that D is l-constructible.*

Proof: Let $D = R_1 t_1 R_2 t_2 \dots R_m t_m$, where each $t_i \geq n - 2d$ and each R_i is a (possibly empty) sequence of terms, all of which are less than $n - 2d$. Thus, each D has a unique representation in this form, up to cyclic permutation. In our example, $n - 2d = 9$. Without loss of generality, assume $t_1 = 20$. In this case, we *must* have $R_2 = \emptyset$, $t_2 = 10$, $R_3 = \emptyset$, $t_3 = 19$, $R_4 = \{2\}$, $t_4 = 9$, $R_5 = \emptyset$, $t_5 = 9$, $R_6 = \{1\}$, $t_6 = 9$, $R_7 = \{1\}$, $t_7 = 9$, and $R_1 = \emptyset$. In other words, we have

$$D = \underbrace{20}_{t_1}, \underbrace{10}_{t_2}, \underbrace{19}_{t_3}, \underbrace{2}_{R_4}, \underbrace{9}_{t_4}, \underbrace{9}_{t_5}, \underbrace{1}_{R_6}, \underbrace{9}_{t_6}, \underbrace{1}_{R_7}, \underbrace{9}_{t_7}.$$

Let $l \geq 0$ be the largest integer such that for any subsequence X of consecutive terms of D, $\sum X \leq d$ if X includes at most l of the t_i's. (In our example, $l < 3$ since $X = \{20, 10, 19\}$ includes three of the t_i's, and $\sum X = 49 > d$. By inspection, it can be checked that $l = 2$). For this $l \geq 0$, we prove that D is l-constructible, and that the assignment of Q_i's and p_i's is unique, up to cyclic permutation. It is important to note that the p_i's and t_i's represent individual terms, while the Q_i's and R_i's represent a sequence of terms.

First suppose that $m \leq 2l$. Note that $R_1 + t_1 + R_2 + t_2 + \ldots + R_l + t_l \leq d$ since this series contains exactly l of the t_i's. Similarly, $R_{l+1} + t_{l+1} + \ldots + R_{2l} + t_{2l} \leq d$. If $m \leq 2l$, then $n = \sum D \leq 2d < n$, a contradiction. Thus, $m \geq 2l + 1$. If $m = 2l + 1$, then we can set $Q_i = R_i$ and $p_i = t_i$ for each i. Then each D is l-constructible, since $\sum D \leq d$ if D contains at most l of the p_i's, and $\sum D \geq n - d$ otherwise. Note that this is the *only* assignment that enables D to be l-constructible, up to cyclic permutation.

So suppose that $m > 2l+1$. In this case, we will assign the p_i's and Q_i's from the set of t_i's and R_i's. All of the p_i's will be chosen from the set of t_i's, while all of the Q_i's will be determined from the R_i's, as well as any leftover t_i's not included among the p_i's. Thus, each p_i will be a single term, and each Q_i will be a (possibly empty) sequence of terms. Note that the p_i's must be chosen from the t_i's, since we require $p_i \geq n - 2d$ for each i. In our proof that the construction is unique, we will formally justify that each p_i must be at least $n - 2d$.

By the definition of the index $l \geq 0$, there must be a subsequence X containing $l+1$ of the t_i's such that its sum exceeds d. Since D is valid, no subsequence of consecutive terms can sum to any number in $[d+1, n-d-1]$. Therefore, $\sum X > d$ implies that $\sum X \geq n - d$.

Cyclically permute the elements of D so that this subsequence X appears at the front of D, i.e., redefine the R_i's and t_i's so that we have

$$t_1 + \sum R_2 + t_2 + \ldots + \sum R_{l+1} + t_{l+1} \geq n - d.$$

Then set $p_i = t_i$ for $1 \leq i \leq l+1$ and $Q_i = R_i$ for $2 \leq i \leq l+1$. In our example, we have $X = \{20, 10, 19\}$, $p_1 = 20$, $Q_2 = \emptyset$, $p_2 = 10$, $Q_3 = \emptyset$, and $p_3 = 19$. Note that this assignment of p_i's and Q_i's is necessary for D to be l-constructible: if any of these Q_i's contains a t_j term, then we will obtain a contradiction because the above subsequence X will have at most l of the p_i's, but its sum will exceed d.

If D is l-constructible, we require the chosen p_i's and Q_i's to satisfy

$$\sum Q_2 + p_2 + \ldots + \sum Q_{l+1} + p_{l+1} + \sum Q_{l+2} \leq d,$$

since this subsequence contains l of the p_i's. Also, we require

$$\sum Q_2 + p_2 + \ldots + \sum Q_{l+1} + p_{l+1} + \sum Q_{l+2} + p_{l+2} \geq n - d,$$

since this subsequence contains $l+1$ of the p_i's.

Let $T = \sum Q_2 + p_2 + \ldots + \sum Q_{l+1} + p_{l+1}$. Then $\sum Q_{l+2} \leq d - T$ and $\sum Q_{l+2} + p_{l+2} \geq n - d - T$. Since each p_i and Q_i has already been assigned for $2 \leq i \leq l+1$, T is a fixed integer. From these two inequalities, we claim that Q_{l+2} is uniquely determined. Note that for some $k \geq 0$, Q_{l+2} must be the first k elements of the sequence $X' = R_{l+2}, t_{l+2}, R_{l+3}, t_{l+3}, \dots R_m, t_m, R_1$. Furthermore, p_{l+2} would have to be the *next* term, i.e., the $(k+1)^{\text{th}}$ term of X'.

We claim that k must be the largest integer such that the first k terms of X' sum to at most $d-T$. This choice is unique because if k were not the largest integer, then $\sum Q_{l+2} + p_{l+2} \leq d-T$, and that contradicts the inequality $\sum Q_{l+2} + p_{l+2} \geq n-d-T$. Since k is uniquely determined, Q_{l+2} *must* represent the first k elements of X', in order for D to be l-constructible. Furthermore, p_{l+2} *must* be the next term in this subsequence. In our example, $T = 29$, $X' = \{2, 9, 9, 1, 9, 1, 9\}$, $Q_4 = \{2, 9\}$, and $p_4 = 9$.

Consider this sum $T + \sum Q_{l+2} + p_{l+2} > d$. By our choice of k, this sum exceeds d. Since D is valid, this sum must be at least $n-d$, since this total represents the sum of a subsequence of consecutive terms in D. Therefore, the fact that D is valid implies that $\sum Q_{l+2} + p_{l+2} \geq n-d-T$. Hence, by our construction, once we fix p_i and Q_i for $2 \leq i \leq l+1$, then Q_{l+2} and p_{l+2} are uniquely determined, and satisfy the properties of l-constructibility. Note that p_{l+2} must satisfy the inequality $p_{l+2} \geq n-2d$ since $T + \sum Q_{l+2} \leq d$ and $T + \sum Q_{l+2} + p_{l+2} \geq n-d$. By the same argument, each $p_i \geq n-2d$. This proves that each p_i is chosen from the set of t_i's.

Similarly, Q_i and p_i are uniquely determined for $i = l+2$, $i = l+3$, and all the way up to $i = 2l+1$. Once Q_{2l+1} and p_{2l+1} are chosen, we are left with k unselected terms for some $k \geq 0$. Then our only choice is to assign these k terms to Q_1. Thus, this assignment of p_i's and Q_i's must be unique, up to cyclic permutation. This completes the proof. ∎

In our example with $(n, d) = (89, 40)$, we have already determined p_i and Q_i for each $1 \leq i \leq 4$. By applying the above method, we see that $Q_5 = \{1\}$, $p_5 = 9$, and $Q_1 = \{1, 9\}$. We can readily verify that this representation of D into p_i's and Q_i's satisfies the properties of an l-constructible sequence. Thus, we have shown that every 2-constructible representation of D *must* be a cyclic permutation of

$$\underbrace{1,9}_{Q_1}, \underbrace{20}_{p_1}, \underbrace{10}_{p_2}, \underbrace{19}_{p_3}, \underbrace{2,9}_{Q_4}, \underbrace{9}_{p_4}, \underbrace{1}_{Q_5}, \underbrace{9}_{p_5}.$$

The next lemma shows that D is l-constructible for *only one* $l \geq 0$.

Lemma 2.15 *If D is l-constructible, then D is not l'-constructible, for any $l' \neq l$.*

Proof: Suppose that D is both l-constructible and l'-constructible. Without loss, suppose $l' < l$. Since D is l-constructible, we know that D can be expressed as

$$D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1},$$

such that $\sum S \leq d$ if S contains at most l of the p_i's, and $\sum S \geq n - d$ otherwise.

If D is l'-constructible, then D can also be expressed as

$$D = Q'_1, p'_1, Q'_2, p'_2, \ldots, Q'_{2l'+1}, p'_{2l'+1},$$

such that $\sum S \leq d$ if S contains at most l' of the p'_i's, and $\sum S \geq n - d$ otherwise.

For each $1 \leq j \leq 2l' + 1$, define X_j to be the subsequence

$$X_j = p'_j, Q'_{j+1}, p'_{j+1}, \ldots, Q'_{j+l'}, p'_{j+l'},$$

where the indices are reduced mod $(2l' + 1)$.

Since X_j contains exactly $l'+1$ of the p'_i's, $\sum X_j \geq n-d$. This sequence X_j appears exactly as a subsequence of consecutive terms in $D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}$. Since $\sum X_j \geq n - d$, it follows that X_j must contain at least $(l + 1)$ of the p_i's, since D is l-constructible.

For each $1 \leq j \leq 2l' + 1$, define $\Gamma(Q'_j)$ to be the number of p_i's that appear in Q'_j, and define $\Gamma(p'_j) = 1$ if $p'_j = p_i$ for some i, and $\Gamma(p'_j) = 0$ otherwise.

Since X_j contains at least $l + 1$ of the p_i's, we must have

$$\Gamma(p'_j) + \Gamma(Q'_{j+1}) + \Gamma(p'_{j+1}) + \ldots + \Gamma(Q'_{j+l'}) + \Gamma(p'_{j+l'}) \geq l + 1.$$

Summing over all $1 \leq j \leq 2l' + 1$, we have

$$l' \sum_{j=1}^{2l'+1} \Gamma(Q'_j) + (l' + 1) \sum_{j=1}^{2l'+1} \Gamma(p'_j) \geq (l + 1)(2l' + 1).$$

This identity follows because each $\Gamma(Q'_j)$ is counted l' times and each $\Gamma(p'_j)$ is counted $l' + 1$ times. This inequality can be rewritten as:

$$\sum_{j=1}^{2l'+1} \Gamma(Q'_j) \geq \frac{(l+1)(2l'+1) - (l'+1)\sum_{j=1}^{2l'+1}\Gamma(p'_j)}{l'}.$$

For each $1 \leq j \leq 2l'+1$, define Y_j to be the subsequence

$$Y_j = Q'_j, p'_j, Q'_{j+1}, p'_{j+1}, \ldots, Q'_{j+l'-1}, p'_{j+l'-1}, Q'_{j+l'},$$

where the indices are reduced mod $(2l'+1)$.

Since Y_j contains exactly l' of the p'_i's, $\sum Y_j \leq d$. This sequence Y_j appears exactly as a subsequence of consecutive terms in $D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}$. Since $\sum Y_j \leq d$, it follows that Y_j contains at most l of the p_i's, since D is l-constructible. Therefore, we have

$$\Gamma(Q'_j) + \Gamma(p'_j) + \Gamma(Q'_{j+1}) + \Gamma(p'_{j+1}) + \ldots + \Gamma(p'_{j+l'-1}) + \Gamma(Q'_{j+l'}) \leq l.$$

Summing over all $1 \leq j \leq 2l'+1$, we have

$$(l'+1)\sum_{j=1}^{2l'+1} \Gamma(Q'_j) + l'\sum_{j=1}^{2l'+1} \Gamma(p'_j) \leq l(2l'+1).$$

This inequality can be rewritten as

$$\sum_{j=1}^{2l'+1} \Gamma(Q'_j) \leq \frac{l(2l'+1) - l'\sum_{j=1}^{2l'+1}\Gamma(p'_j)}{l'+1}.$$

So now we have two inequalities in terms of $\displaystyle\sum_{j=1}^{2l'+1} \Gamma(Q'_j)$ and $\displaystyle\sum_{j=1}^{2l'+1} \Gamma(p'_j)$. From these two inequalities, we have

$$\begin{aligned}
\frac{(l+1)(2l'+1)-(l'+1)\sum_{j=1}^{2l'+1}\Gamma(p'_j)}{l'} &\leq \frac{l(2l'+1)-l'\sum_{j=1}^{2l'+1}\Gamma(p'_j)}{l'+1} \\
(l+1)(l'+1)(2l'+1)-(l'+1)^2\sum_{j=1}^{2l'+1}\Gamma(p'_j) &\leq ll'(2l'+1)-l'^2\sum_{j=1}^{2l'+1}\Gamma(p'_j) \\
(2l'+1)\sum_{j=1}^{2l'+1}\Gamma(p'_j) &\geq (2l'+1)(l+1)(l'+1)-(2l'+1)ll' \\
\sum_{j=1}^{2l'+1}\Gamma(p'_j) &\geq ll'+l+l'+1-ll' \\
\sum_{j=1}^{2l'+1}\Gamma(p'_j) &= l+l'+1 \\
\sum_{j=1}^{2l'+1}\Gamma(p'_j) &> 2l'+1 \quad (\text{since } l>l').
\end{aligned}$$

By the Pigeonhole Principle, we must have $\Gamma(p'_j) > 1$ for some index j. However, each $\Gamma(p'_j) \leq 1$ and this gives us our desired contradiction.

Therefore, we have shown that for any $l' \neq l$, D is not l'-constructible if D is l-constructible. ∎

We require one final result. In the following lemma, we will count the number of m-tuples $(Q_1, Q_2, \ldots, Q_m)$ with a fixed sum that contain a total of t non-zero elements among the Q_i's. In this case, each Q_i is a (possibly empty) sequence of positive integers. We require this lemma when enumerating the number of valid difference sequences.

Lemma 2.16 *Let $a_1, a_2, \ldots, a_m$ be non-negative integers with sum k. Then there are exactly $\binom{k}{t}$ m-tuples $(Q_1, Q_2, \ldots, Q_m)$ that contain a total of t non-zero elements among the Q_i's, where each Q_i is a (possibly empty) sequence of positive integers whose sum is at most a_i.*

<u>Proof:</u> Write down a string of k ones, and place $m-1$ bars in between the ones to create the partition corresponding to the m-tuple $(a_1, a_2, \ldots, a_m)$. Now select any t of the k ones.

As an example, we demonstrate this for the case $(a_1, a_2, a_3) = (5, 6, 4)$, $m = 3$, $k = 15$, and $t = 6$.

$$1, \underline{\mathbf{1}}, 1, \underline{\mathbf{1}}, 1 | \underline{\mathbf{1}}, \underline{\mathbf{1}}, 1, 1, 1, \underline{\mathbf{1}} | 1, \underline{\mathbf{1}}, 1, 1.$$

Clearly, there are $\binom{k}{t}$ ways to select exactly t ones from this string. We map each selection to a unique m-tuple $(Q_1, Q_2, \ldots, Q_m)$ which contains a total of t non-zero elements among the Q_i's, so that the sum of the elements in each Q_i is at most a_i.

Consider the substring of a_i ones in the i^{th} partition. If no elements are selected from this substring, set $Q_i = \emptyset$. Otherwise, let the selected elements in the i^{th} partition be in positions $r_1, r_2, \ldots, r_p$, where $1 \leq r_1 < r_2 < \ldots < r_p \leq a_i$. Now define

$$Q_i = (r_2 - r_1, r_3 - r_2, \ldots, r_p - r_{p-1}, a_i + 1 - r_p).$$

In the above example, our selection of the t's corresponds to the sequences $Q_1 = (2, 2)$, $Q_2 = (1, 4, 1)$, $Q_3 = (3)$, which contain a total of $t = 6$ non-zero elements.

Note that for each i, $\sum Q_i = a_i + 1 - r_1 \leq a_i$. This construction guarantees that each of the $\binom{k}{t}$ selections maps to a unique m-tuple $(Q_1, Q_2, \ldots, Q_m)$ with a total of t non-zero elements, so that $\sum Q_i \leq a_i$. Given such an m-tuple, we now justify that we can determine the unique way the t ones were selected from the string. For each substring of ones in the i^{th} partition, we are given Q_i. From the above definition for Q_i, we can determine the values (or positions) of the r_j's by starting at r_p and calculating backwards. From r_p, we can uniquely compute r_{p-1}, r_{p-2}, and so on, until we have determined all of the r_j's, where $1 \leq j \leq p$. Since we can repeat this process for each i, each selection of the m-tuple $(Q_1, Q_2, \ldots, Q_m)$ corresponds to a unique selection of t elements from a string of k ones. Hence, this construction is bijective, and our proof is complete. ∎

We are finally ready to prove Theorem 2.10.

Proof: By definition, in an l-constructible sequence, every subsequence of consecutive terms has a sum outside the range $[d + 1, n - d - 1]$. Therefore, each l-constructible sequence is valid in B_n, for every $l \geq 0$. By Lemma 2.14 and Lemma 2.15, we have shown that there is a bijection between the set of valid difference sequences of B_n and the union of all l-constructible sequences for $l \geq 0$. Every valid difference sequence D

corresponds to a unique l-constructible sequence, for exactly one $l \geq 0$. To determine the number of valid difference sequences of B_n, it suffices to determine the number of l-constructible sequences for each $l \geq 0$, and then enumerate its union.

Let D be an l-constructible sequence, for some fixed $l \geq 0$. Thus, D is valid in B_n. By definition, any subsequence of consecutive terms containing l of the p_i's must sum to at most d.

Consider an l-constructible sequence $D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}$. We enumerate the number of all possible l-constructible sequences, for this fixed $l \geq 0$. We will show that each l-constructible sequence D must be generated in the following way:

(a) Choose $(a_1, a_2, \ldots, a_{2l+1})$ to be an ordered $(2l+1)$-tuple of non-negative integers with sum $k = (2l+1)d - ln$.

(b) Select $Q_1, Q_2, \ldots, Q_{2l+1}$ so that $\sum Q_j \leq a_{j+l+1}$ for each $1 \leq j \leq 2l+1$. Note that for $j \geq l+1$, the index $j+l+1$ is reduced mod $(2l+1)$.

(c) From this, each p_j is uniquely determined, and satisfies $p_j \geq n - 2d$.

(d) The sequence $D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}$ is l-constructible.

Each of these steps is simple to enumerate, and this will enable us to count the total number of l-constructible difference sequences.

Define $X_j = Q_j, p_j, \ldots, Q_{j+l-1}, p_{j+l-1}$ for each $1 \leq j \leq 2l+1$, where the indices are reduced mod $(2l+1)$. Since X_j contains l of the p_i's, $\sum X_j \leq d$. Let a_j be the integer for which $\sum X_j = d - a_j$. Then each $a_j \geq 0$.

Let $X'_j = X_j, Q_{l+j}$. Then $\sum X'_j \leq d$ because X'_j contains only l of the p_i's. Hence, $\sum X'_j = \sum X_j + \sum Q_{l+j} \leq d$, which implies that $\sum Q_{l+j} \leq a_j$. This is true for each j, so adding $l+1$ to both indices and reducing mod $(2l+1)$, we have $\sum Q_j \leq a_{j+l+1}$.

Note that

$$\begin{aligned}\sum Q_j + p_j &= n - \sum X_{j+1} - \sum X_{j+l+1}\\ &= n - (d - a_{j+1}) - (d - a_{j+l+1})\\ &= n - 2d + a_{j+1} + a_{j+l+1}.\end{aligned}$$

Since $\sum Q_j \leq a_{j+l+1}$, it follows that $p_j \geq n - 2d + a_{j+1} \geq n - 2d$, which is consistent with the definition of l-constructibility.

Let $k = \sum a_j$. We have $\sum X_j = d - a_j$ for each j. Adding these $2l+1$ sums, we have $ln = (2l+1)d - k$, or $k = (2l+1)d - ln \geq 0$. So k is fixed.

A simple combinatorial argument shows that there are $\binom{k+2l}{2l}$ ways to select the $(2l+1)$-tuple $(a_1, a_2, \ldots, a_{2l+1})$ so that each a_j is a non-negative integer with total sum k. For each of these $(2l+1)$-tuples, we select our Q_j's so that $\sum Q_j \leq a_{j+l+1}$ for each $1 \leq j \leq 2l+1$. By Lemma 2.16, if our Q_j's have a *total* of t non-zero elements among them, then our selection of the Q_j's can be made in exactly $\binom{k}{t}$ ways.

This l-constructible sequence D will contain a total of $2l+t+1$ terms, with t of them coming from the union of the Q_j's, and one for each of the $2l+1$ p_i's. So there are $\binom{k+2l}{2l}\binom{k}{t}$ possible l-constructible sequences with $2l+t+1$ terms. Therefore, there are this many valid difference sequences of B_n with $2l+t+1$ terms. Note that some of these sequences are cyclic permutations of others, and we will take this into account when we determine the number of independent sets with $2l+t+1$ vertices.

Let Ψ be the set of pairs (v, D), where v is a vertex of B_n and D is any of the $\binom{k+2l}{2l}\binom{k}{t}$ l-constructible sequences with $2l+t+1$ elements. Each of the $n\binom{k+2l}{2l}\binom{k}{t}$ pairs in Ψ will correspond to an independent set I with $2l+t+1$ vertices:

$$I = \{v, v + d_1, v + d_1 + d_2, \ldots, v + d_1 + d_2 + \ldots + d_{2l+t}\},$$

where the elements are reduced modulo n and arranged in increasing order.

We now justify that each independent set I appears exactly $(2l+1)$ times by this construction. The key insight is that when I is turned into a difference sequence D, this D must be an l-constructible sequence, and hence has the following form:

$$D = Q_1, p_1, Q_2, p_2, \ldots, Q_{2l+1}, p_{2l+1}.$$

Therefore, there are exactly $(2l+1)$ cyclic permutations of D so that it retains the form of an l-constructible sequence: for each cyclic permutation, the sequence begins with the set Q_i, for some $1 \leq i \leq 2l+1$. Thus, we must divide the total number of independent sets by $(2l+1)$, as each one is repeated this many times. In other words, there are $\frac{n}{2l+1}\binom{k+2l}{2l}\binom{k}{t}$ independent sets with $2l+t+1$ vertices.

Since this is true for each $l \geq 0$ and $0 \leq t \leq k = (2l+1)d - ln$, it follows that

$$\begin{aligned} I(B_n, x) &= 1 + \sum_{l \geq 0} \sum_{t=0}^{k} \frac{n}{2l+1} \binom{k+2l}{2l} \binom{k}{t} x^{2l+1+t} \\ &= 1 + \sum_{l \geq 0} \frac{n}{2l+1} \binom{k+2l}{2l} x^{2l+1} \sum_{t=0}^{k} \binom{k}{t} x^t \\ &= 1 + \sum_{l \geq 0} \frac{n}{2l+1} \binom{k+2l}{2l} x^{2l+1} (1+x)^k \\ &= 1 + \sum_{l \geq 0} \frac{n}{2l+1} \binom{(2l+1)d - l(n-2)}{2l} x^{2l+1} (1+x)^{(2l+1)d-ln}. \end{aligned}$$

Note that we require $k = (2l+1)d - ln \geq 0$ for there to be any independent sets. Thus, $l \leq \frac{d}{n-2d}$. Letting $r = n - 2d - 2$, we conclude that

$$I(C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}, x) = 1 + \sum_{l=0}^{\lfloor \frac{d}{r+2} \rfloor} \frac{n}{2l+1} \binom{d-lr}{2l} x^{2l+1} (1+x)^{d-l(r+2)}.$$

This concludes the proof of Theorem 2.10. ∎

Since $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$, we have $B_{2d+2} = C_{2d+2,\{d+1\}}$, which is isomorphic to $d+1$ disjoint copies of K_2. In other words, $I(B_{2d+2}, x) = (1+2x)^{d+1}$. In the following corollary, we verify that our complicated formula for $I(B_n, x)$ is consistent with the observation that $I(B_{2d+2}, x) = (1+2x)^{d+1}$.

Corollary 2.17 *For any fixed d, $I(B_{2d+2}, x) = (1+2x)^{d+1}$.*

Proof: By Theorem 2.10,

$$I(B_{2d+2}, x) - 1 = \sum_{l=0}^{\lfloor \frac{d}{2} \rfloor} \frac{n}{2l+1} \binom{d}{2l} x^{2l+1} (1+x)^{d-2l}.$$

We prove that the right side of the identity equals $(1+2x)^{d+1}-1$. We have

$$\begin{aligned}
(1+2x)^{d+1}-1 &= ((1+x)+x)^{d+1}-((1+x)-x)^{d+1} \\
&= \sum_{i=0}^{d+1}\binom{d+1}{i}(1+x)^i x^{d+1-i} - \sum_{i=0}^{d+1}\binom{d+1}{i}(1+x)^i(-x)^{d+1-i} \\
&= \sum_{i=0}^{d+1}\binom{d+1}{i}(1+x)^i x^{d+1-i}(1+(-1)^{d-i}) \\
&= \sum_{d-i \quad \text{is even}}^{d+1} 2\binom{d+1}{i}(1+x)^i x^{d+1-i} \\
&= \sum_{l=0}^{\lfloor \frac{d}{2} \rfloor} 2\binom{d+1}{d-2l} x^{2l+1}(1+x)^{d-2l} \\
&= \sum_{l=0}^{\lfloor \frac{d}{2} \rfloor} \frac{2(d+1)!}{(2l+1)!(d-2l)!} x^{2l+1}(1+x)^{d-2l} \\
&= \sum_{l=0}^{\lfloor \frac{d}{2} \rfloor} \frac{2d+2}{2l+1}\frac{d!}{(2l)!(d-2l)!} x^{2l+1}(1+x)^{d-2l} \\
&= \sum_{l=0}^{\lfloor \frac{d}{2} \rfloor} \frac{n}{2l+1}\binom{d}{2l} x^{2l+1}(1+x)^{d-2l}.
\end{aligned}$$

This completes our proof. ∎

As an additional corollary, we now have a formula for $\alpha(B_n)$, since this is just the degree of $I(B_n, x)$.

Corollary 2.18 *Let* $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$. *Then,* $\alpha(B_n) = d+1$. *Furthermore,* $[x^{d+1}]I(B_n, x) = 2^{\frac{n}{2}}$ *if* $n = 2d+2$ *and* $[x^{d+1}]I(B_n, x) = n$ *if* $n > 2d+2$.

Proof: If $n = 2d+2$, then $B_n = C_{2d+2,\{d+1\}}$, and so $I(B_n, x) = (1+2x)^{d+1}$. Thus, $[x^{d+1}]I(B_n, x) = 2^{d+1} = 2^{\frac{n}{2}}$. Thus, assume that $n > 2d+2$, i.e., $r = n-2d-2 > 0$.

Theorem 2.10 gives us a formula for $I(B_n, x)$, where $r = n-2d-2 > 0$ is a fixed integer. For each $0 \leq l \leq \lfloor \frac{d}{r+2} \rfloor$, our formula for $I(B_n, x)$ adds a polynomial of degree $2l+1+d-l(r+2) = d-lr+1$. Thus, $\alpha(B_n) = \deg(I(B_n, x)) = d+1$. Furthermore, x^{d+1} terms appear in our polynomial precisely when $l = 0$ or $r = 0$.

From our assumption that $r > 0$, an x^{d+1} term can only appear when $l = 0$. From this, we immediately derive the desired result that $[x^{d+1}]I(B_n, x) = n$. ∎

2.3 Circulants of Degree at Most 3

Armed with these theorems, we now find an explicit formula for $I(C_{n,S}, x)$ for all circulants of degree at most 3. While this may appear to be a straightforward problem, we will discover that calculating the independence polynomials of 3-regular circulants is surprisingly difficult.

The degree 1 case is trivial, as the only 1-regular circulant is $G = C_{2n,\{n\}}$ for some positive integer n. Then, G is a disjoint union of n edges, and so Theorem 1.6 gives us $I(G, x) = I(K_2, x)^n = (1 + 2x)^n$.

Let G be 2-regular. Then $G = C_{n,\{a\}}$ for some $1 \leq a < \frac{n}{2}$. Let $d = \gcd(n, a)$. Then G is a disjoint union of d cycles with $\frac{n}{d}$ vertices [68]. By Corollary 2.4 and Theorem 1.6, it follows that

$$I(G, x) = I(C_{\frac{n}{d}}, x)^d = \left(\sum_{k=0}^{\lfloor \frac{n}{2d} \rfloor} \frac{n}{n - dk} \binom{\frac{n}{d} - k}{k} x^k \right)^d .$$

The interesting case occurs when the circulant graph G is 3-regular. In this case, we must have $G = C_{2n,\{a,n\}}$ for some $1 \leq a < n$. The following result shows that G must be isomorphic to one of two graphs.

Lemma 2.19 ([55]) *Let $t = \gcd(2n, a)$.*

(a) If $\frac{2n}{t}$ is even, then $G = C_{2n,\{a,n\}}$ is isomorphic to t copies of $C_{\frac{2n}{t},\{1,\frac{n}{t}\}}$.

(b) If $\frac{2n}{t}$ is odd, then $G = C_{2n,\{a,n\}}$ is isomorphic to $\frac{t}{2}$ copies of $C_{\frac{4n}{t},\{2,\frac{2n}{t}\}}$.

We now find a formula for $I(C_{2n,\{1,n\}}, x)$ and $I(C_{2n,\{2,n\}}, x)$. By Lemma 2.19, once we find an explicit formula for these two independence polynomials, we can derive a formula for the independence polynomial of all 3-regular circulant graphs. Before proving a lemma that relates our two independence polynomials, we require the following definition.

Definition 2.20 *U_n is the* **ladder graph** *on $2n$ vertices (with the vertices labelled $a_0, \ldots, a_{n-1}, b_0, \ldots, b_{n-1}$) if $a_0b_0, a_{n-1}b_{n-1} \in E(U_n)$, and for each $1 \leq j \leq n-2$, a_j is adjacent to b_{j-1}, b_j, b_{j+1} and b_j is adjacent to a_{j-1}, a_j, a_{j+1}.*

The ladder graph U_n is illustrated in Figure 2.1.

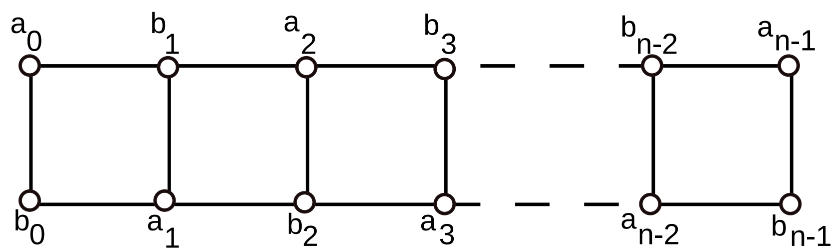

Figure 2.1: The ladder graph U_n.

We now describe a connection between the graphs $G_n = C_{2n,\{1,n\}}$ and $H_n = C_{2n,\{2,n\}}$ (a valid labelling for $n = 9$ is given in Figure 2.2), and the ladder graph U_n.

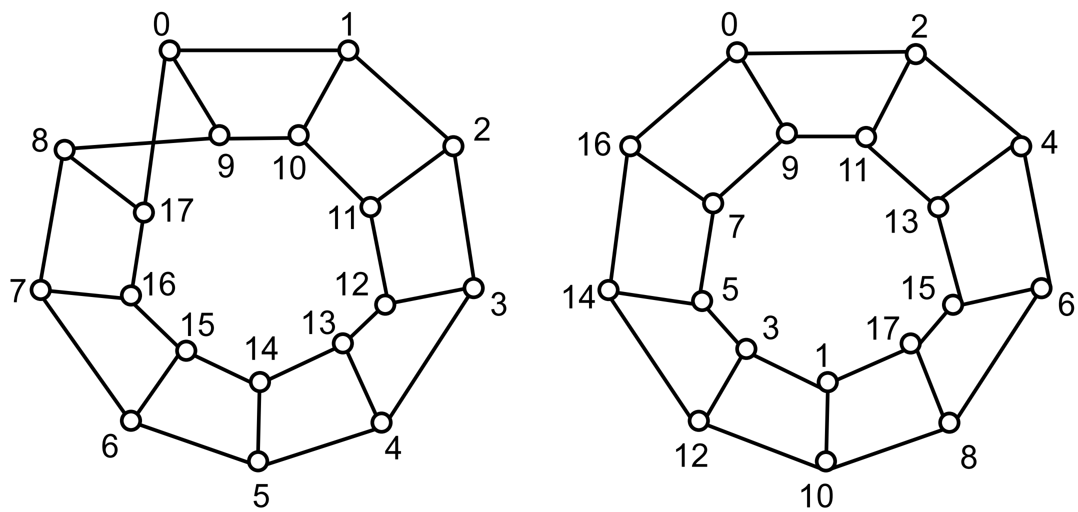

Figure 2.2: The graphs $G_9 = C_{18,\{1,9\}}$ and $H_9 = C_{18,\{2,9\}}$.

The key insight is that U_n is bipartite, and is a subgraph of both G_n and H_n, with exactly two fewer edges. Since n is odd, we have

$$\begin{aligned} G_n &\simeq U_n + \{a_{n-1}b_0, b_{n-1}a_0\} \\ H_n &\simeq U_n + \{a_{n-1}a_0, b_{n-1}b_0\}. \end{aligned}$$

Note that G_9 is bipartite, but H_9 is not. In the above figures comparing U_9 to G_9, we have the following labelling of the a_i's and b_i's to show that $G_9 \simeq U_9 + \{a_8b_0, b_8a_0\}$:

$$(a_0, a_1, a_2, \ldots, a_8) = (0, 10, 2, 12, 4, 14, 6, 16, 8)$$

$$(b_0, b_1, b_2, \ldots, b_8) = (9, 1, 11, 3, 13, 5, 15, 7, 17)$$

And comparing U_9 to H_9, we have the following labelling of the a_i's and b_i's to show that $H_9 \simeq U_9 + \{a_8a_0, b_8b_0\}$:

$$(a_0, a_1, a_2, \ldots, a_8) = (0, 2, 4, 6, 8, 10, 12, 14, 16)$$

$$(b_0, b_1, b_2, \ldots, b_8) = (9, 11, 13, 15, 17, 1, 3, 5, 7)$$

This connection between U_n and the graphs G_n and H_n gives us the following lemma.

Lemma 2.21 *For each odd integer n, let $G_n = C_{2n,\{1,n\}}$ and $H_n = C_{2n,\{2,n\}}$. Then $I(G_n, x) = I(H_n, x) + 2x^n$.*

Proof: We can regard G_n as the Möbius strip of H_n. In fact, G_n is known in the literature as the *Möbius Graph* [82]. We now explain why $G_n - \{a_i, b_i\} \simeq H_n - \{a_i, b_i\}$ for each $0 \leq i \leq n-1$. This can be seen by removing the two vertices a_i and b_i, and then *twisting* the cut Möbius strip $G' := G_n - \{a_i, b_i\}$ so that it becomes isomorphic to $H' := H_n - \{a_i, b_i\}$. More formally, the desired isomorphism $\phi_i : G' \to H'$ is

$$\phi_i(a_j) = \begin{cases} a_j & \text{for } 0 \leq j \leq i-1 \\ b_j & \text{for } i+1 \leq j \leq n-1 \end{cases}$$

$$\phi_i(b_j) = \begin{cases} b_j & \text{for } 0 \leq j \leq i-1 \\ a_j & \text{for } i+1 \leq j \leq n-1 \end{cases}$$

Hence, $G_n - \{a_i, b_i\} \simeq H_n - \{a_i, b_i\}$ for each $0 \leq i \leq n-1$. For a fixed i, it follows that for each $0 \leq k \leq n-1$,

$$[x^k]I(G_n - \{a_i, b_i\}, x) = [x^k]I(H_n - \{a_i, b_i\}, x).$$

Now we count the number of times each independent k-set I' of G_n appears among the n possible subgraphs $G_n - \{a_i, b_i\}$. Among the n possible values of $0 \leq i \leq n-1$, there are k indices where either a_i or b_i is an element of I', since $|I'| = k$ and $a_i \not\sim b_i$. Hence, there are exactly $n-k$ indices i for which I' appears as an independent set of $G_n - \{a_i, b_i\}$. Therefore, for each $0 \leq k \leq n-1$, we have

$$[x^k]I(G_n, x) = \frac{1}{n-k}\sum_{i=0}^{n-1}[x^k]I(G_n - \{a_i, b_i\}, x).$$

By the exact same argument,

$$[x^k]I(H_n, x) = \frac{1}{n-k}\sum_{i=0}^{n-1}[x^k]I(H_n - \{a_i, b_i\}, x).$$

Since we have shown that $[x^k]I(G_n - \{a_i, b_i\}, x) = [x^k]I(H_n - \{a_i, b_i\}, x)$ for each $0 \leq i \leq n-1$, we conclude that $[x^k]I(G_n, x) = [x^k]I(H_n, x)$, for each $0 \leq k \leq n-1$.

Now we prove that $[x^n]I(G_n, x) = 2$ and $[x^n]I(H_n, x) = 0$. Any independent set of cardinality n must be either $\{a_0, a_1, \ldots, a_{n-1}\}$ or $\{b_0, b_1, \ldots, b_{n-1}\}$, since $a_j b_{j+1} \in E(G)$ and $b_j a_{j+1} \in E(G)$. Thus, there are at most two independent sets of cardinality n. We quickly verify that both of these sets are independent in G (and not in H). Thus, $[x^n]I(G_n, x) = 2$ and $[x^n]I(H_n, x) = 0$.

Therefore, we have shown that $I(G_n, x) = I(H_n, x) + 2x^n$, as required. ∎

In Theorem 2.10, we developed a complicated formula for $I(B_n, x)$, from which we obtain the identity for $I(C_{2p,\{p-1,p\}}, x)$, by substituting $n = 2p$ and $d = p-2$.

Corollary 2.22 *Let $p \geq 2$ be an integer. Then,*

$$I(C_{2p,\{p-1,p\}}, x) = 1 + \sum_{l=0}^{\lfloor \frac{p-2}{4} \rfloor} \frac{2p}{2l+1}\binom{p-2l-2}{2l}x^{2l+1}(1+x)^{p-4l-2}.$$

From this, we may extract the x^k coefficient of $I(C_{2p,\{p-1,p\}}, x)$, for any $k \geq 0$. For example,

$$[x^4]I(C_{2p,\{p-1,p\}}, x) = 2p\binom{p-2}{3} + \frac{2p}{3}\binom{p-4}{2}\binom{p-6}{1} = \frac{2p(p-4)(p^2-8p+18)}{3}.$$

In the following two lemmas, we relate $I(C_{2n,\{n-1,n\}}, x)$ to $I(C_{2n,\{1,n\}}, x)$ and $I(C_{2n,\{2,n\}}, x)$, which will allow us to determine an explicit formula for $I(G, x)$, for any circulant graph of degree 3.

Definition 2.23 **([140])** *Let S be any subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. For each integer $r \geq 1$, define $rS = \{|rs|_n : s \in S\}$. If $T = rS$ for some integer r (with $\gcd(r, n) = 1$), then T is a* **multiplier** *of S.*

Lemma 2.24 **([140])** *Consider the circulant graphs $C_{n,S}$ and $C_{n,T}$. If $T = rS$ is a multiplier of S, then $C_{n,S} \simeq C_{n,T}$.*

Lemma 2.25 *If n is odd, then $I(C_{2n,\{2,n\}}, x) = I(C_{2n,\{n-1,n\}}, x)$. If n is even, then $I(C_{2n,\{1,n\}}, x) = I(C_{2n,\{n-1,n\}}, x)$.*

Proof: We first make the following useful observation: to prove $|x|_{2n} = a$ for some $0 \leq a \leq n$, it suffices to prove that either $x + a \equiv 0 \pmod{2n}$ or $x - a \equiv 0 \pmod{2n}$.

The case when n is even follows from Lemma 2.24, with the multiplier being $r = n - 1$. Note that $|n(n-1)|_{2n} = n$, since n is even. Since the two circulants are isomorphic, their independence polynomials must be equal.

Now consider the case when n is odd. We determine an isomorphism from $G = C_{2n,\{2,n\}}$ to $H = C_{2n,\{n-1,n\}}$. (As an example, Figure 2.3 illustrates an isomorphism between the two graphs for the $n = 9$ case, namely the graphs $G = C_{18,\{2,9\}}$ and $H = C_{18,\{8,9\}}$).

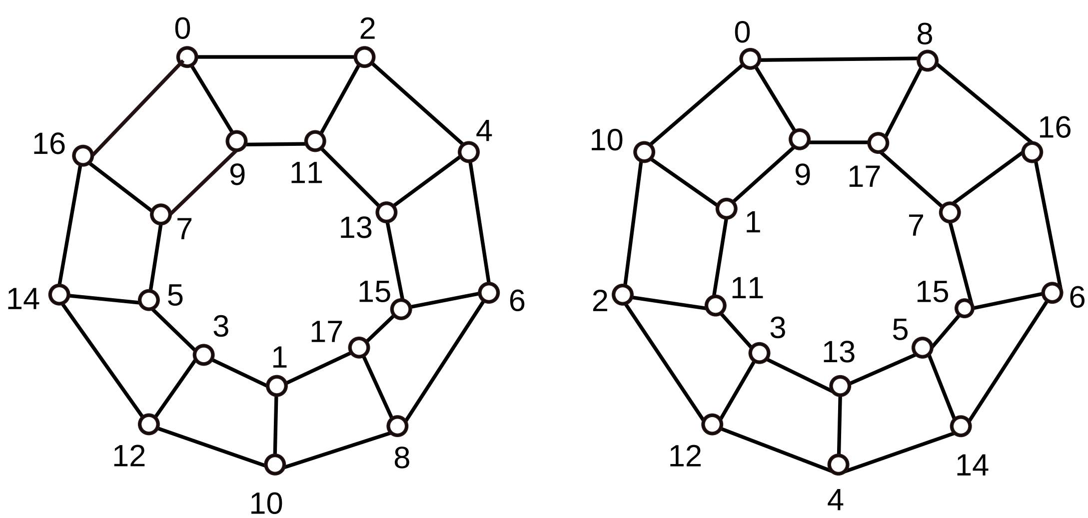

Figure 2.3: The graphs $G = C_{18,\{2,9\}}$ and $H = C_{18,\{8,9\}}$.

Let $\{0, 1, 2, \ldots, 2n-1\}$ be the vertices of $C_{2n,\{2,n\}}$. Define

$$\phi(v) = \begin{cases} \frac{v(n-1)}{2} & \text{if } v \text{ is even} \\ \frac{v(n-1)}{2} + \frac{3n(n+1)}{2} & \text{if } v \text{ is odd} \end{cases}$$

In both cases, we reduce the expression modulo $2n$, if necessary. To prove that ϕ is the desired isomorphism from $G = C_{2n,\{2,n\}}$ to $H = C_{2n,\{n-1,n\}}$, we establish the following.

(a) $\phi(v)$ has the same parity as v, for each $0 \le v \le 2n-1$.

(b) $|u-v|_{2n} = 2$ in G iff $|\phi(u) - \phi(v)|_{2n} = n-1$ in H.

(c) $|u-v|_{2n} = n$ in G iff $|\phi(u) - \phi(v)|_{2n} = n$ in H.

First we establish part (a). If v is even, then $\frac{v}{2}$ is an integer. Since $n-1$ is even, $\phi(v) = \frac{v(n-1)}{2}$ is even. If, on the other hand, v is odd, then $\phi(v) = \frac{v(n-1)}{2} + \frac{3n(n+1)}{2}$. Consider two cases for n: $n = 4k+1$ and $n = 4k+3$. In the former case, $\phi(v) = 2vk + 3(4k+1)(2k+1)$ and in the latter, $\phi(v) = v(2k+1) + 3(4k+3)(2k+2)$. In both cases, $\phi(v)$ is odd, since v is odd. This establishes part (a), since we have shown that $\phi(v)$ and v must have the same parity.

Now we establish part (b). Without loss of generality, assume $0 \le v < u \le 2n-1$. If $|u-v|_{2n} = 2$, then $u - v = 2$ or $u - v = 2n-2$. Since u and v have the same parity, $\phi(u) - \phi(v) \equiv \frac{(u-v)(n-1)}{2} \pmod{2n}$. We have two possible cases for $u - v$, either $u - v = 2$ or $u - v = 2n-2$: in the former case, $\phi(u) - \phi(v) = n-1$, and in the latter case, $\phi(u) - \phi(v) = n+1$, once reduced mod $2n$. In both cases, $|\phi(u) - \phi(v)|_{2n} = n-1$.

Let us establish the converse. If $|\phi(u) - \phi(v)|_{2n} = n-1$, then $\phi(u)$ and $\phi(v)$ have the same parity (since n is odd), implying by part (a) that u and v have the same parity. Thus, $\phi(u) - \phi(v) \equiv \frac{(u-v)(n-1)}{2} \pmod{2n}$, for some $0 \le v < u \le 2n-1$. Define $k = \frac{u-v}{2} \in \mathbb{N}$ so that $u - v = 2k$. Then $n - 1 = |\phi(u) - \phi(v)|_{2n} = |k(n-1)|_{2n}$, which implies that $k(n-1)$ is congruent to either $n-1$ or $-(n-1)$ modulo $2n$. In other words, either $(k-1)(n-1)$ or $(k+1)(n-1)$ is a multiple of $2n$. Since n is odd, we have $\gcd(n-1, 2n) = 2$, and so this implies that $k-1$ or $k+1$ must be a multiple of n. Finally, since $1 \leq k \leq n-1$, we conclude that $k = 1$ or $k = n-1$. Thus, we have shown that $u - v = 2k$ equals 2 or $2n-2$. Therefore, $|u-v|_{2n} = 2$.

Finally, we establish part (c). Without loss of generality, assume $0 \leq v < u \leq 2n-1$. If $|u-v|_{2n} = n$, then $u - v = n$. Since u and v have opposite parity, $\phi(u) - \phi(v) \equiv \frac{(u-v)(n-1)}{2} \pm \frac{3n(n+1)}{2} \pmod{2n}$. Substituting $u - v = n$, we have $\phi(u) - \phi(v) \equiv \frac{n(n-1)}{2} \pm \frac{3n(n+1)}{2} \pmod{2n}$. This simplifies to either $2n^2+n$ or $-n^2-2n$, depending on the sign. Since n is odd, both expressions are congruent to n modulo $2n$. It follows that $|\phi(u) - \phi(v)|_{2n} = n$ in each case.

Let us establish the converse. If $|\phi(u) - \phi(v)|_{2n} = n$, then $\phi(u)$ and $\phi(v)$ have opposite parity, implying by part (a) that u and v do too. Letting $u - v = n + k$ for some $-n < k < n$, we have $n = |\phi(u) - \phi(v)|_{2n} = |\frac{(n+k)(n-1)}{2} \pm \frac{3n(n+1)}{2}|_{2n} = |\frac{k(n-1)}{2} + \frac{n(n-1)}{2} \pm \frac{3n(n+1)}{2}|_{2n}$. In the previous paragraph, we proved that $\frac{n(n-1)}{2} \pm \frac{3n(n+1)}{2}$ is congruent to n modulo $2n$.

Therefore, the above equation simplifies to $n = |\frac{k(n-1)}{2} + n|_{2n}$. This implies that $\frac{k(n-1)}{2}$ must be a multiple of $2n$. Since $-n < k < n$ and $\gcd(n, n-1) = 1$, k must divide n. It follows that $k = 0$, i.e., $u - v = n$. We conclude that $|u-v|_{2n} = n$.

By parts (b) and (c), we have shown that ϕ is an isomorphism from $C_{2n,\{2,n\}}$ to $C_{2n,\{n-1,n\}}$. Therefore, their independence polynomials must be equal. ∎

Applying Corollary 2.22, the following theorem gives us the exact formula for $I(G, x)$, where G is any circulant of degree 3.

Theorem 2.26 *Let $G = C_{2n,\{a,n\}}$ for some $1 \leq a < n$. Let $t = \gcd(2n, a)$. Then,*

(a) If $\frac{n}{t}$ is even, then $I(G, x) = \left(I(C_{\frac{2n}{t},\{\frac{n}{t}-1,\frac{n}{t}\}}, x)\right)^t$.

(b) If $\frac{2n}{t}$ is even and $\frac{n}{t}$ is odd, then $I(G, x) = \left(I(C_{\frac{2n}{t},\{\frac{n}{t}-1,\frac{n}{t}\}}, x) + 2x^{\frac{n}{t}}\right)^t$.

(c) If $\frac{2n}{t}$ is odd, then $I(G, x) = \left(I(C_{\frac{4n}{t},\{\frac{2n}{t}-1,\frac{2n}{t}\}}, x)\right)^{\frac{t}{2}}$.

<u>Proof:</u> Since t divides $2n$, $\frac{2n}{t}$ is an integer; if this quantity is even, then $\frac{n}{t}$ is also an integer. Thus, we have three cases to consider:

(a) $\frac{2n}{t}$ is even and $\frac{n}{t}$ is even. (Trivially, if $\frac{n}{t}$ is even, then $\frac{2n}{t}$ is too).

(b) $\frac{2n}{t}$ is even and $\frac{n}{t}$ is odd.

(c) $\frac{2n}{t}$ is odd.

We consider each of these three cases in order. If $\frac{2n}{t}$ is even, then by Lemma 2.19, G is isomorphic to t copies of $C_{\frac{2n}{t},\{1,\frac{n}{t}\}}$.

If $\frac{n}{t}$ is also even, then $I(C_{\frac{2n}{t},\{1,\frac{n}{t}\}},x) = I(C_{\frac{2n}{t},\{\frac{n}{t}-1,\frac{n}{t}\}},x)$ by Lemma 2.25. Otherwise, $\frac{n}{t}$ is odd, and by Lemma 2.21, $I(C_{\frac{2n}{t},\{1,\frac{n}{t}\}},x) = I(C_{\frac{2n}{t},\{2,\frac{n}{t}\}},x) + 2x^{\frac{n}{t}}$, which equals $I(C_{\frac{2n}{t},\{\frac{n}{t}-1,\frac{n}{t}\}},x) + 2x^{\frac{n}{t}}$, by Lemma 2.25.

If $\frac{2n}{t}$ is odd, then by Lemma 2.19, G is isomorphic to $\frac{t}{2}$ copies of $C_{\frac{4n}{t},\{2,\frac{2n}{t}\}}$. By Lemma 2.25, $I(C_{\frac{4n}{t},\{2,\frac{2n}{t}\}},x) = I(C_{\frac{4n}{t},\{\frac{2n}{t}-1,\frac{2n}{t}\}},x)$. ∎

For example, the above theorem shows that

$$\begin{aligned} I(C_{60,\{18,30\}},x) &= (I(C_{10,\{3,5\}},x))^6 \\ &= (I(C_{10,\{4,5\}},x) + 2x^5)^6 \\ &= (1 + 10x + 30x^2 + 30x^3 + 10x^4 + 2x^5)^6. \end{aligned}$$

We now have a formula for the independence number of any 3-regular circulant graph, since $\alpha(G) = \deg(I(G,x))$.

Corollary 2.27 *Let $G = C_{2n,\{a,n\}}$ for some $1 \le a < n$. Let $t = \gcd(2n,a)$. Then,*

(a) If $\dfrac{n}{t}$ is even, then $\alpha(G) = n - t$.

(b) If $\dfrac{2n}{t}$ is even and $\dfrac{n}{t}$ is odd, then $\alpha(G) = n$.

(c) If $\dfrac{2n}{t}$ is odd, then $\alpha(G) = n - \dfrac{t}{2}$.

Proof: By Corollary 2.18, $\alpha(C_{2m,\{m-1,m\}}) = m - 1$, for any $m \ge 2$. From Theorem 2.26, the result follows. ∎

We have now found a formula for $I(G,x)$, for all circulants of degree at most 3. As noted previously, we will not be able to obtain a general formula for an arbitrary

k-degree circulant, due to the NP-hardness of the problem [46]. Even for the case when G is degree 4, there is no clear method to find an explicit formula for $I(G,x)$, as there is no known characterization or classification of degree 4 circulant graphs. For the degree 3 case, we were able to prove that every 3-regular circulant must be isomorphic to one of three specific families of graphs. This greatly simplified the analysis, as we only needed to determine the independence polynomials for these three families. However, no such result holds for circulants of degree 4. To illustrate, even for the case $n = 12$, there are seven non-isomorphic circulants of degree 4, and all of them have distinct independence polynomials.

$$\begin{aligned}
I(C_{12,\{1,2\}},x) &= 1+12x+42x^2+40x^3+3x^4.\\
I(C_{12,\{1,3\}},x) &= 1+12x+42x^2+52x^3+30x^4+12x^5+2x^6.\\
I(C_{12,\{1,4\}},x) &= 1+12x+42x^2+48x^3+15x^4.\\
I(C_{12,\{1,5\}},x) &= 1+12x+42x^2+52x^3+33x^4+12x^5+2x^6.\\
I(C_{12,\{2,3\}},x) &= 1+12x+42x^2+52x^3+18x^4.\\
I(C_{12,\{2,4\}},x) &= 1+12x+42x^2+36x^3+9x^4.\\
I(C_{12,\{3,4\}},x) &= 1+12x+42x^2+48x^3+18x^4.
\end{aligned}$$

It would be nice if these polynomials were all factorable, so that we could explore deeper connections. However, five of these seven polynomials are irreducible, with the two exceptions being $I(C_{12,\{1,5\}},x) = (1+4x+2x^2)(1+8x+8x^2+4x^3+x^4)$ and $I(C_{12,\{2,4\}},x) = (1+6x+3x^2)^2$. Note that the latter polynomial is trivially factorable, as $C_{12,\{2,4\}}$ is simply two disjoint copies of $C_{6,\{1,2\}}$. While there is no obvious reason to see why $I(C_4,x) = 1+4x+2x^2$ should be a factor of $I(C_{12,\{1,5\}},x)$, we will explain exactly why this must be the case in the following section, when we discuss lexicographic products of graphs and their independence polynomials.

Alas, we suspect that it is intractable to find a general formula for $I(G,x)$, for an arbitrary circulant of degree $d \geq 4$. Nevertheless, we were able to find an explicit formula for $I(G,x)$, for any circulant of degree 3, as well as every graph in the family A_n and B_n. These formulas will be of great help to us throughout the thesis, including the following section, where we develop infinitely many formulas for $I(G,x)$ using products of graphs.

2.4 Graph Products of Circulants

In this section, we apply graph products to generate additional formulas for $I(C_{n,S}, x)$.

Definition 2.28 *For any two graphs G and H, the* **graph product** *is a new graph with vertex set $V(G) \times V(H)$ such that for any two vertices (g, h) and (g', h') in the product, the adjacency of these vertices is determined solely by the adjacency (or non-adjacency) of g and g', and of h and h':*

1. *In the* **Cartesian product graph** *$G \square H$, the vertices (g, h) and (g', h') are adjacent if ($g \sim g'$ and $h = h'$) or ($g = g'$ and $h \sim h'$).*

2. *In the* **categorical product graph** *$G \times H$, the vertices (g, h) and (g', h') are adjacent if $g \sim g'$ and $h \sim h'$.*

3. *In the* **lexicographic product graph** *$G[H]$, the vertices (g, h) and (g', h') are adjacent if ($g \sim g'$) or ($g = g'$ and $h \sim h'$).*

4. *In the* **strong product graph** *$G \otimes H$, the vertices (g, h) and (g', h') are adjacent if ($g \sim g'$ and $h = h'$) or ($g = g'$ and $h \sim h'$) or ($g \sim g'$ and $h \sim h'$).*

If G and H are both regular, so are $G \square H$, $G \times H$, $G[H]$, and $G \otimes H$. Thus, regularity is a property closed under graph products. Due to the symmetry of circulant graphs, a natural conjecture is that circulants are also closed under graph products, i.e., if G and H are both circulants, then so is their product. We now prove that this statement is true for lexicographic products, but false for all of the others.

Proposition 2.29 *Circulant graphs are not closed under the Cartesian, categorical, or strong product.*

Proof: It suffices to find one pair of graphs (G, H) for which the product is not a circulant. We establish our counterexample by comparing independence polynomials. We will prove that circulants are not closed under the Cartesian or categorical product by considering the graphs $C_3 \square C_3$ and $C_3 \times C_3$, and prove that circulants are not closed under the strong product by considering the graph $C_4 \otimes C_4$.

Consider $G = C_3$ and $H = C_3$. Then, $G \square H$ and $G \times H$ are graphs of degree 4 and order 9. These product graphs are isomorphic to the graphs illustrated in Figure 2.4.

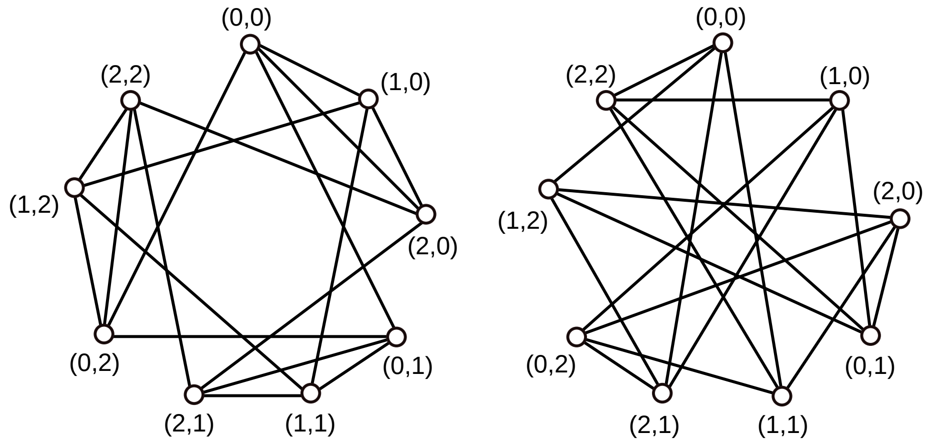

Figure 2.4: The graph products $C_3 \square C_3$ and $C_3 \times C_3$.

Suppose $G \square H$ and $G \times H$ are circulants. Then, we may write $G \square H \simeq C_{9,S_1}$ and $G \times H = C_{9,S_2}$, for some generating sets $S_1, S_2 \subseteq \{1,2,3,4\}$, with $|S_1| = |S_2| = 2$.

By inspection, vertex $(0,0)$ in both $G \square H$ and $G \times H$ appears as a vertex in an independent 2-set four times and an independent 3-set twice. By symmetry, this must be the case for each of the nine vertices, in each of the two graphs. Thus, there are $\frac{9 \cdot 4}{2} = 18$ independent 2-sets and $\frac{9 \times 2}{3} = 6$ independent 3-sets. Also it follows quickly that there exist no independent sets of cardinality 4. Thus,

$$I(G \square H, x) = I(G \times H, x) = 1 + 9x + 18x^2 + 6x^3.$$

Each degree 4 circulant on 9 vertices is isomorphic to either $C_{9,\{1,2\}}$ or $C_{9,\{3,4\}}$, which can easily be checked using Lemma 2.24. (Note that $C_{9,\{1,2\}}$ is isomorphic to $C_{9,\{1,4\}}$ and $C_{9,\{2,4\}}$, while $C_{9,\{3,4\}}$ is isomorphic to $C_{9,\{1,3\}}$ and $C_{9,\{2,3\}}$). By Theorems 2.3 and 2.10, $I(C_{9,\{1,2\}}, x) = 1 + 9x + 18x^2 + 3x^3$ and $I(C_{9,\{3,4\}}, x) = 1 + 9x + 18x^2 + 9x^3$. Therefore, neither $G \square H$ or $G \times H$ is a circulant.

Now consider $G = C_4$ and $H = C_4$. Then, $G \otimes H$ is a degree 8 graph of order 16. Thus, if $G \otimes H \simeq C_{16,S}$ for some $S \subseteq \{1,2,3,4,5,6,7,8\}$, then $|S| = 4$, with

$8 \notin S$. From a computation on Maple, $I(G \otimes H, x) = 1 + 16x + 56x^2 + 48x^3 + 12x^4$. Looking at each of the 35 possible 4-subsets of $\{1, 2, 3, 4, 5, 6, 7\}$, we find (using a Maple computation once again) that only $S = \{1, 2, 6, 7\}$ and $S = \{2, 3, 5, 6\}$ satisfy $I(C_{16,S}, x) = I(G \otimes H, x)$. Let us show that $G \otimes H$ is not isomorphic to either of these circulants. This will enable us to conclude that $G \otimes H$ is not necessarily a circulant, whenever G and H are both circulants.

First consider the case $S = \{1, 2, 6, 7\}$. On the contrary, suppose $G \otimes H \simeq C_{16,S}$. Note that $C_{16,S}$ includes two non-adjacent vertices (namely 0 and 8), which are adjacent to the same set of eight vertices, namely $\{1, 2, 6, 7, 9, 10, 14, 15\}$. Since $G \otimes H$ is assumed to be isomorphic to $C_{16,S}$, there must exist two non-adjacent vertices a and b in $G \otimes H$ that are adjacent to the same set T of eight vertices.

By the symmetry of $G \otimes H = C_4 \otimes C_4$, assume without loss that $a = (0, 0)$. Letting T be the set of vertices in $G \otimes H$ that are adjacent to a, we have

$$T = \{(0, 1), (0, 3), (1, 0), (1, 1), (1, 3), (3, 0), (3, 1), (3, 3)\}.$$

Let $T' = \{(0, 2), (1, 2), (2, 1), (2, 0), (2, 3), (2, 2), (3, 2)\}$ be the set of vertices in $G \otimes H$ that are not adjacent to $a = (0, 0)$. There must exist a vertex $b \in G \otimes H$ that is not adjacent to a, but is adjacent to each vertex in T. Since $b \not\sim a$, we have $b \in T'$. This vertex b, which is of degree 8, must be adjacent to each of the eight vertices of T, and so must be adjacent to no vertices in T'. However, by the definition of the strong product, the following pairs of vertices are adjacent in $G \otimes H = C_4 \otimes C_4$:

$$(0, 2) \sim (1, 2), \quad (2, 1) \sim (2, 0), \quad (2, 3) \sim (2, 2), \quad (2, 2) \sim (3, 2).$$

Therefore, each choice of $b \in T'$ leads to a contradiction. We conclude that $C_{16,S}$ is not isomorphic to $C_4 \otimes C_4$, where $S = \{1, 2, 6, 7\}$. Now the case $S = \{2, 3, 5, 6\}$ follows immediately from the previous case, since Lemma 2.24 implies that $C_{16,\{1,2,6,7\}} \sim C_{16,\{2,3,5,6\}}$, with the desired multiplier being $r = 3$. Therefore, we conclude that $C_4 \otimes C_4$ is not a circulant. $\blacksquare$

Let us now investigate the lexicographic product $G[H]$. The graph $G[H]$ can be thought of as the graph arising from G and H by substituting a copy of H for every vertex of G. We prove that circulants *are* closed under the lexicographic product. We first require the following lemma.

Lemma 2.30 *Let $G = C_{n,S_1}$ and $H = C_{m,S_2}$ be circulant graphs. Construct the lexicographic product graph $G[H]$, and relabel each vertex (g,h) with the integer $g+nh$. Then,*

(a) This relabelling of the vertices ensures that each of the nm vertices in $G[H]$ is assigned a unique integer label between 0 and $nm-1$ inclusive.

(b) Let $x = g_1 + nh_1$ and $y = g_2 + nh_2$ be the new labels assigned to the vertices (g_1,h_1) and (g_2,h_2) in $G[H]$. Suppose that $x > y$ so that $1 \le x-y \le nm-1$. Among these $nm-1$ possible values for $x-y$, $(g_1,h_1) \sim (g_2,h_2)$ in $G[H]$ iff $x - y \equiv \pm r \pmod n$ for some $r \in S_1$, or n divides $x-y$ and $\frac{x-y}{n} \equiv \pm q \pmod m$ for some $q \in S_2$.

Proof: We first prove part (a) of the lemma. Let (g,h) be a vertex of $G[H]$. By definition, $0 \le g \le n-1$ and $0 \le h \le m-1$. Thus, $0 \le g+nh \le (n-1)+n(m-1) = n-1+nm-n = nm-1$. So each of the nm vertices under this labelling is given an integer value between 0 and $nm-1$ inclusive. Now suppose that some integer value is assigned twice, i.e., $g_1 + nh_1 = g_2 + nh_2$ for some $(g_1,h_1) \neq (g_2,h_2)$. Then $g_1 - g_2 = n(h_2 - h_1)$, implying that $g_1 \equiv g_2 \pmod n$. Since $0 \le g_1, g_2 \le n-1$, we must have $g_1 = g_2$. From this it follows that $h_1 = h_2$, contradicting the fact that $(g_1,h_1) \neq (g_2,h_2)$. Hence, each of the nm vertices in $G[H]$ is assigned a unique integer value by this labelling.

Now we prove part (b). Let g_1 and g_2 be two vertices in G. By the definition of adjacency in circulants, as well as the definition of circular distance, we have the following:

(a) $g_1 \sim g_2$ in $G = C_{n,S_1}$ iff $g_1 - g_2 \equiv \pm r \pmod n$, for some $r \in S_1$.

(b) $h_1 \sim h_2$ in $H = C_{m,S_2}$ iff $h_1 - h_2 \equiv \pm q \pmod m$, for some $q \in S_2$.

By definition, $(g_1,h_1) \sim (g_2,h_2)$ in $G[H]$ iff ($g_1 = g_2$ and $h_1 \sim h_2$ in H) or ($g_1 \sim g_2$ in G). We consider the two cases separately. Note that $x - y = (g_1 - g_2) + n(h_1 - h_2)$.

We start with the case ($g_1 = g_2$ and $h_1 \sim h_2$ in H). We prove that this case is equivalent to the condition that n divides $x - y$ and $\frac{x-y}{n} \equiv \pm q \pmod{m}$, for some $q \in S_2$. One direction is clear, since $g_1 = g_2$ and $h_1 \sim h_2$ in H immediately implies the desired result, since $x - y = n(h_1 - h_2)$, i.e., n divides $x - y$ and $\frac{x-y}{n} = h_1 - h_2 \equiv \pm q \pmod{m}$, for some $q \in S_2$. We establish the converse: if n divides $x - y = (g_1 - g_2) + n(h_1 - h_2)$ and $\frac{x-y}{n} \equiv \pm q \pmod{m}$, then $g_1 = g_2$ by the condition $0 \le g_1, g_2 \le n - 1$. Thus, $x - y = n(h_1 - h_2)$, and so $h_1 - h_2 = \frac{x-y}{n} \equiv \pm q \pmod{m}$ for some $q \in S_2$, which from above implies that $h_1 \sim h_2$ in H.

Now consider the case ($g_1 \sim g_2$ in G). We prove that this case is equivalent to the condition that $x - y \equiv \pm r \pmod{n}$ for some $r \in S_1$. One direction is clear, since $g_1 \sim g_2$ in G implies that $x - y = (g_1 - g_2) + n(h_1 - h_2) \equiv \pm r + 0 = \pm r \pmod{n}$ for some $r \in S_1$. The converse follows just as quickly: if $x - y = (g_1 - g_2) + n(h_1 - h_2) \equiv \pm r \pmod{n}$ for some $r \in S_1$, then we must have $g_1 \sim g_2$ in G (note that there is no restriction on h_1 and h_2).

Part (b) of the lemma now follows from the two previous paragraphs. ∎

With this lemma, we can now prove the following theorem, that circulant graphs are closed under the lexicographic product.

Theorem 2.31 *Let $G = C_{n,S_1}$ and $H = C_{m,S_2}$ be circulant graphs. Define*

$$S = \left(\bigcup_{t=0}^{\lfloor \frac{m-1}{2} \rfloor} tn + S_1 \right) \bigcup \left(\bigcup_{t=1}^{\lfloor \frac{m}{2} \rfloor} tn - S_1 \right) \bigcup nS_2,$$

where $tn \pm S_1 = \{tn \pm r : \ r \in S_1\}$ and $nS_2 = \{nq : \ q \in S_2\}$.

Then, $G[H]$ is isomorphic to the circulant $C_{nm,S}$.

Proof: Relabel the vertices of $G[H]$ so that (g, h) is assigned the new vertex $g + nh$. By part (a) of Lemma 2.30, the nm vertices of $G[H]$ are the integers from 0 to $nm - 1$ inclusive. By part (b) of Lemma 2.30, if $x = g_1 + nh_1$ and $y = g_2 + nh_2$ for some $0 \le g_1, g_2 \le n - 1$ and $0 \le h_1, h_2 \le m - 1$, then $x \sim y$ in $G[H]$ iff $x - y \equiv \pm r \pmod{n}$ for some $r \in S_1$, or $\frac{x-y}{n} \equiv \pm q \pmod{m}$ for some $q \in S_2$.

Let S' denote the set of possible values $x - y$ (where $1 \le x - y \le nm - 1$) satisfying the congruence equations above. We note that each integer of the form nq or $n(m - q)$

is in S', where $q \in S_2$. It is simple to check that each such integer lies in the required interval $[1, nm-1]$, since $1 \leq q \leq \lfloor \frac{m}{2} \rfloor$.

In addition to these values already in S', we must also include each value of $cn+r$, over all choices of $0 \leq c \leq m-1$ and $r \in S_1$, and each value of $dn-r$, over all choices of $1 \leq d \leq m$ and $r \in S_1$. We note that all of these values lie in the required interval $[1, nm-1]$, for any choice of c, d, and r. We remark that any c and d not satisfying the given inequality (i.e., $c < 0$, $c > m-1$, $d < 1$, $d > m$) will make $cn+r$ and/or $dn-r$ fall outside of the required interval for any choice of r, since $1 \leq r \leq \lfloor \frac{n}{2} \rfloor$. As a final note, remark that $v \in S'$ iff $nm - v \in S'$. This will make it very easy to compute the set of circular distances $|x-y|_{nm}$.

We have shown that $x \sim y$ in $G[H]$ iff $x-y \in S'$. By letting $S = \{|x-y|_{nm} : \ x-y \in S'\}$ be the generating set produced by computing the circular distance (mod nm) for each value of S', we have $x \sim y$ in $G[H]$ iff $|x-y|_{nm} \in S$. This proves that $G[H]$ is a circulant $C_{nm,S}$, for this generating set S. Given that we know which elements are in S', we can describe exactly the set of elements in S. Since $v \in S'$ iff $nm - v \in S'$, the elements of S are precisely those elements in S' that are in the interval $[1, \lfloor \frac{nm}{2} \rfloor]$. Let us give an explicit characterization of this generating set.

First look at all the multiples of n: each integer of the form nq and $nm - nq$ belong to S', where $q \in S_2$. Clearly each $nq \in S$, since $nq \leq n \lfloor \frac{m}{2} \rfloor \leq \lfloor \frac{nm}{2} \rfloor$. Thus, each of $n, 2n, 3n, \ldots, n\lfloor \frac{m}{2} \rfloor$ are counted in S. Conversely, all of the elements in the latter set are greater than $\lfloor \frac{nm}{2} \rfloor$, and hence do not belong to the set S. The only exception to this occurs when m is even and $q = \frac{m}{2}$; however, this value has already been added to our set S, since $n \cdot \frac{m}{2} = nm - n \cdot \frac{m}{2}$. Among the multiples of n, the only values in S are the elements nq, over all $q \in S_2$.

Define $tn \pm S_1 = \{tn \pm r : \ r \in S_1\}$ and $nS_2 = \{nq : \ q \in S_2\}$. From our analysis above, we have proven that $G[H] \simeq C_{nm,S}$, where

$$S = \left(\bigcup_{t=0}^{c} tn + S_1 \right) \bigcup \left(\bigcup_{t=1}^{d} tn - S_1 \right) \bigcup nS_2,$$

for some indices c and d.

Recall for the full set S', we had $0 \leq c \leq m-1$ and $1 \leq d \leq m$. We will show that for this reduced set S, we require $0 \leq c \leq \lfloor \frac{m-1}{2} \rfloor$ and $1 \leq d \leq \lfloor \frac{m}{2} \rfloor$: given that we are selecting the elements of S' in the "bottom half", this result is completely unsurprising. We do not need to consider the lower bounds $c \geq 0$ and $d \geq 1$, as they have already been dealt with previously. We now prove the upper bounds for c and d, by establishing that all possible values of the form $cn + r$ and $dn - r$ belong to S (for those two bounds), and proving that we have not missed any other values.

If $c \leq \lfloor \frac{m-1}{2} \rfloor$, then $cn + r \leq n \cdot \lfloor \frac{m-1}{2} \rfloor + \lfloor \frac{n}{2} \rfloor \leq \lfloor \frac{nm}{2} \rfloor$ for all choices of r. And if $c > \lfloor \frac{m-1}{2} \rfloor$, this is equivalent to the inequality $c \geq \frac{m}{2}$, since c and m are both integers. Then $cn + r \geq \frac{mn}{2} + r > \lfloor \frac{nm}{2} \rfloor$.

If $d \leq \lfloor \frac{m}{2} \rfloor$, then $dn - r \leq n \cdot \lfloor \frac{m}{2} \rfloor - r < \lfloor \frac{nm}{2} \rfloor$. And if $d > \lfloor \frac{m}{2} \rfloor$, this is equivalent to the inequality $d \geq \frac{m+1}{2}$, since d and m are integers. We have $dn - r \geq \frac{mn}{2} + \frac{n}{2} - r > \lfloor \frac{nm}{2} \rfloor$, except in the one special case when the following four conditions hold: n is even, $r = \frac{n}{2}$, m is odd, and $d = \frac{m+1}{2}$.

However, this case is easily dealt with: we have $dn - r = \frac{mn+n}{2} - \frac{n}{2} = \frac{mn}{2} \in S$. But this value was already taken into account for the case $c = \lfloor \frac{m-1}{2} \rfloor$ and $r = \frac{n}{2}$, since $cn + r = \lfloor \frac{m-1}{2} \rfloor n + r = \frac{m-1}{2} \cdot n + \frac{n}{2} = \frac{mn}{2}$. Hence, the desired upper bound is correct: no elements of S have been omitted, and every element of S has been included.

Therefore, we have proven that $G[H]$ is isomorphic to $C_{nm,S}$, where

$$S = \left(\bigcup_{t=0}^{\lfloor \frac{m-1}{2} \rfloor} tn + S_1 \right) \bigcup \left(\bigcup_{t=1}^{\lfloor \frac{m}{2} \rfloor} tn - S_1 \right) \bigcup nS_2,$$

where $tn \pm S_1 = \{tn \pm r : \ r \in S_1\}$ and $nS_2 = \{nq : \ q \in S_2\}$.

Our proof is now complete. ∎

To illustrate with an example, let $G = C_{10,\{1\}}$ and $H = C_{9,\{4\}}$. Then, $n = 10$, $m = 9$, $S_1 = \{1\}$, and $S_2 = \{4\}$. Therefore,

$$S = \left(\bigcup_{t=0}^{4} 10t + \{1\} \right) \bigcup \left(\bigcup_{t=1}^{4} 10t - \{1\} \right) \bigcup 10 \cdot \{4\},$$

which simplifies to $S = \{1, 9, 11, 19, 21, 29, 31, 39, 40, 41\}$.

Thus, $G[H] = C_{90,\{1,9,11,19,21,29,31,39,40,41\}}$. By a similar analysis, if we were to switch G and H to determine the lexicographic product $H[G]$, we derive

$$S = \left(\bigcup_{t=0}^{4} 9t + \{4\} \right) \bigcup \left(\bigcup_{t=1}^{4} 9t - \{4\} \right) \bigcup 9 \cdot \{1\},$$

which simplifies to $S = \{4, 5, 9, 13, 14, 22, 23, 31, 32, 40, 41\}$.

Thus, $H[G] = C_{90,\{4,5,9,13,14,22,23,31,32,40,41\}}$. As a corollary to Theorem 2.31, we have the following.

Corollary 2.32 *For each n and m, the graph $C_n[\overline{K_m}]$ is a circulant.*

Proof: Note that $C_n = C_{n,\{1\}}$ is a circulant, as is $\overline{K_m} = C_{m,\emptyset}$. From Theorem 2.31, we have $C_n[\overline{K_m}] = C_{nm,S}$, where

$$\begin{aligned} S &= \left(\bigcup_{t=0}^{\lfloor \frac{m-1}{2} \rfloor} tn + \{1\} \right) \bigcup \left(\bigcup_{t=1}^{\lfloor \frac{m}{2} \rfloor} tn - \{1\} \right) \bigcup \emptyset \\ &= \left\{ x : \ 1 \leq x \leq \left\lfloor \frac{nm}{2} \right\rfloor, \ x \equiv \pm 1 \pmod{n} \right\}. \end{aligned}$$

This completes the proof. ∎

The following theorem shows that the independence polynomial of $I(G[H], x)$ can be calculated from $I(G, x)$ and $I(H, x)$.

Theorem 2.33 ([23]) *For any graphs G and H, $I(G[H], x) = I(G, I(H, x) - 1)$.*

As an application of the above identity, consider the independence polynomial $I(C_{12,\{1,5\}}, x) = (1 + 4x + 2x^2)(1 + 8x + 8x^2 + 4x^3 + x^4)$, which was mentioned in the preceding section. At first glance, it is not clear why $I(C_4, x)$ should be a factor of $I(C_{12,\{1,5\}}, x)$. Let us explain why this follows as a direct corollary of Theorem 2.33.

Let $G = C_{6,\{1\}}$ and $H = \overline{C_2} = C_{2,\{\emptyset\}}$. By Theorem 2.31, $C_6[\overline{C_2}] = C_{12,\{1,5\}}$. Also, we have $I(C_6, x) = 1 + 6x + 9x^2 + 2x^3$ from Chapter 1, which factors nicely as $(1 + 2x)(1 + 4x + x^2)$. Therefore, we have

$$\begin{aligned} I(C_{12,\{1,5\}}, x) &= I(C_6[\overline{C_2}], x) \\ &= I(C_6, I(\overline{C_2}, x) - 1) \quad \text{by Theorem 2.33} \\ &= I(C_6, 2x + x^2) \\ &= (1 + 2(2x + x^2))(1 + 4(2x + x^2) + (2x + x^2)^2) \\ &= (1 + 4x + 2x^2)(1 + 8x + 8x^2 + 4x^3 + x^4). \end{aligned}$$

From above, $I(C_4, x)$ divides $I(C_{12,\{1,5\}}, x)$, i.e., $I(C_2[\overline{C_2}], x)$ divides $I(C_6[\overline{C_2}], x)$. In general, if $I(G', x)$ divides $I(G, x)$, then for any graph H, Theorem 2.33 proves that $I(G'[H], x)$ divides $I(G[H], x)$. This theorem enables us to determine formulas for $I(C_{n,S}, x)$ for infinitely many circulants. As an example, we highlight the following result.

Corollary 2.34 *Let (m, n) be an ordered pair of integers with $m, n \geq 2$. Define $S = \{m\} \cup \{x :\ 1 \leq x \leq \lfloor \frac{nm}{2} \rfloor,\ x \equiv \pm 1 \pmod{n}\}$. Then,*

$$I(C_{mn,S}, x) = \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \frac{m}{m-k} \binom{m-k}{k} \left(\sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} \frac{n}{n-j} \binom{n-j}{j} x^j \right)^k$$

Proof: Let $G = C_{m,\{1\}}$ and $H = C_{n,\{1\}}$. By Theorem 2.31, $G[H]$ is a circulant on nm vertices, with $S = \{m\} \cup \{x :\ 1 \leq x \leq \lfloor \frac{nm}{2} \rfloor,\ x \equiv \pm 1 \pmod{n}\}$. Therefore, we may apply Theorem 2.33 to find an explicit formula for $I(C_{nm,S}, x)$. By Corollary 2.4, the result follows. ∎

To illustrate, if we substitute $(m, n) = (7, 5)$ into our corollary, we obtain

$$I(C_{35,\{1,6,7,8,13,15\}}, x) = 1 + 35x + 385x^2 + 1575x^3 + 2975x^4 + 2625x^5 + 875x^6.$$

When Theorem 2.33 is combined with Theorems 2.3 and 2.10, we are able to determine infinitely many formulas for $I(C_{n,S}, x)$. It is highly unlikely that these formulas can be obtained by a direct enumerative approach. Nevertheless, with Theorem 2.33, we can immediately obtain formulas for independence polynomials such as $I(C_{84,\{3,4,10,11,17,18,24,25,28,31,32,35,38,39,42\}}, x)$, since this circulant is the lexicographic product of $C_{7,\{3\}}$ and $C_{12,\{4,5,6\}}$.

As an aside, we mention that the Cartesian product $G \Box H$ of two circulants $G = C_{n,S_1}$ and $H = C_{m,S_2}$ is a circulant whenever $\gcd(m, n) = 1$. We state the following result, which will be proven in Chapter 4 in the context of line graphs.

Theorem 2.35 *Let $G = C_{n,S_1}$ and $H = C_{m,S_2}$ be circulant graphs. Define S to be the set of integers k in $\{1, 2, \ldots, \lfloor \frac{nm}{2} \rfloor\}$ that satisfy one of the following conditions:*

1. $k = im$, for some $i \in S_1$.

2. $k = jn$*, for some* $j \in S_2$*.*

Then, $G \square H$ *is isomorphic to the circulant graph* $C_{nm,S}$*.*

In Chapter 4, we will prove that whenever $\gcd(m, n) = 1$, the line graph of $K_{m,n}$ is a circulant, and is isomorphic to the Cartesian product $K_n \square K_m$. However, as we saw for the $m = n = 3$ case in Proposition 2.29, the Cartesian product of two circulants is not necessarily a circulant when $\gcd(m, n) > 1$.

In Chapter 5, we investigate the roots of independence polynomials, and apply Theorem 2.33 to show that the roots of $I(G, x)$ are dense in the complex plane $\mathbb{C}$, even when G is restricted to the one specific family of circulant graphs, $C_n[\overline{K_m}]$.

2.5 Evaluating the Independence Polynomial at $x = t$

In this chapter, we developed a number of formulas for $I(G, x)$. Computing $I(G, x)$ enables us to determine $[x^k]I(G, x)$, the number of independent sets of cardinality k in G. However, we may also be interested in evaluating $I(G, x)$ at particular points $x = t$. As an example, evaluating $I(G, x)$ at $x = 1$ gives us the *total* number of independent sets in the graph. There are many contexts for which such information is useful. Evaluating a graph polynomial at particular points has been a subject of much interest, especially for chromatic polynomials [60, 103].

To give one illustration, we provide an application from music. The 12-tone music scale consists of the pitch classes $C, C^\#, D, D^\#, E, F, F^\#, G, G^\#, A, A^\#$, and B. Each note is identified with its pitch class (i.e., each C refers to the same note, regardless of its octave). Essentially, these "pitch classes" are the musical analogue of equivalence classes.

Suppose we want to play a chord consisting of k different pitch classes from this scale. Clearly, the number of different possibilities is $\binom{12}{k}$. But if we were to introduce *forbidden intervals* and ask for the number of chords we could play with this restriction, then we can answer this problem using independence polynomials. In particular, if the forbidden intervals correspond to pitch classes that are close together (and hence, dissonant), we show that this problem can be answered from the independence polynomial $I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$.

As a simple example, suppose that we are forbidden to include any chord with two pitch classes separated by a semitone or tone (for example, C and $C^{\#}$, or G and A). In other words, if we were to draw a graph with these 12 pitch classes as our vertices, we would require every pair of pitch classes to be separated by a distance of at least three (i.e., a minor third), to avoid any semitones or tones. Now we can ask how many possible chords can be played with this given restriction.

Mathematically, this is equivalent to the problem of evaluating the independence polynomial $I(C_{12,\{1,2\}}, x)$, and then substituting $x = 1$ to determine our answer. In other words, every possible chord is some independent set of the circulant $C_{12,\{1,2\}}$, since each pair of pitch classes in an independent set is separated by at least a minor third. By Theorem 2.3, $I(C_{12,\{1,2\}}, x) = 1 + 12x + 42x^2 + 40x^3 + 3x^4$, and so $I(C_{12,\{1,2\}}, 1) = 98$. We conclude that there are 98 possible chords that can be played, including the 55 trivial "chords" of less than three pitch classes.

We can generalize the 12-semitone octave to the n-semitone octave. As in the 12-semitone octave, the n-semitone octave is divided into n equally tempered tones, each formed by multiplying the frequency by $2^{\frac{1}{n}}$. Musicians refer to this as the n-tet scale (where "tet" is an acronym of Tone Equal-Tempered). While the 12-tet scale is most common, the 19-tet and 31-tet scales have also been employed by musicians.

In an n-tet scale, the ratio between any two semitones is constant. Since notes with similar frequencies sound dissonant when played together, we can require that no chord include two pitch classes separated by d semitones or less, for some integer $d \geq 1$. Now, if we were to ask how many possible chords can be played with this restriction, we could answer that question directly from our formula for $I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$.

Let $f(n, d)$ be the number of possible chords that can be played with this given restriction. By Theorem 2.3, the answer is simply

$$f(n, d) = \sum_{k=3}^{\lfloor \frac{n}{d+1} \rfloor} \frac{n}{n - dk} \binom{n - dk}{k},$$

which we derive from evaluating $I(C_{n,\{1,2,\ldots,d\}}, x)$ at $x = 1$, and then subtracting the number of trivial chords with less than three pitch classes.

Given a graph G, how difficult is it to evaluate $I(G,1)$? In the above example with $G = A_n = C_{n,\{1,2,\ldots,d\}}$, we first took our known formula for $I(G,x)$ and then substituted $x = 1$. But in general, it is NP-hard to determine $I(G,x)$, since we know that evaluating $\alpha(G)$ is NP-hard [79]. Thus, it is not computationally efficient to solve the problem by first computing the independence polynomial. Possibly we can develop a polynomial-time algorithm to count $I(G,1)$ (i.e., the number of independent sets of G), without actually calculating the independence polynomial. This motivates the problem of determining the computational complexity of evaluating $I(G,x)$ at the point $x = t$. To solve this problem, it is necessary to first introduce some terminology from complexity theory.

A computational problem can be regarded as a function mapping instances to solutions. In the case of graph-theoretic problems, our instance will always be a graph G. Thus, we can investigate the computational complexity of evaluating invariants such as $\alpha(G)$, $\chi(G)$, and $I(G,x)$. If A and B are two computational problems for which A is polynomial time reducible to B, then we denote this as $A \propto B$. Well-known complexity classes include $\boldsymbol{P}$, $\boldsymbol{NP}$, and $\boldsymbol{NP}$**-hard**. For formal definitions on these classes, we refer the reader to [79].

The complexity class **#**$\boldsymbol{P}$ (pronounced "sharp-P") is the class of enumeration problems in which the structures being counted are recognizable in polynomial time, i.e., there exists a constant k for which there is an $O(n^k)$ algorithm to verify whether a given structure has the correct form to be included in the count. While an NP problem is usually of the form, "are there any solutions that satisfy certain constraints?", a $\#P$ problem asks, "how many solutions satisfy certain constraints?".

What makes $\#P$ important is that it contains **#**$\boldsymbol{P}$**-complete** problems which are proven to be at least as hard as any problem in the class. A problem A in $\#P$ is $\#P$-complete if for any problem B in $\#P$, $B \propto A$. As discussed in [103], examples of $\#P$-complete problems include counting the number of Hamiltonian paths in a graph and evaluating the permanent of a square $(0,1)$-matrix.

A problem is **#**$\boldsymbol{P}$**-hard** if some $\#P$-complete problem is polynomial time reducible to it [103]. By definition, the class of $\#P$-complete problems is a subset of the class of $\#P$-hard problems. A $\#P$-hard problem may or may not be in $\#P$ - in fact, a $\#P$-hard problem is in $\#P$ iff it is $\#P$-complete.

If a problem π is $\#P$-hard, then the existence of a polynomial-time algorithm for π would imply the existence of such an algorithm for all problems in the class $\#P$. As mentioned by Jaeger et. al. [103], since $\#P$ contains such notoriously intractable problems, proving that a problem is $\#P$-hard is very strong evidence of its computational intractability.

We wish to determine the complexity of evaluating $I(G, t)$ for an arbitrary number t. We note that the equivalent problem for chromatic polynomials has already been solved.

Theorem 2.36 ([103]) *For a graph G, let $\pi(G, x)$ be the chromatic polynomial of G. Then, $\pi(G, t)$ can be evaluated in polynomial time for $t = 0$, $t = 1$, and $t = 2$. For all other real values of t, evaluating $\pi(G, t)$ is $\#P$-hard.*

We now give a complete solution to the evaluation problem for independence polynomials: we prove that for any complex number $t \neq 0$, it is $\#P$-hard to evaluate $I(G, t)$. Furthermore, if $t = 1$, then the problem is $\#P$-complete. In fact, this latter result follows immediately from a result in [103].

Proposition 2.37 *It is $\#P$-complete to evaluate $I(G, 1)$.*

Proof: By a theorem in [103], it is $\#P$-hard to evaluate the *Tutte polynomial* of a cycle matroid G at the point $(2, 1)$, which counts the total number of independent sets in G. In other words, it is $\#P$-hard to compute $I(G, 1)$. However, $I(G, 1)$ is also in $\#P$, since the structures being counted (i.e., the independent sets of G) are recognizable in polynomial time. Therefore, we conclude that evaluating $I(G, 1)$ is $\#P$-complete. ∎

We now solve the problem for $I(G, t)$ for a general $t \in \mathbb{C}$. We develop an elegant and simple proof, by applying our results on graph products from the previous section.

Theorem 2.38 *Computing $I(G, t)$ for a given number $t \in \mathbb{C}$ is $\#P$-hard iff $t \neq 0$.*

Proof: First, we note that $I(G, 0) = 1$ for any graph G, and so the evaluation is trivial at $t = 0$. Now suppose there exists a number $t \neq 0$ for which $I(G, t)$ can be evaluated in polynomial-time. In other words, given any graph G on n vertices, for this $t \neq 0$ there exists an $O(n^k)$ algorithm to compute the value of $I(G,t)$ (for some constant k).

Let G be a fixed graph on n vertices. For each $1 \leq m \leq n+1$, define H_m to be the lexicographic product graph $G[K_m]$. By our assumption, there is an $O(m^k n^k) \leq O(n^{2k})$ algorithm to compute the value of $I(H_m, t)$.

The construction of each H_m creates $nm \leq n^2+n$ vertices and decides if each pair of vertices is adjacent in H_m. The number of pairs of vertices in H_m is at most $\binom{n^2+n}{2} = O(n^4)$, and so constructing each H_m can be done in polynomial-time.

By Theorem 2.33, $I(H_m,x) = I(G, I(K_m,x)-1) = I(G,mx)$. So $I(H_m,t) = I(G,mt)$ for all $1 \leq m \leq n+1$. We know that there is an $O(m^k n^k) \leq O(n^{2k})$ algorithm to compute the value of $I(H_m,t)$, for each m. Therefore, it takes $O(n^{2k+1})$ steps to evaluate $I(G,x)$ for each $x = mt$. Since $t \neq 0$, these n values of x are distinct.

We know that the independence polynomial of G is $I(G,x) = i_0 + i_1 x + i_2 x^2 + \ldots + i_n x^n$, for some integers i_k. (Note that $\deg(I(G,x)) \leq |G| = n$). Letting $x = mt$ for each $1 \leq m \leq n+1$, we have a system of $n+1$ equations and $n+1$ unknowns.

$$\begin{aligned}
i_0 + i_1 t + i_2 t^2 + \ldots + i_n t^n &= I(G,t) \\
i_0 + i_1(2t) + i_2(2t)^2 + \ldots + i_n(2t)^n &= I(G,2t) \\
&\vdots \quad \vdots \\
i_0 + i_1(n+1)t + i_2((n+1)t)^2 + \ldots + i_n((n+1)t)^n &= I(G,(n+1)t).
\end{aligned}$$

This system has a unique solution iff the matrix

$$M = \begin{pmatrix} 1 & t & t^2 & \cdots & t^n \\ 1 & 2t & (2t)^2 & \cdots & (2t)^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (n+1)t & ((n+1)t)^2 & \cdots & ((n+1)t)^n \end{pmatrix}$$

has a non-zero determinant.

M is an example of a *Vandermonde* matrix, and the formula for its determinant is well-known. It is straightforward to show that

$$\det(M) = t^{\binom{n+1}{2}} \prod_{k=1}^{n} k!$$

Since $\det(M) \neq 0$, this system has a unique solution $(i_0, i_1, \ldots, i_n)$. This system of equations can be solved in $O(n^3)$ time using Gaussian elimination, and so each of the i_k's can be determined in polynomial time, which in turn, gives us the independence polynomial $I(G,x)$.

For any graph G, we have found an $O(n^{2k+1}) + O(n^3)$ algorithm to determine the formula for the independence polynomial $I(G,x)$, where k is some positive integer. Since $\deg(I(G,x)) = \alpha(G)$, we have shown that $\alpha(G)$ can be computed in polynomial-time for any G. This contradicts the well-known result [46, 79] that no such algorithm exists. Since it is NP-hard to evaluate $\alpha(G)$ for an arbitrary graph G [79], we conclude that it is $\#P$-hard to evaluate $I(G,t)$, for all non-zero $t \in \mathbb{C}$. ∎

2.6 Independence Unique Graphs

We conclude this chapter by classifying all circulant graphs that are uniquely characterized by its independence polynomial.

In [68], Farrell and Whitehead investigate circulant graphs that are *chromatically unique* and *matching unique*. In other words, they attempt to characterize circulants that are uniquely defined by their chromatic or matching polynomials. They prove that of the 30 non-isomorphic circulants of order at most eight, 23 are chromatically unique, with the seven exceptions being $C_{4,\{2\}}$, $C_{6,\{2\}}$, $C_{6,\{3\}}$, $C_{8,\{2\}}$, $C_{8,\{4\}}$, $C_{8,\{2,4\}}$, and $C_{8,\{1,3,4\}}$. Then they prove that each of these seven circulants is matching unique, proving that every circulant on $n \leq 8$ vertices is either chromatically unique or matching unique (or both). They conjecture that this result holds for all n.

Their analysis motivates the equivalent problem for independence polynomials. In this section, we provide a full answer to the uniqueness problem for independence polynomials: we prove that a circulant is uniquely characterized by its independence polynomial iff it is the disjoint union of isomorphic complete graphs (e.g. $C_{8,\{1,2,3,4\}}$ and $C_{24,\{3,6,9,12\}}$). In other words, circulants are independence unique only in a handful of cases. More precisely, we will prove that there are exactly $\phi(n)$ non-isomorphic circulants on n vertices, where $\phi(n)$ denotes the number of positive divisors of n.

Definition 2.39 *A graph G is* **independence unique** *if $I(G,x) = I(H,x)$ implies $G \simeq H$.*

Some simple examples of independence unique graphs include K_n and $\overline{K_n}$. To give an example of a graph G that is not independence unique, consider the complement of a tree. For any tree on n vertices, we have $D(G,x) = 1 + nx + (n-1)x^2$, where $D(G,x)$ is the *dependence polynomial* of G, as defined in Chapter 1. Then, $I(\overline{G},x) = D(G,x) = 1 + nx + (n-1)x^2$. So any complement of an n-vertex tree has the same independence polynomial.

It is shown in [60] that two non-isomorphic trees can have the same independence polynomial. An example is illustrated in Figure 2.5. It can be shown that for these two trees,

$$I(T_1,x) = I(T_2,x) = 1 + 10x + 36x^2 + 58x^3 + 42x^4 + 12x^5 + x^6.$$

Figure 2.5: Two trees with the same independence polynomial.

Much work has been done to characterize graphs that are chromatically unique [35, 38, 61, 112, 126, 153, 175], in addition to graphs that are Tutte unique [57] and reliability unique [37]. Since the problem of independence unique graphs was first posed in [98], very few results have been found [120]. Some work has been conducted on classifying independence unique graphs for *spider graphs* [119] and *threshold graphs* [165]. However, other than these two specific families of graphs, not much is known. In the recent survey paper on independence polynomials [120], these are the only two families of graphs that are discussed.

An independence polynomial $I(G,x)$ of the form $1 + nx + \ldots$ corresponds to a graph G on n vertices. To prove that G is independence unique, we must theoretically examine all graphs on n vertices and determine their independence polynomials. For small values of n, the computation is trivial. However, for an arbitrary graph, it is NP-hard [79] to compute the independence polynomial.

Based on our analysis of independence polynomials of circulant graphs, we may naturally ask the following:

Problem 2.40 *Is G independence unique for all circulants?*

We prove that the answer is no, as evidenced by the following counterexample.

Theorem 2.41 *$G = C_n$ is not independence unique, for any $n \geq 4$.*

Proof: Let H be the graph formed by taking the path P_{n-1}, adding a new vertex u, and connecting u to an endpoint v_1 (of P_{n-1}) and its neighbour v_2. Then, $I(G, x) = I(P_{n-1}, x) + x \cdot I(P_{n-3}, x)$ and $I(H, x) = I(P_{n-1}, x) + x \cdot I(P_{n-3}, x)$ by Theorem 1.5. The latter identity follows by removing vertex u from H.

Then, $I(G, x) = I(H, x)$, but clearly $G \not\simeq H$ for $n \geq 4$. Thus, $G = C_n$ is not independence unique, for any $n \geq 4$. ∎

We have just shown that C_n is not independence unique. Are there any circulants that are independence unique, and if so, can we characterize all of them? The analogous question for matching polynomials and chromatic polynomials is partially solved in [68]. As mentioned earlier, Farrell and Whitehead prove that *every* circulant graph on at most 8 vertices is uniquely characterized either by its matching polynomial or chromatic polynomial. They conjecture that this result holds for all circulant graphs. However, they have been unable to solve the problem for any $n \geq 9$.

We will now give a complete solution to the question for independence unique circulants, where we prove the surprising result that a circulant G is independence unique iff G is the disjoint union of isomorphic complete graphs. This result will follow as a corollary of the following theorem.

Theorem 2.42 *Let $G = C_{n,S}$ be a connected circulant graph. Then, G is independence unique iff $G \simeq K_n$.*

We conclude that circulants are not rich in independence unique graphs, even though they are rich in chromatically unique and matching unique graphs. To prove Theorem 2.42, we first require the following definition and lemma.

Definition 2.43 *Let $G = C_{n,S}$ be a circulant graph. Define*

$$S' = \{x : \ |x|_n \in S\} \cup \{0\}.$$

Note that $S' = N_G[0]$, the closed neighbourhood of vertex 0 in G.

For each $i \in S'$, the graph $\boldsymbol{H_i}$ is formed by taking $G - \{0\}$, creating a new vertex u, and then joining u to every vertex $y \in V(G - \{0\})$ for which $y = i + r \pmod{n}$ for some $r \in S'$.

For example, let $G = C_{8,\{3,4\}}$, and $i = 3$. The graphs G and H_3 are illustrated in Figure 2.6.

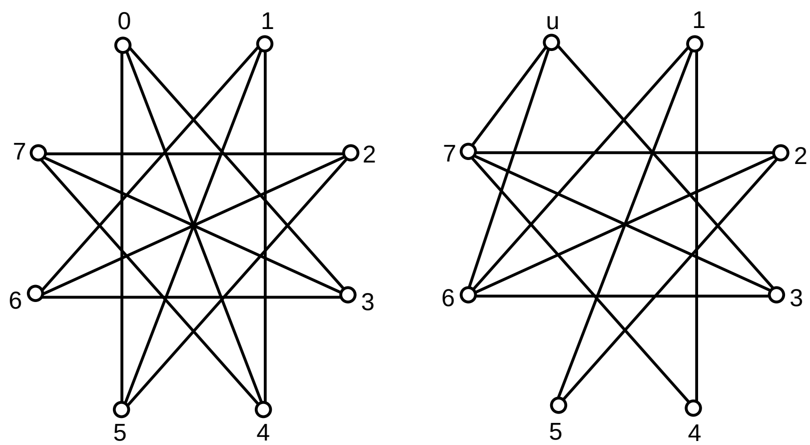

Figure 2.6: The graphs $G = C_{8,\{3,4\}}$ and the corresponding graph H_3.

Now we prove that $I(G, x) = I(H_i, x)$, for each $i \in S'$.

Lemma 2.44 *Consider the set S' and the graph H_i, as described above. For each $i \in S'$, $I(H_i, x) = I(G, x)$.*

Proof: It is clear that $H_i - \{u\} = G - \{0\}$. Note that $x \in V(G - N_G[0])$ iff $x \notin S'$, and $y \in V(H_i - N_{H_i}[u])$ iff $y - i \pmod{n} \notin S'$.

Letting $\phi(x) = x + i \pmod{n}$, we see that ϕ is an isomorphism from $G - N_G[0]$ to $H_i - N_{H_i}[u]$. Therefore, $I(G - N_G[0], x) = I(H_i - N_{H_i}[u], x)$. By Theorem 1.5,

$$\begin{aligned} I(H_i, x) &= I(H_i - \{u\}, x) + x \cdot I(H_i - N_{H_i}[u], x) \\ &= I(G - \{0\}, x) + x \cdot I(G - N_G[0], x) \\ &= I(G, x). \end{aligned}$$

Therefore, we conclude that $I(H_i, x) = I(G, x)$. ∎

By this lemma, G is not independence unique whenever we can find $i \in S$ such that $H_i \not\simeq G$. So in the above example, $G = C_{8,\{3,4\}}$ is not independence unique.

We require one additional result, which is a straightforward observation.

Proposition 2.45 ([17]) *Let $C_{n,S}$ have generating set $S = \{s_1, s_2, \ldots, s_m\}$. Then $C_{n,S}$ is connected iff $d = \gcd(n, s_1, s_2, \ldots, s_m) = 1$.*

We now prove Theorem 2.42, that a connected circulant graph $G = C_{n,S}$ is independence unique iff $G \simeq K_n$.

Proof: If $G \simeq K_n$, then $I(G, x) = 1 + nx$. Clearly G is independence unique, as any graph H with $I(H, x) = 1 + nx$ must have n vertices and satisfy $\alpha(H) = 1$.

Now suppose that G is independence unique, where G is a connected circulant. Define S' to be the closed neighbourhood of vertex 0. For all $i \in S'$, Lemma 2.44 shows that the graph H_i satisfies $I(H_i, x) = I(G, x)$. Since G is independence unique, each H_i must be isomorphic to G.

Since G is a circulant, G must be r-regular, for some r. Then the degree of each vertex in H_i must also be r. By definition, $G - \{0\} = H_i - \{u\}$. It follows that 0 and u must connect to the same set of vertices in $G - \{0\}$ and $H_i - \{u\}$, respectively, as otherwise $\deg_{H_i}(w) \neq \deg_G(w) = r$ for some vertex w. By definition of H_i, this implies that $x \in S'$ iff $x + i \pmod{n} \in S'$. This implication is true for all $i \in S'$.

Let i be the smallest non-zero element of S'. Then, $ki \pmod{n} \in S'$ for all $k \in \mathbb{N}$. By the Euclidean Algorithm, there exists an integer k such that $ki \pmod{n} = \gcd(i, n) \in S'$. By the minimality of i, this implies that $\gcd(i, n) = i$, so $i|n$. If $i = 1$, then $S' = \mathbb{Z}_n$, which implies that $S = \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$, i.e., $G \simeq K_n$.

Now let us assume that $i > 1$. If S' only contains multiples of i, then $G = C_{n,S}$ is disconnected by Proposition 2.45, which contradicts our given assumption that G is connected. So we can assume that there is an element $j \in S'$ with $d = \gcd(i, j) < i$. Since $x \in S'$ implies that $x + i \pmod{n} \in S'$ and $x + j \pmod{n} \in S'$, it follows that $pi + qj \pmod{n} \in S'$ for all pairs of positive integers (p, q). By the Euclidean algorithm, there exists a pair (p, q) for which $pi + qj \pmod{n} = d = \gcd(i, j) < i$, which contradicts the minimality of i.

We conclude that if $G = C_{n,S}$ is a connected circulant graph that is independence unique, then $G \simeq K_n$. This completes the proof. ∎

As a direct corollary of Theorem 2.42, we now establish that a circulant $G = C_{n,S}$ is independence unique iff G is the disjoint union of isomorphic complete graphs.

Corollary 2.46 *The circulant graph $G = C_{n,S}$ is independence unique iff $n = dk$ and $S = \{d, 2d, 3d, \ldots, \lfloor \frac{k}{2} \rfloor d\}$ for some positive integers k and d.*

Proof: Suppose $G = C_{n,S}$ is independence unique, and let $S = \{s_1, s_2, \ldots, s_m\}$. By Proposition 2.45, $C_{n,S}$ is connected iff $d = \gcd(n, s_1, s_2, \ldots, s_m) = 1$. If $d = 1$, then $G = K_n$ by Theorem 2.42. So suppose $d > 1$, and let $n = dk$. Then G is the disjoint union of d isomorphic copies of $G' = C_{n',S'}$, where $n' = \frac{n}{d}$ and $s_i' = \frac{s_i}{d}$ for each $1 \leq i \leq m$. If $G' \not\simeq K_{n'}$, then there exists a graph H' not isomorphic to G' for which $I(G', x) = I(H', x)$. Letting H be the disjoint union of d copies of H', we have $I(G, x) = (I(G', x))^d = (I(H', x))^d = I(H, x)$. In other words, if $G = C_{n,S}$ is independence unique, we must have $G' = K_k$, i.e., $n' = k$ and $S' = \{1, 2, \ldots, \lfloor \frac{k}{2} \rfloor\}$. The desired conclusion follows. ∎

We now enumerate the number of independence unique circulants on n vertices, for each integer $n \geq 1$. From the above theorem, this question is easily answered.

Proposition 2.47 *Define $\phi(n)$ to be the number of positive divisors of n. Then there are $\phi(n)$ independence unique circulants on n vertices, for each $n \geq 1$.*

Proof: From Corollary 2.46, $G = C_{n,S}$ is independence unique iff $n = dk$ for some ordered pair $(d, k) = (d, \frac{n}{d})$. In this case, the generating set S is uniquely defined. Therefore, exactly one independence unique circulant exists for each $d|n$. The desired conclusion follows. ∎

We have now proven that other than disjoint unions of isomorphic complete graphs, circulant graphs are not independence unique. We proved this by constructing a non-circulant graph H with $I(G, x) = I(H, x)$. Let us explore this concept further.

If G and H are both restricted to the family of circulants: must they have different independence polynomials? A variation of this question is posed in [165], where it is shown that if Γ is the family of *threshold graphs* (i.e., graphs with no induced subgraph isomorphic to P_4, C_4, or $\overline{C_4}$), then $I(G,x) \neq I(H,x)$ whenever G and H are non-isomorphic graphs in Γ. If Γ is the family of well-covered *spider graphs* (i.e., trees having at most one vertex of degree ≥ 3), then it is known [119] that $I(G,x) \neq I(H,x)$ for all $G, H \in \Gamma$ with $G \not\simeq H$. In other words, every graph in Γ has a unique independence polynomial within these two families. This motivates the following question, for the family of circulant graphs.

Problem 2.48 *Let G and H be circulants. If $I(G,x) = I(H,x)$, then must this imply that $G \simeq H$?*

We prove that the answer is no. The following is a simple counterexample.

Proposition 2.49 *Let $G = C_{8,\{1,2,4\}}$ and $H = C_{8,\{1,3,4\}}$. Then, $I(G,x) = I(H,x)$ but $G \not\simeq H$.*

Proof: It is easily checked that $I(G,x) = I(H,x) = 1 + 8x + 8x^2$. To prove that $G \not\simeq H$, it suffices to show that $\overline{G} \not\simeq \overline{H}$. But this is clear, since $\overline{G} = C_{8,\{3\}}$ is isomorphic to C_8, and $\overline{H} = C_{8,\{2\}}$ is isomorphic to two disjoint copies of C_4. ∎

To give another example, $G = C_{13,\{1,2,4\}}$ and $H = C_{13,\{1,3,4\}}$ are graphs with $I(G,x) = I(H,x) = 1 + 13x + 39x^2 + 26x^3$ but $G \not\simeq H$. The non-isomorphism of G and H is verified by noting that the 5-wheel W_5 is an induced subgraph of G, but not of H.

Proposition 2.49 can also be proved by comparing the sets of eigenvalues of G and H, and showing that they are different. To compute the eigenvalues of a graph, we find its adjacency matrix A, and then the eigenvalues correspond to all scalars λ such that $Ax = \lambda x$ for some non-zero vector x.

In a circulant $G = C_{n,S}$, each row of the adjacency matrix A is a cyclic permutation of every other row. Let $a = [a_0, a_1, \ldots, a_{n-1}]$ be the first row of A, where $a_i = a_{n-i} = 1$ iff $i \in S$. Several papers and books have been written on circulant matrices and their properties [12, 46, 56, 115, 156]. In all of these works, the eigenvalues of these matrices are studied. Here is the formula for the set of eigenvalues of $C_{n,S}$.

Theorem 2.50 ([46]) *If n is odd, the eigenvalues of G are*

$$\lambda_0 = \sum_{k=1}^{(n-1)/2} 2a_k, \quad \lambda_j = \lambda_{n-j} = \sum_{k=1}^{(n-1)/2} 2a_k \cos\left(\frac{2jk\pi}{n}\right) \qquad \text{for } 1 \le j \le \frac{n-1}{2}.$$

If n is even, then for all $1 \le j \le \frac{n}{2}$,

$$\lambda_0 = a_{n/2} + \sum_{k=1}^{n/2-1} 2a_k, \quad \lambda_j = \lambda_{n-j} = a_{n/2}\cos(j\pi) + \sum_{k=1}^{n/2-1} 2a_k \cos\left(\frac{2jk\pi}{n}\right).$$

From Theorem 2.50, we can manually verify that the set of eigenvalues of $G = C_{8,\{1,2,4\}}$ is different from those of $H = C_{8,\{1,3,4\}}$. Hence, we must have $G \not\simeq H$.

Therefore, we conclude that there are pairs of non-isomorphic circulants that have the same independence polynomial. There are several techniques to verify that two circulants are (not) isomorphic. For example, the techniques discussed in Proposition 2.49 and Theorem 2.50 are straightforward, but tedious. Is there a simpler method to determine whether two circulants $C_{n,S}$ and $C_{n,T}$ are isomorphic?

In Lemma 2.24, we gave a sufficient condition for isomorphism. In [1], Ádám conjectured that this multiplier condition is also necessary. This was later disproved [65]. To give one counterexample, $C_{16,\{1,2,7\}} \simeq C_{16,\{2,3,5\}}$, yet there is no r for which $\{2,3,5\} \equiv \{r, 2r, 7r\} \pmod{16}$. It is known that the conjecture is false if n is divisible by 8 or is the square of an odd prime [140]. However, Ádám's conjecture is true whenever n is square-free, i.e., there is no integer $d > 1$ with $d^2 | n$.

Theorem 2.51 ([140]) *If n is square-free, then $C_{n,S} \simeq C_{n,T}$ iff there exists an integer r with $\gcd(r,n) = 1$ such that $T = rS$.*

By Theorem 2.51, we immediately have another proof that $C_{13,\{1,2,4\}} \not\simeq C_{13,\{1,3,4\}}$. A complete solution to the isomorphism problem for circulant graphs was recently given by Muzychuk [141]. The results are developed in the context of Schur rings, and an efficient algorithm is given for recognizing isomorphism between two circulant graphs.

In this section, we proved that a circulant graph is independence unique iff it is the disjoint union of isomorphic complete graphs. The problem of classifying all independence unique graphs G remains open.

Chapter 3

Analysis of a Recursive Family of Circulant Graphs

Due to the structure and symmetry of a circulant graph, one might expect that there is a simple algorithm to compute $\alpha(G)$ when G is restricted to circulants. But as we discussed earlier, determining the independence number of an arbitrary circulant is NP-hard. Moreover, it is shown in [46] that it is NP-hard even to get a good approximation for $\alpha(G)$. A formula for $\alpha(C_{n,S})$ is known only for a handful of generating sets. We gave several examples in Chapter 2, where we directly computed $\alpha(C_{n,S})$ from a formula for $I(C_{n,S}, x)$. But even for these "simple" cases, determining a formula for $I(G, x)$ is an extremely complicated task.

While it may be computationally intractable to determine $I(C_{n,S}, x)$ for an arbitrary generating set S, we may be able to determine families of sets S for which $\alpha(C_{n,S}) = \deg(I(C_{n,S}, x))$ can be calculated without determining its independence polynomial. In this section, we will determine an infinite family of generating sets S for which this is the case. Our formula for $\alpha(C_{n,S})$ will be a simple recurrence relation, from which the independence number can easily be computed.

This infinite class of circulants will feature prominently in four important and varied applications: a new classification of star extremal graphs; a generalization of known results on the chromatic number of integer distance graphs; an explicit formula for the generalized fractional Ramsey number; and the optimal Nordhaus-Gaddum inequalities for the fractional chromatic and circular chromatic numbers. In each of these four applications, using the formula for $\alpha(C_{n,S})$ will be the key step.

3.1 Calculating the Independence Number $\alpha(C_{n,S})$

Let $S \subseteq \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ be the generating set for some circulant $G = C_{n,S}$. Define

$$\pm S \pmod{n} = \{x \in \mathbb{Z} : \quad x \in S \text{ or } n - x \in S\}.$$

For each k-tuple of integers $(a_1, a_2, \ldots, a_k)$ with each $a_i \geq 3$, we construct the graphs $G_j(a_1, a_2, \ldots, a_k)$ as follows.

Definition 3.1 *Let $k \geq 1$ and let $(a_1, a_2, \ldots, a_k)$ be a k-tuple of integers with each $a_i \geq 3$.*

Define $n_0 = 1$, and $n_i = a_i n_{i-1} - 1$, for $1 \leq i \leq k$. Then for each $1 \leq j \leq i \leq k$, set

$$S_{j,i} = \begin{cases} \pm S_{j,i-1} \pmod{n_{i-1}} & \text{for all } 1 \leq j < i \\ \left\{1, 2, \ldots, \left\lfloor \frac{n_i}{2} \right\rfloor \right\} - \bigcup_{j=1}^{i-1} S_{j,i} & \text{for } j = i \end{cases}$$

Then $\boldsymbol{G_j(a_1, a_2, \ldots, a_k) := C_{n_k, S_{j,k}}}$, the circulant graph on n_k vertices with generating set $S_{j,k}$.

For notational convenience, we will now abbreviate $G_j(a_1, a_2, \ldots, a_k)$ as $G_{j,k}$, where the a_i's are assumed to be fixed integers with each $a_i \geq 3$. To illustrate our construction, let $(a_1, a_2, a_3) = (5, 6, 8)$. Then, we get $(n_1, n_2, n_3) = (4, 23, 183)$. We have

$$\begin{aligned} S_{1,1} &= \{1, 2\} \\ S_{1,2} &= \{1, 2, 3\} \\ S_{2,2} &= \{4, 5, 6, \ldots, 11\} \\ S_{1,3} &= \{1, 2, 3, 20, 21, 22\} \\ S_{2,3} &= \{4, 5, \ldots, 19\} \\ S_{3,3} &= \{23, 24, \ldots, 91\}. \end{aligned}$$

Therefore, we have $G_{1,3} = C_{183,\{1,2,3,20,21,22\}}$, $G_{2,3} = C_{183,\{4,5,\ldots,19\}}$, and $G_{3,3} = C_{183,\{23,24,\ldots,91\}}$ for the ordered triplet $(a_1, a_2, a_3) = (5, 6, 8)$.

Note that in our example, the $S_{j,k}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$ for $k = 3$. We prove that this is always the case, for any fixed k. This will show that the $G_{j,k}$'s form an edge partition of K_{n_k}, i.e., the $G_{j,k}$'s induce a k-edge colouring of K_{n_k}.

Lemma 3.2 *The $S_{j,k}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$. In other words, given any $1 \le x \le \lfloor \frac{n_k}{2} \rfloor$, there is a unique index $1 \le j \le k$ such that $x \in S_{j,k}$.*

Proof: We proceed by induction on k. The result is trivial for $k = 1$, so assume $k \ge 2$. Suppose that the $S_{j,k-1}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_{k-1}}{2} \rfloor\}$, where $1 \le j \le k-1$.

By definition, $S_{j,k} = \pm S_{j,k-1} \pmod{n_{k-1}}$. Therefore, every element in the set $\{1, 2, \ldots, n_{k-1} - 1\}$ will appear in exactly one $S_{j,k}$, for some $1 \le j \le k-1$. Clearly no other elements will appear. By definition, it follows that $S_{k,k} = \{n_{k-1}, n_{k-1} + 1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$. Hence, the $S_{j,k}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$, which completes the proof. ∎

Definition 3.3 *For any generating set $S = \{s_1, s_2, \ldots, s_t\}$ with $1 \le s_1 < s_2 < \ldots < s_t \le \lfloor \frac{n}{2} \rfloor$, the* **end sum** *is $\Omega(S) = \min(S) + \max(S) = s_1 + s_t$.*

Definition 3.4 *A generating set $S = \{s_1, s_2, \ldots, s_t\}$ is* **reversible** *if $s_i + s_{t+1-i} = \Omega(S)$ for all $1 \le i \le t$.*

In our example, $S_{1,3}$ and $S_{2,3}$ are both reversible sets with end sum $n_2 = 23$. The following results are all straightforward to prove; we will constantly refer to them throughout this chapter.

Proposition 3.5 *For any k-tuple of positive integers $(a_1, a_2, \ldots, a_k)$ with each $a_i \ge 3$, the $S_{j,k}$'s satisfy the following conditions:*

(a) $S_{j,k} = S_{j,k-1} \bigcup \{n_{k-1} - x : \quad x \in S_{j,k-1}\}$, *for all* $1 \le j < k$.

(b) $S_{j,i-1} \subset S_{j,i}$ *for each* $1 \le j < i \le k$.

(c) $0 \le n_{k-1} - 1 < \lfloor \frac{n_k}{2} \rfloor$, *with equality iff* $k = 1$.

(d) $S_{k,k} = \{n_{k-1}, n_{k-1} + 1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$.

(e) $S_{k-1,k} = \{n_{k-2}, n_{k-2} + 1, \ldots, n_{k-1} - n_{k-2}\}$.

(f) For every $1 \le j \le k$, the connection set $S_{j,k}$ is reversible. Furthermore, if $1 \le j \le k-1$, then $\Omega(S_{j,k}) = n_{k-1}$.

(g) For all $1 \leq j \leq k-1$, $\max(S_{j,k}) \leq n_{k-1} - 1$.

<u>Proof:</u> By definition, $S_{j,k} = \pm S_{j,k-1} \pmod{n_{k-1}}$. So each $y \in S_{j,k}$ satisfies $y \in S_{j,k-1}$ or $n_{k-1} - y \in S_{j,k-1}$. Therefore, $S_{j,k} = S_{j,k-1} \bigcup \{n_{k-1} - x : \ x \in S_{j,k-1}\}$. This proves part (a).

By the same argument as part (a), $S_{j,i} = S_{j,i-1} \bigcup \{n_{i-1} - x : \ x \in S_{j,i-1}\}$, for each $1 \leq j < i \leq k$. Thus, $S_{j,i-1} \subset S_{j,i}$, proving part (b).

We note that part (c) is trivial for $k = 1$, since $n_0 = 1$ and $n_1 = a_1 - 1 \geq 2$. If $k \geq 2$, then $n_{k-1} = a_{k-1} n_{k-2} - 1 \geq a_{k-1} - 1 > 1$. Finally, $\lfloor \frac{n_k}{2} \rfloor = \lfloor \frac{a_k n_{k-1} - 1}{2} \rfloor \geq \frac{a_k n_{k-1}}{2} - 1 > n_{k-1} - 1$, since each $a_k \geq 3$. This proves part (c).

Part (d) was established in the proof of Lemma 3.2. From part (d), $S_{k-1,k-1} = \{n_{k-2}, n_{k-2}+1, \ldots, \lfloor \frac{n_{k-1}}{2} \rfloor\}$. By part (a),

$$S_{k-1,k} = S_{k-1,k-1} \bigcup \{n_{k-1} - x : \ x \in S_{k-1,k-1}\} = \{n_{k-2}, n_{k-2}+1, \ldots, n_{k-1} - n_{k-2}\},$$

which proves part (e).

Now we prove part (f). Fix $1 \leq j \leq k-1$. Let $S_{j,k-1} = \{s_1, s_2, \ldots, s_t\}$. Then, $S_{j,k} = \pm S_{j,k-1} \pmod{n_{k-1}} = \{s_1, s_2, \ldots, s_t, s_{t+1}, s_{t+2}, \ldots, s_{2t}\}$, where $s_i + s_{2t+1-i} = n_{k-1}$ for all $1 \leq i \leq 2t$. To confirm that $S_{j,k}$ is reversible, we must verify that these elements appear in non-decreasing order. Since $s_t = \max(S_{j,k-1}) \leq \lfloor \frac{n_{k-1}}{2} \rfloor$, we have $s_t \leq s_{t+1}$, which implies that $S_{j,k}$ is non-decreasing. It follows that $S_{j,k}$ is reversible, with $\Omega(S_{j,k}) = n_{k-1}$. Note that if $j = k$, then $S_{k,k} = \{n_{k-1}, n_{k-1}+1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$, which is also reversible, but has a different end sum.

Finally, part (g) follows from the observation that $\min(S_{j,k}) = s_1 \geq 1$, and so by part (f), $\max(S_{j,k}) = s_{2t} = \Omega(S_{j,k}) - s_1 = n_{k-1} - s_1 \leq n_{k-1} - 1$. ∎

Each result in Proposition 3.5 holds for any k-tuple of integers $(a_1, a_2, \ldots, a_k)$, where each $a_i \geq 3$. Consider the truncation of the k-tuple to the first $m \leq k$ elements, i.e., the m-tuple $(a_1, a_2, \ldots, a_m)$. By the same argument, each of the results in Proposition 3.5 hold for this m-tuple, which we derive by simply replacing k by m. For example, $S_{j,m} = S_{j,m-1} \bigcup \{n_{m-1} - x : \ x \in S_{j,m-1}\}$. We refer to this as the **Truncation Principle**. Although it will not be explicitly stated, the Truncation Principle will be applied repeatedly throughout this chapter, especially in our analysis of star extremal graphs in Section 3.2.

Definition 3.6 *We say that an* **interval** *of a generating set $S_{j,k}$ is a maximum sequence of consecutive terms.*

For example, $S_{1,3} = \{1, 2, 3, 20, 21, 22\}$ consists of two intervals of length 3, namely the intervals $\{1, 2, 3\}$ and $\{20, 21, 22\}$. For any integer $k \geq 1$, the generating set $S_{k,k} = \{n_{k-1}, n_{k-1} + 1, \dots, \lfloor \frac{n_k}{2} \rfloor\}$ consists of one interval of length $\lfloor \frac{n_k}{2} \rfloor - n_{k-1} + 1$.

Lemma 3.7 *Let $1 \leq j \leq k-1$. Then $S_{j,k}$ consists of 2^{k-j-1} intervals of equal length.*

<u>Proof:</u> We proceed by induction on k. The base case $k = 2$ is trivial, as $S_{1,2} = \{1, 2, \dots, n_1 - 1\}$. Let $k \geq 3$ and suppose the lemma is true for $k - 1$. Then, for all $1 \leq j \leq k-2$, the set $S_{j,k-1}$ consists of 2^{k-j-2} intervals of equal length. As noted earlier in the proof of Proposition 3.5 (f), if $S_{j,k-1} = \{s_1, s_2, \dots, s_t\}$, then $S_{j,k} = \{s_1, s_2, \dots, s_t, s_{t+1}, s_{t+2}, \dots, s_{2t}\}$ where $s_i + s_{2t+1-i} = n_{k-1}$ for all $1 \leq i \leq 2t$. Each half of $S_{j,k}$ (namely the first t elements and the last t elements) consists of exactly 2^{k-j-2} intervals of equal length, by the induction hypothesis. Now we show that no elements overlap, and that these intervals are disjoint. By Proposition 3.5 (g), $\max(S_{j,k-1}) = s_t \leq n_{k-2} - 1$, and so

$$
\begin{aligned}
s_{t+1} - s_t &= (n_{k-1} - s_t) - s_t \\
&= n_{k-1} - 2s_t \\
&\geq n_{k-1} - 2(n_{k-2} - 1) \\
&= (a_{k-1}n_{k-2} - 1) - 2n_{k-2} + 2 \\
&= (a_{k-1} - 2)n_{k-2} + 1 \\
&> 1.
\end{aligned}
$$

It follows that all of these intervals are disjoint. Thus, $S_{j,k}$ consists of 2^{k-j-1} intervals of equal length, completing the induction. Finally, if $j = k-1$, then we need to show that $S_{k-1,k}$ consists of just $2^{k-j-1} = 1$ interval. This follows as $S_{k-1,k} = \{n_{k-2}, n_{k-2} + 1, \dots, n_{k-1} - n_{k-2}\}$, by Proposition 3.5 (e). ∎

Now we state the main theorem of this section.

Theorem 3.8 *Let $a_1, a_2, \ldots, a_k$ be integers such that $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-2} \leq a_{k-1} \leq a_k + 1$. Then,*

$$\alpha(G_{j,k}) = \begin{cases} a_k \alpha(G_{j,k-1}) - 1 & \text{for } 1 \leq j \leq k-1 \\ n_{k-1} & \text{for } j = k \end{cases}$$

This theorem gives us a formula for each $\alpha(G_{j,k})$, for any k-tuple $(a_1, a_2, \ldots, a_k)$ satisfying the given conditions. This powerful theorem gives us a simple recurrence relation to compute exact values of $\alpha(G)$ for an infinite family of circulant graphs, rather than just upper and lower bounds. Past papers [30, 46, 48, 78, 99, 121, 123] have established many bounds on $\alpha(G)$ for various families of circulants, but only a few formulas for $\alpha(G)$ have been found. In all of these known examples, the generating set S has either consisted of at most two intervals of equal length, or has been a set of at most 4 singleton elements (e.g. $S = \{x, y, x+y, x-y\}$ for some $x > y$). By Lemma 3.7, this theorem will give us the exact value of $\alpha(G)$ for families of circulants with 2^k intervals, for any integer $k \geq 1$. Therefore, Theorem 3.8 extends much of what is currently known about the values of $\alpha(C_{n,S})$.

Theorem 3.8 gives us a simple polynomial time recurrence to determine $\alpha(G)$ for any graph in this infinite family. To illustrate, we compute the independence number for the graph $G = C_{183,\{1,2,3,20,21,22\}}$. Recall that this graph is $G_{1,3}$, where $(a_1, a_2, a_3) = (5, 6, 8)$.

$$\begin{aligned} \alpha(C_{183,\{1,2,3,20,21,22\}}) &= 8\alpha(C_{23,\{1,2,3\}}) - 1 \\ &= 8(6\alpha(C_{4,\{1,2\}}) - 1) - 1 \\ &= 8(6 \cdot 1 - 1) - 1 \\ &= 39. \end{aligned}$$

In fact, we can find an explicit formula for $\alpha(G_{j,k})$ from Theorem 3.8.

Corollary 3.9 *For each $1 \leq j < k$,*

$$\alpha(G_{j,k}) = n_{j-1} \prod_{p=j+1}^{k} a_p - \sum_{i=j+2}^{k} \left(\prod_{p=i}^{k} a_p \right) - 1.$$

Proof: Fix $a_1, a_2, \ldots, a_k$, and let $g(k)$ equal the right side of the above identity. Then $g(k) = a_k g(k-1) - 1$. Also, $\alpha(G_{j,k}) = a_k \alpha(G_{j,k-1}) - 1$. The desired result then follows by a simple induction argument. ∎

Now we prove Theorem 3.8. First, we prove the $j = k$ case directly. Then we establish the $1 \leq j \leq k-1$ case by proving the upper bound, then the lower bound.

Proposition 3.10 *Let $k \geq 1$. Then, $\alpha(G_{k,k}) = n_{k-1}$.*

Proof: By Proposition 3.5 (d), $S_{k,k} = \{n_{k-1}, n_{k-1}+1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$. The set $I = \{0, 1, 2, \ldots, n_{k-1} - 1\}$ is independent in $G_{k,k}$, which shows that $\alpha(G_{k,k}) \geq |I| = n_{k-1}$. But if I is an independent set with $|I| > n_{k-1}$, then there must be two elements with a circular distance of at least n_{k-1}, which is a contradiction. ∎

Now we prove that $\alpha(G_{j,k}) \leq a_k \alpha(G_{j,k-1}) - 1$, for each $1 \leq j \leq k-1$. The result will follow immediately from two lemmas. The first lemma is a result of Collins [48].

Lemma 3.11 ([48]) *Let $G = C_{n,S}$. Let G_S be the subgraph of G induced by taking any set of $\Omega(S)$ consecutive vertices in G. Then, $\frac{\alpha(G)}{|G|} \leq \frac{\alpha(G_S)}{|G_S|}$.*

Lemma 3.12 *Let $1 \leq j \leq k-1$ be fixed. Let H be the subgraph of $G_{j,k}$ induced by taking any set of $\Omega(S_{j,k})$ consecutive vertices in $G_{j,k}$. Then, $H \simeq G_{j,k-1}$.*

Proof: By Proposition 3.5 (f), $S_{j,k}$ is reversible with $\Omega(S_{j,k}) = n_{k-1}$. Since $G_{j,k}$ is a circulant, all induced subgraphs of $G_{j,k}$ with n_{k-1} consecutive vertices will be isomorphic. So without loss, we can take H to be the subgraph of $G_{j,k}$ induced by the vertices $0, 1, 2, \ldots, n_{k-1} - 1$. To show $H \simeq G_{j,k-1}$, we prove that $uv \in E(H)$ iff $uv \in E(G_{j,k-1})$. The latter is equivalent to the condition $|u - v|_{n_{k-1}} \in S_{j,k-1}$.

Let $0 \leq u < v \leq n_{k-1} - 1$. Since $n_k = a_k n_{k-1} - 1 > 2(n_{k-1} - 1)$, $uv \in E(H)$ iff $|u-v|_{n_k} = v-u \in S_{j,k}$. By Proposition 3.5 (a), $S_{j,k} = S_{j,k-1} \bigcup \{n_{k-1} - x : \ x \in S_{j,k-1}\}$, and so $v - u \in S_{j,k}$ iff $v - u \in S_{j,k-1}$ or $n_{k-1} - (v-u) \in S_{j,k-1}$. In other words, $uv \in E(H)$ iff $|u - v|_{n_{k-1}} \in S_{j,k-1}$. This proves that $H \simeq G_{j,k-1}$, and our proof is complete. ∎

Proposition 3.13 *For each $1 \leq j \leq k-1$, we have $\alpha(G_{j,k}) \leq a_k \alpha(G_{j,k-1}) - 1$.*

Proof: From Lemmas 3.11 and 3.12, $\frac{\alpha(G_{j,k})}{|G_{j,k}|} \leq \frac{\alpha(G_{j,k-1})}{|G_{j,k-1}|}$. Since $|G_{j,k}| = n_k$ and $|G_{j,k-1}| = n_{k-1}$, we have

$$\alpha(G_{j,k}) \leq \frac{n_k}{n_{k-1}}\alpha(G_{j,k-1}) = \frac{a_k n_{k-1} - 1}{n_{k-1}}\alpha(G_{j,k-1}) < a_k\alpha(G_{j,k-1}).$$

Since $\alpha(G_{j,k}) < a_k\alpha(G_{j,k-1})$, this implies that $\alpha(G_{j,k}) \leq a_k\alpha(G_{j,k-1}) - 1$, as required. ∎

Now we prove that $\alpha(G_{j,k}) \geq a_k\alpha(G_{j,k-1}) - 1$, for each $1 \leq j \leq k-1$. We will require two lemmas. Once again, the first lemma is a result of Collins [48].

Lemma 3.14 ([48]) *Let $H_1 = C_{n,S}$ have a reversible generating set S, and suppose $n \geq \Omega(S) + \max(S)$. For $k \geq 2$, define H_k to be the circulant with $n + (k-1)\Omega(S)$ vertices and generating set S. Let H_S be the subgraph induced by taking any set of $\Omega(S)$ vertices from H_1. Then, $\alpha(H_k) \geq \alpha(H_1) + (k-1)\alpha(H_S)$ for all $k \geq 1$.*

In the actual lemma found in [48], the given condition is $n > \Omega(S) + \max(S)$. However, Lemma 3.14 is also correct when $n = \Omega(S) + \max(S)$, as the proof just requires that there is no element $x \in S$ such that $0 \leq n - x \leq \Omega(S) - 1$. And if $n = \Omega(S) + \max(S)$, then $n - x \geq n - \max(S) = \Omega(S)$. Thus, Lemma 3.14 also holds in this special case, and so we include this in the statement of the lemma.

Lemma 3.15 *Let $i \in S_{j,k}$, where $1 \leq j \leq k-2$. Then $i = x$ or $i = n_{k-1} - n_{k-2} + x$ for some $x \in S_{j,k-1}$.*

Proof: By Proposition 3.5 (f), $S_{j,k-1}$ is a reversible set with $\Omega(S_{j,k-1}) = n_{k-2}$. Let $S_{j,k-1} = \{s_1, s_2, \ldots, s_t\}$. Then the reversibility of $S_{j,k-1}$ implies that $s_{t-q+1} = n_{k-2} - s_q$ for any $1 \leq q \leq t$.

Since $S_{j,k} = \pm S_{j,k-1} \pmod{n_{k-1}}$, we have $S_{j,k} = \{s_1, s_2, \ldots, s_t, s_{t+1}, \ldots, s_{2t}\}$, which is also reversible. Therefore, for any $1 \leq q \leq t$, we have $s_{t+q} = n_{k-1} - s_{t-q+1} = n_{k-1} - (n_{k-2} - s_q)$, and so $s_{t+q} = n_{k-1} - n_{k-2} + s_q$.

Let $x \in S_{j,k-1} = \{s_1, s_2, \ldots, s_t\}$. By our analysis, we conclude that $i = x$ or $i = n_{k-1} - n_{k-2} + x$ for some $x \in S_{j,k-1}$. ∎

Lemma 3.16 *Let $k \geq 3$, and fix $1 \leq j \leq k-2$. Define $H = C_{a_{k-1}(n_{k-1}-n_{k-2}),S_{j,k}}$ and $H' = C_{n_{k-1}-n_{k-2},S_{j,k-1}}$. Then, $\alpha(H) \geq a_{k-1}\alpha(H')$.*

Proof: Let $\alpha(H') = t$, and let $I' = \{v_1, v_2, \ldots, v_t\}$ be a maximum independent set of H'. We will prove that $\alpha(H) \geq ta_{k-1}$.

Since I' is independent, for any $v_a, v_b \in I'$, we have $|v_a - v_b|_{|V(H')|} \notin S_{j,k-1}$, which implies that $v_a - v_b \not\equiv \pm r' \pmod{n_{k-1} - n_{k-2}}$, for all $r' \in S_{j,k-1}$. This holds because $|V(H')| = n_{k-1} - n_{k-2}$.

By Lemma 3.15, every $r \in S_{j,k}$ satisfies $r \equiv r' \pmod{n_{k-1} - n_{k-2}}$, for some $r' \in S_{j,k-1}$.

Let us construct an independent set of H with ta_{k-1} vertices. Define

$$I = \{p(n_{k-1} - n_{k-2}) + v_q : \quad 0 \leq p \leq a_{k-1} - 1, \quad 1 \leq q \leq t\}.$$

We show that I is independent, which will prove that $\alpha(H) \geq |I| = ta_{k-1}$. Let $x, y \in I$. Then $|x - y|_{|V(H)|} = z(n_{k-1} - n_{k-2}) + (v_a - v_b)$, for some integer z and $v_a, v_b \in I'$. Since $|V(H)| = a_{k-2}(n_{k-1} - n_{k-2})$, it follows that $|x - y|_{|V(H)|} \equiv v_a - v_b \pmod{n_{k-1} - n_{k-2}}$. From above, this implies that $|x - y|_{|V(H)|} \not\equiv \pm r' \pmod{n_{k-1} - n_{k-2}}$, for any $r' \in S_{j,k-1}$. But we just showed that every element in $S_{j,k}$ is congruent modulo $n_{k-1} - n_{k-2}$ to some $r' \in S_{j,k-1}$. Therefore, $|x - y|_{|V(H)|} \notin S_{j,k}$, i.e, $x, y \in I$ implies that $xy \notin E(H)$. Thus, I is independent, and our proof is complete. ∎

To illustrate Lemma 3.16, let us use our earlier example of $(a_1, a_2, a_3) = (5, 6, 8)$. For this ordered triplet, we have $n_1 = 4$, $n_2 = 23$, and $n_3 = 183$. This lemma states that $\alpha(C_{114,\{1,2,3,20,21,22\}}) \geq 6\alpha(C_{19,\{1,2,3\}})$. We have $\alpha(C_{19,\{1,2,3\}}) = 4$, and a maximal independent set is $\{0, 4, 8, 12\}$. By our lemma, the set $I = \{19p + 4q : 0 \leq p \leq 5, 0 \leq q \leq 3\}$ is an independent set in $C_{114,\{1,2,3,20,21,22\}}$ with 24 vertices.

Now we are ready to prove the upper bound.

Proposition 3.17 *Let $a_1, a_2, \ldots, a_k$ be integers such that $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-2} \leq a_{k-1} \leq a_k + 1$. Then, $\alpha(G_{j,k}) \geq a_k\alpha(G_{j,k-1}) - 1$, for each $1 \leq j \leq k-1$.*

Proof: First, we prove that the result is true for $j = k-1$. By Proposition 3.5 (e), $S_{k-1,k} = \{n_{k-2}, n_{k-2} + 1, \ldots, n_{k-1} - n_{k-2}\}$. Now define

$$I = \{pn_{k-1} + q : \quad 0 \leq p \leq a_k - 1, \quad 0 \leq q \leq n_{k-2} - 1\}.$$

Then, it is straightforward to check that $I-\{0\}$ is an independent set of $S_{k-1,k}$, which proves that $\alpha(G_{k-1,k}) \geq |I|-1 = a_k n_{k-2}-1 = a_k\alpha(G_{k-1,k-1})-1$, by Proposition 3.10.

Now let $1 \leq j \leq k-2$. We proceed by induction on k. There is nothing to prove for the case $k=2$, so let $k \geq 3$, and suppose that the statement is true for all indices less than k.

By definition, $n_k = a_k n_{k-1} - 1$ and $n_{k-1} = a_{k-1}n_{k-2} - 1$. Hence,

$$\begin{aligned} n_k &= a_k n_{k-1} + n_{k-1} - a_{k-1}n_{k-2} \\ &= a_{k-1}(n_{k-1} - n_{k-2}) + (a_k - a_{k-1} + 1)n_{k-1} \\ &= a_{k-1}(n_{k-1} - n_{k-2}) + (a_k - a_{k-1} + 1)\Omega(S_{j,k}). \end{aligned}$$

For each $k \geq 1$, define H_k to be the circulant on $a_{k-1}(n_{k-1} - n_{k-2}) + (k-1)n_{k-1}$ vertices, with generating set $S_{j,k}$. We wish to apply Lemma 3.14. Before we apply the lemma, we must check that the required conditions are satisfied. We require $(a_k - a_{k-1} + 1) \geq 0$ and $a_{k-1}(n_{k-1} - n_{k-2}) \geq \Omega(S_{j,k}) + \max(S_{j,k})$. The former is satisfied because of the given inequality $a_1 \leq a_2 \leq \ldots \leq a_{k-2} \leq a_{k-1} \leq a_k + 1$. Now we verify the latter inequality. Since $a_{k-1} \geq 3$, we have

$$\begin{aligned} (a_{k-1} - 3)n_{k-1} &\geq 0 \\ \Longrightarrow a_{k-1}n_{k-1} - (n_{k-1} + 1) &\geq 2n_{k-1} - 1 \\ \Longrightarrow a_{k-1}n_{k-1} - a_{k-1}n_{k-2} &\geq n_{k-1} + (n_{k-1} - 1) \\ \Longrightarrow a_{k-1}(n_{k-1} - n_{k-2}) &\geq \Omega(S_{j,k}) + (n_{k-1} - 1) \\ \Longrightarrow a_{k-1}(n_{k-1} - n_{k-2}) &\geq \Omega(S_{j,k}) + \max(S_{j,k}), \quad \text{by Proposition 3.5 (g).} \end{aligned}$$

Therefore, the conditions of the lemma are indeed met. By Lemma 3.14 and Lemma 3.12, we have

$$\alpha(G_{j,k}) = \alpha(C_{n_k,S_{j,k}}) \geq \alpha(C_{a_{k-1}(n_{k-1}-n_{k-2}),S_{j,k}}) + (a_k - a_{k-1} + 1)\alpha(G_{j,k-1}).$$

We claim that $\alpha(C_{n_{k-1}-n_{k-2},S_{j,k-1}}) = \alpha(G_{j,k-1}) - \alpha(G_{j,k-2})$. By the induction hypothesis, Proposition 3.17 holds for all $(k-1)$-tuples of integers $(b_1, b_2, \ldots, b_{k-1})$ for which $3 \leq b_1 \leq b_2 \leq \ldots \leq b_{k-2} \leq b_{k-1} + 1$. Therefore, by the given condition $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-2} \leq a_{k-1}$, the corollary holds for both the k-tuples $(a_1, a_2, \ldots, a_{k-2}, a_{k-1})$ and $(a_1, a_2, \ldots, a_{k-2}, a_{k-1} - 1)$.

This translates to the following inequalities, by the induction hypothesis:

$$\begin{aligned}\alpha(C_{a_{k-1}n_{k-2}-1,S_{j,k-1}}) = \alpha(G_{j,k-1}) &\geq a_{k-1}\alpha(G_{j,k-2}) - 1.\\ \alpha(C_{(a_{k-1}-1)n_{k-2}-1,S_{j,k-1}}) = \alpha(C_{n_{k-1}-n_{k-2},S_{j,k-1}}) &\geq (a_{k-1}-1)\alpha(G_{j,k-2}) - 1.\end{aligned}$$

But by Proposition 3.13, equality is reached in both cases. Note that in the second case, equality follows by replacing a_{k-1} by $a_{k-1}-1$ in the statement of Proposition 3.13.

Subtracting one identity from the other, we have $\alpha(G_{j,k-1}) - \alpha(C_{n_{k-1}-n_{k-2},S_{j,k-1}}) = \alpha(G_{j,k-2})$, which is equivalent to $\alpha(C_{n_{k-1}-n_{k-2},S_{j,k-1}}) = \alpha(G_{j,k-1}) - \alpha(G_{j,k-2})$.

Therefore, by Lemma 3.16,

$$\begin{aligned}\alpha(G_{j,k}) &\geq \alpha(C_{a_{k-1}(n_{k-1}-n_{k-2}),S_{j,k}}) + (a_k - a_{k-1} + 1)\alpha(G_{j,k-1})\\ &\geq a_{k-1}\alpha(C_{n_{k-1}-n_{k-2},S_{j,k-1}}) + (a_k - a_{k-1} + 1)\alpha(G_{j,k-1})\\ &= a_{k-1}(\alpha(G_{j,k-1}) - \alpha(G_{j,k-2})) + (a_k - a_{k-1} + 1)\alpha(G_{j,k-1})\\ &= a_k\alpha(G_{j,k-1}) + \alpha(G_{j,k-1}) - a_{k-1}\alpha(G_{j,k-2})\\ &\geq a_k\alpha(G_{j,k-1}) - 1, \quad \text{by the induction hypothesis.}\end{aligned}$$

This completes the proof. ∎

Now Theorem 3.8 follows immediately from Propositions 3.10, 3.13, and 3.17.

3.2 Application 1: Star Extremal Graphs

A graph G is *star extremal* if its fractional chromatic number equals its circular chromatic number. Let us now define these two graph invariants. First, we provide a brief introduction to fractional graph theory.

For invariants such as $\omega(G)$ and $\chi(G)$, we may define a corresponding *fractional* invariant [158], where we no longer require our solution to consist of whole pieces. For example, in the case of the *fractional chromatic number*, denoted by $\chi_f(G)$, we will require that each vertex get a *total* of one colour, allowing cases such as a vertex being coloured $\frac{1}{2}$ red, $\frac{1}{3}$ blue, and $\frac{1}{6}$ white. We will still require that no two adjacent vertices share any amount of the same colour, i.e., we want a *proper* fractional colouring. If no vertex gets assigned a red part of more than $\frac{1}{2}$, then this colour contributes $\frac{1}{2}$ to the "total" number of colours used. The fractional chromatic number $\chi_f(G)$ is defined to be the smallest number of "total" colours used in a proper fractional colouring of G.

For example, it can be shown that $\chi_f(C_5) = \frac{5}{2}$. Figure 3.1 illustrates a proper fractional $\frac{5}{2}$-colouring of C_5. Our colours are denoted by the letters A, B, C, D, E. By definition, $\chi_f(G) \leq \chi(G)$.

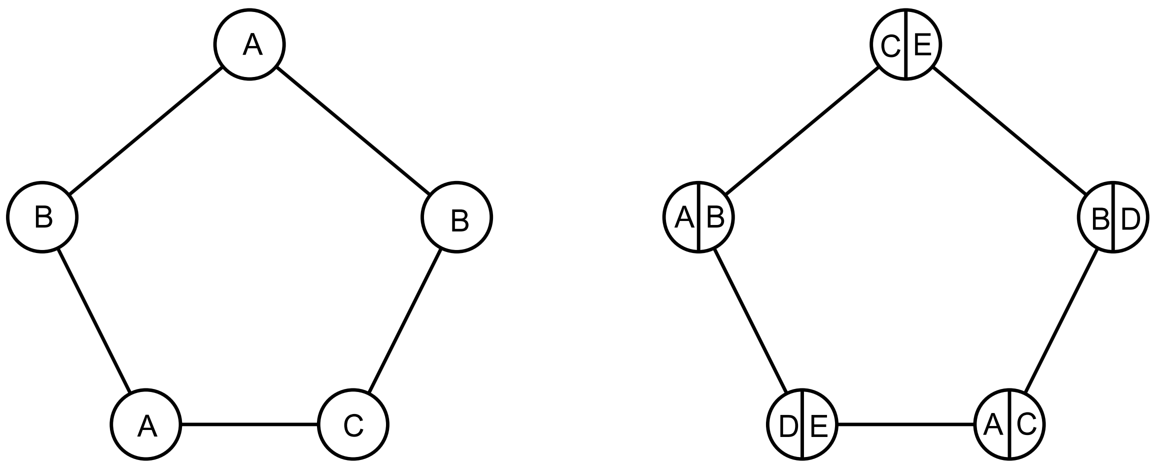

Figure 3.1: A 3-colouring of C_5 and a fractional $\frac{5}{2}$-colouring of C_5.

The chromatic number $\chi(G)$ can be alternatively defined as the smallest cardinality of a vertex cover of G by independent sets. For example, in the above 3-colouring of C_5, the vertices that are assigned to each colour form an independent set. Since three independent sets are required to cover all of the vertices, $\chi(C_5) = 3$. In this context, we can define $\chi(G)$ using concepts from linear programming. This, in turn, motivates the definition for $\chi_f(G)$.

Let M denote the vertex-independent set incidence matrix of G. The rows of M are indexed by the vertices $\{v_1, v_2, \ldots, v_n\}$, and the columns are indexed by the independent subsets of the vertices, $\{I_1, I_2, \ldots, I_m\}$. The (i, j) entry of M is 1 when $v_i \in I_j$, and is 0 otherwise.

Definition 3.18 ([158]) *The chromatic number* $\chi(G) = \min \mathbf{1}^{\mathrm{T}} x$*, where* $Mx \geq \mathbf{1}$*,* $x \geq 0$*, and* $x \in \mathbb{Z}^m$*. (Here,* $\mathbf{1}$ *denotes the* m *by* 1 *vector of all* 1*'s).*

The **fractional chromatic number** $\chi_f(G)$ *is the relaxation of the integer program into a linear program:*

$\chi_f(G) = \min \mathbf{1}^{\mathrm{T}} x$, *where* $Mx \geq \mathbf{1}$, $x \geq 0$, *and* $x \in \mathbb{R}^m$.

A comprehensive reference on fractional graph theory is found in [158]. Using the idea of relaxing integer programs of graph invariants to the linear case, they similarly define invariants such as the fractional matching number, the fractional edge colouring number, and the fractional arboricity number. It is shown that these invariants always take on rational (or fractional) values, hence the name. The topic of fractional graph theory makes important connections between graph theory and combinatorial optimization. Now we define the *circular chromatic number* $\chi_c(G)$.

Definition 3.19 ([169]) *Let k and d be positive integers such that $k \geq 2d$. A* **(k, d)-colouring** *of a graph $G = (V, E)$ is a mapping $C : V \to \{0, 1, \ldots, k-1\}$ such that the circular distance $|C(x) - C(y)|_k \geq d$ for any $xy \in E(G)$. Then, the* **circular chromatic number** *$\chi_c(G)$ is the infimum of $\frac{k}{d}$ for which there exists a (k, d)-colouring of G.*

For any non-trivial graph, $\chi(G)$ is just the smallest k for which there exists a $(k, 1)$-colouring of G. So $\chi_c(G)$ is a generalization of $\chi(G)$. The circular chromatic number is sometimes referred to as the *star chromatic number* [169, 181]. The following theorems are known.

Theorem 3.20 ([169]) *For any graph G, $\chi(G) = \lceil \chi_c(G) \rceil$.*

Theorem 3.21 ([102]) *For any circulant graph G, $\chi_f(G) = \frac{|G|}{\alpha(G)}$. More generally, this identity holds for every vertex transitive graph G.*

Theorem 3.22 ([121]) *$\chi_f(G)$ and $\chi_c(G)$ are rational numbers satisfying*

$$\max\left\{\omega(G), \frac{|G|}{\alpha(G)}\right\} \leq \chi_f(G) \leq \chi_c(G) \leq \chi(G).$$

Since $\chi_f(G) \leq \chi_c(G)$ for all G, a natural question is to investigate when these two invariants are equal. This motivates the definition of *star extremality*.

Definition 3.23 ([78]) *A graph G is* **star extremal** *if $\chi_f(G) = \chi_c(G)$.*

The notion of star extremality in graphs is first introduced in the study of the chromatic number and the circular chromatic number of the lexicographic product of graphs [78]. In all of the examples that follow, knowing that a graph is star extremal enables us to quickly determine the circular chromatic number $\chi_c(G)$, which is equal to the fractional chromatic number $\chi_f(G)$. By Lemma 3.20, this immediately gives us the chromatic number $\chi(G)$. For many graphs, it is extremely difficult to compute $\chi(G)$. However, in some cases, the value of $\chi_f(G)$ is known, or can be quickly computed. Thus, proving the star extremality of G enables us to determine $\chi(G)$.

Therefore, star extremal graphs are highly useful and important as it provides a powerful technique to compute $\chi(G)$. In all of the papers on star extremal graphs, the focus has been to characterize families of star extremal *circulant* graphs.

While several papers [30, 99, 111, 121, 123, 124, 125, 177, 178] have been written on this topic, only a few examples of star extremal circulants are known. Gao and Zhu [78] prove that $C_{n,\{1,2,\ldots,d\}}$ is star extremal for any $n \geq 2d$. This is generalized by Lih et. al., who show in [121] that $C_{n,\{a,a+1,\ldots,b\}}$ is star extremal for any ordered triplet (n, a, b) satisfying $n \geq 2b$ and $b \geq \frac{5a}{4}$. Other families of star extremal graphs are given in [123], where S is of the form $\{1, 2, \ldots, m-1, k, k+1, \ldots, k+m-2\}$ and $\{k, k+1, \ldots, k_1, k_2, k_2+1, \ldots, \lfloor \frac{n}{2} \rfloor\}$. In each of the known families of star extremal graphs, the generating set consists of at most two intervals. Even for these relatively simple cases, it is extremely technical to prove that these circulant graphs are star extremal, as the proof requires a great deal of case work. In this section, we will prove the star extremality of an infinite family of circulant graphs, where these circulants have 2^k intervals of arbitrary length, for any $k \geq 0$. The main theorem presented in this section will greatly extend (or generalize) many of the currently known results.

Before we proceed further, let us mention that there are infinitely many circulant graphs G that are *not* star extremal. The construction [181] is as follows: take any circulant H with $\chi_f(H) \neq \chi(H)$ (e.g. an odd cycle). Then let $\overline{G}$ be the disjoint union of k copies of $\overline{H}$, for some $k \geq 2$. Then, $\overline{G}$ is a circulant, which implies that G is a circulant. Zhu [181] proves that for this G, $\chi_f(G) < \chi_c(G)$. Therefore, we know that infinitely many non star extremal graphs exist. To give one example of this construction, $G = C_{10,\{1,3,4,5\}}$ is not star extremal. For this graph, we have $\chi_f(G) = 5$ and $\chi_c(G) = 6$.

Given $G = C_{n,S}$, and a positive integer t, let

$$\lambda_t(G) = \min\{|ti|_n : i \in S\},$$

where the product ti is reduced modulo n. Then define

$$\lambda(G) = \max\{\lambda_t(G) : t = 1, 2, 3, \ldots, n\}.$$

Unlike $\alpha(G)$, we note that $\lambda(G)$ can be determined in polynomial-time for any $G = C_{n,S}$.

The following lemma provides a sufficient condition for a graph to be star extremal.

Lemma 3.24 ([78]) *Let $G = C_{n,S}$. Then, $\lambda(G) \leq \alpha(G)$. Furthermore, if $\lambda(G) = \alpha(G)$, then $\chi_f(G) = \chi_c(G) = \frac{n}{\alpha(G)}$, i.e., G is star extremal.*

In any graph G satisfying $\lambda(G) = \alpha(G)$, the value of $\chi(G)$ can be calculated by Theorem 3.20, namely $\chi(G) = \lceil \frac{n}{\alpha(G)} \rceil$.

Lemma 3.24 is the main technique used to verify that a circulant $G = C_{n,S}$ is star extremal, and every paper on star extremal graphs has relied on this lemma. But as we noted earlier, it is NP-hard to compute $\alpha(G)$ explicitly [46], even when G is restricted to circulants. That is why so few star extremal graphs are known. However, by Theorem 3.8, we know the exact value of $\alpha(G)$ for an infinite family of circulants $G_{j,k}$ with 2^k intervals (for any $k \geq 0$). Thus, it is a natural question to consider the star extremality of these graphs. If we can calculate a formula for $\lambda(G)$ for each $G = G_{j,k}$ in our infinite family, we can compare it to $\alpha(G)$ and check if these values are equal.

In this section, we just restrict our analysis to the family of circulants $G_{j,k}$, where $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-1} \leq a_k$. We make this restriction as the condition $a_{k-1} = a_k + 1$ was just a special case we introduced to prove Theorem 3.8.

Using Lemma 3.24, we will prove the following theorem, which proves the surprising result that *every* graph in our infinite family is star extremal. This is the main result in this section of the thesis, and we will devote the next 30 pages to formally justify this theorem.

Theorem 3.25 *Let $k \geq 2$ be an integer, and let $(a_1, a_2, \ldots, a_k)$ be a k-tuple of integers satisfying the inequality*

$$3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-1} \leq a_k.$$

Consider the circulant $G_{j,k} = G_j(a_1, a_2, \ldots, a_k)$, as introduced in Definition 3.1. Then $G_{j,k}$ is star extremal for all j satisfying $1 \leq j \leq k$.

Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-1} \leq a_k$. For notational convenience, we now refer to all such k-tuples as satisfying the **non-decreasing condition**. Note that in all these k-tuples, we require $a_1 \geq 3$.

Theorem 3.25 encompasses many of the known families of star extremal graphs that were highlighted earlier. For example, $G_{k-1,k}$ is a one-interval set of the form $\{a, a+1, \ldots, b\}$, and $G_{1,3}$ is a two-interval set of the form $\{1, 2, \ldots, a-1, b, b+1, \ldots, b+a-2\}$. For many of the known examples of circulant star extremal graphs, we can determine the k-tuple $(a_1, a_2, \ldots, a_k)$ corresponding to that graph. And as we noted earlier, our construction for $S_{j,k}$ (see Definition 3.1) generates infinitely many examples of circulant graphs with 2^k intervals, for any $k \geq 0$. Therefore, Theorem 3.25 represents a completely new classification of star extremal circulants, significantly extending currently known results.

In the following definition, we introduce the ordered pair i $(p_{i,m}, q_{i,m})$, for each $j+1 \leq m \leq k$ and $i \in S_{j,m}$. We will repeatedly use this definition in our inductive proof that $S_{j,k}$ is star extremal, for each $1 \leq j \leq k-1$. (Note: the $j = k$ case is trivial, and will be handled as a separate case).

Definition 3.26 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition, and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$, for each $j+1 \leq m \leq k$. Define $\boldsymbol{t_j = 1}$ and $\boldsymbol{t_m = a_{j+1} a_{j+2} \cdots a_m}$ for each $j+1 \leq m \leq k$. For each m satisfying $j+1 \leq m \leq k$, define for each $i \in S_{j,m}$ the ordered pair $\boldsymbol{(p_{i,m}, q_{i,m})}$, where $(p_{i,m}, q_{i,m})$ is the unique pair of integers satisfying*

$$t_m i = p_{i,m} n_m + q_{i,m}$$

and

$$-\frac{n_m}{2} < q_{i,m} \leq \frac{n_m}{2}.$$

By definition, $|q_{i,m}| = |t_m i|_{n_m}$ for all $i \in S_{j,m}$.

Let us illustrate this definition with a specific example.

Consider the ordered triplet $(a_1, a_2, a_3) = (5, 6, 8)$, and fix $j = 1$. As described previously, $n_0 = 1$, $n_1 = 4$, $n_2 = 23$, and $n_3 = 183$, from which we derive $S_{1,2} = \{1, 2, 3\}$, and $S_{1,3} = \{1, 2, 3, 20, 21, 22\}$. By definition, $t_1 = 1$, $t_2 = a_2 = 6$, and $t_3 = a_2 a_3 = 48$.

We calculate $(p_{i,m}, q_{i,m})$ for $m = 2$ and $m = 3$. For $m = 2$, each $i \in S_{1,2}$ satisfies $6i = 23p_{i,2} + q_{i,2}$, and for $m = 3$, each $i \in S_{1,3}$ satisfies $48i = 183p_{i,3} + q_{i,3}$. We have

$$\begin{aligned} 6 \cdot 1 &= 0 \cdot 23 + 6 \\ 6 \cdot 2 &= 1 \cdot 23 - 11 \\ 6 \cdot 3 &= 1 \cdot 23 - 5 \end{aligned}$$

$$\begin{aligned} 48 \cdot 1 &= 0 \cdot 183 + 48 \\ 48 \cdot 2 &= 1 \cdot 183 - 87 \\ 48 \cdot 3 &= 1 \cdot 183 - 39 \\ 48 \cdot 20 &= 5 \cdot 183 + 45 \\ 48 \cdot 21 &= 6 \cdot 183 - 90 \\ 48 \cdot 22 &= 6 \cdot 183 - 42 \end{aligned}$$

We derive the following ordered pairs, from the condition that $-\frac{n_m}{2} < q_{i,m} \leq \frac{n_m}{2}$.

$$\begin{aligned} (p_{1,2}, q_{1,2}) &= (0, 6) \\ (p_{2,2}, q_{2,2}) &= (1, -11) \\ (p_{3,2}, q_{3,2}) &= (1, -5) \end{aligned}$$

$$
\begin{aligned}
(p_{1,3}, q_{1,3}) &= (0, 48) \\
(p_{2,3}, q_{2,3}) &= (1, -87) \\
(p_{3,3}, q_{3,3}) &= (1, -39) \\
(p_{20,3}, q_{20,3}) &= (5, 45) \\
(p_{21,3}, q_{21,3}) &= (6, -90) \\
(p_{22,3}, q_{22,3}) &= (6, -42)
\end{aligned}
$$

By definition, $\lambda_{t_m}(G_{j,m}) = \min\{|q_{i,m}| : i \in S_{j,m}\}$. In the above example, we have $\lambda_6(G_{1,2}) = \min\{6, 11, 5\} = 5$ and $\lambda_{48}(G_{1,3}) = \min\{48, 87, 39, 45, 90, 42\} = 39$.

By Theorem 3.8, $\alpha(G_{1,2}) = 6 \cdot 1 - 1 = 5$ and $\alpha(G_{1,3}) = 8 \cdot 5 - 1 = 39$. By Lemma 3.24, both of these circulants are star extremal since $5 = \lambda_6(G_{1,2}) \leq \lambda(G_{1,2}) \leq \alpha(G_{1,2}) = 5$ and $39 = \lambda_{48}(G_{1,3}) \leq \lambda(G_{1,3}) \leq \alpha(G_{1,3}) = 39$.

We will prove that $\lambda_{t_k}(G_{j,k}) = \alpha(G_{j,k})$ for each $1 \leq j \leq k-1$, and prove that $\lambda_1(G_{k,k}) = \alpha(G_{k,k})$. By Lemma 3.24, this will establish that every $G_{j,k}$ is star extremal.

To prove Theorem 3.25, we will require several technical lemmas. The first result just highlights some trivial inequalities, and reiterates the definitions of some key variables that will be applied repeatedly in the following proofs.

Proposition 3.27 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple of integers satisfying the non-decreasing condition. Let $1 \leq j \leq k-1$ be fixed. Then, the following inequalities hold for each $j+1 \leq m \leq k$.*

(a) $3 \leq a_{m-1} \leq a_m$.

(b) $n_m = a_m n_{m-1} - 1$.

(c) $t_m = a_m t_{m-1}$.

(d) $n_m > n_{m-1} \geq 2$.

(e) $t_m > t_{m-1} > 0$.

Proof: Parts (a), (b), and (c) follow by definition.

Since $a_m \geq 3$, we have $n_m = a_m n_{m-1} - 1 > n_{m-1}$. Also, $n_{m-1} \geq n_j \geq n_1 = a_1 - 1 \geq 2$. This proves part (d).

Since $a_m \geq 3$, we have $t_m = a_m t_{m-1} > t_{m-1}$. Also, $t_{m-1} \geq t_j = 1$. This proves part (e). ∎

The following lemma provides a bound on $p_{i,m}$, which will be essential when proving our recursive formula for $(p_{i,m}, q_{i,m})$, for each $i \in S_{j,m}$.

Lemma 3.28 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$ for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Then, $0 \leq p_{i,m} \leq t_{m-1}$, for all $i \in S_{j,m}$. Furthermore, if $q_{i,m} \geq 0$, then $p_{i,m} \leq t_{m-1} - 1$.*

Proof: By definition, $q_{i,m} = t_m i - p_{i,m} n_m \leq \frac{n_m}{2}$. Since each $i \geq 1$, we must have $p_{i,m} \geq 0$, or else $q_{i,m} \geq t_m \cdot 1 + n_m > \frac{n_m}{2}$, a contradiction. This establishes the lower bound. Now suppose that $p_{i,m} \geq t_{m-1} + 1$ for some $i \in S_{j,m}$. Then

$$
\begin{aligned}
t_m i &= p_{i,m} n_m + q_{i,m} \\
&\geq (t_{m-1} + 1) n_m + q_{i,m} \\
&> (t_{m-1} + 1) n_m - \frac{n_m}{2} \\
&> t_{m-1} n_m \\
&= t_{m-1}(a_m n_{m-1} - 1) \\
&= t_m n_{m-1} - t_{m-1} \\
&> t_m n_{m-1} - t_m \\
&= t_m (n_{m-1} - 1).
\end{aligned}
$$

It follows that $i > n_{m-1} - 1$. However, by Proposition 3.5 (g), $i \leq \max(S_{j,m}) \leq n_{m-1} - 1$, which is a contradiction. Hence, $0 \leq p_{i,m} \leq t_{m-1}$, as required.

Now we prove that $p_{i,m} \leq t_{m-1} - 1$ whenever $q_{i,m} \geq 0$. Since $i \leq n_{m-1} - 1$, we have $q_{i,m} = t_m i - p_{i,m} n_m \leq t_m(n_{m-1} - 1) - p_{i,m} n_m$. If $p_{i,m} = t_{m-1}$, then

$$\begin{aligned} q_{i,m} &\leq t_m(n_{m-1} - 1) - p_{i,m} n_m \\ &= t_m n_{m-1} - t_m - t_{m-1} n_m \\ &= a_m t_{m-1} n_{m-1} - t_m - t_{m-1}(a_m n_{m-1} - 1) \\ &= t_{m-1} - t_m < 0. \end{aligned}$$

Thus, if $q_{i,m} \geq 0$, we must have $p_{i,m} \leq t_{m-1} - 1$. ∎

The next three results are technical algebraic proofs, which we will require to prove the key lemmas that imply Theorem 3.25.

Lemma 3.29 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition, and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$, for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Then, for $j+2 \leq m \leq k$, we have*

$$n_m > 2t_{m-2} a_m + 2t_{m-2} + 1.$$

Proof: We prove the inequality by induction on m.

The base case $m = j+2$ is equivalent to $n_{j+2} > 2t_j a_{j+2} + 2t_j + 1 = 2a_{j+2} + 3$. Since $n_{j+1} = a_{j+1} n_j - 1 \geq 3 \cdot 2 - 1 = 5$, we have $n_{j+2} = a_{j+2} n_{j+1} - 1 \geq 5a_{j+2} - 1 > 2a_{j+2} + 3$, since $a_{j+2} \geq 3$. This establishes the base case.

Now suppose the inequality is true for all indices less than m, for some $m \geq j+3$. By the induction hypothesis, we have

$$\begin{aligned} n_{m-1} &> 2t_{m-3} a_{m-1} + 2t_{m-3} + 1 \\ a_m n_{m-1} &> 2a_m t_{m-3} a_{m-1} + 2a_m t_{m-3} + a_m \\ a_m n_{m-1} &\geq 2a_m t_{m-3} a_{m-2} + 2a_{m-2} t_{m-3} + a_m \\ n_m + 1 &\geq 2a_m t_{m-2} + 2t_{m-2} + a_m \\ n_m &\geq 2a_m t_{m-2} + 2t_{m-2} + (a_m - 1) \\ n_m &> 2t_{m-2} a_m + 2t_{m-2} + 1. \end{aligned}$$

This completes the induction, and so we are done. ∎

Lemma 3.30 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition, and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$, for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Then $n_m > 2t_{m-1} + 1$ for $j+1 \leq m \leq k$.*

Proof: For $j+2 \leq m \leq k$, the lemma follows as a direct corollary of Lemma 3.29, since $n_m > 2t_{m-2}a_m + 2t_{m-2} + 1 \geq 2t_{m-2}a_{m-1} + 0 + 1 = 2t_{m-1} + 1$. It remains to prove part the lemma for the case $m = j+1$. However, this is trivial since $n_{j+1} = a_{j+1}n_j - 1 \geq 3 \cdot 2 - 1 > 3 = 2t_j + 1$. ∎

Lemma 3.31 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition. Then*

$$t_k(n_{k-1} - n_{k-2}) = (t_{k-1} - t_{k-2})n_k - t_{k-2}(a_k - a_{k-1} + 1).$$

Proof: This proof follows directly from our established identities.

$$\begin{aligned}
& t_k(n_{k-1} - n_{k-2}) \\
= \;& a_k t_{k-1}(n_{k-1} - n_{k-2}) \\
= \;& t_{k-1}a_k n_{k-1} - a_k t_{k-1} n_{k-2} \\
= \;& t_{k-1}(n_k + 1) - t_{k-2}n_k + t_{k-2}n_k - a_k t_{k-1} n_{k-2} \\
= \;& (t_{k-1} - t_{k-2})n_k + t_{k-1} + t_{k-2}n_k - a_k t_{k-1} n_{k-2} \\
= \;& (t_{k-1} - t_{k-2})n_k + t_{k-2}a_{k-1} + t_{k-2}(a_k n_{k-1} - 1) - a_k t_{k-2} a_{k-1} n_{k-2} \\
= \;& (t_{k-1} - t_{k-2})n_k + t_{k-2}a_{k-1} + t_{k-2}(a_k n_{k-1} - 1) - a_k t_{k-2}(n_{k-1} + 1) \\
= \;& (t_{k-1} - t_{k-2})n_k + t_{k-2}a_{k-1} - t_{k-2} - t_{k-2}a_k \\
= \;& (t_{k-1} - t_{k-2})n_k - t_{k-2}(a_k - a_{k-1} + 1).
\end{aligned}$$

This completes the proof. ∎

By Lemma 3.15, if $i \in S_{j,k}$, then either $i = x$ or $i = n_{k-1} - n_{k-2} + x$, for some $x \in S_{j,k-1}$. In our earlier example with $(a_1, a_2, a_3) = (5, 6, 8)$, we showed that $S_{1,2} = \{1, 2, 3\}$ and $S_{1,3} = \{1, 2, 3, 20, 21, 22\}$. Hence, each $i \in S_{1,3}$ equals x or $19 + x$ for some $x \in S_{1,2}$. Note that $n_2 - n_1 = 23 - 4 = 19$.

Now we prove that each pair $(p_{i,k}, q_{i,k})$ can be recursively generated from some previous term $(p_{x,k-1}, q_{x,k-1})$, where $i \in S_{j,k}$ and $x \in S_{j,k-1}$. There are four possible representations for $(p_{i,k}, q_{i,k})$, depending on the value of $i \in S_{j,k}$. We will define a term $r_{x,k}$, which is a particular function of $p_{x,k-1}$ and $q_{x,k-1}$. This term $r_{x,k}$ is *not* to be confused with a remainder function; it is simply a term we introduce for notational convenience.

To avoid confusion in the following proof, i will always refer to an element in $S_{j,k}$, and x will always refer to an element in $S_{j,k-1}$.

Lemma 3.32 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-2$. Consider the generating set $S_{j,k}$. Select any $i \in S_{j,k}$. Then $i = x$ or $i = n_{k-1} - n_{k-2} + x$, for some $x \in S_{j,k-1}$. Let $\boldsymbol{r_{x,k} = p_{x,k-1} + a_k q_{x,k-1}}$ for this value of x.*

Then, there are four possible representations of $(p_{i,k}, q_{i,k})$ as a function of $p_{x,k-1}$ and $q_{x,k-1}$.

$$\begin{aligned}
&\text{Type I}: && (p_{i,k}, q_{i,k}) = (p_{x,k-1}, r_{x,k}) \\
&\text{Type II}: && (p_{i,k}, q_{i,k}) = (p_{x,k-1} + 1, r_{x,k} - n_k) \\
&\text{Type III}: && (p_{i,k}, q_{i,k}) = (p_{x,k-1} + t_{k-1} - t_{k-2}, r_{x,k} - t_{k-2}(a_k - a_{k-1} + 1)) \\
&\text{Type IV}: && (p_{i,k}, q_{i,k}) = (p_{x,k-1} + t_{k-1} - t_{k-2} - 1, r_{x,k} - t_{k-2}(a_k - a_{k-1} + 1) + n_k)
\end{aligned}$$

If $i = x \in S_{j,k-1}$, then we have a Type I or Type II pair. And if $i = n_{k-1} - n_{k-2} + x$ for some $x \in S_{j,k-1}$, then we have a Type III or Type IV pair.

<u>Proof:</u> For each $i \in S_{j,k}$, $(p_{i,k}, q_{i,k})$ is the unique ordered pair satisfying $t_k i = p_{i,k} n_k + q_{i,k}$, where $-\frac{n_k}{2} < q_{i,k} \leq \frac{n_k}{2}$.

Also, for each $x \in S_{j,k-1}$, $(p_{x,k-1}, q_{x,k-1})$ is the unique ordered pair satisfying $t_{k-1} x = p_{x,k-1} n_{k-1} + q_{x,k-1}$, where $-\frac{n_{k-1}}{2} < q_{x,k-1} \leq \frac{n_{k-1}}{2}$.

In the following proof, we will find all possible ways that $(p_{i,k}, q_{i,k})$ can be expressed recursively as a function of $(p_{x,k-1}, q_{x,k-1})$.

We split our analysis into two cases.

<u>*Case 1:*</u> $i = x$, where $x \in S_{j,k-1}$.

If $i = x \in S_{j,k-1}$, we have $t_{k-1} i = t_{k-1} x = p_{x,k-1} n_{k-1} + q_{x,k-1}$ for some pair of integers $(p_{x,k-1}, q_{x,k-1})$ with $-\frac{n_{k-1}}{2} < q_{x,k-1} \leq \frac{n_{k-1}}{2}$. Multiplying both sides of the identity by a_k, we have

$$\begin{aligned} a_k t_{k-1} x &= p_{x,k-1} a_k n_{k-1} + a_k q_{x,k-1} \\ t_k x &= p_{x,k-1}(n_k + 1) + a_k q_{x,k-1} \\ t_k i &= p_{x,k-1} n_k + (p_{x,k-1} + a_k q_{x,k-1}) \\ t_k i &= p_{x,k-1} n_k + r_{x,k}. \end{aligned}$$

Since $t_k i = t_k x = p_{x,k} n_k + q_{x,k}$, we have $r_{x,k} \equiv q_{x,k} \pmod{n_k}$. Thus, $q_{x,k} = r_{x,k} + l n_k$, for some integer l. We now show that $l = 0$ or $l = -1$.

Since $q_{x,k-1} > -\frac{n_{k-1}}{2}$, this implies that $q_{x,k-1} \geq -\frac{n_{k-1}}{2} + \frac{1}{2}$. Also, $p_{x,k-1} \geq 0$ by Lemma 3.28. Therefore,

$$\begin{aligned} r_{x,k} &= p_{x,k-1} + a_k q_{x,k-1} \\ &\geq 0 - \frac{a_k n_{k-1}}{2} + \frac{a_k}{2} \\ &= -\frac{n_k + 1}{2} + \frac{a_k}{2} \\ &= -\frac{n_k}{2} + \frac{a_k - 1}{2} \\ &> -\frac{n_k}{2}. \end{aligned}$$

Thus, each $r_{x,k} > -\frac{n_k}{2}$. Now we show that $r_{x,k} < n_k$. By definition, $q_{x,k-1} \leq \frac{n_{k-1}}{2}$, and by Lemma 3.28, $p_{x,k-1} \leq t_{k-2}$. By Lemma 3.30, $n_k > n_{k-1} > 2t_{k-2}+1$. Therefore, $r_{x,k} = p_{x,k-1} + a_k q_{x,k-1} \leq t_{k-2} + a_k \cdot \frac{n_{k-1}}{2} = t_{k-2} + \frac{n_k}{2} + \frac{1}{2} < \frac{n_k - 1}{2} + \frac{n_k}{2} + \frac{1}{2} = n_k$.

So we have shown that $-\frac{n_k}{2} < r_{x,k} < n_k$. Since $q_{i,k} = q_{x,k} = r_{x,k} + l n_k$ must be in the interval $(-\frac{n_k}{2}, \frac{n_k}{2}]$, we must have $l = 0$ or $l = -1$.

If $-\frac{n_k}{2} < r_{x,k} \leq \frac{n_k}{2}$, then $l = 0$. In this case, $q_{i,k} = r_{x,k}$, and so $(p_{i,k}, q_{i,k}) = (p_{x,k-1}, p_{x,k-1} + a_k q_{x,k-1})$. This is a Type I pair.

If $\frac{n_k}{2} < r_{x,k} < n_k$, then $l = -1$. In this case, $q_{i,k} = r_{x,k} - n_k$, and so $(p_{i,k}, q_{i,k}) = (p_{x,k-1} + 1, p_{x,k-1} + a_k q_{x,k-1} - n_k)$. This is a Type II pair.

Therefore, we conclude that $(p_{i,k}, q_{i,k})$ must be a Type I or Type II pair, when $i = x \in S_{j,k-1}$.

<u>*Case 2:*</u> $i = n_{k-1} - n_{k-2} + x$, where $x \in S_{j,k-1}$.

By Lemma 3.31, we have

$$\begin{aligned} t_k i &= t_k(n_{k-1} - n_{k-2}) + t_k x \\ &= (t_{k-1} - t_{k-2})n_k - t_{k-2}(a_k - a_{k-1} + 1) + t_k x \\ &= (t_{k-1} - t_{k-2})n_k - t_{k-2}(a_k - a_{k-1} + 1) + (p_{x,k}n_k + q_{x,k}) \\ &= (p_{x,k} + t_{k-1} - t_{k-2})n_k + (q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1)). \end{aligned}$$

Let $v_{i,k} = q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1)$. By definition, $t_k i = p_{i,k}n_k + q_{i,k}$, and so $q_{i,k} \equiv v_{i,k} \pmod{n_k}$.

Note that $x \in S_{j,k-1} \subseteq S_{j,k}$. From Case 1, we know that $x \in S_{j,k}$ and $-\frac{n_k}{2} < q_{x,k} \leq \frac{n_k}{2}$.

We prove that $-n_k < v_{i,k} \leq \frac{n_k}{2}$. The upper bound is clear, since $q_{x,k} \leq \frac{n_k}{2}$, $t_{k-2} > 0$, and $a_{k-1} \leq a_k$. Now we show that $v_{i,k} > -n_k$. By Lemma 3.30, $n_{k-1} > 2t_{k-2} + 1$. Also, $q_{x,k} > -\frac{n_k}{2}$. Thus,

$$\begin{aligned} v_{i,k} &= q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1) \\ &> -\frac{n_k}{2} - t_{k-2}(a_k - a_{k-1} + 1) \\ &= -\frac{n_k}{2} - t_{k-2}a_k + t_{k-2}(a_{k-1} - 1) \\ &> -\frac{n_k}{2} - t_{k-2}a_k \\ &> -\frac{n_k}{2} + \frac{a_k}{2}(-n_{k-1} + 1) \quad \text{by Lemma 3.30} \\ &= -\frac{n_k}{2} - \frac{n_k + 1}{2} + \frac{a_k}{2} \\ &= -n_k + \frac{a_k - 1}{2} \\ &> -n_k. \end{aligned}$$

Hence, $-n_k < v_{i,k} \leq \frac{n_k}{2}$. From above, $t_k i = (p_{x,k} + t_{k-1} - t_{k-2})n_k + v_{i,k}$. Since $q_{i,k} \equiv v_{i,k} \pmod{n_k}$, $q_{i,k} = v_{i,k} + ln_k$ for some integer l. Since $-n_k < v_{i,k} \leq \frac{n_k}{2}$, l must be 0 or 1, so that $q_{i,k}$ falls in the desired range $(-\frac{n_k}{2}, \frac{n_k}{2}]$.

If $-\frac{n_k}{2} < v_{i,k} \leq \frac{n_k}{2}$, then $l = 0$. In this case, $q_{i,k} = v_{i,k}$ and so

$$(p_{i,k}, q_{i,k}) = (p_{x,k} + t_{k-1} - t_{k-2}, v_{i,k}).$$

If $-n_k < v_{i,k} \leq -\frac{n_k}{2}$, then $l = 1$. In this case, $q_{i,k} = v_{i,k} + n_k$, and so

$$(p_{i,k}, q_{i,k}) = (p_{x,k} + t_{k-1} - t_{k-2} - 1, v_{i,k} + n_k).$$

Our motivation is to express $p_{i,k}$ and $q_{i,k}$ recursively in terms of $p_{x,k-1}$ and $q_{x,k-1}$. To do this, we first express $q_{i,k}$ in terms of $v_{i,k}$, which is a function of $q_{x,k}$. We then express $q_{x,k}$ as a function of $r_{x,k} = p_{x,k-1} + a_k q_{x,k-1}$.

Note that $v_{i,k} = q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1)$ is a function of $q_{x,k}$, and from the earlier analysis of Type I and Type II pairs, $q_{x,k} = r_{x,k}$ or $q_{x,k} = r_{x,k} - n_k$. In all, there are four possible subcases that we need to consider for $(p_{i,k}, q_{i,k})$.

(a) $q_{i,k} = v_{i,k}$, with $q_{x,k} = r_{x,k}$.

(b) $q_{i,k} = v_{i,k}$ with $q_{x,k} = r_{x,k} - n_k$.

(c) $q_{i,k} = v_{i,k} + n_k$, with $q_{x,k} = r_{x,k}$.

(d) $q_{i,k} = v_{i,k} + n_k$, with $q_{x,k} = r_{x,k} - n_k$.

Consider subcase (a). We have $t_k i = (p_{x,k} + t_{k-1} - t_{k-2})n_k + v_{i,k}$. In this case, $q_{i,k} = v_{i,k}$, i.e., $-\frac{n_k}{2} < q_{i,k} = v_{i,k} \leq \frac{n_k}{2}$. Therefore, we have

$$\begin{aligned}
p_{i,k} &= p_{x,k} + t_{k-1} - t_{k-2} \\
q_{i,k} &= v_{i,k} \\
&= q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1) \\
&= r_{x,k} - t_{k-2}(a_k - a_{k-1} + 1).
\end{aligned}$$

Hence, this subcase corresponds to a Type III pair.

By a similar argument, subcase (c) corresponds to a Type IV pair, and subcase (d) corresponds to a Type III pair. To conclude the proof, it suffices to prove that subcase (b) leads to a contradiction, i.e., $q_{i,k}$ falls outside of the required range $(-\frac{n_k}{2}, \frac{n_k}{2}]$.

In subcase (b), $q_{i,k} = r_{x,k} - n_k - t_{k-2}(a_k - a_{k-1} + 1)$. We prove that $q_{i,k} < -\frac{n_k}{2}$, which establishes the desired contradiction. First assume that $q_{x,k-1} \geq 0$. By Lemma 3.28, this implies that $p_{x,k-1} \leq t_{k-2} - 1$. We have

$$\begin{aligned}
q_{i,k} &= v_{i,k} \\
&= q_{x,k} - t_{k-2}(a_k - a_{k-1} + 1) \\
&= r_{x,k} - n_k - t_{k-2}(a_k - a_{k-1} + 1) \\
&= p_{x,k-1} + a_k q_{x,k-1} - n_k - t_{k-2}(a_k - a_{k-1} + 1) \\
&\leq (t_{k-2} - 1) + a_k \cdot \frac{n_{k-1}}{2} - n_k - t_{k-2}(a_k - a_{k-1} + 1) \\
&= t_{k-2} - 1 + \frac{n_k + 1}{2} - n_k - t_{k-2}(a_k - a_{k-1} + 1) \\
&= \frac{-n_k - 1}{2} - t_{k-2}(a_k - a_{k-1}) \\
&< -\frac{n_k}{2} \quad \text{since } a_k \geq a_{k-1} \text{ and } t_{k-2} \geq 0.
\end{aligned}$$

The case $q_{x,k-1} < 0$ follows just as easily: we have

$$\begin{aligned}
q_{i,k} &= p_{x,k-1} + a_k q_{x,k-1} - n_k - t_{k-2}(a_k - a_{k-1} + 1) \\
&< t_{k-2} + 0 - n_k - t_{k-2}(a_k - a_{k-1} + 1) \quad \text{by Lemma 3.28} \\
&= -n_k - t_{k-2}(a_k - a_{k-1}) \\
&< -\frac{n_k}{2}.
\end{aligned}$$

Therefore, subcase (b) leads to a contradiction.

Our proof is now complete. In the first case $i = x \in S_{j,k-1}$, we established that $(p_{i,k}, q_{i,k})$ must be Type I or Type II. In the second case $i = n_{k-1} - n_{k-2} + x$ with $x \in S_{j,k-1}$, we established that $(p_{i,k}, q_{i,k})$ must be Type III or Type IV. This concludes the proof. ∎

This lemma generalizes to all $j + 2 \leq m \leq k$ by the same argument: $(p_{i,m}, q_{i,m})$ can be represented as a function of $p_{x,m-1}$ and $q_{x,m-1}$ in exactly four ways, where $i \in S_{j,m}$ and $x \in S_{j,m-1}$. These four representations correspond to the four types given in Lemma 3.32 (by replacing k by m). The proof follows in exactly the same way.

Now we introduce the element the element $y = n_j - n_{j-1}$. By Proposition 3.5 (e), $y \in S_{j,j+1}$. (Also by Proposition 3.5 (d), $y \notin S_{j,j}$). Hence, Proposition 3.5 (b) implies that $y \in S_{j,m}$ for all $j+1 \leq m \leq k$. We will prove that $i = y$ is the element for which $|q_{i,k}|$ is minimized over all $i \in S_{j,k}$. As we will refer to this constant element y throughout the next few lemmas, we formally define it here.

Definition 3.33 *Let $1 \leq j \leq k-1$ be a fixed integer. Then set $\boldsymbol{y = n_j - n_{j-1}}$.*

The following three lemmas deal with the value of $q_{y,k}$, and will be extremely useful in proving our key result that $q_{y,k}$ is a negative number satisfying the inequality $|q_{i,k}| \geq -q_{y,k}$ for all $i \in S_{j,k}$. This will imply that for $t = t_k$, $\lambda_t(G_{j,k}) = -q_{y,k}$. We will then prove that $\alpha(G_{j,k}) = -q_{y,k}$, immediately implying that $\lambda(G_{j,k}) = \alpha(G_{j,k})$. Thus, the star extremality of $G_{j,k}$ will be formally established, and this will conclude the proof of Theorem 3.25.

Lemma 3.34 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$ for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Let $y = n_j - n_{j-1}$. Then*

$$p_{y,j+1} = 1 \text{ and } q_{y,j+1} = -a_{j+1} n_{j-1} + 1.$$

Proof: By definition, $t_{j+1} y = p_{y,j+1} n_{j+1} + q_{y,j+1}$. Since $t_{j+1} = a_{j+1}$ and $y = n_j - n_{j-1}$, we have $q_{y,j+1} = a_{j+1}(n_j - n_{j-1}) - l n_{j+1}$, for some integer $l = p_{y,j+1}$.

There is a unique integer l for which $-\frac{n_{j+1}}{2} < q_{y,j+1} \leq \frac{n_{j+1}}{2}$. We will prove that $l = 1$.

First, we establish that $n_j - n_{j-1} \geq \frac{n_j}{2}$. This inequality is equivalent to $n_j = a_j n_{j-1} - 1 \geq 2n_{j-1}$, or $(a_j - 2) n_{j-1} \geq 1$, which holds since $a_j \geq 3$ and $n_{j-1} \geq n_0 = 1$.

If $l \leq 0$, then the above identity shows that $q_{y,j+1} \geq a_{j+1}(n_j - n_{j-1}) \geq \frac{a_{j+1} n_j}{2} = \frac{n_{j+1}+1}{2} > \frac{n_{j+1}}{2}$, a contradiction.

If $l \geq 2$, then $q_{y,j+1} \leq a_{j+1}(n_j - n_{j-1}) - 2n_{j+1} < a_{j+1} n_j - 2n_{j+1} = n_{j+1} + 1 - 2n_{j+1} < -\frac{n_{j+1}}{2}$, a contradiction.

It follows that $l = 1$, and so $q_{y,j+1} = a_{j+1}(n_j - n_{j-1}) - n_{j+1} = a_{j+1} n_j - a_{j+1} n_{j-1} - n_{j+1} = (n_{j+1} + 1) - a_{j+1} n_{j-1} - n_{j+1} = -a_{j+1} n_{j-1} + 1$. ∎

We now prove that $(p_{y,m}, q_{y,m})$ is a Type I pair for each $j+2 \leq m \leq k$. By induction, we prove that if $(p_{y,m}, q_{y,m})$ is a Type I pair for the base case $m = j+2$, then it must be a Type I pair for all $m \geq j+2$.

Lemma 3.35 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$ for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Let $y = n_j - n_{j-1}$. Then for each $j+2 \leq m \leq k$,*

(a) $(p_{y,m}, q_{y,m})$ *is a Type I pair with* $p_{y,m} = 1$.

(b) $q_{y,m} = 1 + a_m q_{y,m-1} < 0$.

Proof: We first prove that $\frac{n_m}{2} < t_m y = t_m(n_j - n_{j-1}) < n_m$, for all $j+1 \leq m \leq k$. We proceed by induction on m.

We establish the base case $m = j+1$. By definition, $t_{j+1} = a_{j+1}$. We have $t_{j+1}(n_j - n_{j-1}) = a_{j+1} n_j - a_{j+1} n_{j-1} < a_{j+1} n_j - 1 = n_{j+1}$, which proves the upper bound. The lower bound holds since $t_{j+1}(n_j - n_{j-1}) = a_{j+1}(n_j - n_{j-1}) = a_{j+1}\left(n_j - \frac{n_j+1}{a_j}\right) \geq a_{j+1}\left(n_j - \frac{n_j+1}{3}\right) > a_{j+1} \cdot \frac{n_j}{2} > \frac{a_{j+1}n_j - 1}{2} = \frac{n_{j+1}}{2}$.

Now suppose the inequality is true for all indices less than m, for some $m \geq j+2$. By the induction hypothesis, we have

$$\begin{aligned}
t_{m-1}(n_j - n_{j-1}) &\leq n_{m-1} - 1 \\
a_m t_{m-1}(n_j - n_{j-1}) &\leq a_m n_{m-1} - a_m \\
t_m(n_j - n_{j-1}) &< a_m n_{m-1} - 1 \\
t_m(n_j - n_{j-1}) &= n_m.
\end{aligned}$$

This establishes the upper bound. The lower bound follows just as easily, since

$$\begin{aligned}
t_{m-1}(n_j - n_{j-1}) &> \frac{n_{m-1}}{2} \\
a_m t_{m-1}(n_j - n_{j-1}) &> \frac{a_m n_{m-1}}{2} \\
t_m(n_j - n_{j-1}) &> \frac{a_m n_{m-1}}{2} \\
t_m(n_j - n_{j-1}) &> \frac{a_m n_{m-1} - 1}{2} \\
t_m(n_j - n_{j-1}) &= \frac{n_m}{2}.
\end{aligned}$$

Hence, we have proven the desired inequality by induction.

By definition, $t_m y = t_m(n_j - n_{j-1}) = p_{y,m}n_m + q_{y,m}$, where $-\frac{n_m}{2} < q_{y,m} \leq \frac{n_m}{2}$. From the above inequality, $-\frac{n_m}{2} < t_m y - n_m < 0 \leq \frac{n_m}{2}$.

Therefore, it follows that $t_m y - p_{y,m}n_m = q_{y,m} = t_m y - n_m$, implying that $p_{y,m} = 1$ for all $j+2 \leq m \leq k$.

Note that $(p_{y,m}, q_{y,m})$ is one of four possible types by Lemma 3.32. By this Lemma, $(p_{y,m}, q_{y,m})$ must be Type I or Type II, since $y \in S_{j,m-1}$ as well.

Since Type I is the only case where $p_{y,m} = p_{y,m-1}$, it follows that $(p_{y,m}, q_{y,m})$ must be Type I, since $p_{y,j+1} = p_{y,j+2} = \ldots = p_{y,k} = 1$.

By the definition of a Type I pair, $q_{y,m} = r_{y,m} = p_{y,m-1} + a_m q_{y,m-1} = 1 + a_m q_{y,m-1}$. Since $q_{y,j+1} < 0$ by Lemma 3.34, a trivial induction shows that each $q_{y,m} < 0$. ∎

We have now proven that each $q_{y,m}$ is negative. Now we find a bound on this value of $q_{y,m}$.

Lemma 3.36 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$ for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m}n_m + q_{i,m}$, for each $i \in S_{j,m}$. Let $y = n_j - n_{j-1}$. Then $-q_{y,m} > t_{m-2} - 1$, for all $j+2 \leq m \leq k$.*

Proof: We prove a slightly stronger result, that $-q_{y,m} > t_{m-2} + 1$. We proceed by induction on m.

First, we establish the base case $m = j+2$. The desired inequality is equivalent to $-q_{y,j+2} > t_j + 1 = 2$, or $q_{y,j+2} < -2$. By Lemma 3.34, $q_{y,j+1} = -a_{j+1}n_{j-1} + 1 \leq -3 \cdot 1 + 1 = -2$. By Lemma 3.35, $q_{y,j+2} = 1 + a_{j+2}q_{y,j+1} \leq 1 + 3 \cdot (-2) < -2$.

This establishes the base case. Now suppose the inequality is true for all indices less than m, for some $m \geq j+3$. By the induction hypothesis,

$$\begin{aligned}
-q_{y,m-1} &> t_{m-3}+1 \\
-a_m q_{y,m-1} &> a_m t_{m-3}+a_m \\
-q_{y,m}+1 &> a_m t_{m-3}+a_m \quad \text{by Lemma 3.35} \\
-q_{y,m} &> a_m t_{m-3}+(a_m-1) \\
-q_{y,m} &\geq a_{m-2} t_{m-3}+(a_m-1) \\
-q_{y,m} &= t_{m-2}+(a_m-1) \\
-q_{y,m} &> t_{m-2}+1.
\end{aligned}$$

This completes the induction, and so we are done. ∎

Now we will prove a major lemma that will require multiple pages to justify rigorously. Part (a) of the lemma will determine the maximum value of $q_{i,m}$ when $q_{i,m} < 0$ and Part (b) will determine the minimum value of $q_{i,m}$ when $q_{i,m} \geq 0$. Combining both parts, this will enable us to determine the minimum value of $|q_{i,m}|$ over all $i \in S_{j,m}$. We will prove that this minimum value is $-q_{y,m}$, where $y = n_j - n_{j-1}$.

Lemma 3.37 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition and fix $1 \leq j \leq k-1$. Consider the generating set $S_{j,m}$ for each $j+1 \leq m \leq k$. Let $t_m i = p_{i,m} n_m + q_{i,m}$, for each $i \in S_{j,m}$. Let $y = n_j - n_{j-1}$. Then, the following statements hold for all $j+1 \leq m \leq k$.*

(a) If $q_{i,m} < 0$, then

$$0 \leq p_{i,m} - p_{y,m} \leq (a_m - 1)(q_{y,m} - q_{i,m}).$$

In other words, $q_{i,m} \leq q_{y,m}$, whenever $q_{i,m} < 0$. Equality occurs when $i = y$.

(b) If $q_{i,m} \geq 0$, then

$$q_{i,m} \geq -q_{y,m} + t_{m-1}.$$

Equality occurs when $i = n_{m-1} - y$.

<u>Proof:</u> We will prove the lemma by induction on m. We first establish the base case $m = j+1$ for both Parts (a) and (b). Then we will prove Part (a) of the lemma, by splitting the analysis into the four types described in Lemma 3.32. For each of these four cases, we prove the lemma via the induction hypothesis. We use the exact same technique to prove Part (b) of the lemma. Thus, all in all, we must prove the base case, and then consider *eight* different cases to justify the lemma.

We first establish the base case $m = j+1$.

By Proposition 3.5 (e), $S_{j,j+1} = \{n_{j-1}, n_{j-1}+1, \ldots, n_j - n_{j-1}\}$. For each $i \in S_{j,j+1}$, we calculate the pair $(p_{i,j+1}, q_{i,j+1})$. We have $0 < t_{j+1}i = a_{j+1}i \leq a_{j+1}(n_j - n_{j-1}) \leq a_{j+1}(n_j - 1) = a_{j+1}n_j - a_{j+1} = n_{j+1} + 1 - a_{j+1} < n_{j+1}$. Therefore, $0 < t_{j+1}i < n_{j+1}$.

Since $t_{j+1}i = p_{i,j+1}n_{j+1} + q_{i,j+1}$ satisfies $-\frac{n_{j+1}}{2} < q_{i,j+1} \leq \frac{n_{j+1}}{2}$, we must have $p_{i,j+1} = 0$ or $p_{i,j+1} = 1$. In the former case, $q_{i,j+1} > 0$, and in the latter case, $q_{i,j+1} < 0$.

To illustrate the proof that follows, we introduce the example given at the beginning of this section. In this example, recall that $(a_1, a_2, a_3) = (5, 6, 8)$, $n_3 = 183$, and $S_{2,3} = \{4, 5, 6, \ldots, 19\}$. For $j = 2$, we also have $t_3 = a_3 = 8$. Letting $j = 2$, the following table generates the values of $q_{i,3}$ for each $i \in S_{2,3}$.

$$\begin{array}{rcl}
8 \cdot 4 & = & 0 \cdot 183 + 32 \\
8 \cdot 5 & = & 0 \cdot 183 + 40 \\
8 \cdot 6 & = & 0 \cdot 183 + 48 \\
\vdots & & \vdots \\
8 \cdot 10 & = & 0 \cdot 183 + 80 \\
8 \cdot 11 & = & 0 \cdot 183 + 88 \\
8 \cdot 12 & = & 1 \cdot 183 - 87 \\
\vdots & & \vdots \\
8 \cdot 17 & = & 1 \cdot 183 - 47 \\
8 \cdot 18 & = & 1 \cdot 183 - 39 \\
8 \cdot 19 & = & 1 \cdot 183 - 31
\end{array}$$

If $q_{i,3} < 0$, then $|q_{i,3}| = -q_{i,3} \geq 31$, where the minimum value is attained at the endpoint $i = 19$. If $q_{i,3} \geq 0$, then $q_{i,3} \geq 32$, where the minimum value is attained at the endpoint $i = 4$. We prove that in the general case, these minimum values of $|q_{i,j+1}|$ always occur at the endpoints.

Among all the values of i for which $q_{i,j+1} < 0$ (i.e., $p_{i,j+1} = 1$), the minimum value of $|q_{i,j+1}|$ occurs at the endpoint $i = n_j - n_{j-1}$. This follows from the identity $-q_{i,j+1} = n_{j+1} - t_{j+1}i$, which is minimized when $i \in S_{j,j+1}$ is maximized. Thus, the minimum value of $-q_{i,j+1}$ (i.e., the maximum of $q_{i,j+1}$) occurs at $i = n_j - n_{j-1} = y$.

By Lemma 3.34, $q_{y,j+1} = -a_{j+1}n_{j-1} + 1$. From the previous paragraph, we have $q_{y,j+1} - q_{i,j+1} > 0$ for all $i \neq y$ with $q_{i,j+1} < 0$. Since $p_{i,j+1} = p_{y,j+1} = 1$, we have

$$0 = p_{i,j+1} - p_{y,j+1} \leq (a_{j+1} - 1)(q_{y,j+1} - q_{i,j+1}).$$

This proves Part (a) of the base case $m = j + 1$. Now we prove Part (b). Among all the values of i for which $q_{i,j+1} \geq 0$ (i.e., $p_{i,j+1} = 0$), the minimum value of $q_{i,j+1}$ occurs at the endpoint $i = n_{j-1}$. This follows from the identity $q_{i,j+1} = t_{j+1}i$, which is minimized when $i \in S_{j,j+1}$ is minimized. Thus, the minimum value of $q_{i,j+1}$ occurs at $i = n_{j-1} = n_j - (n_j - n_{j-1}) = n_j - y$.

Therefore, if $q_{i,j+1} \geq 0$, then $q_{i,j+1} \geq t_{j+1}n_{j-1} = a_{j+1}n_{j-1} = -q_{y,j+1} + 1$, by Lemma 3.34. Since $t_j = 1$, we have shown that $q_{i,j+1} \geq -q_{y,j+1} + t_j$, with equality occurring when $i = n_j - y$. This proves Part (b) of the base case.

This establishes the base case $m = j+1$. Now let $m \geq j+2$, and suppose that the lemma holds for all indices less than m. By the induction hypothesis, the following identities hold for each $x \in S_{j,m-1}$.

(a) If $q_{x,m-1} < 0$, then $0 \leq p_{x,m-1} - p_{y,m-1} \leq (a_{m-1} - 1)(q_{y,m-1} - q_{x,m-1})$.

(b) If $q_{x,m-1} \geq 0$, then $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$.

In proving Part (a) of Lemma 3.37, we will constantly refer to this induction hypothesis.

Proof of Part (a)

We split our analysis into the four cases corresponding to the types determined in Lemma 3.32. In all four possibilities for part (a), **we are only interested in the case** $q_{i,m} < 0$, since there is nothing to prove when $q_{i,m} \geq 0$. By Lemma 3.32, each $q_{i,m}$ can be expressed recursively as a function of $r_{x,m} = p_{x,m-1} + a_m q_{x,m-1}$, where $x \in S_{j,m-1}$ satisfies $i = x$ or $i = x + n_{m-1} - n_{m-2}$. Recall that the $i = x$ case corresponds to the Type I and Type II pairs, while the $i = x + n_{m-1} - n_{m-2}$ case corresponds to the Type III and Type IV pairs.

For each of our four types, either $q_{x,m-1} < 0$ or $q_{x,m-1} \geq 0$. We will determine which inequality holds for each of our four types (there will be only one), which then enables us to use the correct statement of the induction hypothesis.

Recall by Lemma 3.35 that $(p_{y,m}, q_{y,m})$ is a Type I pair with $p_{y,m} = p_{y,m-1} = 1$ and $q_{y,m} = r_{y,m} = p_{y,m-1} + a_m q_{y,m-1} = 1 + a_m q_{y,m-1} < 0$.

Case 1: $(p_{i,m}, q_{i,m})$ is a Type I pair.

In this case, $p_{i,m} = p_{x,m-1}$ and $q_{i,m} = r_{x,m} = p_{x,m-1} + a_m q_{x,m-1}$, where $i = x \in S_{j,m-1} \subseteq S_{j,m}$.

As discussed above, either $q_{x,m-1} \geq 0$ or $q_{x,m-1} < 0$. We prove that in this case, the former leads to a contradiction.

If $q_{x,m-1} \geq 0$, then Lemma 3.28 tells us that $q_{i,m} = p_{x,m-1} + a_m q_{x,m-1} \geq 0 + a_m \cdot 0 = 0$, contradicting the assumption that $q_{i,m} < 0$. Thus, $q_{x,m-1} < 0$. Since $q_{x,m-1} < 0$, we may apply the induction hypothesis on the pair $(p_{x,m-1}, q_{x,m-1})$. By the first statement of the induction hypothesis, we have

$$p_{i,m} - p_{y,m} = p_{x,m-1} - p_{y,m-1} \geq 0.$$

Now we prove the second half of our desired inequality. We have

$$\begin{aligned}
q_{y,m} - q_{i,m} &= (p_{y,m-1} + a_m q_{y,m-1}) - (p_{x,m-1} + a_m q_{x,m-1}) \\
&= a_m(q_{y,m-1} - q_{x,m-1}) + (p_{y,m-1} - p_{x,m-1}) \\
&\geq \frac{a_m}{a_{m-1}-1}(p_{x,m-1} - p_{y,m-1}) - (p_{x,m-1} - p_{y,m-1}) \quad \text{by the Ind. Hyp.} \\
&= \frac{a_m - a_{m-1} + 1}{a_{m-1}-1}(p_{x,m-1} - p_{y,m-1}) \\
&\geq \frac{p_{x,m-1} - p_{y,m-1}}{a_{m-1}-1} \quad \text{since } a_m \geq a_{m-1} \\
&= \frac{p_{i,m} - p_{y,m}}{a_{m-1}-1} \quad \text{since } (p_{i,m}, q_{i,m}) \text{ and } (p_{y,m}, q_{y,m}) \text{ are Type I pairs} \\
&\geq \frac{p_{i,m} - p_{y,m}}{a_m - 1} \quad \text{since } a_m \geq a_{m-1}.
\end{aligned}$$

Multiplying both sides by $a_m - 1$, we obtain the desired conclusion.

Case 2: $(p_{i,m}, q_{i,m})$ is a Type II pair.

In this case, $p_{i,m} = p_{x,m-1} + 1$ and $q_{i,m} = r_{x,m} - n_m = p_{x,m-1} + a_m q_{x,m-1} - n_m$, where $i = x \in S_{j,m-1} \subseteq S_{j,m}$.

First, we must determine whether $q_{x,m-1} \geq 0$ or $q_{x,m-1} < 0$.

Suppose that $q_{x,m-1} < 0$. Then

$$\begin{aligned}
q_{i,m} &= p_{x,m-1} + a_m q_{x,m-1} - n_m \\
&< p_{x,m-1} - n_m \\
&\leq t_{m-2} - n_m \quad \text{by Lemma 3.28} \\
&< \frac{n_{m-1} - 1}{2} - n_m \quad \text{by Lemma 3.30} \\
&< \frac{n_m}{2} - n_m \\
&= -\frac{n_m}{2}.
\end{aligned}$$

This contradicts the inequality $-\frac{n_m}{2} < q_{i,m} \leq \frac{n_m}{2}$. Therefore, we must have $q_{x,m-1} \geq 0$.

By the second statement of the induction hypothesis, we have $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$, i.e., $q_{y,m-1} \geq -q_{x,m-1} + t_{m-2}$.

By Lemma 3.28, we have $p_{i,m} - p_{y,m} = (p_{x,m-1} + 1) - 1 = p_{x,m-1} \geq 0$, which proves the first inequality.

Now we prove that $(a_m - 1)(q_{y,m} - q_{i,m}) \geq p_{i,m} - p_{y,m} = p_{x,m-1}$. We have

$$\begin{aligned}
& (a_m - 1)(q_{y,m} - q_{i,m}) \\
\geq\; & q_{y,m} - q_{i,m} \quad \text{since } a_m \geq 3 \\
=\; & (p_{y,m-1} + a_m q_{y,m-1}) - (p_{x,m-1} + a_m q_{x,m-1} - n_m) \\
=\; & (p_{y,m-1} + n_m) + a_m(q_{y,m-1} - q_{x,m-1}) - p_{x,m-1} \\
=\; & (1 + n_m) + a_m(q_{y,m-1} - q_{x,m-1}) - p_{x,m-1} \quad \text{by Lemma 3.35} \\
\geq\; & a_m n_{m-1} + a_m(-q_{x,m-1} + t_{m-2} - q_{x,m-1}) - p_{x,m-1} \quad \text{by the I.H.} \\
=\; & a_m(n_{m-1} - 2q_{x,m-1}) + a_m t_{m-2} - p_{x,m-1} \\
\geq\; & a_m \cdot 0 + a_m t_{m-2} - p_{x,m-1} \quad \text{by the inequality } q_{x,m-1} \leq \tfrac{n_{m-1}}{2} \\
>\; & 2t_{m-2} - p_{x,m-1} \quad \text{since } a_m \geq 3 \\
\geq\; & p_{x,m-1} \quad \text{by Lemma 3.28} \\
=\; & (p_{x,m-1} + 1) - 1 \\
=\; & p_{i,m} - p_{y,m} \quad \text{by Lemma 3.35 .}
\end{aligned}$$

We have proven the desired inequality.

Case 3: $(p_{i,m}, q_{i,m})$ is a Type III pair.

Let $x = i - (n_{m-1} - n_{m-2}) \in S_{j,m-1}$. In this case, $p_{i,m} = p_{x,m-1} + (t_{m-1} - t_{m-2})$ and $q_{i,m} = r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) = p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1)$.

First assume that $q_{x,m-1} \geq 0$. By the second statement of the Induction Hypothesis, this implies that $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$. In this case, we have

$$\begin{aligned}
q_{i,m} &= p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) \\
&\geq 0 + a_m(-q_{y,m-1} + t_{m-2}) - t_{m-2}(a_m - a_{m-1} + 1) \quad \text{by the I.H.} \\
&= -a_m q_{y,m-1} + a_m t_{m-2} - a_m t_{m-2} + a_{m-1} t_{m-2} - t_{m-2} \\
&= -a_m q_{y,m-1} + a_{m-1} t_{m-2} - t_{m-2} \\
&> a_m(t_{m-2} - 1) + a_{m-1} t_{m-2} - t_{m-2} \quad \text{by Lemma 3.36} \\
&\geq 3(t_{m-2} - 1) + a_{m-1} t_{m-2} - t_{m-2} \quad \text{since } a_m \geq 3 \\
&= t_{m-2}(a_{m-1} + 2) - 3 \\
&\geq 1(3 + 2) - 3 \\
&> 0.
\end{aligned}$$

Hence, we have $q_{i,m} > 0$, contradicting the assumption that $q_{i,m} < 0$.

Therefore, we have shown that $q_{x,m-1} < 0$. Hence, we can use the first statement of the induction hypothesis. Since $t_{m-1} = a_{m-1} t_{m-2} > t_{m-2}$, we have

$$p_{i,m} - p_{y,m} = (p_{x,m-1} - p_{y,m-1}) + (t_{m-1} - t_{m-2}) > 0,$$

by the induction hypothesis. We now establish the second half of our desired inequality. We have

$$\begin{aligned}
& q_{y,m} - q_{i,m} \\
= \;& q_{y,m} - (p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1)) \\
= \;& (p_{y,m-1} + a_m q_{y,m-1}) - (p_{x,m-1} + a_m q_{x,m-1}) + t_{m-2}(a_m - a_{m-1} + 1) \\
= \;& a_m(q_{y,m-1} - q_{x,m-1}) + (p_{y,m-1} - p_{x,m-1}) + t_{m-2}(a_m - a_{m-1} + 1) \\
\geq \;& \frac{a_m(p_{x,m-1} - p_{y,m-1})}{a_{m-1} - 1} - (p_{x,m-1} - p_{y,m-1}) + t_{m-2}(a_m - a_{m-1} + 1) \;\; \text{by the I.H.} \\
= \;& \frac{a_m - a_{m-1} + 1}{a_{m-1} - 1}(p_{x,m-1} - p_{y,m-1}) + t_{m-2}(a_m - a_{m-1} + 1) \\
\geq \;& \frac{p_{x,m-1} - p_{y,m-1}}{a_{m-1} - 1} + t_{m-2}(a_m - a_{m-1} + 1) \;\; \text{since } a_m \geq a_{m-1} \\
= \;& \frac{1}{a_{m-1} - 1}((p_{i,m} - p_{y,m}) - (t_{m-1} - t_{m-2})) + t_{m-2}(a_m - a_{m-1} + 1) \;\; \text{from above} \\
= \;& \frac{p_{i,m} - p_{y,m}}{a_{m-1} - 1} - \frac{t_{m-1} - t_{m-2}}{a_{m-1} - 1} + t_{m-2}(a_m - a_{m-1} + 1) \\
= \;& \frac{p_{i,m} - p_{y,m}}{a_{m-1} - 1} - \frac{a_{m-1}t_{m-2} - t_{m-2}}{a_{m-1} - 1} + t_{m-2}(a_m - a_{m-1} + 1) \\
= \;& \frac{p_{i,m} - p_{y,m}}{a_{m-1} - 1} - t_{m-2} + t_{m-2}(a_m - a_{m-1} + 1) \\
= \;& \frac{p_{i,m} - p_{y,m}}{a_{m-1} - 1} + t_{m-2}(a_m - a_{m-1}) \\
\geq \;& \frac{p_{i,m} - p_{y,m}}{a_{m-1} - 1} \;\; \text{since } a_m \geq a_{m-1} \\
\geq \;& \frac{p_{i,m} - p_{y,m}}{a_m - 1} \;\; \text{since } a_m \geq a_{m-1}.
\end{aligned}$$

Multiplying both sides by $a_m - 1$, we obtain the desired conclusion.

Case 4: $(p_{i,m}, q_{i,m})$ is a Type IV pair.

Let $x = i - (n_{m-1} - n_{m-2}) \in S_{j,m-1}$. In this case, $p_{i,m} = p_{x,m-1} + (t_{m-1} - t_{m-2} - 1)$ and $q_{i,m} = r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) + n_m$.

We now prove that $q_{i,m} > 0$, which is irrespective of the sign of $q_{x,m-1}$, i.e., the induction hypothesis is unnecessary in this case.

This result will then contradict our assumption that $q_{i,m} < 0$. We have

$$\begin{aligned}
q_{i,m} &= r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \\
&> r_{x,m} - t_{m-2}a_m + n_m \quad \text{since } a_m \geq 3 \\
&= p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}a_m + n_m \\
&> 0 + a_m \cdot \frac{-n_{m-1}}{2} - t_{m-2}a_m + n_m \\
&> -\frac{a_m n_{m-1}}{2} + \frac{a_m(-n_{m-1}+1)}{2} + n_m \quad \text{by Lemma 3.30} \\
&= -a_m n_{m-1} + \frac{a_m}{2} + n_m \\
&= -(n_m + 1) + \frac{a_m}{2} + n_m \\
&= \frac{a_m}{2} - 1 \\
&> 0 \quad \text{since } a_m \geq 3.
\end{aligned}$$

This yields the desired contradiction.

We have considered all four possibilities, and completed the induction in each case. Therefore, we have proven Part (a) of Lemma 3.37. Now we prove Part (b). Recall that by the induction hypothesis, we have the following.

(a) If $q_{x,m-1} < 0$, then $q_{x,m-1} \leq q_{y,m-1}$, with equality occurring when $x = y = n_j - n_{j-1}$.

(b) If $q_{x,m-1} \geq 0$, then $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$, with equality occurring when $x = n_{m-2} - y = n_{m-2} - (n_j - n_{j-1})$.

We will require both parts of the induction hypothesis in the following proof.

Proof of Part (b)

We have already proven the result for the base case $m = j + 1$. So suppose part (b) of the lemma is true for all indices less than m, for some $m \geq j + 2$. Since our desired inequality requires the condition $q_{i,m} \geq 0$, we will now assume that $q_{i,m} \geq 0$.

For $i \in S_{j,m} \subseteq \{1, 2, \ldots, n_{m-1} - 1\}$, define $\bar{i} = n_{m-1} - i$. Note that by Proposition 3.5 (a), $\bar{i} \in S_{j,m}$ for each $i \in S_{j,m}$. We will now prove that

$$q_{i,m} + q_{\bar{i},m} = t_{m-1}.$$

Immediately thereafter, we will show that $q_{i,m} \geq 0$ implies $q_{\bar{i},m} < 0$. By part (a) of the lemma, which we just proved, we must have $q_{\bar{i},m} \leq q_{y,m}$. Note that we may apply this inequality in part (a), since $\bar{i} \in S_{j,m}$.

Combining these two results, we will have $q_{i,m} = -q_{\bar{i},m} + t_{m-1} \geq -q_{y,m} + t_{m-1}$, proving part (b) for the case $q_{i,m} \geq 0$.

First we prove that $q_{i,m} + q_{\bar{i},m} = t_{m-1}$ for all $i \in S_{j,m}$, where $\bar{i} = n_{m-1} - i$. Since $t_m i = p_{i,m} n_m + q_{i,m}$ and $t_m \bar{i} = p_{\bar{i},m} n_m + q_{\bar{i},m}$, we have

$$\begin{aligned}
(p_{i,m} + p_{\bar{i},m}) n_m + (q_{i,m} + q_{\bar{i},m}) &= t_m (i + \bar{i}) \\
&= t_m n_{m-1} \\
&= t_{m-1} a_m n_{m-1} \\
&= t_{m-1}(n_m + 1) \\
&= t_{m-1} + t_{m-1} n_m.
\end{aligned}$$

It follows that $q_{i,m} + q_{\bar{i},m} \equiv t_{m-1} \pmod{n_m}$, for all $i \in S_{j,m}$. Therefore, $q_{i,m} + q_{\bar{i},m} = t_{m-1} + l n_m$ for some integer l.

We know that $0 \leq q_{i,m} \leq \frac{n_m}{2}$ and $-\frac{n_m}{2} < q_{\bar{i},m} \leq \frac{n_m}{2}$. The former inequality holds since $i \in S_{j,m}$, and the latter inequality holds by the definition of $q_{\bar{i},m}$, since $\bar{i} \in S_{j,m}$.

If $l \leq -1$, then $q_{i,m} + q_{\bar{i},m} \leq t_{m-1} - n_m$. In this case, $q_{\bar{i},m} \leq t_{m-1} - n_m - q_{i,m} \leq t_{m-1} - n_m < \left(\frac{n_m}{2} - \frac{1}{2}\right) - n_m = -\frac{n_m}{2} - \frac{1}{2}$, by Lemma 3.30. However, this contradicts the inequality $q_{\bar{i},m} > -\frac{n_m}{2}$, which holds by definition.

If $l \geq 1$, then $q_{i,m} + q_{\bar{i},m} \geq t_{m-1} + n_m > n_m$. However, both $q_{i,m} \leq \frac{n_m}{2}$ and $q_{\bar{i},m} \leq \frac{n_m}{2}$. Adding these two inequalities, we arrive at our desired contradiction.

Therefore, we must have $l = 0$, i.e., $q_{i,m} + q_{\bar{i},m} = t_{m-1}$.

For any $i \in S_{j,m}$ with $q_{i,m} \geq 0$, we have either $q_{\bar{i},m} < 0$ or $q_{\bar{i},m} \geq 0$. We now explain how the former inequality implies part (b) of the lemma.

In the case $q_{\bar{i},m} < 0$, we may directly quote the result of part (a), which we just proved, since $\bar{i} \in S_{j,m}$. By replacing i with $\bar{i}$, we have $q_{\bar{i},m} \leq q_{y,m}$.

Therefore, if $q_{\bar{i},m} < 0$, we have $q_{i,m} = -q_{\bar{i},m} + t_{m-1} \geq -q_{y,m} + t_{m-1}$, with equality occurring when $\bar{i} = y$, i.e., $i = n_{m-1} - y$. This establishes Part (b) of Lemma 3.37 for all $i \in S_{j,m}$ satisfying $q_{\bar{i},m} < 0$.

It remains to consider the case $q_{\bar{i},m} \geq 0$. We now prove that this case will never occur (i.e., *every* possibility leads to a contradiction), which will complete the proof of Lemma 3.37. We prove that this $i \in S_{j,m}$ cannot satisfy both $q_{i,m} \geq 0$ and $q_{\bar{i},m} \geq 0$.

Suppose the contrary. Then by the identity $q_{i,m} + q_{\bar{i},m} = t_{m-1}$, we must have $0 \leq q_{i,m} \leq t_{m-1}$. Let us consider all four of the possible types for $(p_{i,m}, q_{i,m})$ given in the proof of Lemma 3.32, and prove that in no case can the inequality $0 \leq q_{i,m} \leq t_{m-1}$ hold. This will give us our desired contradiction.

Let us consider each of the four types and derive a contradiction in each case. This will complete the proof of Lemma 3.37.

<u>*Case 1:*</u> $(p_{i,m}, q_{i,m})$ is a Type I pair.

In this case, $i = x \in S_{j,m-1}$, and $q_{i,m} = r_{x,m} = p_{x,m-1} + a_m q_{x,m-1}$.

As we did previously, we must consider the two possibilities: either $q_{x,m-1} \geq 0$ or $q_{x,m-1} < 0$. We will derive a contradiction in each case.

If $q_{x,m-1} \geq 0$, then by the second statement of the induction hypothesis, we have $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$. Therefore,

$$\begin{aligned}
q_{i,m} &= p_{x,m-1} + a_m q_{x,m-1} \\
&\geq 0 + a_m q_{x,m-1} \quad \text{by Lemma 3.28} \\
&\geq a_m(-q_{y,m-1} + t_{m-2}) \quad \text{by the induction hypothesis} \\
&= -a_m q_{y,m-1} + a_m t_{m-2} \\
&= -q_{y,m} + 1 + a_m t_{m-2} \quad \text{by Lemma 3.35} \\
&> t_{m-2} + a_m t_{m-2} \quad \text{by Lemma 3.36} \\
&\geq t_j + a_m t_{m-2} \quad \text{since } m \geq j+2 \\
&\geq 1 + a_{m-1} t_{m-2} \quad \text{since } a_m \geq a_{m-1} \text{ and } t_j = 1 \\
&> a_{m-1} t_{m-2} \\
&= t_{m-1}.
\end{aligned}$$

If $q_{x,m-1} < 0$, then we have

$$\begin{aligned}
q_{i,m} &= p_{x,m-1} + a_m q_{x,m-1} \\
&\leq p_{x,m-1} + a_m q_{y,m-1} \quad \text{by the induction hypothesis} \\
&\leq t_{m-2} + a_m q_{y,m-1} \quad \text{by Lemma 3.28} \\
&= t_{m-2} + (q_{y,m} - 1) \quad \text{by Lemma 3.35} \\
&< 0 \quad \text{by Lemma 3.36}\ .
\end{aligned}$$

In both situations, we have shown that $q_{i,m}$ cannot lie in the interval $[0, t_{m-1}]$, giving us our desired contradiction.

<u>*Case 2:*</u> $(p_{i,m}, q_{i,m})$ is a Type II pair.

In this case, $i = x \in S_{j,m-1}$, and $q_{i,m} = r_{x,m} - n_m = p_{x,m-1} + a_m q_{x,m-1} - n_m$. We will prove that $q_{i,m} < 0$, irrespective of the sign of $q_{x,m-1}$. We have

$$\begin{aligned}
q_{i,m} &= r_{x,m} - n_m \\
&= p_{x,m-1} + a_m q_{x,m-1} - n_m \\
&\leq t_{m-2} + a_m \cdot \frac{n_{m-1}}{2} - n_m \quad \text{by Lemma 3.28} \\
&< t_{m-1} + \frac{a_m n_{m-1}}{2} - n_m \\
&< \frac{n_m - 1}{2} + \frac{n_m + 1}{2} - n_m \quad \text{by Lemma 3.30} \\
&= 0.
\end{aligned}$$

Therefore, we have proven that $q_{i,m} < 0$, a contradiction.

<u>*Case 3:*</u> $(p_{i,m}, q_{i,m})$ is a Type III pair.

Let $x = i - (n_{m-1} - n_{m-2}) \in S_{j,m-1}$. In this case, $q_{i,m} = r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1)$. We consider two cases: either $q_{x,m-1} \geq 0$ or $q_{x,m-1} < 0$. We derive a contradiction in each case.

If $q_{x,m-1} \geq 0$, then by the second statement of the induction hypothesis, $q_{x,m-1} \geq -q_{y,m-1} + t_{m-2}$. We have

$$\begin{aligned}
q_{i,m} &= r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) \\
&= p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) \\
&\geq 0 + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) \quad \text{by Lemma 3.28} \\
&\geq 0 + a_m(-q_{y,m-1} + t_{m-2}) - t_{m-2}(a_m - a_{m-1} + 1) \quad \text{by the Ind Hyp.} \\
&= -a_m q_{y,m-1} + a_m t_{m-2} - a_m t_{m-2} + a_{m-1} t_{m-2} - t_{m-2} \\
&= -a_m q_{y,m-1} + a_{m-1} t_{m-2} - t_{m-2} \\
&= (-q_{y,m} + 1) + t_{m-1} - t_{m-2} \quad \text{by Lemma 3.35} \\
&> t_{m-2} + t_{m-1} - t_{m-2} \quad \text{by Lemma 3.36} \\
&= t_{m-1}.
\end{aligned}$$

On the other hand, if $q_{x,m-1} < 0$, then by the first statement of the induction hypothesis, $q_{x,m-1} \leq q_{y,m-1}$. We have

$$\begin{aligned}
q_{i,m} &= r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) \\
&= p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) \\
&\leq t_{m-2} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) \ \text{ by Lemma 3.28} \\
&< t_{m-2} + a_m q_{x,m-1} \ \text{ since } a_m \geq a_{m-1} \text{ and } t_{m-2} > 0 \\
&\leq t_{m-2} + a_m q_{y,m-1} \ \text{ by the induction hypothesis} \\
&= t_{m-2} + (q_{y,m} - 1) \ \text{ by Lemma 3.35} \\
&< 0 \ \text{ by Lemma 3.36.}
\end{aligned}$$

In both situations, we have shown that $q_{i,m}$ does not lie in the interval $[0, t_{m-1}]$, giving us our desired contradiction.

Case 4: $(p_{i,m}, q_{i,m})$ is a Type IV pair.

Let $x = i - (n_{m-1} - n_{m-2}) \in S_{j,m-1}$. In this case, $q_{i,m} = r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) + n_m$.

We prove that $q_{i,m} > t_{m-1}$, irrespective of the sign of $q_{x,m-1}$. We have

$$\begin{aligned}
q_{i,m} &= r_{x,m} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \\
&= p_{x,m-1} + a_m q_{x,m-1} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \\
&\geq 0 + a_m \cdot \frac{-n_{m-1}}{2} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \ \text{ by Lemma 3.28} \\
&= -\frac{a_m n_{m-1}}{2} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \\
&= -\frac{n_m + 1}{2} - t_{m-2}(a_m - a_{m-1} + 1) + n_m \\
&= \frac{n_m}{2} - t_{m-2}(a_m - a_{m-1} + 1) - \frac{1}{2} \\
&> \left(t_{m-2} a_m + t_{m-2} + \frac{1}{2}\right) - t_{m-2}(a_m - a_{m-1} + 1) - \frac{1}{2} \ \text{ by Lemma 3.29} \\
&= t_{m-2} a_m + t_{m-2} - t_{m-2} a_m + t_{m-2} a_{m-1} - t_{m-2} \\
&= t_{m-2} a_{m-1} \\
&= t_{m-1}.
\end{aligned}$$

Therefore, we have proven that $q_{i,m} > t_{m-1}$, a contradiction.

In all four cases, we have shown that there exists no $i \in S_{j,m}$ for which $q_{i,m} \geq 0$ and $q_{\bar{i},m} \geq 0$. If $q_{i,m} \geq 0$, then we *must* have $q_{\bar{i},m} < 0$. As discussed before, we may now directly quote part (a) of the lemma which states that $q_{\bar{i},m} \leq q_{y,m}$, with equality occurring when $\bar{i} = y$, i.e., $i = n_{m-1} - y$.

Combined with our earlier proof that $q_{i,m} + q_{\bar{i},m} = t_{m-1}$, we conclude that $q_{i,m} \geq -q_{y,m} + t_{m-1}$, with equality occurring when $i = n_{m-1} - y$. This establishes Part (b) of Lemma 3.37.

We have now examined every possible case for both Parts (a) and (b), and completed the induction. This concludes the proof of Lemma 3.37. ∎

With these results, we are finally able to prove Theorem 3.25, the main theorem of this section.

<u>Proof:</u> Before proceeding, we recall some definitions. Given $G = C_{n,S}$, and a positive integer t,

$$\lambda_t(G) = \min\{|ti|_n : i \in S\},$$

where the product ti is reduced modulo n. In addition,

$$\lambda(G) = \max\{\lambda_t(G) : t = 1, 2, 3, \ldots, n\}.$$

By Lemma 3.24, $\lambda(G) \leq \alpha(G)$. Furthermore, to prove that G is star extremal, it suffices to prove that $\lambda(G) = \alpha(G)$. Specifically, to prove G is star extremal, we only need to find *one* integer t for which $\lambda_t(G) = \alpha(G)$.

For $j = k$, we have $\lambda_1(G_{j,k}) = \min\{n_{k-1}, n_{k-1}+1, \ldots, \lfloor \frac{n_k}{2} \rfloor\} = n_{k-1}$, which equals $\alpha(G_{k,k})$, by Theorem 3.8. Thus, $t = 1$ satisfies the desired identity.

For $1 \leq j \leq k-1$, we require a more sophisticated strategy, and that is the reason why we introduced the ordered pair $(p_{i,k}, q_{i,k})$. As discussed earlier, to prove that each $G_{j,k}$ is star extremal, it suffices to find one integer t for which

$$\lambda_t(G_{j,k}) = \min\{|ti|_{n_k} : i \in S_{j,k}\} = \min\{|q_{i,k}| : i \in S_{j,k}\} = \alpha(G_{j,k}).$$

Finding such a t for each $1 \leq j \leq k-1$ will complete the proof of Theorem 3.25.

We now prove that $t_k = a_{j+1}a_{j+2}\cdots a_k$ is the desired value of t. Recall that by our definition of $q_{i,k}$, we have $|t_k i|_{n_k} = |q_{i,k}|$. For this index $t = t_k$, we prove that $i = n_j - n_{j-1} = y$ gives us the minimum value of $|ti|_{n_k} = |q_{i,k}|$, and we will show that this minimum value equals $\alpha(G_{j,k})$.

By Theorem 3.8, recall that

$$\alpha(G_{j,k}) = \begin{cases} a_k\alpha(G_{j,k-1}) - 1 & \text{for } 1 \leq j \leq k-1 \\ n_{k-1} & \text{for } j = k \end{cases}$$

If $q_{i,k} < 0$, Lemmas 3.35 and 3.37 give us $q_{i,k} \leq q_{y,k} < 0$, or $|q_{i,k}| \geq |q_{y,k}| = -q_{y,k}$. Equality occurs when $i = y$.

If $q_{i,k} \geq 0$, Lemmas 3.35 and 3.37 give us $q_{i,k} \geq -q_{y,k} + t_{k-1} > 0$, with equality when $i = n_{k-1} - y$. In other words, $|q_{i,k}| \geq -q_{y,k} + t_{k-1}$.

This proves that $\min\{|q_{i,k}| : i \in S_{j,k}\} = \min\{-q_{y,k}, -q_{y,k} + t_{k-1}\} = -q_{y,k}$.

This implies that for $t = t_k$, $\lambda_t(G_{j,k}) = -q_{y,k}$, where $y = n_j - n_{j-1}$. By Lemma 3.35, $q_{y,k} = 1 + a_k q_{y,k-1}$, from which it follows that $|q_{y,k}| = a_k|q_{y,k-1}| - 1$. In other words, $\lambda_{t_k}(G_{j,k}) = a_k\lambda_{t_{k-1}}(G_{j,k-1}) - 1$. This identity holds for any k-tuple satisfying $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$, with $1 \leq j \leq k-1$. This argument easily generalizes to the identity $\lambda_{t_m}(G_{j,m}) = a_m\lambda_{t_{m-1}}(G_{j,m-1}) - 1$ for each $j+1 \leq m \leq k$.

By Theorem 3.8, $\alpha(G_{j,m}) = a_m\alpha(G_{j,m-1}) - 1$, which is the exact same recurrence relation. So to prove that $\lambda_{t_k}(G_{j,k}) = \alpha(G_{j,k})$, it suffices to verify that the functions have the same value for the base case $m = j+1$. But this is trivial, since $\lambda_{t_{j+1}}(G_{j,j+1}) = -q_{y,j+1} = a_{j+1}n_{j-1} - 1 = a_{j+1}\alpha(G_{j,j}) - 1 = \alpha(G_{j,j+1})$, by Lemma 3.34 and Theorem 3.8.

We have thus shown that every $G_{j,k}$ is star extremal, for all k-tuples satisfying $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$. Our proof is finally complete. ∎

3.3 Application 2: Integer Distance Graphs

If S is a subset of the positive integers, then the *integer distance graph* $G(\mathbb{Z}, S)$ is defined to be the graph with vertex set $\mathbb{Z}$, where two vertices u and v are adjacent iff $|u - v| \in S$. As with other families of graphs, a natural question is to determine the *chromatic number* of $G(\mathbb{Z}, S)$, the minimum number of colours required to colour the vertices of $G(\mathbb{Z}, S)$, so that no two adjacent vertices receive the same colour.

Thus, S is the set of forbidden distances with respect to colouring the integers on the real line. In a way, we can regard the integer distance graph $G(\mathbb{Z}, S)$ as the infinite analogue of the circulant $C_{n,S}$.

The distance graph, first introduced by Eggleton, Erdös and Skilton [63], is motivated by the well-known Hadwiger-Nelson problem which asks for the minimum number of colours needed to colour all points of the plane such that points at unit distances receive different colours. This problem is equivalent to determining the chromatic number of $G(\mathbb{R}^2, \{1\})$, which is known to be at least 4 and at most 7. A comprehensive survey of this well-studied problem appears in [40].

Motivated by the plane colouring problem, we can consider the analogue to the one-dimensional case by investigating the chromatic numbers of distance graphs on the real line $\mathbb{R}$ and the integer set $\mathbb{Z}$. A particularly interesting problem is determining the value of $\chi(G(\mathbb{Z}, S))$ for a given set S. Much work has been done on this problem [30, 34, 63, 64, 99, 107, 108, 109, 110, 123, 125, 170, 171, 172], and we now highlight some of the known results from these papers. For notational convenience, we abbreviate $\chi(G(\mathbb{Z}, S))$ by $\boldsymbol{\chi(\mathbb{Z}, S)}$.

If $|S| \leq 3$, then an explicit formula for $\chi(\mathbb{Z}, S)$ is known [34, 170] for all possible sets S. For sets with $|S| \geq 4$, only some partial results have been solved [107, 171]. For example, a formula is known for $S = \{x, y, x+y, y-x\}$ with $y > x > 0$ and also for $S = \{1, 2, 3, 4n\}$. If S $= \{2, 3, x, x+y\}$, then $\chi(\mathbb{Z}, S)$ is known for many pairs (x, y). It is shown [109] that $\chi(\mathbb{Z}, S) \leq |S| + 1$, for an arbitrary S, and so a natural question is to classify the sets S for which equality is reached. However, a full classification has not yet been found.

If S is of a particular form, then several results are known. For example, it is proven [125] that $\chi(\mathbb{Z}, S) = m$ if $S = \{1, 2, \ldots, n\} \backslash \{m, 2m, \ldots, sm\}$, for some $n \geq (s+1)m$. If $S = \{x, 2x, \ldots, nx, y\}$ where (x, y, n) is an ordered triplet of positive integers, then it is known [110] that $\chi(\mathbb{Z}, S) = |S| + 1$ if $x = 1$ and $(n+1)$ divides y; otherwise, $\chi(\mathbb{Z}, S) = |S|$.

We highlight one final result, as we will employ it later in this section.

Theorem 3.38 ([108]) *Let a and d be positive integers so that $S = \{a + kd : k = 0, 1, 2, \ldots\}$ is an arithmetic sequence (either finite or infinite). Then*

$$\chi(\mathbb{Z}, S) = \begin{cases} \left\lceil \dfrac{|S|-1}{a} \right\rceil + 2 & \textit{if } d = 1 \\ 2 & \textit{if } d \textit{ is even or } |S| = 1 \\ 3 & \textit{otherwise} \end{cases}$$

Most of the known formulas for $\chi(\mathbb{Z}, S)$ occur when S is a small set of singleton elements, or when S is a highly structured set, such as an arithmetic sequence. We generalize many of these results in this section, by determining a formula for $\chi(\mathbb{Z}, S)$, for *every* generating set $S = S_{j,k}$ in our infinite family of circulants. This gives us explicit values of $\chi(\mathbb{Z}, S)$ for a new (infinite) family of sets S, which extends much of what is currently known. For example, if $(a_1, a_2, a_3, a_4) = (5, 6, 8, 10)$, then

$$S_{1,4} = \{1, 2, 3, 20, 21, 22, 161, 162, 163, 180, 181, 182\}.$$

And from the main theorem in this section, we will derive that $\chi(\mathbb{Z}, S_{1,4}) = 10$. Our theorem will calculate $\chi(\mathbb{Z}, S)$ for sets S with 2^k intervals of arbitrary length, for any $k \geq 0$. This is a significant extension of previously published results. In this main theorem, we give the correct formula for $\chi(\mathbb{Z}, S)$, for every $S = S_{j,k}$. As an immediate corollary, we can determine the formula for the chromatic number $\chi(G_{j,k})$, for each $1 \leq j \leq k$. As we will see at the end of this section, the formula is remarkably simple.

Recall how the $S_{j,k}$'s are defined. Given any k-tuple of non-decreasing integers $(a_1, a_2, \ldots, a_k)$, we first define $n_0 = 1$, and $n_i = a_i n_{i-1} - 1$, for $1 \leq i \leq k$. Then for each $1 \leq j \leq i \leq k$, we define

$$S_{j,i} = \begin{cases} \pm S_{j,i-1} \pmod{n_{i-1}} & \text{for all } 1 \leq j < i \\ \\ \left\{1, 2, \ldots, \left\lfloor \dfrac{n_i}{2} \right\rfloor \right\} - \displaystyle\bigcup_{j=1}^{i-1} S_{j,i} & \text{for } j = i \end{cases}$$

We now state the main theorem of this section.

Theorem 3.39 *Let $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-1} \leq a_k$, and let $S_{j,k}$ be defined as above. Then,*

$$\chi(\mathbb{Z}, S_{j,k}) = \begin{cases} a_j & \text{if } 1 \leq j \leq k-1 \text{ and } k \geq 3 \\ \left\lfloor \dfrac{a_j+3}{2} \right\rfloor & \text{if } j = k \geq 3 \text{ or if } j = k = 2 \text{ and } a_1 > 3 \\ \left\lfloor \dfrac{a_2+2}{2} \right\rfloor & \text{if } j = k = 2 \text{ and } a_1 = 3 \\ \left\lfloor \dfrac{a_1+1}{2} \right\rfloor & \text{if } j = k = 1 \\ a_1 - 1 & \text{if } (j,k) = (1,2) \end{cases}$$

Before we prove Theorem 3.39, we will require two lemmas.

Lemma 3.40 *Let $C_{n,S}$ be a circulant, where $S \subseteq \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. Then, $\chi(\mathbb{Z}, S) \leq \chi(C_{n,S})$.*

Proof: Define $S' = S \bigcup \{n - x : \ x \in S\}$. Since $S \subseteq S'$, it follows that $\chi(\mathbb{Z}, S) \leq \chi(\mathbb{Z}, S')$, as $|u - v| \notin S'$ implies that $|u - v| \notin S$. In other words, any k-colouring of $G(\mathbb{Z}, S')$ must also be a k-colouring of $G(\mathbb{Z}, S)$.

We now prove that $\chi(\mathbb{Z}, S') = \chi(C_{n,S})$. Combined with the inequality $\chi(\mathbb{Z}, S) \leq \chi(\mathbb{Z}, S')$, this will complete the proof. By definition, any proper colouring of $G(\mathbb{Z}, S')$ must satisfy $u - v \notin S'$ whenever $u > v$. By the definition of S', any proper colouring of $C_{n,S}$ must satisfy $u - v \notin S'$ whenever $u > v$. The condition for a proper colouring is identical for both graphs: the only difference is that $G(\mathbb{Z}, S')$ is an infinite graph, while $C_{n,S}$ is not.

We now justify that $\chi(\mathbb{Z}, S') = \chi(C_{n,S})$. First note that any k-colouring of $G(\mathbb{Z}, S')$ can be made into a k-colouring of $C_{n,S}$ by taking its restriction to just the n vertices of the circulant. Now we establish the converse: start with any k-colouring of $C_{n,S}$. We explain how this generates a k-colouring of $G(\mathbb{Z}, S')$.

For a particular k-colouring of $C_{n,S}$, let $\{V_1, V_2, \ldots, V_k\}$ be the set of colour classes produced. We define the following *tiling* of the k colour classes:

$$W_i = V_i + n\mathbb{Z} = \{x + ny : \quad x \in V_i,\ y \in \mathbb{Z}.\}$$

We now justify that each W_i is independent in $G(\mathbb{Z}, S')$, thus proving that the set $\{W_1, W_2, \ldots, W_k\}$ represents the colour classes corresponding to a proper k-colouring of $G(\mathbb{Z}, S')$.

Suppose on the contrary that a and b are not independent in some W_i, where $a > b$. Then $|a - b| = a - b = pn + v_1 - v_2 \in S'$, where $v_1, v_2 \in V_i$ and p is some non-negative integer. Since $0 \leq v_1, v_2 \leq n-1$ and $1 \leq pn + v_1 - v_2 \leq n-1$, it follows that $p = 0$ or $p = 1$.

If $p = 0$, then $v_1 - v_2 \in S'$, from above. So $v_1 > v_2$. By definition of S', this implies that $v_1 - v_2 \in S$ or $n - (v_1 - v_2) \in S$. In other words, v_1 and v_2 are not independent in $C_{n,S}$, and thus cannot belong to the same colour class V_i. We have a contradiction.

If $p = 1$, then $n + v_1 - v_2 \in S'$. So $v_2 > v_1$. By definition of S', this implies that $n + v_1 - v_2 = n - (v_2 - v_1) \in S$ or $n - (n + v_1 - v_2) = v_2 - v_1 \in S$. In other words, v_1 and v_2 are not independent in $C_{n,S}$, and thus cannot belong to the same colour class V_i. We have a contradiction.

This establishes the converse, that every k-colouring of $C_{n,S}$ can be extended to a k-colouring of $G(\mathbb{Z}, S')$. Hence we conclude that $\chi(\mathbb{Z}, S') = \chi(C_{n,S})$. Since we have already proven that $\chi(\mathbb{Z}, S) \leq \chi(\mathbb{Z}, S')$, the proof is complete. ∎

There are infinitely many sets S for which equality does not hold. As a simple example, consider the case $n = 4$ and $S = \{1, 2\}$. Then $\chi(\mathbb{Z}, S) = 3$, while $\chi(C_{n,S}) = \chi(K_4) = 4$.

Lemma 3.41 *Let* $(a_1, a_2, \ldots, a_k)$ *be a* k*-tuple of integers such that* $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$. *Then,* $\frac{n_k}{\alpha(G_{j,k})} < a_j$ *for all* $1 \leq j \leq k$.

<u>Proof:</u> Let $1 \leq m \leq k$ be an integer. By induction on m, we will prove that the inequality $a_j \alpha(G_{j,m}) - n_m \geq 1$ holds for all $1 \leq j \leq m$. Letting $m = k$, this will establish the lemma.

We proceed by induction on m, proving the inequality for each $1 \le j \le m$. The base case $m = 1$ is trivial, as $n_1 = a_1 - 1$, and $\alpha(G_{1,1}) = 1$. So let $m \ge 2$, and suppose the lemma is true for all indices less than m. Then, by the induction hypothesis, $a_j\alpha(G_{j,m-1}) - n_{m-1} \ge 1$ for each $1 \le j \le m-1$. We have

$$\begin{aligned}
a_j\alpha(G_{j,m-1}) - n_{m-1} &\ge 1 \\
a_j a_m \alpha(G_{j,m-1}) - a_m n_{m-1} &\ge a_m \\
a_j(\alpha(G_{j,m}) + 1) - n_m - 1 &\ge a_m, \quad \text{by Theorem 3.8.} \\
a_j\alpha(G_{j,m}) - n_m &\ge a_m - a_j + 1 \\
a_j\alpha(G_{j,m}) - n_m &\ge 1, \quad \text{since } a_m \ge a_j.
\end{aligned}$$

This proves the lemma for each $1 \le j \le m-1$. Finally for $j = m$, we have $\alpha(G_{m,m}) = n_{m-1}$, by Theorem 3.8. And so $a_m\alpha(G_{m,m}) - n_m = a_m n_{m-1} - n_m = 1$, and our induction is complete.

Thus, letting $m = k$, we have shown that $a_j\alpha(G_{j,k}) - n_k \ge 1$, from which the desired conclusion follows. ∎

Now we are ready to prove Theorem 3.39.

Proof: We first deal with the most difficult (and most interesting!) case $1 \le j \le k-1$, with $k \ge 3$. We prove that $\chi(\mathbb{Z}, S_{j,k}) = a_j$ in this case.

By Theorem 3.25, $G_{j,k}$ is star extremal. By Lemma 3.24 and Lemma 3.41, $\chi_c(G_{j,k}) = \frac{n_k}{\alpha(G_{j,k})} < a_j$. Therefore, $\chi(G_{j,k}) = \lceil \chi_c(G_{j,k}) \rceil \le a_j$, by Theorem 3.20. Finally, Lemma 3.40 implies that $\chi(\mathbb{Z}, S_{j,k}) \le \chi(C_{n_k, S_{j,k}}) = \chi(G_{j,k}) \le a_j$.

To complete the proof, we need to prove that there is no $(a_j - 1)$ colouring of $\chi(\mathbb{Z}, S_{j,k})$. We split our analysis into two subcases: when $j = 1$, and when $2 \le j \le k-1$.

Subcase 1: $j = 1$.

On the contrary, suppose there is an $(a_1 - 1)$-colouring of $G(\mathbb{Z}, S_{1,k})$. We note that $S_{1,2} = \{1, 2, \ldots, a_1 - 2\}$. Note that an $(a_1 - 1)$-colouring of $G(\mathbb{Z}, S_{1,2})$ must be unique, up to a permutation of colours. In fact, the colouring can be characterized very easily as follows: u and v have the same colour iff $u \equiv v \pmod{a_1 - 1}$.

By Proposition 3.5 (b), $S_{1,2} \subseteq S_{1,k}$, and so any $(a_1 - 1)$-colouring of $G(\mathbb{Z}, S_{1,k})$ must have the property that u and v have the same colour iff $u \equiv v \pmod{a_1 - 1}$. So in any proper colouring, the vertices 0 and $(a_1 - 1)(a_2 - 1)$ must be coloured the same, and hence $(a_1 - 1)(a_2 - 1) \notin S_{1,k}$, for all $k \geq 2$.

We claim that $n_2 - n_1 + 1 \in S_{1,3}$. To see this, note that $a_1 - 2 = n_1 - 1 \in S_{1,2}$. Since $S_{1,3} = \pm S_{1,2} \pmod{n_2}$, we have $n_2 - (n_1 - 1) \in S_{1,3}$. Thus, $n_2 - n_1 + 1 \in S_{1,k}$ for all $k \geq 3$.

However, $n_2 - n_1 + 1 = (a_2 n_1 - 1) - n_1 + 1 = n_1(a_2 - 1) = (a_1 - 1)(a_2 - 1) \notin S_{1,k}$. And this is a contradiction for all $k \geq 3$. Therefore, no such $(a_1 - 1)$-colouring exists.

Subcase 2: $2 \leq j \leq k - 1$.

On the contrary, suppose there is an $(a_j - 1)$-colouring of $G(\mathbb{Z}, S_{j,k})$. Let H_j be the restriction of this graph to the vertices $\{0, 1, 2, \ldots, (a_j - 1)n_{j-1}\}$. By the Pigeonhole Principle, there must be $n_{j-1} + 1$ vertices in H_j that appear in the same colour class. Let these vertices be $v_1, v_2, \ldots, v_m$, arranged in increasing order, where $m = n_{j-1} + 1$. Thus, $v_m - v_1 \leq (a_j - 1)n_{j-1}$.

Let $u_i = v_{i+1} - v_i$ for each $1 \leq i \leq m - 1$. Since v_i and v_{i+1} belong to the same colour class, $u_i \notin S_{j,k}$. By Proposition 3.5 (b), $S_{j,j+1} \subseteq S_{j,k}$, and so $u_i \notin S_{j,j+1}$. By Proposition 3.5 (e), $S_{j,j+1} = \{n_{j-1}, n_{j-1} + 1, \ldots, n_j - n_{j-1}\}$, so either $1 \leq u_i < n_{j-1}$ or $u_i > n_j - n_{j-1}$. First, suppose some $u_p \geq n_j - n_{j-1} + 1$, for some $1 \leq p \leq m - 1$. Since each of the other u_i's are at least 1, we have

$$\begin{aligned} v_m - v_1 &= \sum_{i=1}^{m-1} u_i \\ &\geq (n_j - n_{j-1} + 1) + (m - 2) \cdot 1 \\ &= (n_j - n_{j-1} + 1) + (n_{j-1} + 1 - 2) \\ &= n_j \\ &= a_j n_{j-1} - 1 \\ &> (a_j - 1)n_{j-1}. \end{aligned}$$

Since $v_m - v_1 \leq (a_j - 1)n_{j-1}$, we have our desired contradiction. This shows that

$u_i < n_{j-1}$, for each $1 \leq i \leq m-1$.

For each $1 \leq i \leq m$, define $w_i = v_i - v_1$. Since v_1 and v_i belong to the same colour class, $w_i = v_i - v_1 \notin S_{j,j+1}$. Consider the strictly increasing sequence $\{w_1, w_2, \ldots, w_m\}$. Since $w_m = v_m - v_1 \geq m-1 = n_{j-1}$ and $w_m \notin S_{j,j+1}$, we must have $w_m > n_j - n_{j-1}$.

Since $w_1 = 0 < n_{j-1}$ and $w_m > n_j - n_{j-1}$, there must exist a unique index r for which $w_r < n_{j-1}$ and $w_{r+1} > n_j - n_{j-1}$. For this r, we have $u_r = v_{r+1} - v_r = w_{r+1} - w_r \geq (n_j - n_{j-1} + 1) - (n_{j-1} - 1) = n_j - 2n_{j-1} + 2 = (a_j - 2)n_{j-1} + 1 > n_{j-1}$. And this contradicts our claim that every $u_i < n_{j-1}$.

In both subcases, we have proven that no $(a_j - 1)$-colouring exists in $G(\mathbb{Z}, S_{j,k})$. Therefore, we have shown that $\chi(\mathbb{Z}, S_{j,k}) = a_j$ for all $k \geq 3$ and $1 \leq j \leq k-1$.

To complete the proof of Theorem 3.39, we must consider the cases $j = k$ and $(j,k) = (1,2)$. We split these cases into further subcases.

In all of these cases, we remark that $S_{j,k}$ is a sequence of consecutive integers. If $j = k \geq 1$, then by Proposition 3.5 (d), $S_{k,k} = \{n_{k-1}, n_{k-1}+1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$. And if $(j,k) = (1,2)$, then $S_{1,2} = \{1, 2, \ldots, a_1 - 2\}$, by Proposition 3.5 (e).

By Theorem 3.38, we have $\chi(\mathbb{Z}, S_{1,2}) = \lceil \frac{(a_1-2)-1}{1} \rceil + 2 = a_1 - 1$, which proves the final case of Theorem 3.39.

Also by Theorem 3.38, $\chi(\mathbb{Z}, S_{k,k}) = \lceil \frac{|S|-1}{n_{k-1}} \rceil + 2$, where $|S| = \lfloor \frac{n_k}{2} \rfloor - n_{k-1} + 1$. From this, it follows that for all $k \geq 1$,

$$\begin{aligned} \chi(\mathbb{Z}, S_{k,k}) &= \left\lceil \frac{|S|-1}{n_{k-1}} \right\rceil + 2 \\ &= \left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} - 1 \right\rceil + 2 \\ &= \left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil + 1. \end{aligned}$$

We now determine a simple formula for $\left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil$ for each $k \geq 1$.

If $j = k = 1$, we have $n_0 = 1$ and $n_1 = a_1 - 1$. Thus,

$$\begin{aligned}
\chi(\mathbb{Z}, S_{1,1}) &= \left\lceil \frac{\lfloor \frac{n_1}{2} \rfloor}{n_0} \right\rceil + 1 \\
&= \left\lceil \left\lfloor \frac{a_1 - 1}{2} \right\rfloor \right\rceil + 1 \\
&= \left\lfloor \frac{a_1 - 1}{2} \right\rfloor + 1 \\
&= \left\lfloor \frac{a_1 + 1}{2} \right\rfloor .
\end{aligned}$$

If $j = k = 2$ and $a_1 = 3$, we have $n_0 = 1$, $n_1 = a_1 - 1 = 2$, and $n_2 = a_2 n_1 - 1 = 2a_2 - 1$. Thus,

$$\begin{aligned}
\chi(\mathbb{Z}, S_{2,2}) &= \left\lceil \frac{\lfloor \frac{n_2}{2} \rfloor}{n_1} \right\rceil + 1 \\
&= \left\lceil \frac{\lfloor \frac{2a_2 - 1}{2} \rfloor}{2} \right\rceil + 1 \\
&= \left\lceil \frac{a_2 - 1}{2} \right\rceil + 1 \\
&= \left\lfloor \frac{a_2}{2} \right\rfloor + 1 \\
&= \left\lfloor \frac{a_2 + 2}{2} \right\rfloor .
\end{aligned}$$

We have two cases remaining: when $j = k \geq 3$, and when $j = k = 2$ and $a_1 > 3$. Note that in both of these cases, n_{k-1} is at least 3. Since $n_k = a_k n_{k-1} - 1$, we have

$$\frac{a_k n_{k-1} - 2}{2} \leq \left\lfloor \frac{n_k}{2} \right\rfloor = \left\lfloor \frac{a_k n_{k-1} - 1}{2} \right\rfloor \leq \frac{a_k n_{k-1} - 1}{2}.$$

This implies that

$$\frac{a_k}{2} - \frac{1}{n_{k-1}} \leq \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \leq \frac{a_k}{2} - \frac{1}{2n_{k-1}}.$$

If a_k is even, then the above inequality shows that $\frac{a_k}{2} - 1 \leq \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \leq \frac{a_k}{2}$, implying that $\left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil = \frac{a_k}{2}$.

And if a_k is odd, then the above inequality shows that $\frac{a_k - 1}{2} \leq \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \leq \frac{a_k + 1}{2}$, since $n_{k-1} \geq 3$. This implies that $\left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil = \frac{a_k + 1}{2}$.

Consolidating both of these case into one identity, we have $\left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil = \left\lfloor \frac{a_k+1}{2} \right\rfloor$. Therefore,

$$\begin{aligned} \chi(\mathbb{Z}, S_{k,k}) &= \left\lceil \frac{\lfloor \frac{n_k}{2} \rfloor}{n_{k-1}} \right\rceil + 1 \\ &= \left\lfloor \frac{a_k+1}{2} \right\rfloor + 1 \\ &= \left\lfloor \frac{a_k+3}{2} \right\rfloor \\ &= \left\lfloor \frac{a_j+3}{2} \right\rfloor \quad \text{since } j = k. \end{aligned}$$

Therefore, we have shown that

$$\chi(\mathbb{Z}, S_{j,k}) = \begin{cases} a_j & \text{if } 1 \leq j \leq k-1 \text{ and } k \geq 3 \\ \left\lfloor \frac{a_j+3}{2} \right\rfloor & \text{if } j = k \geq 3 \text{ or if } j = k = 2 \text{ and } a_1 > 3 \\ \left\lfloor \frac{a_2+2}{2} \right\rfloor & \text{if } j = k = 2 \text{ and } a_1 = 3 \\ \left\lfloor \frac{a_1+1}{2} \right\rfloor & \text{if } j = k = 1 \\ a_1 - 1 & \text{if } (j,k) = (1,2) \end{cases}$$

This completes the proof of Theorem 3.39. ∎

Therefore, we have successfully verified our formula for $\chi(\mathbb{Z}, S_{j,k})$, for every possible generating set $S_{j,k}$ in our construction. As a corollary of Theorem 3.39, we can quickly derive the chromatic number for every graph in this infinite family $G_{j,k} = C_{n_k, S_{j,k}}$.

Theorem 3.42 *Let $3 \leq a_1 \leq a_2 \leq \ldots \leq a_{k-1} \leq a_k$, and $1 \leq j \leq k$. Then,*

$$\chi(G_{j,k}) = \begin{cases} a_j - 1 & \textit{if } j = k = 1 \\ a_j & \textit{otherwise} \end{cases}$$

Proof: By Theorem 3.21, $\chi_f(G_{j,k}) = \frac{n_k}{\alpha(G_{j,k})}$. Since $G_{j,k}$ is star extremal by Theorem 3.25, $\chi_c(G_{j,k}) = \chi_f(G_{j,k}) < a_j$ by Lemma 3.41. By Theorem 3.20, $\chi(G_{j,k}) = \lceil \chi_c(G_{j,k}) \rceil \leq a_j$. This identity holds for all $1 \leq j \leq k$.

In Theorem 3.39, we showed that $\chi(\mathbb{Z}, S_{j,k}) = a_j$ whenever $1 \leq j \leq k-1$ and $k \geq 3$. In this case, we must have $\chi(G_{j,k}) = a_j$, since $\chi(G_{j,k}) = \chi(C_{n_k, S_{j,k}}) \geq \chi(\mathbb{Z}, S_{j,k}) = a_j$ by Lemma 3.40.

Now consider the other cases. If $j = k \geq 1$, then by Theorems 3.21 and 3.8, $\chi_c(G_{j,k}) = \chi_f(G_{j,k}) = \frac{n_k}{\alpha(G_{j,k})} = \frac{n_j}{\alpha(G_{j,j})} = \frac{a_j n_{j-1} - 1}{n_{j-1}} = a_j - \frac{1}{n_{j-1}}$.

If $j = k = 1$, then $n_{j-1} = 1$ and so $\chi_c(G_{j,k}) = a_1 - 1$ in this case. Hence, $\chi(G_{j,k}) = \lceil \chi_c(G_{j,k}) \rceil = a_1 - 1$. And if $j = k > 1$, then $n_{j-1} > 1$ and so $\chi(G_{j,k}) = \lceil \chi_c(G_{j,k}) \rceil = \lceil a_j - \frac{1}{n_{j-1}} \rceil = a_j$.

Finally, consider the case $(j,k) = (1,2)$. By Theorem 3.8, $\alpha(G_{1,2}) = a_2\alpha(G_{1,1}) - 1 = a_2 - 1$. Therefore, $\chi_c(G_{j,k}) = \chi_f(G_{j,k}) = \frac{n_2}{\alpha(G_{1,2})} = \frac{a_2 n_1 - 1}{a_2 - 1} = \frac{a_2(a_1-1)-1}{a_2-1}$. Since $3 \leq a_1 \leq a_2$, we have $a_1 - 1 < \frac{a_2(a_1-1)-1}{a_2-1} < a_1$. This implies that $\chi(G_{j,k}) = \lceil \chi_c(G_{j,k}) \rceil = \lceil \frac{a_2(a_1-1)-1}{a_2-1} \rceil = a_1$.

Therefore, in all cases, we have shown that $\chi(G_{j,k}) = a_j$, with the exceptional case $\chi(G_{j,k}) = a_1 - 1$ when $j = k = 1$. ∎

3.4 Application 3: Fractional Ramsey Numbers

In this section, we determine an explicit formula for the generalized fractional Ramsey number $r_{\omega_f}(a_1, a_2, \ldots, a_k)$, solving an open problem from [102, 117].

Stated in its most general form, Ramsey Theory claims that within any sufficiently large system, some regularity must always exist. In other words, "complete disorder is impossible" [83]. Ramsey Theory is the study of regularity in complex random structures. This branch of mathematics has laid the groundwork for many important areas of current combinatorial research, which have applications to diverse areas of pure and applied mathematics. Ramsey theorists have made significant contributions to fields such as dynamical systems and ergodic theory.

This branch of mathematics grew out of the seminal paper by Frank Ramsey [152] in 1930, which constituted a first step in an unsuccessful attempt to prove the continuum hypothesis [132]. The motivation for Ramsey Theory originates from the so-called "party problem" [83], which is stated as follows.

Problem 3.43 *If six people attend a party, prove that there must be a group of three mutual acquaintances, or a group of three mutual strangers.*

The proof is a straightforward application of the Pigeonhole Principle. We now define the Ramsey number $r(a, b)$.

Definition 3.44 *The* **Ramsey number** $r(a, b)$ *is the smallest positive integer* n *such that if* H_1 *and* H_2 *are any graphs for which* $K_n = H_1 \oplus H_2$*, then* $\omega(H_1) \geq a$ *or* $\omega(H_2) \geq b$*.*

In other words, in any 2-edge decomposition of K_n, either the first subgraph has a clique of cardinality a or the second subgraph has a clique of cardinality b. We can generalize this to a k-edge decomposition $H_1 \oplus H_2 \oplus \cdots \oplus H_k$.

Definition 3.45 *The* **generalized Ramsey number** $r(a_1, a_2, \ldots, a_k)$ *is the smallest positive integer* n *such that if* H_1*,* H_2*, …,* H_k *are any graphs for which* $K_n = H_1 \oplus H_2 \oplus \cdots \oplus H_k$*, then* $\omega(H_i) \geq a_i$ *for some* $1 \leq i \leq k$*.*

Ramsey's celebrated theorem [83, 152] states that $r(a_1, a_2, \ldots, a_k)$ is well-defined, for any choice of the a_i's.

Problem 3.43 tells us that $r(3, 3) \leq 6$. To show that $r(3, 3) > 5$, it suffices to find two K_3-free graphs H_1 and H_2 with $K_5 = H_1 \oplus H_2$. A solution is $H_1 = C_{5,\{1\}}$ and $H_2 = C_{5,\{2\}}$. Both H_1 and H_2 are isomorphic to C_5, and hence, contain no K_3 subgraph. Thus, $r(3, 3) = 6$.

Since $H_2 = \overline{H_1}$ and $\omega(H_2) = \omega(\overline{H_1}) = \alpha(H_1)$, we can alternatively define $r(a, b)$ to be the smallest n such that for any graph G on n vertices, either $\omega(G) \geq a$ or $\alpha(G) \geq b$.

Definition 3.46 ([83]) *A graph* G *is* **Ramsey (a, b)-critical** *if* $|G| = r(a, b) - 1$*, and* G *contains neither a clique of order* a *or an independent set of order* b*.*

For example, it can be shown that the only Ramsey $(3, 3)$-critical graph is $G = C_5$. We will assume that in the generalized Ramsey number $r(a_1, a_2, \ldots, a_k)$, each $a_i \geq 2$, as the case $\min\{a_1, a_2, \ldots, a_k\} = 1$ implies that $r(a_1, a_2, \ldots, a_k) = 1$ (since a single vertex is a clique of cardinality 1). Also we will assume that $k \geq 2$, since $r(a_1) = a_1$. The following observations are trivial.

1. If $a_i \leq b_i$ for each $1 \leq i \leq k$, then $r(a_1, a_2, \ldots, a_k) \leq r(b_1, b_2, \ldots, b_k)$.

2. If σ is a permutation of $\{a_i\}$, then $r(a_1, a_2, \ldots, a_k) = r(a_{\sigma(1)}, a_{\sigma(2)}, \ldots, a_{\sigma(k)})$.

3. $r(a_1, a_2, \ldots, a_k, 2) = r(a_1, a_2, \ldots, a_k)$.

Thus, we will assume that $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$. Remarkably, $r(3, 3, 3) = 17$ is the only non-trivial Ramsey number known for $k > 2$. All other known Ramsey numbers are of the form $r(a, b)$, and only nine have been determined. An excellent survey of known results and bounds appears in [151]. Table 3.1 lists the nine known non-trivial Ramsey numbers of the form $r(a, b)$.

(a, b)	$r(a, b)$
$(3, 3)$	6
$(3, 4)$	9
$(3, 5)$	14
$(3, 6)$	18
$(3, 7)$	23
$(3, 8)$	28
$(3, 9)$	36
$(4, 4)$	18
$(4, 5)$	25

Table 3.1: The nine known Ramsey numbers of the form $r(a, b)$.

The proofs for the cases $(a, b) = (3, 6), (3, 7), (3, 8), (3, 9), (4, 5)$ require computer analysis and elaborate case-checking. More details can be found in [151]. But the other four cases require no case-checking at all. We provide a new proof of these results, by involving independence polynomials to prove our lower bounds.

We first state a lemma that can be proven using a simple parity argument.

Lemma 3.47 ([83]) *Suppose $r(a, b-1)$ and $r(a-1, b)$ are both even. Then $r(a, b) \leq r(a, b-1) + r(a-1, b) - 1$. If they are not both even, then $r(a, b) \leq r(a, b-1) + r(a-1, b)$.*

Now we compute the exact values of three Ramsey numbers. All of these results were known to Greenwood and Gleason [85] in 1955, and were cited in [83]. However, our proofs for the lower bounds are slightly different, as we will apply our work on independence polynomials.

Theorem 3.48 *$r(3,4) = 9$, $r(3,5) = 14$, and $r(4,4) = 18$.*

<u>Proof:</u> We know that $r(3,3) = 6$ and $r(2,4) = r(4) = 4$. By Lemma 3.47, $r(3,4) \leq r(3,3)+r(2,4)-1 = 9$. By Lemma 3.47, we have $r(3,5) \leq r(2,5)+r(3,4) = 5+r(3,4) \leq 14$ and $r(4,4) \leq r(3,4)+r(3,4) \leq 18$. This establishes the upper bounds.

To complete the proof that $r(a,b) = n$, we must construct a Ramsey (a,b)-critical graph G. All of our critical graphs will be circulants.

Let $G = C_{8,\{1,4\}}$. Then, $\overline{G} = C_{8,\{2,3\}}$. By Theorems 2.10 and 2.26, $I(G,x) = 1+8x+16x^2+8x^3$. By Theorem 1.5, $I(\overline{G},x) = 1+8x+12x^2$. Thus, $\omega(G) = \alpha(\overline{G}) = \deg(I(\overline{G},x)) = 2 < 3$ and $\omega(\overline{G}) = \alpha(G) = \deg(I(G,x)) = 3 < 4$.

Let $G = C_{13,\{1,5\}}$. Then, $\overline{G} = C_{13,\{2,3,4,6\}}$. By Theorem 1.5, $I(G,x) = 1 + 13x + 52x^2 + 78x^3 + 39x^4$ and $I(\overline{G},x) = 1 + 13x + 26x^2$. Thus, $\omega(G) = \alpha(\overline{G}) = 2 < 3$ and $\omega(\overline{G}) = \alpha(G) = 4 < 5$.

Let $G = C_{17,\{1,2,4,8\}}$. By Lemma 2.24, $\overline{G} = C_{17,\{3,5,6,7\}} \simeq C_{17,\{1,2,4,8\}}$, with the multiplier $r = 3$. By Theorem 1.5, $I(G,x) = I(\overline{G},x) = 1 + 17x + 68x^2 + 68x^3$, so $\omega(G) = \omega(\overline{G}) = 3 < 4$. ∎

This technique of calculating the independence polynomial is more rigorous than the approach where we can determine the graph invariants by simply drawing the diagram. For small graphs, the "by inspection" method is sufficient, but we will require a more formal approach for graphs of larger order.

In [104], it is proven that the Ramsey $(3,3)$-critical, $(3,5)$-critical, and $(4,4)$-critical graphs are unique. In addition to $G = C_{8,\{1,4\}}$ and its complement, there are two other Ramsey $(3,4)$-critical graphs. However, neither graph is a circulant.

Unfortunately, not all Ramsey (a,b)-critical graphs are circulants. It would be very convenient if that were the case, as that would produce better lower bounds for the Ramsey numbers than the ones currently known. But to quote [83], "it appears likely (though not certain) that the structure of these maximal Ramsey graphs is illusory. Perhaps combinatorialists have again been victimized by the Law of Small Numbers: patterns discovered for small k evaporate for k sufficiently large to make calculation difficult". Despite extensive research, hardly anything is known about the Ramsey numbers, and it has become increasingly difficult to improve the currently known bounds.

While it appears intractable to calculate an explicit formula for $r(a_1, a_2, \ldots, a_k)$, we now introduce the generalized *fractional* Ramsey number $r_{\omega_f}(a_1, a_2, \ldots, a_k)$, and determine an explicit formula for this function.

Earlier in this chapter, we defined the fractional chromatic number $\chi_f(G)$ as the linear relaxation of the IP for $\chi(G)$. We do the same for the fractional clique number $\omega_f(G)$.

Definition 3.49 ([158]) *Let M be the vertex-independent set incidence matrix of G. The dual IP of $\chi(G)$ gives us the value of the clique number $\omega(G)$.*

$\omega(G) = \max \mathbf{1} \cdot y$, *where* $M^t y \leq \mathbf{1}$, $y \geq 0$, *and* $y \in \mathbb{Z}^n$.

Then the **fractional clique number** $\omega_f(G)$ *is*

$\omega_f(G) = \max \mathbf{1} \cdot y$, *where* $M^t y \leq \mathbf{1}$, $y \geq 0$, *and* $y \in \mathbb{R}^n$.

For any graph G, we have $\omega(G) \leq \omega_f(G) = \chi_f(G) \leq \chi(G)$, by the duality theorem of linear programming [45]. In [102, 117], the *fractional* Ramsey number $r_{\omega_f}(a_1, a_2, \ldots, a_k)$ is introduced as an analogue to the Ramsey number.

Definition 3.50 *The* **fractional Ramsey function** *is the smallest positive integer n such that if $H_1, \ldots, H_k$ are any graphs for which $K_n = H_1 \oplus H_2 \oplus \cdots \oplus H_k$, then $\omega_f(H_i) \geq a_i$ for some i.*

Note that $r_{\omega_f}(a_1, a_2, \ldots, a_k)$ must exist for any choice of the a_i's, as it is bounded above by $r(a_1, a_2, \ldots, a_k)$. This follows because $\omega(H_i) \leq \omega_f(H_i)$, for each subgraph H_i.

Since $\chi_f(G) = \omega_f(G)$ for all G, $r_{\chi_f}(a_1, a_2, \ldots, a_k) = r_{\omega_f}(a_1, a_2, \ldots, a_k)$. Hence, we make the important note that these two functions are interchangeable. For notational consistency, we will only refer to the function $r_{\omega_f}(a_1, a_2, \ldots, a_k)$.

Trivially, we have $r_{\omega_f}(a) = a$ and $r_{\omega_f}(2, a_2, a_3, \ldots, a_k) = r_{\omega_f}(a_2, a_3, \ldots, a_k)$. So we will assume that $(a_1, a_2, \ldots, a_k)$ is a k-tuple of integers with $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$, and $k \geq 2$. The following formulas are known:

Theorem 3.51 ([102, 117]) *Let a and b be positive integers with $3 \leq a \leq b$. Then $r_{\omega_f}(a, b) = ab - b$.*

Theorem 3.52 ([102, 117]) *Let $a \geq 3$ be an integer. Then for any integer $k \geq 2$,*

$$r_{\omega_f}(\underbrace{a,\ a,\ \ldots,\ a}_{k\ times}) = a^k - a^{k-1} - a^{k-2} - \ldots - a^2 - a.$$

These are the only known results for the fractional Ramsey function, where the a_i's are all integers. In this section, we apply Theorem 3.8 to prove a complete generalization, for any k-tuple of integers $(a_1, a_2, \ldots, a_k)$. As with other Ramsey functions, this formula is invariant under any permutation of the a_i's. However, in this formula, there is a slight twist: to get the desired Ramsey number, one must first order the a_i's in increasing order. Nevertheless, this does not change the invariance of our generalized formula.

Note that by Theorem 3.21, $\omega_f(G) = \chi_f(G) = \frac{|G|}{\alpha(G)}$ for any circulant graph G.

Theorem 3.53 *Let $a_1, a_2, \ldots, a_k$ be integers with $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$. Then,*

$$r_{\omega_f}(a_1, a_2, \ldots, a_k) = \prod_{j=1}^{k} a_j - \sum_{i=2}^{k} \left(\prod_{j=i}^{k} a_j \right).$$

Proof: Recall that we defined $n_0 = 1$ and $n_i = a_i n_{i-1} - 1$ for each $1 \leq i \leq k$. By the same argument as Corollary 3.9, the right side of the identity is equal to $n_k + 1$.

We first prove the upper bound $r_{\omega_f}(a_1, a_2, \ldots, a_k) \leq n_k + 1$. We proceed by induction on k. The case $k = 1$ is trivial. By the induction hypothesis, suppose that the result is true for the index $k - 1$, where $k \geq 2$. Let $n = n_k + 1 = a_k n_{k-1}$. Let $K_n = H_1 \oplus H_2 \oplus \cdots \oplus H_k$. We will show that $\omega_f(H_i) \geq a_i$ for some $1 \leq i \leq k$. This will prove the upper bound.

Consider $G' = H_1 \oplus H_2 \oplus \cdots \oplus H_{k-1}$. If $\omega(G') \geq n_{k-1} + 1$, then G' contains a clique of cardinality $n_{k-1} + 1$. Restricting G' to the set of vertices belonging to this clique, we have a $(k-1)$-edge colouring of $K_{n_{k-1}+1}$. By the induction hypothesis, $r_{\omega_f}(a_1, a_2, \ldots, a_{k-1}) \leq n_{k-1}+1$, and so we must have $\omega_f(H_i) \geq a_i$ for some $1 \leq i \leq k-1$.

Now consider the case that $\omega(G') \leq n_{k-1}$. Then by Theorem 3.21, we have

$$\omega_f(H_k) \geq \frac{|H_k|}{\alpha(H_k)} = \frac{n}{\omega(\overline{H_k})} = \frac{n}{\omega(G')} \geq \frac{a_k n_{k-1}}{n_{k-1}} = a_k.$$

In any k-edge colouring of K_n, we have shown that $\omega_f(H_i) \geq a_i$, for some $1 \leq i \leq k$. This proves that $r_{\omega_f}(a_1, a_2, \ldots, a_k) \leq n_k + 1$.

To complete the proof, we need to find a k-edge colouring of K_{n_k} such that if H_j is the subgraph induced by colour j, then $\omega_f(H_j) < a_j$, for all j. This will establish the lower bound $r_{\omega_f}(a_1, a_2, \ldots, a_k) > n_k$. Conveniently, the earlier construction of the $G_{j,k}$'s is *exactly* what we need for our k-edge colouring (i.e., k-edge decomposition) of K_{n_k}.

Let $H_j = G_j(a_1, a_2, \ldots, a_k) = G_{j,k}$ for each $1 \leq j \leq k$. By Lemma 3.2, the $S_{j,k}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$, and so the H_j's induce a k-edge colouring of K_{n_k}. We wish to prove that $\omega_f(G_{j,k}) < a_j$, for each $1 \leq j \leq k$. But this follows immediately, since $\omega_f(G_{j,k}) = \frac{n_k}{\alpha(G_{j,k})} < a_j$, by Theorem 3.21 and Lemma 3.41.

Therefore, we have proven that $r_{\omega_f}(a_1, a_2, \ldots, a_k) = n_k + 1$, as required. ∎

This completes the main theorem of this section.

We now introduce a generalized class of Ramsey numbers, which we will call π-Ramsey functions. This definition first appeared in the literature as f-Ramsey functions in [33], and was developed further in [116].

Definition 3.54 ([33]) *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple of positive real numbers. Then for any parameter π, the* **π-Ramsey function** *$r_\pi(a_1, a_2, \ldots, a_k)$ is the smallest integer n such that in any k-edge decomposition $G_1 \oplus G_2 \oplus \cdots \oplus G_k$ of K_n, $\pi(G_i) \geq a_i$ for at least one index i.*

Hence, the ω-Ramsey function is $r(a_1, a_2, \ldots, a_k)$. Similarly, $r_{\omega_f}(a_1, a_2, \ldots, a_k)$ is the π-Ramsey function for the fractional clique number (i.e., the fractional chromatic number).

We note that for some graph parameters π, the π-Ramsey function is not well-defined. For example, if we let $\pi(G)$ be the number of components of G, then $r_\pi(2,2)$ does not exist. To see this, note that C_n and $\overline{C_n}$ are both connected for every $n \geq 5$, and so we have $\pi(C_n) = \pi(\overline{C_n}) = 1 < 2$. But by a theorem in [116], if $\lim_{n\to\infty} \pi(K_n) = \infty$ and $\pi(H) \leq \pi(G)$ whenever $H \subseteq G$, then $r_\pi(a_1, a_2, \ldots, a_k)$ is well-defined.

Thus, we may define $r_\pi(a_1, a_2, \ldots, a_k)$ for any parameter π satisfying these two conditions. Three such parameters are $\chi(G)$, $\chi_c(G)$, and $\chi_f(G) = \omega_f(G)$. Having already determined a formula for $r_{\chi_f}(a_1, a_2, \ldots, a_k) = r_{\omega_f}(a_1, a_2, \ldots, a_k)$, we turn our attention to the corresponding Ramsey functions for the first two parameters.

Let us consider the Ramsey functions $r_\chi(a_1, a_2, \ldots, a_k)$ and $r_{\chi_c}(a_1, a_2, \ldots, a_k)$. The former appears in [116].

Theorem 3.55 ([116]) *Let $a_1, a_2, \ldots, a_k$ be integers with $a_i \geq 3$ for each i. Then,*

$$r_\chi(a_1, a_2, \ldots, a_k) = (a_1 - 1)(a_2 - 1)\cdots(a_k - 1) + 1.$$

Like with other Ramsey functions, this formula is invariant under permutation of the a_i's. As discussed earlier, this invariance property also holds for our formula for $r_{\omega_f}(a_1, a_2, \ldots, a_k)$, proven in Theorem 3.53.

To our surprise, the circular chromatic Ramsey number equals the fractional Ramsey number. The proof is essentially a corollary of our previous theorems.

Theorem 3.56 *Let $a_1, a_2, \ldots, a_k$ be integers with $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$. Then,*

$$r_{\chi_c}(a_1, a_2, \ldots, a_k) = \prod_{j=1}^{k} a_j - \sum_{i=2}^{k} \left(\prod_{j=i}^{k} a_j \right).$$

<u>Proof:</u> As we showed in the proof of Theorem 3.53, the right side of the identity is equal to $n_k + 1$, where $n_0 = 1$ and $n_i = a_i n_{i-1} - 1$ for each $1 \leq i \leq k$. Since $\chi_f(G) \leq \chi_c(G)$ for all G, it follows by definition that

$$r_{\chi_c}(a_1, a_2, \ldots, a_k) \leq r_{\chi_f}(a_1, a_2, \ldots, a_k).$$

Therefore, $r_{\chi_c}(a_1, a_2, \ldots, a_k) \leq n_k + 1$, by Theorem 3.53.

To complete the proof, we need to find a k-edge colouring of K_{n_k} such that if H_j is the subgraph induced by colour j, then $\chi_c(H_j) < a_j$, for all j. We use the same k-edge partition as in Theorem 3.53. Let $H_j = G_j(a_1, a_2, \ldots, a_k) = G_{j,k}$ for each $1 \leq j \leq k$. By Lemma 3.2, the $S_{j,k}$'s form a partition of $\{1, 2, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$, and so the H_j's induce a k-edge colouring of K_{n_k}. It suffices to prove that $\chi_c(G_{j,k}) < a_j$, for each $1 \leq j \leq k$.

In Theorem 3.25, we proved that each $G_{j,k}$ is star extremal, i.e., $\chi_f(G_{j,k}) = \chi_c(G_{j,k})$. Therefore, we have $\chi_c(G_{j,k}) = \chi_f(G_{j,k}) = \frac{n_k}{\alpha(G_{j,k})} < a_j$, by Theorem 3.21 and Lemma 3.41. This completes the proof. ∎

Our analysis of π-Ramsey functions will be continued in the following section, where we use π-Ramsey functions to determine the optimal Nordhaus-Gaddum inequalities for the fractional chromatic and fractional clique number.

3.5 Application 4: Nordhaus-Gaddum Inequalities

In [143], Nordhaus and Gaddum determined bounds for the sum and product of the chromatic numbers of a graph and its complement.

Theorem 3.57 ([143]) *Let G be a graph on n vertices. Then,*

$$\lceil 2\sqrt{n} \rceil \leq \chi(G) + \chi(\overline{G}) \leq n + 1,$$

$$n \leq \chi(G) \cdot \chi(\overline{G}) \leq \left\lfloor \left(\frac{n+1}{2} \right)^2 \right\rfloor.$$

Nordhaus and Gaddum also showed that these bounds are optimal by finding examples of graphs for which equality is reached. Since then, various papers have been published on determining optimal bounds for $\pi(G) + \pi(\overline{G})$ and $\pi(G) \cdot \pi(\overline{G})$, for other graph parameters π. In the literature, these results are known as *Nordhaus-Gaddum inequalities.*

Since the notion of an *optimal* bound is ambiguous, let us formally define our notion of optimality. We say that the function $f(n)$ is an *optimal lower bound* for $\pi(G) + \pi(\overline{G})$ if for every integer n, $f(n) \leq \pi(G) + \pi(\overline{G})$ for any graph G on n vertices, and the value $f(n)$ cannot be replaced by any larger real number.

Since there are only finitely many graphs on n vertices, the optimal bound $f(n)$ is simply the minimum value of $\pi(G)+\pi(\overline{G})$ over all possible graphs G on n vertices. Thus, there must be at least one graph G (with $|G|=n$) for which equality is attained.

In all cases, the function $f(n)$ is uniquely defined. As a specific example, $f(n)=\lceil 2\sqrt{n}\rceil$ is *the* optimal lower bound for $\chi(G)+\chi(\overline{G})$. In some papers, it is written that $2\sqrt{n}\leq\pi(G)+\pi(\overline{G})$ is the optimal lower bound; by our definition, that will not be the case.

Nordhaus-Gaddum inequalities have been established for many other graph parameters, such as the independence and edge-independence number [32, 67], list-colouring number [54, 77], diameter, girth, circumference, and edge-covering number [179], connectivity and edge-connectivity number [51], achromatic and pseudoachromatic number [7, 180], and arboricity [136, 173]. In some cases, bounds are found, yet it is unknown if they are optimal. A survey of known theorems (pre-1971) is given in [31]. Two such results are as follows.

Let $\alpha_1(G)$ be the edge-independence number of G. Then, it is shown [32] that

$$\left\lfloor\frac{n}{2}\right\rfloor\leq\alpha_1(G)+\alpha_1(\overline{G})\leq 2\cdot\left\lfloor\frac{n}{2}\right\rfloor,$$

$$0\leq\alpha_1(G)\cdot\alpha_1(\overline{G})\leq\left\lfloor\frac{n}{2}\right\rfloor^2.$$

Let $\beta_1(G)$ be the edge-covering number of G. Then, it is shown [179] that

$$2\cdot\left\lceil\frac{n}{2}\right\rceil\leq\beta_1(G)+\beta_1(\overline{G})\leq 2n-2-\left\lfloor\frac{n}{2}\right\rfloor,$$

$$\left\lfloor\frac{n}{2}\right\rfloor^2\leq\beta_1(G)\cdot\beta_1(\overline{G})\leq\frac{n(n-1)}{2}.$$

$G\oplus\overline{G}$ is a 2-edge decomposition of K_n, i.e., a partition of the edges of K_n into two subgraphs. (For convenience, we will now refer to all edge decompositions as **decompositions**). We can generalize this to examine all k-decompositions of K_n, and determine bounds for $\sum_{i=1}^{k}\pi(G_i)$ and $\prod_{i=1}^{k}\pi(G_i)$. We refer to these as *generalized* Nordhaus-Gaddum inequalities. Generalized bounds have been found when π is the chromatic number [51, 77, 146], the clique number, list colouring number, and Szekeres-Wilf number [77].

In this section, we apply the π-Ramsey function, introduced at the end of the previous section. Using π-Ramsey functions, we derive a theorem that gives us the optimal lower bound of $\sum_{i=1}^{k} \pi(G_i)$, for *any* graph parameter π for which $\lim_{n\to\infty} \pi(K_n) = \infty$ and $\pi(H) \leq \pi(G)$ whenever $H \subseteq G$.

As an application, we derive an explicit formula for this optimal lower bound, when π is the chromatic number $\chi(G)$ and the vertex arboricity $\rho(G)$.

In all of the known examples in the literature, the parameter $\pi(G)$ is *integer*-valued. In this section, we also provide the first instances of Nordhaus-Gaddum inequalities where the parameters are *rational*-valued, and our optimal bounds are non-integers. We will determine the optimal bounds for $\pi(G) + \pi(\overline{G})$ and $\pi(G) \cdot \pi(\overline{G})$, when $\pi(G)$ is the fractional chromatic number $\chi_f(G)$ and when $\pi(G)$ is the circular chromatic number $\chi_c(G)$. For the most difficult of the four inequalities, we will establish the optimality by finding a star extremal circulant graph G for which $\chi_f(G) + \chi_f(\overline{G}) = \chi_c(G) + \chi_c(\overline{G})$ attains the desired lower bound. Our result will follow as an immediate consequence of theorems proven earlier in this chapter.

We will first prove our optimal lower bound of $\sum_{i=1}^{k} \pi(G_i)$, for *any* graph parameter π. As an application, we determine the exact lower bound for the parameters $\chi(G)$ and $\rho(G)$. Following that, we will determine the optimal Nordhaus-Gaddum inequalities for $\chi_f(G)$ and $\chi_c(G)$. Thus, the remainder of this section will be separated into two parts.

In the previous section, we defined the π-Ramsey function $r_\pi(a_1, a_2, \ldots, a_k)$. In the following theorem, we make an important connection showing that the lower bound for *any* generalized Nordhaus-Gaddum inequality can be expressed in terms of the corresponding π-Ramsey function. Note that in the following theorem, $\pi(G)$ is not restricted to be an integer; in fact, $\pi(G)$ can be any positive real number. This result will enable us to determine the correct Nordhaus-Gaddum inequalities for $\chi_f(G)$ and $\chi_c(G)$.

Theorem 3.58 *Let π be a graph parameter, with $\lim_{n\to\infty} \pi(K_n) = \infty$ and $\pi(H) \leq$*

$\pi(G)$ whenever $H \subseteq G$. Then, for any k-decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n,

$$\sum_{i=1}^{k} \pi(G_i) \geq \inf \left\{ \sum_{i=1}^{k} a_i \;\;|\;\; r_\pi(a_1+\varepsilon, a_2+\varepsilon, \ldots, a_k+\varepsilon) > n \quad \forall \varepsilon > 0 \right\}.$$

Moreover, this lower bound is optimal.

<u>Proof:</u> Let S be the set of real numbers t for which there is a k-tuple $(a_1, a_2, \ldots, a_k)$ of real numbers with $t = \sum_{i=1}^{k} a_i$ and $r_\pi(a_1+\varepsilon, a_2+\varepsilon, \ldots, a_k+\varepsilon) > n$, for all $\varepsilon > 0$.

First we justify that S is non-empty. Let r be the smallest number for which $\pi(H) \leq r$ for every subgraph $H \subseteq K_n$. Then for any k-decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n, we must have $\pi(G_i) \leq r$. Then $(r, r, \ldots, r)$ is a k-tuple satisfying the above conditions, and so $kr \in S$.

Thus S is non-empty and it must have a finite-valued infimum. In fact, it is straightforward to see that $S = (m, \infty)$ or $S = [m, \infty)$, where $m = \inf S$. We wish to prove that $\sum_{i=1}^{k} \pi(G_i) \geq m$.

On the contrary, suppose that there exists a k-decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n for which $\sum_{i=1}^{k} \pi(G_i) = m' < m$. Let $\pi(G_i) = b_i$ for each i. Now consider the π-Ramsey number $r_\pi(b_1+\varepsilon, b_2+\varepsilon, \ldots, b_k+\varepsilon)$.

If there exists an $\varepsilon > 0$ such that $r_\pi(b_1+\varepsilon, b_2+\varepsilon, \ldots, b_k+\varepsilon) \leq n$, then by definition, there must exist an index i such that $\pi(G_i) \geq b_i + \varepsilon$. But then $b_i \geq b_i + \varepsilon$, a contradiction. Therefore, we must have $r_\pi(b_1+\varepsilon, b_2+\varepsilon, \ldots, b_k+\varepsilon) > n$ for all $\varepsilon > 0$. But then $\sum_{i=1}^{k} b_i = m' < m \leq \sum_{i=1}^{k} a_i$, contradicting the minimality of m. Hence, no such m' exists, and we conclude that $\sum_{i=1}^{k} \pi(G_i) \geq m$ for all k-decompositions $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n.

By the definition of the π-Ramsey function, $r_\pi(a_1+\varepsilon, a_2+\varepsilon, \ldots, a_k+\varepsilon) > n$ implies the existence of a k-decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n with $\pi(G_i) < a_i + \varepsilon$ for each i. So in this decomposition, $\sum_{i=1}^{k} \pi(G_i) < m + k\varepsilon$. Since such a decomposition exists for any $\varepsilon > 0$, we conclude that $\sum_{i=1}^{k} \pi(G_i)$ can be made as close to m as we wish. Therefore, we conclude that $\sum_{i=1}^{k} \pi(G_i) \geq m$, and that this lower bound cannot be reduced any further. ∎

As a specific case of Theorem 3.58, we have the following result.

Corollary 3.59 *Let π be a graph parameter such that $\pi(G) \in \mathbb{N}$ for all G. Then, for any decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n,*

$$\sum_{i=1}^{k} \pi(G_i) \geq \min\left\{\sum_{i=1}^{k} a_i \;\mid\; r_\pi(a_1+1, a_2+1, \ldots, a_k+1) > n, \quad a_i \in \mathbb{N}\right\}.$$

Moreover, this is the optimal lower bound.

Proof: Observe that for any small $\varepsilon > 0$, we have $\pi(G_i) \geq a_i + 1$ iff $\pi(G_i) \geq a_i + \varepsilon$. Since $\pi(G)$ is an integer-valued function, we must have $r_\pi(a_1+1, a_2+1, \ldots, a_k+1) = r_\pi(a_1+\varepsilon, a_2+\varepsilon, \ldots, a_k+\varepsilon)$ for any k-tuple $(a_1, a_2, \ldots, a_k)$, with $0 < \varepsilon \leq 1$. The conclusion follows from Theorem 3.58. ∎

Using Corollary 3.59, we now determine the optimal lower bounds for $\sum_{i=1}^{k} \pi(G_i)$ for two parameters, namely the chromatic number $\chi(G)$, and the vertex arboricity number $\rho(G)$. The *vertex arboricity* is the minimum number of subsets that $V(G)$ can be partitioned into so that each subset induces an acyclic subgraph.

First, we require additional definitions and a theorem from Lesniak-Foster and Roberts [116].

Definition 3.60 *Let P be a graphical property that is possessed by the trivial graph K_1. Then the* **vertex partition number** *$\nu(G)$ of a graph G is the minimum number of subsets into which the vertex set of G can be partitioned so that each subset induces a subgraph having property P.*

As an example, if we let P be the property that a graph is edge-free, then $\nu(G)$ is simply the chromatic number $\chi(G)$. Hence, $\chi(G)$ is a vertex partition parameter. Note that every vertex partition parameter is integer-valued.

Definition 3.61 *If ν is a vertex partition parameter, then for each positive integer k, let $\overline{\nu}(k)$ denote the largest integer m for which there exists a k-decomposition of K_m such that $\nu(H_i) = 1$ for all $1 \leq i \leq k$.*

As a simple example, $\chi(G)$ is a vertex partition parameter for which $\overline{\chi}(k) = 1$ for all k.

Definition 3.62 *A graphical property P is* **co-hereditary** *if P is closed under subgraphs and disjoint unions.*

To be more specific, if P is co-hereditary, then every subgraph of a graph having property P also has property P, and the graph consisting of disjoint subgraphs each having property P, also has property P. As an example, the property that a graph is edge-free is co-hereditary, but the property that a graph is connected is not.

Letting π be a vertex partition parameter ν, we can investigate the ν-Ramsey function $r_\nu(a_1, a_2, \ldots, a_k)$, defined the same way as our π-Ramsey function. The following result is proved by Lesniak [116].

Theorem 3.63 ([116]) *Let $a_1, a_2, \ldots, a_k$ be positive integers and let ν be a vertex partition parameter for which $\lim\limits_{n\to\infty} \nu(K_n) = \infty$ and the corresponding property P is co-hereditary. Then,*

$$r_\nu(a_1, a_2, \ldots, a_k) = 1 + \overline{\nu}(k) \cdot \prod_{i=1}^{k}(a_i - 1).$$

From Corollary 3.59 and Theorem 3.63, we can derive the optimal lower bound of $\sum_{i=1}^k \pi(G_i)$, for the parameter $\pi = \nu$.

Theorem 3.64 *Let ν be a vertex partition parameter for which $\lim\limits_{n\to\infty} \nu(K_n) = \infty$ and the corresponding property P is co-hereditary. If $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ is any k-decomposition of K_n, then*

$$\sum_{i=1}^{k} \nu(G_i) \geq \left\lceil k \cdot \sqrt[k]{\frac{n}{\overline{\nu}(k)}} \right\rceil.$$

Moreover, this is the optimal lower bound.

<u>Proof:</u> From Theorem 3.63 and Corollary 3.59, we have

$$\begin{aligned}
\sum_{i=1}^{k} \nu(G_i) &\geq \min\left\{ \sum_{i=1}^{k} a_i \;\middle|\; r_\nu(a_1+1, a_2+1, \ldots, a_k+1) > n, \quad a_i \in \mathbb{N} \right\} \\
&= \min\left\{ \sum_{i=1}^{k} a_i \;\middle|\; \overline{\nu}(k) a_1 a_2 \ldots a_k + 1 > n, \quad a_i \in \mathbb{N} \right\} \\
&= \min\left\{ \sum_{i=1}^{k} a_i \;\middle|\; \overline{\nu}(k) a_1 a_2 \ldots a_k \geq n, \quad a_i \in \mathbb{N} \right\} \\
&\geq k \cdot \sqrt[k]{\frac{n}{\overline{\nu}(k)}}, \quad \text{by the AM-GM inequality.}
\end{aligned}$$

Note that equality occurs iff $n = \overline{\nu}(k)m^k$ for some $m \in \mathbb{N}$, and each $\nu(G_i) = m$. Such a decomposition $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ of K_n must exist, since

$$r_\nu(m+1, m+1, \ldots, m+1) > \overline{\nu}(k)m^k = n.$$

Also, if $\frac{n}{\overline{\nu}(k)}$ is not a perfect k^{th} power, then we apply a discrete smoothing argument, to establish the following claim: given a fixed product $a_1 a_2 \ldots a_k$, the sum $a_1 + a_2 + \ldots + a_k$ is maximized when the a_i's are as close as possible. If the a_i's are all integers, we require each a_i to be $\lfloor r \rfloor$ or $\lceil r \rceil$, where $r = \sqrt[k]{\frac{n}{\overline{\nu}(k)}}$. From this, one must have

$$\sum_{i=1}^{k} \nu(G_i) \geq \left\lceil k \cdot \sqrt[k]{\frac{n}{\overline{\nu}(k)}} \right\rceil.$$

Moreover, this must be the optimal lower bound. ∎

In [116], it is shown that $\overline{\chi}(k) = 1$ and $\overline{\rho}(k) = 2k$. Also, it is straightforward to verify that both $\chi(G)$ and $\rho(G)$ satisfy the conditions of Theorem 3.64. Therefore, by Theorem 3.64, we have

Corollary 3.65 *Let $G_1 \oplus G_2 \oplus \ldots \oplus G_k$ be any k-decomposition of K_n. Then,*

$$\sum_{i=1}^{k} \chi(G_i) \geq k \cdot \sqrt[k]{n} \quad \text{and} \quad \sum_{i=1}^{k} \rho(G_i) \geq k \cdot \sqrt[k]{\frac{n}{2k}}.$$

The first result on $\sum_{i=1}^{k} \chi(G_i)$ appeared in [146] with a different proof, while the second result is original. Our lower bound on $\sum_{i=1}^{k} \rho(G_i)$ is a generalization of the $k = 2$ case, which was shown in [136].

By determining a formula for $\overline{\nu}(k)$ for other co-hereditary vertex partition parameters, we will immediately derive a formula for the lower bound of $\sum_{i=1}^{k} \nu(G_i)$. It is hoped that several other Nordhaus-Gaddum inequalities can be established through this process.

We can also determine optimal lower bounds for various generalized Nordhaus-Gaddum inequalities by computing formulas for various π-Ramsey functions. For some parameters (such as the clique number $\omega(G)$), it seems intractable to determine values for $r_\pi(a_1, a_2, \ldots, a_k)$, even for the case $k = 2$. That is why the optimal lower bound for the Nordhaus-Gaddum inequality $\alpha(G)+\alpha(\overline{G}) = \omega(G)+\omega(\overline{G})$ is a formula in terms of Ramsey functions [32].

We now state the main theorem of this section, which determines the optimal Nordhaus-Gaddum inequalities for both $\chi_f(G)$ and $\chi_c(G)$. We note that two of the trivial bounds were established by Wang and Zhou [174], who proved that $\chi_c(G) + \chi_c(\overline{G}) \leq n + 1$ and $\chi_c(G) \cdot \chi_c(\overline{G}) \geq n$. We now provide all of the correct optimal bounds, for both graph invariants.

To simplify the proof, we split the main result into two separate theorems; first we establish our desired bounds, and then we prove the optimality of these bounds by constructing for each n, a graph G of order n for which equality is attained.

Theorem 3.66 *Let G be a graph on n vertices. Then,*

$$\min\left\{\lceil 2\sqrt{n}\rceil, \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}\right\} \leq \chi_f(G) + \chi_f(\overline{G}) \leq \chi_c(G) + \chi_c(\overline{G}) \leq n+1,$$

$$n \leq \chi_f(G) \cdot \chi_f(\overline{G}) \leq \chi_c(G) \cdot \chi_c(\overline{G}) \leq \left\lfloor \left(\frac{n+1}{2}\right)^2 \right\rfloor.$$

Theorem 3.67 *All four bounds given in the statement of Theorem 3.66 are optimal.*

Note the similarity of Theorem 3.66 to Theorem 3.57: in three of the four cases, the bounds are identical. However, the lower bound for $\chi_f(G)+\chi_f(\overline{G})$ is different. For example, if $n = 7$, then Theorem 3.66 implies that $\chi_f(G)+\chi_f(\overline{G}) \geq \min\{6, \frac{35}{6}\} = \frac{35}{6}$, whereas Theorem 3.57 shows that $\chi(G) + \chi(\overline{G}) \geq \lceil 2\sqrt{7}\rceil = 6$. For this lower bound of $\chi_f(G) + \chi_f(\overline{G})$, we will prove the optimality by finding a star extremal circulant graph G attaining the desired bound.

In the previous section, we discussed the generalized *fractional Ramsey function* $r_{\omega_f}(a_1, a_2, \ldots, a_k)$, which is the π-Ramsey function for the parameter $\omega_f(G) = \chi_f(G)$. By Theorem 3.22, $\omega_f(G) = \chi_f(G) \geq \omega(G)$, and so $r_{\omega_f}(a_1, a_2, \ldots, a_k)$ is well-defined, since it is bounded above by $r(a_1, a_2, \ldots, a_k)$.

Theorem 3.68 ([102, 117]) *Let $r_{\omega_f}(x,y)$ be the ω_f-Ramsey function for two variables. Let $x, y \geq 2$ be any real numbers. Then,*

$$r_{\omega_f}(x,y) = \min\left\{\lceil(\lceil x\rceil - 1)y\rceil, \lceil(\lceil y\rceil - 1)x\rceil\right\}.$$

Knowing this formula for $r_{\omega_f}(x,y) = r_{\chi_f}(x,y)$ is the key to proving Theorem 3.66, since Theorem 3.58 provides the optimal lower bound for $\chi_f(G) + \chi_f(\overline{G})$ in terms of this Ramsey function.

Corollary 3.69

$$\chi_f(G) + \chi_f(\overline{G}) \geq \inf\left\{a_1 + a_2 \;\middle|\; r_{\omega_f}(a_1+\varepsilon, a_2+\varepsilon) > n \quad \forall \varepsilon > 0\right\}.$$

We now determine the minimum value of $a_1 + a_2$ for which $r_{\omega_f}(a_1+\varepsilon, a_2+\varepsilon) > n$ for all $\varepsilon > 0$. This will establish the optimal lower bound for $\chi_f(G) + \chi_f(\overline{G})$, which in turn will give us the optimal lower bound for $\chi_c(G) + \chi_c(\overline{G})$.

Before we proceed with the proof of Theorem 3.66, we require a definition and several lemmas. To simplify notation, we introduce the function $\boldsymbol{t(n)}$.

Definition 3.70 *For each integer $n \geq 1$, set*

$$t(n) = \min\left\{\lceil 2\sqrt{n}\rceil, \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}\right\}.$$

The following lemmas will all include this definition of $t(n)$. Our main theorem, Theorem 3.66, will follow quickly from these three results.

Lemma 3.71 *Let $p = \lfloor\sqrt{n}\rfloor$. Then $n = p^2 + q$ for some $0 \leq q \leq 2p$. Then, $t(n)$ can be represented as the following piecewise function.*

$$t(n) = \begin{cases} \dfrac{2n}{p} & \text{if } p^2 \leq n < p^2 + \frac{p}{2} \\[2ex] \lceil 2\sqrt{n}\rceil = 2p+1 & \text{if } p^2 + \frac{p}{2} \leq n \leq p^2 + p \\[2ex] \dfrac{n(2p+1)}{p^2+p} & \text{if } p^2 + p + 1 \leq n \leq p^2 + \frac{3p}{2} \\[2ex] \lceil 2\sqrt{n}\rceil = 2p+2 & \text{if } p^2 + \frac{3p+1}{2} \leq n \leq p^2 + 2p \end{cases}$$

Proof: Since $p^2+p<(p+\frac{1}{2})^2<p^2+p+1$, we can readily verify the following identities.

$$\lceil 2\sqrt{n}\rceil = \begin{cases} 2p & \text{if } n=p^2 \\ 2p+1 & \text{if } p^2<n\le p^2+p \\ 2p+2 & \text{if } p^2+p+1\le n\le p^2+2p \end{cases}$$

$$\frac{n}{\lfloor\sqrt{n}\rfloor}+\frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor} = \begin{cases} \dfrac{n}{p}+\dfrac{n}{p} & \text{if } p^2\le n\le p^2+p \\[2ex] \dfrac{n}{p}+\dfrac{n}{p+1} & \text{if } p^2+p+1\le n\le p^2+2p \end{cases}$$

If $n\le p^2+\frac{3p}{2}$, then $n<p^2+\frac{3p}{2}+\frac{p}{4p+2}=\frac{(4p^3+2p^2)+3p(2p+1)+p}{4p+2}=\frac{2p^3+4p^2+2p}{2p+1}=\frac{(2p+2)(p^2+p)}{2p+1}$, which implies that $\frac{n}{p}+\frac{n}{p+1}=\frac{n(2p+1)}{p^2+p}<2p+2$. Similarly, if $n\ge p^2+\frac{3p+1}{2}$, then $n>p^2+\frac{3p}{2}+\frac{p}{4p+2}=\frac{(2p+2)(p^2+p)}{2p+1}$, which implies that $\frac{n}{p}+\frac{n}{p+1}=\frac{n(2p+1)}{p^2+p}>2p+2$. We will use these inequalities in our case analysis below.

If $n=p^2$, then $\lceil 2\sqrt{n}\rceil=\frac{n}{\lfloor\sqrt{n}\rfloor}+\frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}$, and so $t(n)=2p=\frac{2n}{p}$.
If $p^2<n<p^2+\frac{p}{2}$, then $2p+1>\frac{2n}{p}$, and so $t(n)=\frac{n}{\lfloor\sqrt{n}\rfloor}+\frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}=\frac{2n}{p}$.
If $p^2+\frac{p}{2}\le n\le p^2+p$, then $2p+1\le\frac{2n}{p}$, and so $t(n)=\lceil 2\sqrt{n}\rceil=2p+1$.
If $p^2+p+1\le n\le p^2+\frac{3p}{2}$, then $2p+2>\frac{n}{p}+\frac{n}{p+1}$, and so $t(n)=\frac{n}{\lfloor\sqrt{n}\rfloor}+\frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}=\frac{n}{p}+\frac{n}{p+1}=\frac{n(2p+1)}{p^2+p}$.
If $p^2+\frac{3p+1}{2}\le n\le p^2+2p$, then $2p+2<\frac{n}{p}+\frac{n}{p+1}$, and so $t(n)=\lceil 2\sqrt{n}\rceil=2p+2$.
This completes the proof. ∎

By inspection, we can verify that $2\sqrt{n}\le t(n)<2\sqrt{n}+1$ in each of the four cases above. Therefore, $\lceil 2\sqrt{n}\rceil$ and $\frac{n}{\lfloor\sqrt{n}\rfloor}+\frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}$ are "close" in the sense that for any n, these two expressions differ by at most 1.

Lemma 3.72 *Let n be a fixed positive integer. For each integer $1\le k\le n$, define $f_1(k)=k+\lceil\frac{n}{k}\rceil$ and $f_2(k)=\frac{n}{k}+\frac{n}{\lfloor\frac{n}{k}\rfloor}$. Then, $\min\{f_1(k),f_2(k)\}\ge t(n)$, for all k. Moreover, this is the optimal lower bound, i.e., there exists at least one index $1\le k\le n$ with $\min\{f_1(k),f_2(k)\}=t(n)$.*

Proof: Fix n. We first prove that $f_1(k) \geq \lceil 2\sqrt{n} \rceil$ for all $1 \leq k \leq n$, which implies by definition that $f_1(k) \geq t(n)$ for each k. Let $n = p^2 + q$, where $0 \leq q \leq 2p$.

If $q = 0$, then $f_1(k) \geq \lceil 2\sqrt{n} \rceil = 2p$ is equivalent to $k + \lceil \frac{n}{k} \rceil \geq 2p$, or $\lceil \frac{n}{k} \rceil \geq 2p - k$. Since $(p-k)^2 \geq 0$, $n = p^2 \geq 2pk - k^2 = k(2p-k)$. Therefore, $\lceil \frac{n}{k} \rceil \geq \frac{n}{k} \geq 2p - k$.

If $1 \leq q \leq p$, then $f_1(k) \geq \lceil 2\sqrt{n} \rceil = 2p + 1$ is equivalent to $\lceil \frac{n}{k} \rceil \geq 2p - k + 1$. Since $(p-k)^2 \geq 0$, $n > p^2 \geq 2pk - k^2 = k(2p-k)$, and so $\frac{n}{k} > 2p - k$. It follows that $\lceil \frac{n}{k} \rceil \geq 2p - k + 1$.

If $p + 1 \leq q \leq 2p$, then $f_1(k) \geq \lceil 2\sqrt{n} \rceil = 2p + 2$ is equivalent to $\lceil \frac{n}{k} \rceil \geq 2p - k + 2$. Since p and k are integers, $(p-k)(p-k+1) \geq 0$, and so $p^2 + p \geq 2pk - k^2 + k = k(2p-k+1)$, from which we get $\frac{n}{k} > \frac{p^2+p}{k} \geq 2p-k+1$. It follows that $\lceil \frac{n}{k} \rceil \geq 2p-k+2$.

Note that in all three cases, equality occurs if $k = p = \lfloor \sqrt{n} \rfloor$. Therefore, we have shown that $f_1(k) \geq \lceil 2\sqrt{n} \rceil$ for all $1 \leq k \leq n$, with at least one value of k for which equality occurs.

Now let us prove that $f_2(k) \geq t(n)$ for each k. This will conclude the proof of the lemma. We split our analysis into the four cases described in Lemma 3.71, which conveniently allows us to apply the formula for $t(n)$.

Case 1: $p^2 \leq n < p^2 + \frac{p}{2}$.

The desired inequality $f_2(k) \geq \frac{2n}{p}$ is equivalent to $\frac{n}{k} + \frac{n}{\lfloor \frac{n}{k} \rfloor} \geq \frac{2n}{p}$, which simplifies to $\lfloor \frac{n}{k} \rfloor (\frac{2k}{p} - 1) \leq k$. If $2k - p \leq 0$, the result is trivial, so assume otherwise. We divide both sides by $2k - p > 0$, and so it suffices to prove that $\lfloor \frac{n}{k} \rfloor \leq \frac{kp}{2k-p}$. We consider two further subcases: when $p^2 + \frac{p}{2} \geq (2p+1)k - k^2$, and when $p^2 + \frac{p}{2} < (2p+1)k - k^2$. In fact, for each of our four cases, we will separate our analysis into two subcases.

If $p^2 + \frac{p}{2} \geq (2p+1)k - k^2$, then

$$\begin{aligned}
(2p+1)k - \left(p^2 + \frac{p}{2}\right) &\leq k^2 \\
\left(p + \frac{1}{2}\right)(2k-p) &\leq k^2 \\
\left(p^2 + \frac{p}{2}\right)(2k-p) &\leq k^2 p \\
\frac{p^2 + \frac{p}{2}}{k} &\leq \frac{kp}{2k-p}.
\end{aligned}$$

Therefore, $\left\lfloor \dfrac{n}{k} \right\rfloor \leq \dfrac{n}{k} < \dfrac{p^2 + \frac{p}{2}}{k} \leq \dfrac{kp}{2k-p}$.

If $p^2 + \frac{p}{2} < (2p+1)k - k^2$, then $\lfloor \frac{n}{k} \rfloor \leq \lfloor \frac{p^2+\frac{p}{2}}{k} \rfloor \leq 2p - k$. Since $2(k-p)^2 \geq 0$, we have $4pk - 2k^2 - 2p^2 + kp \leq kp$, which is equivalent to $2p - k \leq \frac{kp}{2k-p}$. Therefore, we have $\lfloor \frac{n}{k} \rfloor \leq 2p - k \leq \frac{kp}{2k-p}$, with equality iff $k = p = \lfloor \sqrt{n} \rfloor$.

Case 2: $p^2 + \frac{p}{2} \leq n \leq p^2 + p$.

The desired inequality $f_2(k) \geq 2p+1$ is equivalent to $\lfloor \frac{n}{k} \rfloor (\frac{(2p+1)k}{n} - 1) \leq k$. If $(2p+1)k \leq n$, the inequality is trivial, so assume that $\frac{(2p+1)k}{n} - 1 > 0$. Then, it suffices to prove that $\lfloor \frac{n}{k} \rfloor \leq \frac{kn}{(2p+1)k-n}$.

If $n \geq (2p+1)k - k^2$, then

$$\begin{aligned}
n &\geq (2p+1)k - k^2 \\
(2p+1)k - n &\leq k^2 \\
n((2p+1)k - n) &\leq k^2 n \\
\frac{n}{k} &\leq \frac{kn}{(2p+1)k - n}.
\end{aligned}$$

Therefore, $\left\lfloor \dfrac{n}{k} \right\rfloor \leq \dfrac{n}{k} \leq \dfrac{kn}{(2p+1)k-n}$.

If $n < (2p+1)k - k^2$, then $\lfloor \frac{n}{k} \rfloor \leq 2p - k$. From $n \geq p^2 + \frac{p}{2}$ and $p^2 \geq k(2p-k)$, we have

$$\begin{aligned}
n &\geq p^2 + \frac{p}{2} \\
n &= \frac{p^2(2p+1)}{2p} \\
n &\geq \frac{k(2p-k)(2p+1)}{2p} \\
2pn &\geq k(2p-k)(2p+1) \\
(2p-k)(2p+1)k - 2pn + kn &\leq kn \\
(2p-k)((2p+1)k - n) &\leq kn \\
2p - k &\leq \frac{kn}{(2p+1)k - n}.
\end{aligned}$$

Therefore, $\left\lfloor \frac{n}{k} \right\rfloor \leq 2p - k \leq \dfrac{kn}{(2p+1)k - n}$.

<u>*Case 3:*</u> $p^2 + p < n \leq p^2 + \frac{3p}{2}$.

The desired inequality $f_2(k) \geq \frac{n(2p+1)}{p^2+p}$ is equivalent to $\lfloor \frac{n}{k} \rfloor (\frac{(2p+1)k}{p^2+p} - 1) \leq k$.

If $(2p+1)k \leq p^2 + p$, the inequality is trivial, so assume otherwise. Then, it suffices to prove that $\lfloor \frac{n}{k} \rfloor \leq \frac{k(p^2+p)}{(2p+1)k-(p^2+p)}$.

Since $(2p+3)(2p+1) = (2p+2)^2 - 1$, we have $\frac{(2p+3)(2p+1)}{2p+2} < 2p+2$, which is equivalent to $2p + 2 > \frac{\left(p+\frac{3}{2}\right)(2p+1)}{p+1}$.

If $p^2 + \frac{3p}{2} \geq (2p+2)k - k^2$, then

$$\begin{aligned}
p^2 + \frac{3p}{2} &\geq (2p+2)k - k^2 \\
p^2 + \frac{3p}{2} &> \frac{\left(p+\frac{3}{2}\right)(2p+1)}{p+1} k - k^2 \\
\left(p^2 + \frac{3p}{2}\right)(p+1) &> \left(p + \frac{3}{2}\right)(2p+1)k - k^2(p+1) \\
\left(p + \frac{3}{2}\right)((2p+1)k - (p^2+p)) &< k^2(p+1) \\
\left(p^2 + \frac{3p}{2}\right)((2p+1)k - (p^2+p)) &< k^2(p^2+p) \\
\frac{p^2 + \frac{3p}{2}}{k} &< \frac{k(p^2+p)}{(2p+1)k - (p^2+p)}.
\end{aligned}$$

Therefore, $\left\lfloor \dfrac{n}{k} \right\rfloor \leq \dfrac{n}{k} \leq \dfrac{p^2 + \frac{3p}{2}}{k} < \dfrac{k(p^2+p)}{(2p+1)k - (p^2+p)}$.

If $p^2 + \frac{3p}{2} < (2p+2)k - k^2$, then $\lfloor \frac{n}{k} \rfloor \leq \lfloor \frac{p^2 + \frac{3p}{2}}{k} \rfloor \leq 2p - k + 1$.

Since k and p are both integers, $(k-p)(k-p-1) \geq 0$, with equality iff $k = p = \lfloor \sqrt{n} \rfloor$ or when $k = p+1 = \lfloor \sqrt{n} \rfloor + 1$. Thus, we have

$$\begin{aligned}
(k-p)(k-p-1) &\geq 0 \\
(k-p)^2 - (k-p) &\geq 0 \\
2pk + k - p^2 - p &\leq k^2 \\
(2p+1)k - (p^2+p) &\leq k^2 \\
(2p+1)((2p+1)k - (p^2+p)) &\leq k^2(2p+1) \\
(2p+1)((2p+1)k - (p^2+p)) - k^2(2p+1) + k(p^2+p) &\leq k(p^2+p) \\
(2p+1-k)((2p+1)k - (p^2+p)) &\leq k(p^2+p) \\
2p - k + 1 &\leq \frac{k(p^2+p)}{(2p+1)k - (p^2+p)}.
\end{aligned}$$

Therefore, $\left\lfloor \dfrac{n}{k} \right\rfloor \leq 2p - k + 1 \leq \dfrac{k(p^2+p)}{(2p+1)k - (p^2+p)}$, with equality holding iff $k = \lfloor \sqrt{n} \rfloor$ or $k = \lfloor \sqrt{n} \rfloor + 1$.

Case 4: $\quad p^2 + \frac{3p+1}{2} \leq n \leq p^2 + 2p$.

The desired inequality $f_2(k) \geq 2p + 2$ is equivalent to $\lfloor \frac{n}{k} \rfloor (\frac{(2p+2)k}{n} - 1) \leq k$. If $(2p+2)k \leq n$, the inequality is trivial, so assume otherwise. Then, it suffices to prove that $\lfloor \frac{n}{k} \rfloor \leq \frac{kn}{(2p+2)k - n}$.

If $n \geq (2p+2)k - k^2$, then

$$\begin{aligned}
(2p+2)k - k^2 &\leq n \\
(2p+2)kn - k^2 n &\leq n^2 \\
(2p+2)kn - n^2 &\leq k^2 n \\
\frac{n}{k} &\leq \frac{kn}{(2p+2)k - n}.
\end{aligned}$$

Therefore, $\left\lfloor \dfrac{n}{k} \right\rfloor \leq \dfrac{n}{k} \leq \dfrac{kn}{(2p+2)k - n}$.

If $n < (2p+2)k - k^2$, then $\lfloor \frac{n}{k} \rfloor \leq 2p - k + 1$. Since $(k-p)(k-p-1) \geq 0$, we have $k^2 - (2p+1)k + p(p+1) \geq 0$, or $p^2 + p \geq (2p+1)k - k^2$. Also, $\frac{(2p+2)(p^2+p)}{2p+1} = p^2 + \frac{3p}{2} + \frac{p}{4p+2} < p^2 + \frac{3p+1}{2}$. Thus, we have

$$\begin{aligned}
n &\geq p^2 + \frac{3p+1}{2} \\
n &> \frac{(2p+2)(p^2+p)}{2p+1} \\
(2p+1)n &> (2p+2)(p^2+p) \\
(2p+1)n &\geq (2p+2)((2p+1)k - k^2) \\
(2p+1)(2p+2)k - (2p+1)n &\leq k^2(2p+2) \\
(2p+1)((2p+2)k - n) &\leq k^2(2p+2) \\
(2p+1)((2p+2)k - n) - k^2(2p+2) + kn &\leq kn \\
(2p+1-k)((2p+2)k - n) &\leq kn \\
2p - k + 1 &\leq \frac{kn}{(2p+2)k - n}.
\end{aligned}$$

Therefore, we have $\left\lfloor \dfrac{n}{k} \right\rfloor \leq 2p - k + 1 \leq \dfrac{kn}{(2p+2)k - n}$.

This clears all of the cases, and so we have shown that $f_2(k) \geq t(n)$ for each $1 \leq k \leq n$. Earlier we showed that $f_1(k) \geq \lceil 2\sqrt{n} \rceil \geq t(n)$. Therefore, we conclude that $\min\{f_1(k), f_2(k)\} \geq t(n)$, for all $1 \leq k \leq n$. Furthermore, we showed that in Cases 1 and 3, $f_2(\lfloor \sqrt{n} \rfloor) = t(n)$ and in Cases 2 and 4, $f_1(\lfloor \sqrt{n} \rfloor) = \lceil 2\sqrt{n} \rceil = t(n)$. Therefore, for any integer n, there is at least one index $1 \leq k \leq n$ for which $\min\{f_1(k), f_2(k)\} = t(n)$, which implies that our lower bound is indeed optimal. ∎

Lemma 3.73 *Let $n \geq 2$ be a fixed integer. Say that a pair (x, y) of real numbers is* ***n-amicable*** *if $(\lceil y \rceil - 1)x > n$ and $(\lceil x \rceil - 1)y > n$, where $x, y \geq 2$. If (x, y) is an n-amicable pair, then $x + y > t(n)$. Moreover, this is the optimal lower bound, i.e., $\inf(x + y) = t(n)$, where the infimum is taken over all n-amicable pairs.*

Proof: Given any fixed $x \geq 2$, (x, y) is amicable if y satisfies $\lceil y \rceil > \frac{n}{x} + 1$ and $y > \frac{n}{\lceil x \rceil - 1}$. Let Y denote the set of real numbers y satisfying both inequalities. Then, $\inf Y = m$ or $\inf Y = \frac{n}{m}$, for some positive integer $1 \leq m \leq n$. We have the same result for x: for a fixed $y \geq 2$, the infimum of x must be k or $\frac{n}{k}$, for some integer $1 \leq k \leq n$.

So let us consider two cases: when $x = k + \varepsilon$ and when $x = \frac{n}{k} + \varepsilon$, where ε is some infinitely small positive real number. In each case, we will determine the infimum of $x + y$ such that (x, y) is n-amicable. Note that for any fixed x, (x, y) is amicable iff $\lceil y \rceil > \frac{n}{x} + 1$ and $y > \frac{n}{\lceil x \rceil - 1}$.

If $x = k + \varepsilon$, then we require $\lceil y \rceil > \frac{n}{k+\varepsilon} + 1$ and $y > \frac{n}{k}$. Then, (x, y) is not n-amicable when $y = \lceil \frac{n}{k} \rceil$, but is n-amicable when $y = \lceil \frac{n}{k} \rceil + \varepsilon'$, for any $\varepsilon' > 0$. Hence, in this case, $\inf(x + y) = k + \lceil \frac{n}{k} \rceil$, for some $1 \leq k \leq n$.

If $x = \frac{n}{k} + \varepsilon$, then we require $\lceil y \rceil > \frac{n}{\frac{n}{k}+\varepsilon} + 1$ and $y > \frac{n}{\lceil \frac{n}{k}+\varepsilon \rceil - 1} = \frac{n}{\lfloor \frac{n}{k} \rfloor}$. The latter inequality does not hold if $y = \frac{n}{\lfloor \frac{n}{k} \rfloor}$, but does if $y = \frac{n}{\lfloor \frac{n}{k} \rfloor} + \varepsilon'$, for any $\varepsilon' > 0$. We check that this value of y also satisfies the former inequality: if $y = \frac{n}{\lfloor \frac{n}{k} \rfloor} + \varepsilon' \geq \frac{n}{\frac{n}{k}} + \varepsilon' = k + \varepsilon'$, then $\lceil y \rceil \geq k + 1$, implying that $\lceil y \rceil \geq k + 1 = \frac{n}{\frac{n}{k}} + 1 > \frac{n}{\frac{n}{k}+\varepsilon} + 1$.

Thus, (x, y) is n-amicable when $y = \frac{n}{\lfloor \frac{n}{k} \rfloor} + \varepsilon'$, for any $\varepsilon' > 0$. Hence, in this case, $\inf(x + y) = \frac{n}{k} + \frac{n}{\lfloor \frac{n}{k} \rfloor}$ for some $1 \leq k \leq n$.

In Lemma 3.72, we defined $f_1(k) = k + \lceil \frac{n}{k} \rceil$ and $f_2(k) = \frac{n}{k} + \frac{n}{\lfloor \frac{n}{k} \rfloor}$. We just proved that there exists a pair (x, y) with $\inf(x+y) = \min\{f_1(k), f_2(k)\}$ for some $1 \leq k \leq n$. But in Lemma 3.72, we proved that there exists a k for which $\min\{f_1(k), f_2(k)\}$ attains the minimum value of $t(n)$. Thus, we conclude that $\inf(x + y) = t(n)$, and our proof is complete. ∎

We are finally ready to prove Theorem 3.66. In addition to our lemmas, we will repeatedly apply Theorem 3.22, which states that for any graph G on n vertices,

$$\max\left\{\omega(G), \frac{n}{\alpha(G)}\right\} \leq \chi_f(G) \leq \chi_c(G) \leq \chi(G).$$

We now prove Theorem 3.66.

Proof: By Theorems 3.22 and 3.57, $\chi_f(G)+\chi_f(\overline{G}) \leq \chi_c(G)+\chi_c(\overline{G}) \leq \chi(G)+\chi(\overline{G}) \leq n+1$. Similarly, $\chi_f(G)\chi_f(\overline{G}) \leq \chi_c(G)\chi_c(\overline{G}) \leq \chi(G)\chi(\overline{G}) \leq \left\lfloor \left(\frac{n+1}{2}\right)^2 \right\rfloor$. From three applications of Theorem 3.22, $\chi_c(G)\chi_c(\overline{G}) \geq \chi_f(G)\chi_f(\overline{G}) \geq \frac{n\chi_f(G)}{\alpha(\overline{G})} = \frac{n\chi_f(G)}{\omega(G)} \geq n$. Thus, we have justified three of the four bounds.

Finally, we prove that $t(n) \leq \chi_f(G) + \chi_f(\overline{G})$. Let $x = a_1 + \varepsilon$ and $y = a_2 + \varepsilon$. By Corollary 3.69, the optimal lower bound of $\chi_f(G) + \chi_f(\overline{G})$ is the infimum of the set of possible sums $a_1 + a_2$ such that $r_{\chi_f}(x, y) = r_{\chi_f}(a_1 + \varepsilon, a_2 + \varepsilon) > n$, for any $\varepsilon > 0$. Thus, we require x and y to be chosen so that $(\lceil x \rceil - 1)y > n$ and $(\lceil y \rceil - 1)x > n$. In other words, we seek to find the n-amicable pair (x, y) so that its sum $x + y$ is as small as possible. By Lemma 3.73, the infimum of all possible sums $x + y$ equals $t(n)$, implying that $\inf(a_1 + a_2) = t(n)$, taken over all possible sums $a_1 + a_2$. Therefore, we have proven that $\chi_f(G) + \chi_f(\overline{G}) \geq t(n)$. By Theorem 3.22, we also have $\chi_c(G) + \chi_c(\overline{G}) \geq t(n)$. This completes the proof of Theorem 3.66. ∎

To verify Theorem 3.67, we only need to establish the existence of *one* extremal graph for each of our four bounds.

We require the following definition and theorem.

Definition 3.74 ([73]) *For each ordered triplet (n, x, y) with $x + y - 1 \leq n \leq xy$, the set $\boldsymbol{T(n, x, y)}$ of graphs is defined as follows: consider a rectangular array M with x rows and y columns, where we place at most one dot in each of the xy entries of M. We place a dot in each entry of the first row and first column of M, which accounts for $x + y - 1$ dots. Now place $n - (x + y - 1)$ dots in any of the remaining entries of M. Then a graph G in the family $T(n, x, y)$ is formed by taking the n dots of M as the vertices of G, and defining adjacency as follows:*

(a) Any two dots in the same column are adjacent.

(b) No two dots in the same row are adjacent.

(c) Any two dots which belong to distinct rows and columns may or may not be adjacent.

Note that for any $G \in T(n, x, y)$, we have $\chi(G) = \omega(G) = x$ and $\chi(\overline{G}) = \omega(\overline{G}) = y$. By Theorem 3.22, this implies that $\chi_c(G) = \chi_f(G) = x$ and $\chi_c(\overline{G}) = \chi_f(\overline{G}) = y$.

Theorem 3.75 ([73]) *Let G be a graph on n vertices. Then, $\chi(G)+\chi(\overline{G}) = \lceil 2\sqrt{n}\rceil$ iff $G \in T(n,x,y)$, where $x+y = \lceil 2\sqrt{n}\rceil$.*

To finish this section, we prove Theorem 3.67, which enables us to conclude that the Nordhaus-Gaddum inequalities found in Theorem 3.66 are indeed optimal. For the most difficult case among our four bounds, our extremal graph will be a star extremal circulant.

<u>Proof:</u> For each of our four bounds, it suffices to find one graph on n vertices for which equality is attained. This will complete the proof of Theorem 3.67.

Let $G = K_n$. Then, $\omega(G) = \chi(G) = n$, which implies that $\chi_f(G) = \chi_c(G) = n$, by Theorem 3.22. By the same argument, $\chi_f(\overline{G}) = \chi_c(\overline{G}) = 1$. Hence, for this graph G, $\chi_f(G) + \chi_f(\overline{G}) = \chi_c(G) + \chi_c(\overline{G}) = n+1$, and $\chi_f(G)\chi_f(\overline{G}) = \chi_c(G)\chi_c(\overline{G}) = n$.

Let $G = K_m \cup \overline{K_{n-m}}$ be the disjoint union of K_m and $n-m$ isolated vertices, where $m = \lfloor \frac{n+1}{2} \rfloor$. Then, $\omega(G) = \chi(G) = m$, implying that $\chi_f(G) = \chi_c(G) = m$. Also, $\overline{G}$ consists of a complete K_{n-m} subgraph, of which every vertex is joined to each of the other m vertices of the graph. Thus, $\omega(\overline{G}) = \chi(\overline{G}) = n-m+1$, implying that $\chi_f(\overline{G}) = \chi_c(\overline{G}) = n-m+1$. Since $m = \lfloor \frac{n+1}{2} \rfloor$, we have

$$\begin{aligned}
\chi_f(G)\cdot\chi_f(\overline{G}) &= \chi_c(G)\cdot\chi_c(\overline{G}) \\
&= \left\lfloor \frac{n+1}{2} \right\rfloor \cdot \left(n+1 - \left\lfloor \frac{n+1}{2} \right\rfloor \right) \\
&= \left\lfloor \left(\frac{n+1}{2} \right)^2 \right\rfloor .
\end{aligned}$$

The last line follows from a simple case analysis (n even and n odd).

Finally, we verify the existence of a graph G for which $\chi_f(G) + \chi_f(\overline{G}) = \chi_c(G) + \chi_c(\overline{G}) = t(n)$. Since $t(n)$ is defined to be the minimum of two functions, we consider both possibilities separately.

<u>*Case 1:*</u> $t(n) = \lceil 2\sqrt{n} \rceil$.

By Theorem 3.75, $\chi(G) + \chi(\overline{G}) = \lceil 2\sqrt{n}\rceil = t(n)$ iff $G \in T(n,x,y)$. In any such graph G, $\chi(G) = \omega(G)$ and $\chi(\overline{G}) = \omega(\overline{G})$. By Theorem 3.22, we must have $\chi_f(G)+\chi_f(\overline{G}) = \chi_c(G)+\chi_c(\overline{G}) = \chi(G)+\chi(\overline{G}) = t(n)$. Any such graph $G \in T(n,x,y)$ is an extremal graph.

<u>*Case 2:*</u> $t(n) = \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}$.

By Lemma 3.71, this case only occurs when $p^2 \le n < p^2 + \frac{p}{2}$ or $p^2 + p + 1 \le n \le p^2 + \frac{3p}{2}$. For the values of n for which $\lceil 2\sqrt{n}\rceil = \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor}$, an extremal graph must exist from the analysis in Case 1.

Thus, we may assume that $t(n) = \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor} > \lceil 2\sqrt{n}\rceil$. It is easy to check that this requires $n \ge 7$. Let $G = C_{n,\{1,2,\ldots,d\}}$, where $d = \lfloor\sqrt{n}\rfloor - 1$. Then, $\overline{G} = C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}}$. By Theorem 2.3 and Corollary 2.18, $\alpha(G) = \lfloor\frac{n}{d+1}\rfloor$ and $\alpha(\overline{G}) = d+1$. We now prove that both G and $\overline{G}$ are star extremal.

To prove that G is star extremal, we cite theorem by Gao and Zhu [78] which states that $C_{n,\{1,2,\ldots,d\}}$ is star extremal for any $n \ge 2d$. By this theorem, G is star extremal for each $n \ge 7$ since $n \ge 2d = 2\lfloor\sqrt{n}\rfloor - 2$. To prove that $\overline{G}$ is star extremal, we cite the theorem by Lih et. al. [121] which states that $C_{n,\{a,a+1,\ldots,b\}}$ is star extremal for any $n \ge 2b$ and $b \ge \frac{5a}{4}$. By this theorem, $\overline{G} = C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}}$ is star extremal for each $n \ge 7$, since $n \ge 2\cdot\lfloor\frac{n}{2}\rfloor$ and $\lfloor\frac{n}{2}\rfloor \ge \frac{5(d+1)}{4} = \frac{5\lfloor\sqrt{n}\rfloor}{4}$. Therefore, we have proven that both G and $\overline{G}$ are star extremal.

By Lemma 3.21, we have

$$\chi_f(G) = \chi_c(G) = \frac{n}{\alpha(G)} = \frac{n}{\lfloor\frac{n}{d+1}\rfloor} = \frac{n}{\lfloor\frac{n}{\lfloor\sqrt{n}\rfloor}\rfloor}$$
$$\chi_f(\overline{G}) = \chi_c(\overline{G}) = \frac{n}{\alpha(\overline{G})} = \frac{n}{d+1} = \frac{n}{\lfloor\sqrt{n}\rfloor}$$

From above, note that $p^2 \le n < p^2 + \frac{p}{2}$ or $p^2 + p + 1 \le n \le p^2 + \frac{3p}{2}$. In both these cases, a simple case analysis shows that

$$\left\lfloor\frac{n}{\lfloor\sqrt{n}\rfloor}\right\rfloor = \left\lfloor\sqrt{n+\sqrt{n}}\right\rfloor.$$

Therefore, $\chi_f(G) + \chi_f(\overline{G}) = \chi_c(G) + \chi_c(\overline{G}) = \frac{n}{\lfloor\sqrt{n}\rfloor} + \frac{n}{\lfloor\sqrt{n+\sqrt{n}}\rfloor} = t(n)$, as required.

Thus, for all four bounds, we have determined the existence of an extremal graph. This completes the proof of Theorem 3.67, and hence our Nordhaus-Gaddum inequalities are indeed optimal. ∎

Chapter 4

Properties and Applications of Circulant Graphs

In this chapter, we study various properties and applications of circulants. First, we investigate line graphs, and give a full characterization of all graphs G for which its line graph $L(G)$ is a circulant. Then we determine the list colouring number of a particular family of circulants, by making an elegant connection to independence polynomials. We then characterize families of circulant graphs that are well-covered, and show that it is co-NP complete to determine if an arbitrary circulant is well-covered. To conclude the chapter, we study independence complexes of circulant graphs, and characterize pure complexes that are shellable.

4.1 Line Graphs of Circulants

Recall that the *line graph* of G, denoted $L(G)$, is the graph with vertex set $E(G)$, where vertices x and y are adjacent in $L(G)$ iff edges x and y share a common vertex in G. As an example, we can readily verify that if $G = K_4$, then $L(K_4) \simeq C_{6,\{1,2\}}$. This example was also presented in the introductory chapter of the thesis.

Line graphs make connections between many important areas of graph theory. For example, determining a maximum matching in a graph is equivalent to finding a maximum independent set in the corresponding line graph. Similarly, edge colouring is equivalent to vertex colouring in the line graph. Much research has been done on the study and application of line graphs; a comprehensive survey of results is found in [149].

In [176], Whitney solves the determination problem for line graphs, by showing that with the exception of the graphs $K_{1,3}$ and K_3, a graph is uniquely characterized by its line graph.

Theorem 4.1 ([176]) *Let G and H be two graphs for which $L(G) \simeq L(H)$. If $\{G, H\} \neq \{K_{1,3}, K_3\}$, then $G \simeq H$.*

By Whitney's Theorem, we will refer to G as *the* corresponding graph of $L(G)$, whenever $L(G) \not\simeq K_3$.

Let Φ be any mapping from the set of finite graphs to itself. For example, the line graph operator L is such a mapping. A natural question is to determine all families of graphs Γ for which Γ is closed under Φ.

This question is investigated in [149] for $\Phi = L$, where the author surveys known families of graphs Γ for which $G \in \Gamma$ implies $L(G) \in \Gamma$. As a simple example, the family of regular graphs is closed under L, since the line graph of an r-regular graph G is a $(2r-2)$-regular graph. Other L-closed families include k-connected graphs, non-chordal graphs, non-perfect graphs, non-comparability graphs [2], and Eulerian graphs [95].

Since a circulant is regular and vertex transitive, a natural conjecture is that $L(G)$ is a circulant whenever G is a circulant. As discussed above, such is the case for $G = K_4 = C_{4,\{1,2\}}$. It is also true for $C_n = C_{n,\{1\}}$, since $L(C_n) \simeq C_n$. However, a counterexample to the conjecture is found for $G = K_5$.

Theorem 4.2 $L(K_5)$ *is not a circulant graph.*

Proof: Since K_5 has 10 edges, $L(K_5)$ has 10 vertices. Suppose on the contrary that $L(K_5)$ is a circulant. Then, $L(K_5) = C_{10,S}$ for some generating set $S \subseteq \{1,2,3,4,5\}$. Since K_5 is 4-regular, this implies that $L(K_5)$ is 6-regular, and hence $|S| = 3$. Furthermore, $5 \notin S$, as otherwise $L(K_5)$ would have odd degree. Thus, S must be one of $\{1,2,3\}$, $\{1,3,4\}$, $\{1,2,4\}$, or $\{2,3,4\}$. We may reject the latter two cases since $C_{10,S}$ has a 5-clique (namely the set $\{0,2,4,6,8\}$), while $L(K_5)$ clearly has no 5-clique.

Therefore, $S = \{1,2,3\}$ or $S = \{1,3,4\}$. By Lemma 2.24, $C_{10,\{1,2,3\}} \simeq C_{10,\{1,3,4\}}$ with the multiplier $r = 3$, which implies that $L(K_5)$ must be isomorphic to $C_{10,\{1,2,3\}}$. This circulant contains ten distinct 4-cliques, namely the cliques $\{i, i+1, i+2, i+3\}$ for $0 \le i \le 9$, where each element is reduced mod 10. This implies that $L(K_5)$ must also have ten 4-cliques. However, $L(K_5)$ has only 5 cliques of cardinality 4, since a 4-clique must arise from four pairwise adjacent edges in K_5, and this occurs iff all four edges share a common vertex in K_5. Therefore, no such set S exists. ∎

We have given examples of graphs G for which $L(G)$ is a circulant, and shown that

$G = K_5$ does not satisfy this property. A natural question is to characterize all graphs G such that $L(G)$ is a circulant. A complete characterization theorem is the main result of this section. Before we proceed with the main theorem, let us characterize a specific family of graphs (which appeared in the proof of Theorem 2.35) for which its line graph is always a circulant.

Lemma 4.3 *Let $G = K_{a,b}$, where* $\gcd(a,b) = 1$. *Then,* $L(G) \simeq C_{ab,S}$, *where*

$$S = \left\{1 \le k \le \left\lfloor \frac{ab}{2} \right\rfloor : a|k \text{ or } b|k\right\}.$$

Proof: Let (X,Y) be the bipartition of G, with $|X| = a$ and $|Y| = b$. Represent each edge in G by an ordered pair (x,y), where $0 \le x \le a-1$ and $0 \le y \le b-1$. We will label each edge xy in G with the integer $e_{x,y} := bx + ay \pmod{ab}$. Thus, edge (x,y) in G will correspond to the *vertex* $e_{x,y}$ in $L(G)$.

We claim that $e_{x,y}$ is one-to-one. On the contrary, suppose that $e_{x,y} = e_{x',y'}$ for some $(x,y) \ne (x',y')$. Then $b(x-x') \equiv a(y'-y) \pmod{ab}$. Since $\gcd(a,b) = 1$, we must have $a|(x-x')$ and $b|(y'-y)$. But $0 \le x, x' \le a-1$ and $0 \le y, y' \le b-1$, and so this implies that $(x,y) = (x',y')$, a contradiction. Therefore, the vertices of $L(G)$ are the integers from 0 to $ab-1$, inclusive.

Vertices $e_{x,y}$ and $e_{x',y'}$ are adjacent in $L(G)$ iff $x = x'$ or $y = y'$. In the former case, we have $|e_{x,y} - e_{x',y'}|_{ab} = |ay - ay'|_{ab} = a|y-y'|_b$, and in the latter case, $|e_{x,y} - e_{x',y'}|_{ab} = |bx - bx'|_{ab} = b|x-x'|_a$. Hence, $e_{x,y} \sim e_{x',y'}$ in $L(G)$ iff $|e_{x,y} - e_{x',y'}|_{ab} \in S$, where S is the union of all possible values of $a|y-y'|_b$ and $b|x-x'|_a$. Note that $1 \le |y-y'|_b \le \lfloor \frac{b}{2} \rfloor$ and $1 \le |x-x'|_a \le \lfloor \frac{a}{2} \rfloor$. Then this implies that S takes on every multiple of a and b less than or equal to $\lfloor \frac{ab}{2} \rfloor$. Hence,

$$S = \left\{1 \le k \le \left\lfloor \frac{ab}{2} \right\rfloor : a|k \text{ or } b|k\right\}.$$

We conclude that $L(G)$ is isomorphic to the circulant $C_{ab,S}$. ∎

To give an example, if $G = K_{7,12}$, then $L(G) \simeq C_{84,\{7,12,14,21,24,28,35,36,42\}}$. We note that Lemma 4.3 fails when $\gcd(a,b) \ne 1$. As an example, consider $G = K_{3,3}$. Then $L(G)$ is the Cartesian product $K_3 \square K_3$, which is not a circulant by the proof of Theorem 2.29.

As an aside, we can easily compute the independence polynomial $I(L(K_{a,b}), x)$. Even though our line graph may not be a circulant when $\gcd(a, b) \neq 1$, the following theorem holds for all ordered pairs (a, b).

Theorem 4.4 *Let $G = K_{a,b}$, for any positive integers a and b. Then,*

$$I(L(G), x) = \sum_{k=0}^{\min(a,b)} k! \binom{a}{k} \binom{b}{k} x^k.$$

Proof: By definition, $I(L(G), x) = \sum_{k \geq 0} i_k x^k$, where i_k is the number of independent sets of cardinality k in $L(G)$. But an independent set with k vertices in $L(G)$ corresponds to a unique matching of k edges in G. Thus, if we let m_k be the number of matchings with k edges in G, then $I(L(G), x) = \sum_{k \geq 0} m_k x^k$.

So it remains to compute the number of matchings in $K_{a,b}$ with k edges. The first edge can be any of the ab edges in $K_{a,b}$. Other edges in our matching cannot include either endpoint of this edge, so we can delete all edges incident with these two vertices. So the second edge can be any of the $(a-1)(b-1)$ edges remaining. We continue this process, and find that there are $(a-k+1)(b-k+1)$ choices for the k^{th} edge. Therefore, m_k is the product of all of these terms, divided by $k!$ to account for each of the permutations of selecting our k edges. Therefore, we have

$$m_k = \frac{a(a-1)\ldots(a-k+1)b(b-1)\ldots(b-k+1)}{k!} = k! \binom{a}{k} \binom{b}{k}.$$

Since $I(L(G), x) = \sum_{k \geq 0} m_k x^k$, our proof is complete. ∎

We remark that a special case of Theorem 4.4 (when $a = b$) appears in [81].

Theorem 4.4 gives us an additional family of building blocks from which we may derive even more explicit formulas for independence polynomials of circulants. For example, letting $(a, b) = (4, 9)$ gives us

$$I(C_{36,\{4,8,9,12,16,18\}}, x) = 1 + 36x + 432x^2 + 2016x^3 + 3024x^4.$$

Now taking the lexicographic product of $G = C_{36,\{4,8,9,12,16,18\}}$ with any other circulant H for which $I(H, x)$ is known, we can determine $I(G[H], x)$. For example, if $H = C_{5,\{1\}}$, then Theorems 2.31 and 2.33 enable us to determine the independence polynomial $I(G[H],x) = I(C_{180,S},x)$, where S is the following generating set on 29 elements.

$$\begin{aligned} S &= \{4, 8, 9, 12, 16, 18, 20, 24, 27, 28, 32, 36, 40, 44, 45, 48, \\ &\quad 52, 54, 56, 60, 63, 64, 68, 76, 80, 81, 84, 88, 90\}. \end{aligned}$$

Therefore, the independence polynomial of circulants with "seemingly random" generating sets can be exactly determined by this process of taking the lexicographic product.

We have now shown that $L(G)$ is a (connected) circulant if $G = K_4$, $G = C_n$, or $G = K_{a,b}$ for some $\gcd(a,b) = 1$. What is surprising is that these are the *only* such possibilities. The rest of this section is devoted to proving this theorem.

Theorem 4.5 *Let G be a connected graph such that $L(G)$ is a circulant. Then G must either be C_n, K_4, or $K_{a,b}$ for some a and b with* $\gcd(a,b) = 1$.

Proof: If G is connected, then so is $L(G)$. So let us assume that $L(G) = C_{n,S}$ is a connected circulant graph.

If i is a vertex of $L(G)$, then the corresponding edge in G will be denoted e_i. Thus, $x \sim y$ in $L(G)$ iff e_x and e_y share a common vertex in G.

First, we consider the case when 1 is an element of the generating set S. We will prove that if $1 \in S$, then G must be $K_{1,n}$, C_n, or K_4.

If $S = \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$, then $L(G) = K_n$. This implies that $G = K_{1,n}$ for all n (and in the special case $n = 3$, we could also have $G = K_3 = C_3$). So assume $L(G) \neq K_n$. Then, there must exist a *smallest* index k such that $1, 2, \ldots, k \in S$ and $k + 1 \notin S$. Note that $k \leq \lfloor \frac{n}{2} \rfloor - 1$. We split our analysis into three subcases.

Case 1: $3 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$.

The vertices $\{0, 1, 2, \ldots, k\}$ induce a copy of K_{k+1} in $L(G)$, since $1, 2, \ldots, k \in S$. Therefore, the edges in $\{e_0, e_1, e_2, \ldots, e_k\}$ must be pairwise adjacent in G. Since $k \geq 3$, these $k + 1$ edges must share a common vertex u in G. Now consider edge e_{k+1}. This edge is adjacent to e_i for each $1 \leq i \leq k$, and thus, shares a common vertex with each of these k edges. Since $k \geq 3$, u must also be an endpoint of e_{k+1}. But then $e_0 \sim e_{k+1}$, which contradicts the assumption that $k+1 \notin S$. Thus, no graph G exists in this case.

<u>*Case 2:*</u> $k = 2$.

First note that if $n \leq 5$, then $L(G) = K_n$, so suppose that $n \geq 6$. If $n = 6$, then $L(G) = C_{6,\{1,2\}}$, from which we immediately derive $G = K_4$ (this result was also quoted in the introduction to this section). So assume that $n \geq 7$. Consider the subgraph of G induced by the edges $\{e_0, e_1, e_2, e_3, e_{n-3}, e_{n-2}, e_{n-1}\}$.

If $1, 2 \in S$ and $3 \notin S$, we claim that this subgraph of G must be isomorphic to one of the graphs in Figure 4.1. For notational convenience, we represent edge e_k by just the index k.

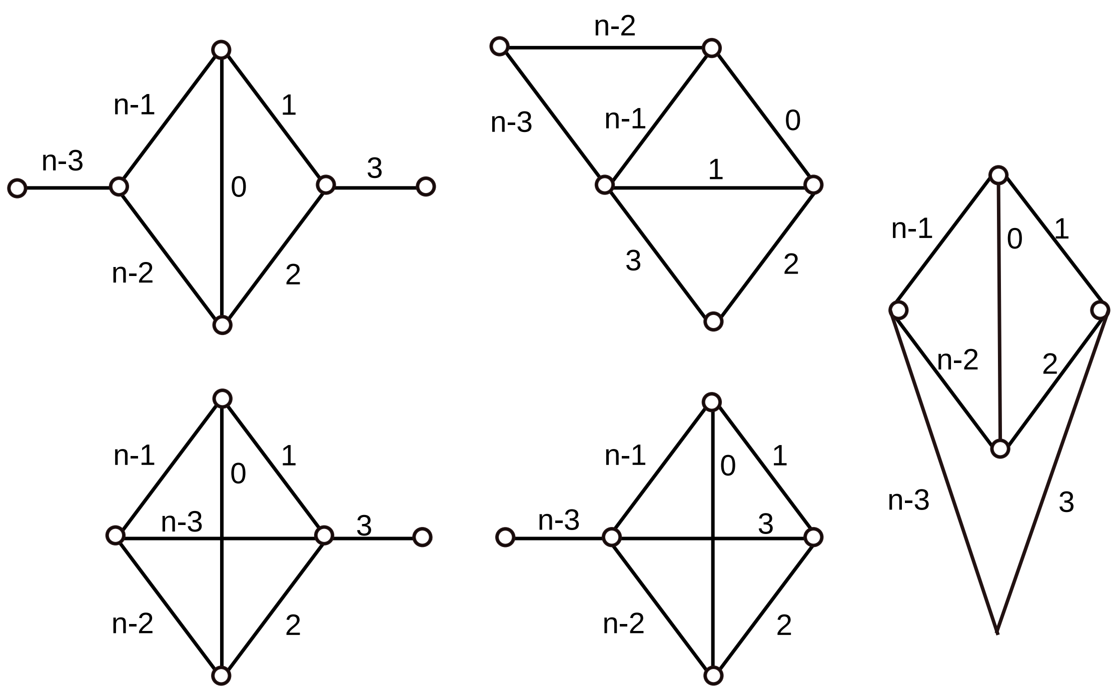

Figure 4.1: Possible subgraphs of G induced by these 7 edges.

To explain why this subgraph of G must be isomorphic to one of these five graphs, we perform a step-by-step case analysis. Start with the edges e_0, e_1, and e_2. Either these three edges induce a K_3 or a $K_{1,3}$. In each case, add edge e_3. Since $3 \notin S$, e_3 is adjacent to e_1 and e_2, but not e_0. Now add e_{n-1}. This edge is adjacent to e_0 and e_1, but not e_2. At this stage, we have three possible cases, as illustrated in Figure 4.2.

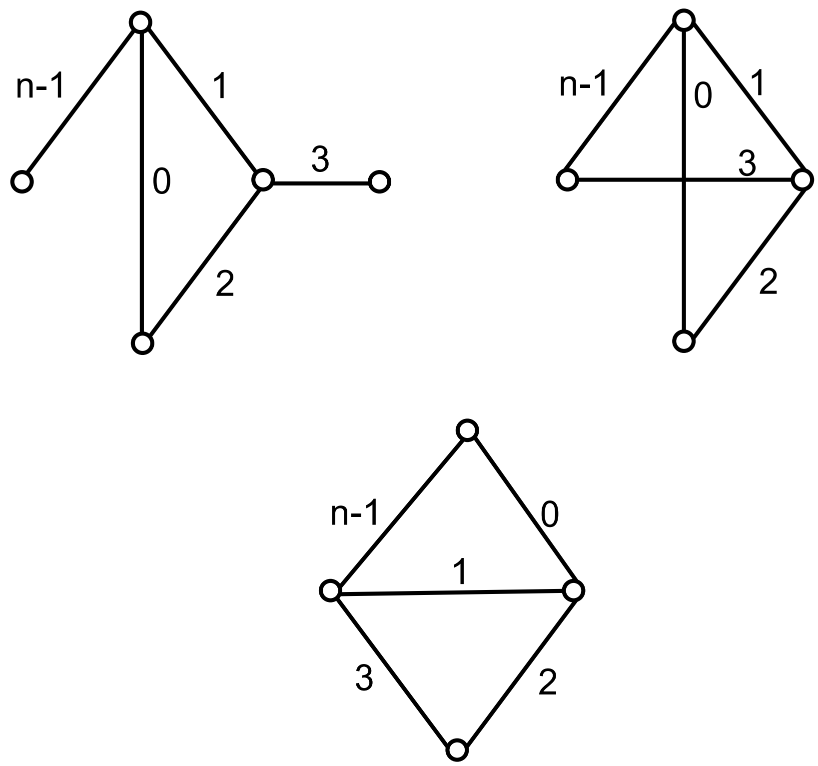

Figure 4.2: Possible subgraphs of G induced by $\{e_0, e_1, e_2, e_3, e_{n-1}\}$.

Now add edge e_{n-2}, which is adjacent to e_0 and e_{n-1}, but not e_1. Finally, add edge e_{n-3}, which is adjacent to e_{n-2} and e_{n-1}, but not e_0. Adding these two edges in all possible ways to our three graphs in Figure 4.2, we find that there are five possible subgraphs. These five subgraphs correspond to the graphs in Figure 4.1.

If $n = 7$, then $e_1 \sim e_4$ in the second graph of Figure 4.1 (top centre) and $e_2 \sim e_5$ in other four. But this contradicts the assumption that $3 \notin S$. So assume $n \geq 8$. In the second graph, $e_{n-3} \sim e_1$ and $e_{n-2} \nsim e_2$, which shows that $4 \sim S$ and $4 \nsim S$, a contradiction. We get a similar contradiction for the other four graphs: $e_{n-2} \sim e_2$ and either $e_{n-3} \nsim e_1$ or $e_{n-1} \nsim e_3$.

So in the case $k = 2$, we *must* have $n = 6$. Thus, $L(G) = C_{6,\{1,2\}}$, implying that $G = K_4$.

<u>*Case 3:*</u> $k = 1$.

If $S = \{1\}$, then $L(G) = C_n$, and so $G = C_n$ (in the special case that $n = 3$, we could also have $G = K_{1,n}$). So we may assume that $|S| > 1$ and that $n \geq 4$. We know that $2 \notin S$ since $k = 1$. Let l be the smallest index for which $1 \in S$, $2, 3, \ldots, l \notin S$, and $l + 1 \in S$. Note that $2 \leq l \leq \lfloor \frac{n}{2} \rfloor - 1$.

The vertices $\{0, 1, \ldots, l + 1\}$ induce a copy of C_{l+2} in $L(G)$, since $2, 3, \ldots, l \notin S$. Since $l \geq 2$, the edges $\{e_0, e_1, \ldots, e_{l+1}\}$ must induce an $(l + 2)$-cycle in G. Let x be the vertex shared by e_0 and e_1, and let y be the vertex shared by e_{l+1} and e_0.

Now consider e_{l+2}. Since $e_{l+2} \sim e_{l+1}$ and $e_{l+2} \nsim e_l$, one of the endpoints of e_{l+2} must be y. Since $e_{l+2} \sim e_1$ and $e_{l+2} \nsim e_2$, one of the endpoints of e_{l+2} must be x. But then this forces $e_{l+2} = xy = e_0$, which is a contradiction, since $l + 2 \leq \lfloor \frac{n}{2} \rfloor + 1 < n$. Thus, no graph G exists in this case.

We have proven that if $1 \in S$ and $L(G)$ is a circulant, then G must be $K_{1,n}$, K_4 or C_n. Now consider all generating sets S with $1 \notin S$.

Suppose we have $L(G) = C_{n,S}$ with some element $x \in S$ such that $\gcd(x, n) = 1$. There must exist an integer y with $xy \equiv 1 \pmod{n}$. Then the set $yS = \{|yi|_n : i \in S\}$ is a generating set with $|S|$ elements, and by Lemma 2.24, $C_{n,S} \simeq C_{n,yS}$. Since $1 \in yS$, we have reduced the problem to the previously-solved case of $1 \in S$.

Therefore, we may assume that every $i \in S$ satisfies $\gcd(i, n) > 1$. We now prove that in such a generating set S, if $L(G) = C_{n,S}$, then G *must* be the complete bipartite graph $K_{a,b}$, where a and b are integers for which $\gcd(a, b) = 1$ and $n = ab$. The remaining details of the proof are quite technical as we require multiple subcases, and a very careful treatment of the Extreme Principle.

Let $S = \{s_1, s_2, \ldots, s_m\}$. By Proposition 2.45, $\gcd(n, s_1, s_2, \ldots, s_m) = 1$, or else $G = C_{n,S}$ is disconnected. For every integer t with $\gcd(t, n) = 1$, define

$$tS = \{|tx|_n \ : \ x \in S\} = \{t_1, t_2, \ldots, t_m\}.$$

We claim that there exists an integer $t \geq 1$ so that $\gcd(t_1, t_2, \ldots, t_m) = 1$.

If $\gcd(s_1, s_2, \ldots, s_m) = 1$, then this claim is trivial, since we can set $t = 1$. So suppose $\gcd(s_1, s_2, \ldots, s_m) = d > 1$. Note that $\gcd(n, s_1, s_2, \ldots, s_m) = \gcd(n, d) = 1$. Therefore, there must exist an integer $t \geq 1$ such that $td \equiv 1 \pmod{n}$. Then, $ts_i = td \cdot \frac{s_i}{d} \equiv \frac{s_i}{d} \pmod{n}$ for each $1 \leq i \leq m$, implying that $t_i = |ts_i|_n = \frac{s_i}{d}$. Hence, $\gcd(t_1, t_2, \ldots, t_m) = \frac{1}{d} \gcd(s_1, s_2, \ldots, s_m) = 1$.

Hence, we have proven the existence of such an index t. Therefore, by Lemma 2.24, $L(G) = C_{n,S} \simeq C_{n,tS}$, with $\gcd(t_1, t_2, \ldots, t_m) = 1$.

For each $2 \leq k \leq m$, consider all k-tuples $(a_1, a_2, \ldots, a_k)$ comprised of the elements of tS so that $\gcd(a_1, a_2, \ldots, a_k) = 1$. Clearly such a k-tuple exists for $k = m$ by setting $a_i = t_i$ for each $1 \leq i \leq k = m$. Of all k-tuples satisfying $\gcd(a_1, a_2, \ldots, a_k) = 1$ (over all $k \geq 2$), select a k-tuple for which the sum $a_1 + a_2 + \ldots + a_k$ is minimized.

We will show that $k = 2$, i.e., there exists an ordered pair (a_1, a_2) such that $a_1, a_2 \in tS$ and $\gcd(a_1, a_2) = 1$. Suppose on the contrary that the minimum k-tuple satisfies $k \geq 3$. Then $L(G) = C_{n,tS}$ is a connected circulant graph with vertex 0 adjacent to each of a_1, a_2, and a_3. Consider e_0 in the corresponding graph G. We know that e_{a_1}, e_{a_2}, and e_{a_3} share a common vertex with e_0. By the Pigeonhole Principle, two of these three edges must share the same common vertex, and hence $|a_j - a_i|_n \in tS$ for some $1 \leq i < j \leq 3$.

Without loss, suppose that $a_2 - a_1 \in tS$. We have $\gcd(a_1, a_2) = \gcd(a_1, a_2 - a_1)$. If $a_2 - a_1 = a_j$ for some $1 \leq j \leq k$, then $\gcd(a_1, a_3, a_4, \ldots, a_k) = 1$, contradicting the minimality of our chosen k-tuple. If $a_2 - a_1$ does not already appear as some a_j in our minimum k-tuple, then $\gcd(a_1, a_2 - a_1, a_3, a_4, \ldots, a_k) = 1$, and once again we have contradicted our minimality assumption.

Therefore, in a minimum k-tuple satisfying the given conditions, we must have $k = 2$. This minimum k-tuple must be a pair (a, b), where $a + b$ is minimized over all pairs such that $a, b \in tS$ and $\gcd(a, b) = 1$. Without loss, assume $a < b$. Specifically, this choice of (a, b) implies that $b - a \notin tS$, as otherwise the pair $(a, b - a)$ satisfies $\gcd(a, b - a) = 1$ and contradicts the minimality of (a, b). Since $1 \notin tS$, we have $2 \leq a < b \leq \lfloor \frac{n}{2} \rfloor$.

We now show that $|a + b|_n \notin tS$. On the contrary, suppose that $|a + b|_n \in tS$. Consider the subgraph of G induced by the edges in the set $\{e_0, e_a, e_b, e_{b-a}, e_{a+b}, e_{2a}\}$.

Since $2a < a + b < n$ and $\gcd(a, b) = 1$, these six edges are distinct.

From $a, b, |a + b|_n \in tS$ and $b - a \notin tS$, a simple case analysis shows that this subgraph must be isomorphic to K_4, with one of two possible edge labellings, as shown in Figure 4.3. We arrive at this conclusion by considering the edges in the following order: e_0, e_a, e_b, e_{a+b}, e_{b-a}, and e_{2a}. After we have included five edges, there are four possible subgraphs. But after we include e_{2a}, we must eliminate the two cases with $e_{b-a} \not\sim e_a$, and this leaves us with the two labellings in Figure 4.3. As before, we represent edge e_k by just the index k for notational convenience.

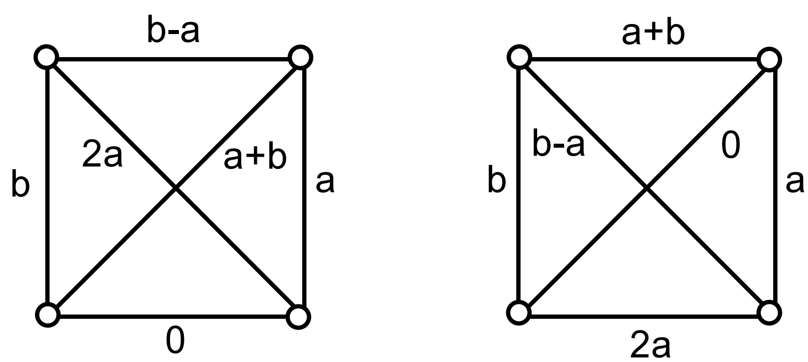

Figure 4.3: Two possible edge labellings of K_4.

In both valid labellings, $e_0 \sim e_{2a}$. Therefore, if $|a + b|_n \in tS$, this implies that $|2a|_n \in tS$ as well.

Now consider the edge e_{n-a}. We claim that edge e_{n-a} is distinct from the other six edges. Note that $\gcd(a, n) > 1$, $\gcd(b, n) > 1$, and $\gcd(a, b) = 1$, with $2 \leq a < b \leq \frac{n}{2}$. If $n-a$ equals 0, a, b or $b-a$, then we have an immediate contradiction. If $n-a = a+b$, then $n = 2a + b$, so that $\gcd(a, n) = \gcd(a, 2a + b) = \gcd(a, b) = 1$, by the Euclidean algorithm. But then $\gcd(a, n) = 1$, which is a contradiction. Finally, if $n - a = 2a$ (i.e., $n = 3a$), we argue that (a, b) is not the *minimum* pair satisfying the given conditions. Let $b' = |a + b|_n \in tS$. Since $a < b$, we have $a + b > 2a > \frac{n}{2}$, and so $b' = |a+b|_n = n - (a+b) = 2a - b$. Then, $\gcd(a, b') = \gcd(a, 2a - b) = \gcd(a, b) = 1$. Note that $b' = 2a - b < b$. So (a, b') is a pair satisfying $\gcd(a, b') = 1$ and $a, b' \in tS$, thus contradicting the minimality of (a, b).

Thus, edge e_{n-a} is distinct from the six other edges in this K_4 subgraph, and is adjacent to each of e_0, e_a, and e_b. But the three edges $\{e_b, e_0, e_a\}$ induce the path P_4, and so e_{n-a} must coincide with one of the edges e_{a+b}, e_{b-a}, or e_{2a}. This establishes our desired contradiction, and so we have shown that $|a+b|_n \notin tS$.

We have now shown that $a, b \in tS$, $\gcd(a,b) = 1$, $b - a \notin tS$, and $|a+b|_n \notin tS$. We will now prove that in our circulant $L(G) = C_{n,tS}$, n must equal ab, and that the generating set tS must equal

$$tS = \left\{ 1 \leq k \leq \left\lfloor \frac{ab}{2} \right\rfloor : a|k \text{ or } b|k \right\}.$$

By Lemma 4.3 and Theorem 4.1, this will immediately establish our desired conclusion that $G = K_{a,b}$. Hence, it suffices to prove that $n = ab$, and that $1 \leq k \leq \lfloor \frac{ab}{2} \rfloor$ is an element of tS iff k is a multiple of a or b.

Now consider the subgraph of $L(G)$ induced by the vertices $\{0, a, b, n-a, n-b\}$. It is well-known (and straightforward to show) that any line graph $L(G)$ is *claw-free*, i.e., $L(G)$ has no induced $K_{1,3}$ subgraph. This implies that $|2a|_n \in tS$, as otherwise $\{0, a, b, n-a\}$ induces a $K_{1,3}$ subgraph in $L(G)$, since $b - a \notin tS$ and $|a+b|_n \notin tS$. Similarly, if $n > 2b$, then $|2b|_n \in tS$ as well. In the exceptional case that $n = 2b$ (i.e., $b = \frac{n}{2} = \lfloor \frac{n}{2} \rfloor$), we have $b = n - b$, and we will deal with this case separately.

We have shown that in our generating set tS, if $a \in tS$, then $|2a|_n \in tS$. We now prove that n must be a multiple of a. Since $a < \lfloor \frac{n}{2} \rfloor$, we know that $n > 2a$. Consider two cases.

Case 1: $|3a|_n \in tS$.

We will show that n must be a multiple of a, and that $ka \in tS$ for each $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$. The subgraph of G induced by the edges $\{e_0, e_a, e_{2a}, e_{3a}\}$ must be isomorphic to $K_{1,4}$, since these edges are pairwise adjacent. Let u be the vertex common to each edge. Since e_{4a} is adjacent to e_a, e_{2a}, and e_{3a}, it follows that u must also be an endpoint of e_{4a}, which implies that $|4a|_n \in tS$ since $e_0 \sim e_{4a}$. Continuing in this manner, we see that each $|ka|_n \in tS$, for all $k \geq 4$. Now, let $d = \gcd(a, n)$. Then, there exists an integer m for which $|ma|_n = d$, which implies that $d \in tS$. If $d < a$, then (d, b) is a pair with $\gcd(d, b) = 1$ since $d = \gcd(a, n)|a$. And this contradicts the minimality of (a, b). Therefore, we must have $d = a$, which implies that $a|n$. Hence, $|ka|_n \in tS$ for each $k \geq 1$. In other words, $ka \in tS$ for each $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$.

<u>*Case 2:*</u> $|3a|_n \notin tS$.

We prove that if $|3a|_n \notin tS$, then $n = ka$ for some $3 \leq k \leq 6$. Consider the subgraph of G induced by the edges $\{e_0, e_a, e_{2a}, e_{3a}, e_{4a}, e_{5a}, e_{6a}\}$, where the indices are reduced mod n (if necessary). We now split our analysis into two subcases: when n does not divide ma for any $m \leq 6$, and when $n|ma$ for some $m \leq 6$.

If n does not divide ma for any $m \leq 6$, then these seven edges must be distinct. We claim that if $|3a|_n \notin tS$, then the edges $\{e_0, e_a, e_{2a}, e_{3a}, e_{4a}, e_{5a}\}$ must induce a copy of K_4, with one of two possible edge-labellings as shown in Figure 4.4. In both possible edge labellings, $e_0 \sim e_{4a}$, i.e., $|4a|_n \in tS$.

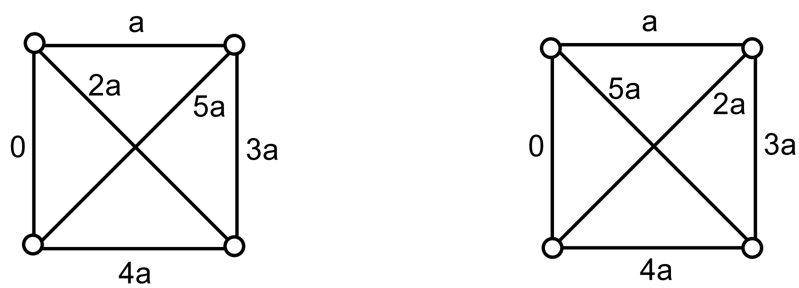

Figure 4.4: Two possible K_4 subgraphs induced by $\{e_0, e_a, e_{2a}, e_{3a}, e_{4a}, e_{5a}\}$.

This is justified by doing a case analysis, considering the edges in the following order: e_0, e_a, e_{2a}, e_{3a}, e_{4a}, and e_{5a}. After the first five edges have been included, there are three possible subgraphs. But after we include e_{5a}, we see that we must eliminate the subgraph with $e_0 \not\sim e_{4a}$. This leaves us with the two subgraphs in Figure 4.4.

Now consider e_{6a}. We know that $e_{6a} \nsim e_{3a}$, while e_{6a} is adjacent to each of e_{2a}, e_{4a}, and e_{5a}. And this implies that e_{6a} and e_0 coincide, which is a contradiction.

Therefore, n must divide ma for some $m \leq 6$. If $n < 6a$, then this reduces to the previously solved Case 1, where we showed that $ka \in tS$ for $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$. Thus, Case 2 only adds one possible scenario not previously considered, namely the case $n = 6a$ and $3a \notin tS$.

Therefore, we have shown that $n \equiv 0 \pmod{a}$ and that $ka \in tS$ for each $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$, with the only possible exception being the case when $3a \notin tS$ and $n = 6a$. We have an analogous result when we replace a by b, except in the special case $n = 2b$. Thus, we have shown that $L(G) = C_{n,tS}$ *must* satisfy one of the following four cases.

1. $n = 6a$, with $a, 2a \in tS$, $3a \notin tS$, and $lb \in tS$ for $1 \leq l \leq \lfloor \frac{n}{2b} \rfloor$.

2. $n = 6b$, with $b, 2b \in tS$, $3b \notin tS$, and $ka \in tS$ for $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$.

3. $n = 2b$, with $b \in tS$, and $ka \in tS$ for $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$.

4. $n = mab$ for some integer m, with $ka \in tS$ for $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$ and $lb \in tS$ for $1 \leq l \leq \lfloor \frac{n}{2b} \rfloor$.

Note that the third case is a special instance of the fourth case (when $m = 1$ and $a = 2$), so we may disregard this case as we will include it in our analysis of the fourth case. We first prove that the first two cases cannot occur, leaving us with only Case 4 to consider. In this remaining final case, we will prove that n must equal ab and that

$$tS = \left\{1 \leq k \leq \left\lfloor \frac{ab}{2} \right\rfloor : a|k \text{ or } b|k \right\}.$$

As mentioned previously, this enables us to conclude that $G = K_{a,b}$, by Lemma 4.3 and Theorem 4.1.

We show that the first two cases are impossible. By symmetry, we will just disprove the first case. As mentioned before, the subgraph of G induced by the edges $\{e_0, e_a, e_{2a}, e_{3a}, e_{4a}, e_{5a}\}$ must be isomorphic to K_4, since $a, 2a \in tS$ and $3a \notin tS$. There are two possible labellings of the edges on K_4, as shown in Figure 4.4. Now consider the edges e_b and e_{a+b}, which are distinct from the six edges of the subgraph since $\gcd(a, b) = 1$ and $a, b > 1$. Since $b - a \notin tS$, we must have $e_b \nsim e_a$ and $e_{a+b} \nsim e_{2a}$. Also, we must have $e_b \sim e_{a+b}$, $e_b \sim e_0$, and $e_{a+b} \sim e_a$. Therefore, the only possible edge labellings are given in Figure 4.5.

The first graph has $e_{a+b} \sim e_{3a}$ and $e_b \nsim e_{2a}$, and the second graph has $e_{a+b} \nsim e_{3a}$ and $e_b \sim e_{2a}$. Therefore, in both graphs, $|2a - b|_n \sim tS$ and $|2a - b|_n \nsim tS$, a

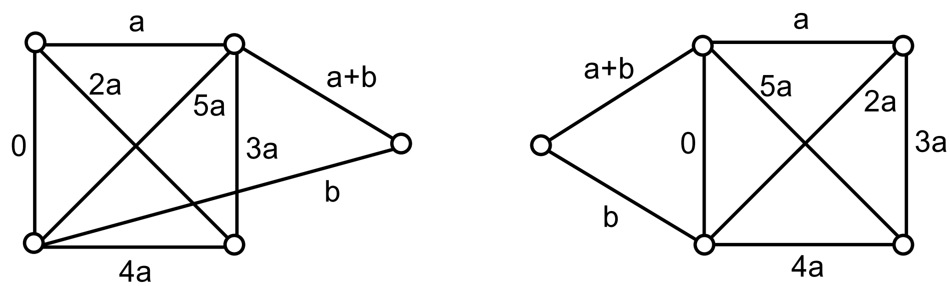

Figure 4.5: Two possible subgraphs induced by this set of eight edges.

contradiction. Thus, we have proven that the first two possible cases for $L(G) = C_{n,tS}$ are impossible, and so we only need to consider the fourth and final case.

We have $n = mab$ for some integer m, where $ka \in tS$ for $1 \leq k \leq \lfloor \frac{n}{2a} \rfloor$ and $lb \in tS$ for $1 \leq l \leq \lfloor \frac{n}{2b} \rfloor$. We now prove that $n = ab$, i.e., $m = 1$.

Suppose that $m > 1$. Since $b > a > 1$, we have $a \geq 2$ and $b \geq 3$. Therefore, the edges $\{e_0, e_a, e_{2a}, e_b, e_{ab}, e_{(a+1)b}\}$ are distinct. The edges $\{e_0, e_a, e_{2a}, e_{ab}\}$ are pairwise adjacent in G, and so they must induce a copy of $K_{1,4}$. Let u be the vertex common to all four edges. Since the edges $\{e_0, e_b, e_{ab}, e_{(a+1)b}\}$ are pairwise adjacent in G, these four edges must also induce a copy of $K_{1,4}$. It follows that e_b and $e_{(a+1)b}$ must also have vertex u as one of its endpoints. But then $e_a \sim e_b$, which implies that $b-a \in tS$, a contradiction. Thus, we must have $m = 1$.

If $m = 1$, then $L(G) = C_{ab,tS}$, where the generating set tS includes every element $ka \in tS$ for $1 \leq k \leq \lfloor \frac{b}{2} \rfloor$, and $lb \in tS$ for $1 \leq l \leq \lfloor \frac{a}{2} \rfloor$. First assume that tS contains no other elements. Then this implies that $tS = \{1 \leq k \leq \lfloor \frac{ab}{2} \rfloor : a|k \text{ or } b|k\}$. From Lemma 4.3, this is precisely the line graph for $G = K_{a,b}$, where $\gcd(a, b) = 1$. By Theorem 4.1, $L(G) = C_{ab,tS}$ implies that $G = K_{a,b}$.

Therefore, suppose that tS contains other elements than the multiples of a and b. Let c be the *smallest* element of tS that is not a multiple of a or b. Note that $c > a$ and $c > b$ since (a, b) is the smallest pair with $\gcd(a, b) = 1$, and $a, b \in tS$.

Let $e_0 = xy$ in G. Since each multiple of a is an element of tS, the edges

$e_0, e_a, e_{2a}, e_{3a}, \ldots$ all share the same vertex in G. Without loss, assume this vertex is x. Similarly, the edges $e_0, e_b, e_{2b}, e_{3b}, \ldots$ all share the same vertex in G. This common vertex must be y, since $b-a \notin tS$. Now consider e_c, which shares a common vertex with e_0. Without loss, assume e_c has an endpoint x. Then, e_c is adjacent to e_{ka} for all $k \geq 1$, where the index is reduced mod n. Thus, $|c-ka|_n = |c-ka|_{ab}$ is an element of tS for all $k \geq 1$.

Let $c = pa+q$, where (p,q) is the unique integer pair with $0 \leq q \leq a-1$. Letting $k = p$ and $k = p+1$, we have $|c-pa|_n = q \in tS$ and $|c-(p+1)a|_n = a-q \in tS$. By the minimality of c, both q and $a-q$ must be multiples of a or b. Clearly neither is a multiple of a. Thus, q and $a-q$ must both be multiples of b. But then its sum, $q+(a-q) = a$, must be a multiple of b. This contradicts the fact that $\gcd(a,b) = 1$.

We have shown that if tS contains some element c other than multiples of a or b, we obtain a contradiction. Thus, tS cannot contain any other elements than the multiples of a and b. We have proven that if $L(G) = C_{n,tS}$ is a circulant, then we must have $n = ab$ and $tS = \{1 \leq k \leq \lfloor \frac{ab}{2} \rfloor : a|k \text{ or } b|k\}$. From our earlier analysis, $L(G) = C_{ab,tS}$ implies that $G = K_{a,b}$.

In conclusion, we have proven that if $L(G)$ is a circulant, then G *must* be one of K_4, C_n, or $K_{a,b}$ where $\gcd(a,b) = 1$. We have now given a complete characterization of all circulant line graphs. This completes the proof of Theorem 4.5. ∎

4.2 List Colourings

In this section, we investigate the *list colouring number* $\chi_l(G)$ of a graph, and cleverly utilize the formula for the independence polynomial $I(C_n, x)$ to calculate the values of $\chi_l(G)$ for a particular family of circulant graphs. To our knowledge, the main result in this section provides the first example of a graph family whose list colouring number can be determined directly from its independence polynomial.

Definition 4.6 *The* **list colouring number** $\chi_l(G)$ *is the smallest integer* n *such that if each vertex* v *of* G *is assigned any list* $L(v)$ *of possible colours with* $|L(v)| = n$*, then* G *has a proper colouring.*

The list colouring number is introduced in [66], and is also known in the literature as the *choice number*. Since a list colouring is a generalization of the usual colouring (i.e., assigning the list $L(v) = \{1, 2, \ldots, n\}$ for each vertex), it follows that $\chi_l(G) \geq \chi(G)$, for all G.

We often have $\chi_l(G) = \chi(G)$, but this is not always the case. For example, $\chi(K_{2,4}) = 2$ and $\chi_l(K_{2,4}) = 3$. The former is clear since $K_{2,4}$ is bipartite. To prove the latter, we first note that any 3-list colouring of $K_{2,4}$ admits a proper colouring (select any colour for each of the vertices of degree 4, and then there is at least one colour left to properly colour each of the remaining four vertices). To show that $\chi_l(G) = 3$, we exhibit a list of two colours for each vertex of $K_{2,4}$, such that the lists do not admit a proper colouring. This is illustrated in Figure 4.6.

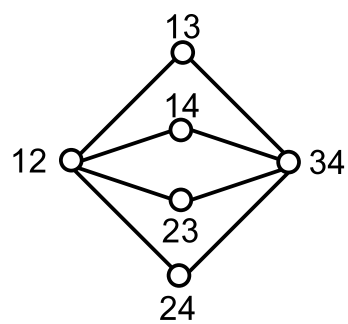

Figure 4.6: A 2-list colouring of $K_{2,4}$ that is not proper.

We also give the following example, where $\chi(K_{7,7}) = 2$ and $\chi_l(K_{7,7}) = 4$. Figure 4.7 gives a 3-list colouring that is not proper, showing that $\chi_l(K_{7,7}) > 3$. We remark that the lists correspond to the edges of the Fano Plane.

We now show that the difference $\chi_l(G) - \chi(G)$ can be made as large as we wish.

Proposition 4.7 *The difference $\chi_l(G) - \chi(G)$ can take on infinitely large values, even when G is restricted to circulants.*

<u>Proof:</u> First, we establish that $\chi_l(K_{n,n}) > k$, for $n = \binom{2k-1}{k}$. To find the desired k-list colouring of $K_{n,n}$, let (X, Y) be the bipartition of $K_{n,n}$ and assign each of the $\binom{2k-1}{k}$ k-subsets of $\{1, 2, \ldots, 2k-1\}$ to a vertex of X. We do the same for Y. Any proper colouring of $K_{n,n}$ must consist of at least k distinct colours assigned to the

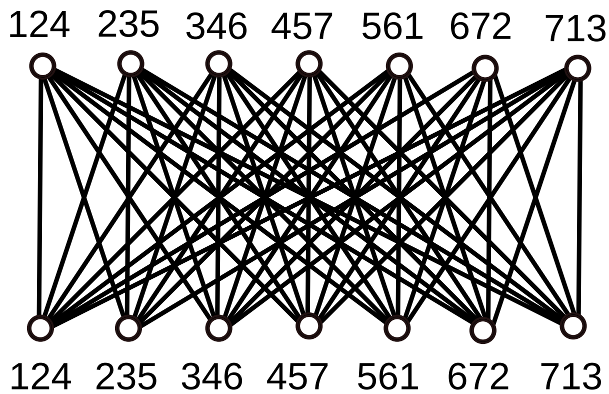

Figure 4.7: A 3-list colouring of $K_{7,7}$ that is not proper.

vertices of X and at least k distinct colours assigned to the vertices of Y (which must all be different from the colours used to colour X). Therefore, any proper colouring of $K_{n,n}$ must require at least $2k$ distinct colours. Hence, we conclude that no proper colouring exists with this assignment of $2k-1$ total colours.

Letting $G = K_{n,n}$, we have $\chi_l(G) > k$, implying that $\chi_l(G) - \chi(G) > k-2$. Thus, $\chi_l(G) - \chi(G)$ can be made arbitrarily large. Even when G is restricted to circulants, $\chi_l(G) - \chi(G)$ can take on infinitely large values: this is immediate from the previous paragraph, since $K_{n,n} = C_{2n,\{1,3,5,\ldots,2n-1\}}$. ∎

We now develop more properties of $\chi_l(G)$ by investigating graph orientations, where we direct each edge uv in E.

Definition 4.8 *A directed graph (digraph)* $\overrightarrow{G}$ *is* **Eulerian** *if its in-degree equals the out-degree for each vertex of* G*.*

This digraph $\overrightarrow{G}$ is not required to be connected, and is allowed to have any number of isolated vertices.

Definition 4.9 *Let* $\boldsymbol{ee(\overrightarrow{G})}$ *be the number of Eulerian subgraphs of* $\overrightarrow{G}$ *which have an even number of edges, and let* $\boldsymbol{eo(\overrightarrow{G})}$ *be the number of Eulerian subgraphs which have an odd number of edges.*

For convenience, we say that the empty graph is an even Eulerian subgraph. Our results will involve applications of the following theorem by Alon and Tarsi [4] that relates Eulerian subgraphs of $\overrightarrow{G}$ to the list colouring number $\chi_l(G)$. This theorem is extremely surprising and powerful, as it connects two topics that appear to have no connection.

Theorem 4.10 ([4]) *Let $\overrightarrow{G}$ be an orientation of G such that the out-degree of each vertex is $k-1$. If $ee(\overrightarrow{G}) \neq eo(\overrightarrow{G})$, then $\chi_l(G) \leq k$.*

To illustrate Theorem 4.10, we calculate the list colouring number of the circulant $G = C_{9,\{1,2\}}$.

Proposition 4.11 *Let $G = C_{9,\{1,2\}}$. Then $\chi_l(G) = 3$.*

Proof: Since G contains a K_3-subgraph, we have $\chi_l(G) \geq \chi(G) \geq 3$. Now we show that $\chi_l(G) \leq 3$, which will complete the proof.

We remark that G is the union of two edge-disjoint 9-cycles, $C_{9,\{1\}}$ and $C_{9,\{2\}}$. Let $\overrightarrow{G}$ be the orientation of G where each of these 9-cycles is oriented clockwise. Specifically, the orientation will have $v \to v+1$ and $v \to v+2$ for each $0 \leq v \leq 8$, where addition is computed mod 9. For example, $1 \to 3 \to 4 \to 6 \to 8 \to 0 \to 1$ is an example of a 6-cycle in $\overrightarrow{G}$, and hence is an Eulerian subgraph of $\overrightarrow{G}$.

We determine the number of Eulerian subgraphs in $\overrightarrow{G}$. Define u_k to be the number of Eulerian subgraphs of $\overrightarrow{G}$ with k edges. (Later in this section, we will prove that each k-edge Eulerian subgraph with $k \leq 9$ must be a directed k-cycle). With the aid of Maple, we calculate the following values of u_k, for each $0 \leq k \leq 9$.

k	0	1	2	3	4	5	6	7	8	9
u_k	1	0	0	0	0	9	30	27	9	2

Table 4.1: Eulerian subgraphs for the circulant $C_{9,\{1,2\}}$.

Since $\overrightarrow{G}$ is Eulerian, the complement of an Eulerian subgraph of $\overrightarrow{G}$ is also Eulerian. Because $|E(\overrightarrow{G})| = 18$, it follows that $u_k = u_{18-k}$ for $0 \leq k \leq 9$. Therefore, we have $ee(\overrightarrow{G}) = 1+30+9+9+30+1 = 80$ and $eo(\overrightarrow{G}) = 9+27+2+27+9 = 74$. Since $ee(\overrightarrow{G}) \neq eo(\overrightarrow{G})$, Theorem 4.10 implies that $\chi_l(G) \leq 3$. ∎

Later in this section, we will provide a generalization to Proposition 4.11, by proving that $\chi_l(C_{3m,\{1,2\}}) = 3$ for any $m \geq 2$.

Our proof above is extremely unsatisfying, as we have relied on a Maple procedure to enumerate our Eulerian subgraphs. However, there is no known algorithm to enumerate Eulerian subgraphs of an arbitrary digraph $\overrightarrow{G}$. We should note that counting Eulerian orientations and Eulerian cycles in a general (undirected) graph is $\#P$-complete [19, 134], and so it is possible that counting the number of Eulerian subgraphs of $\overrightarrow{G}$ is also $\#P$-complete. We conjecture that this is indeed the case.

However, if the graph has a certain structure, then combinatorial techniques can be used to count the number of Eulerian subgraphs. As an example, we prove the following theorem which is a generalization of the above result. But first we require a technical combinatorial lemma and a corollary.

Lemma 4.12 *For each* $k \geq 1$, *define* $S(k) = \displaystyle\sum_{i=0}^{\lfloor \frac{k-1}{2} \rfloor} (-1)^i \cdot \binom{k-i}{k-2i-1}$. *Then for all* $k \geq 1$,

$$S(k+2) - S(k+1) + S(k) = 1.$$

Proof: Let $k \geq 1$. Then,

$$\begin{aligned}
& S(k+1) - S(k) \\
= \; & \sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^i \cdot \binom{k-i+1}{k-2i} - \sum_{i=0}^{\lfloor \frac{k-1}{2} \rfloor} (-1)^i \cdot \binom{k-i}{k-2i-1} \\
= \; & \binom{k+1}{k} + \sum_{i=1}^{\lfloor \frac{k}{2} \rfloor} (-1)^i \cdot \binom{k-i+1}{k-2i} - \sum_{i=0}^{\lfloor \frac{k-1}{2} \rfloor} (-1)^i \cdot \binom{k-i}{k-2i-1} \\
= \; & \binom{k+1}{k} + \sum_{i=0}^{\lfloor \frac{k}{2} \rfloor - 1} (-1)^{i+1} \cdot \binom{k-(i+1)+1}{k-2(i+1)} - \sum_{i=0}^{\lfloor \frac{k-1}{2} \rfloor} (-1)^i \cdot \binom{k-i}{k-2i-1}
\end{aligned}$$

$$
\begin{aligned}
&= \binom{k+1}{k} - \sum_{i=0}^{\lfloor\frac{k-1}{2}\rfloor} (-1)^i \cdot \left[\binom{k-i}{k-2i-2} + \binom{k-i}{k-2i-1}\right] \\
&= \binom{k+1}{k} - \sum_{i=0}^{\lfloor\frac{k-1}{2}\rfloor} (-1)^i \cdot \binom{k-i+1}{k-2i-1} \quad \text{, by Pascal's Identity} \\
&= -1 + \binom{k+2}{k+1} - \sum_{i=1}^{\lfloor\frac{k+1}{2}\rfloor} (-1)^{i-1} \cdot \binom{k-(i-1)+1}{k-2(i-1)-1} \\
&= -1 + \binom{k+2}{k+1} + \sum_{i=1}^{\lfloor\frac{k+1}{2}\rfloor} (-1)^{i} \cdot \binom{k-i+2}{k-2i+1} \\
&= -1 + \sum_{i=0}^{\lfloor\frac{k+1}{2}\rfloor} (-1)^{i} \cdot \binom{k-i+2}{k-2i+1} \\
&= -1 + S(k+2).
\end{aligned}
$$

Therefore, we have proven that $S(k+2) - S(k+1) + S(k) = 1$, for all $k \geq 1$. ■

Corollary 4.13 *$S(u) = S(v)$ whenever $u \equiv v \pmod 6$.*

Proof: By Lemma 4.12, we have

$$
\begin{aligned}
S(k+6) - S(k+5) + S(k+4) &= 1 \\
S(k+5) - S(k+4) + S(k+3) &= 1 \\
-S(k+3) + S(k+2) - S(k+1) &= -1 \\
-S(k+2) + S(k+1) - S(k) &= -1
\end{aligned}
$$

Adding the four equations, we have $S(k+6) - S(k) = 0$. This identity holds for any $k \geq 1$, and hence the sequence $\{S(k)\}_{k=1}^{\infty}$ has period 6. It is easy to show that $S(5) = S(6) = 0$, $S(1) = S(4) = 1$, and $S(2) = S(3) = 2$. Thus, we can use these initial values to compute $S(k)$, for any $k \geq 1$. ■

Having established Lemma 4.12 and Corollary 4.13, we now determine an infinite family of circulants for which $\chi_l(G) = 3$ for every graph in this family. We provide two proofs: the first will be a combinatorial enumeration, and the second will use independence polynomials. The following theorem is a generalization of Proposition 4.11.

Theorem 4.14 *Let G be the circulant $C_{3m,\{1,2\}}$, where $m \geq 2$ is an integer. Then, $\chi_l(G) = 3$.*

Proof: Since K_3 is a subgraph of G, we have $\chi_l(G) \geq \chi(G) = 3$. We now use Theorem 4.10 to prove that $\chi_l(G) \leq 3$. Given an orientation $\overrightarrow{G}$, define u_k to be the number of Eulerian subgraphs of $\overrightarrow{G}$ with k edges. We determine a formula for u_k.

Case 1: $m = 2n+1$ is odd.

Note that G is the union of two disjoint Hamiltonian cycles, namely $C_{3m,\{1\}}$ and $C_{3m,\{2\}}$. Orient each edge of these cycles clockwise, i.e., $v \to v+1$ and $v \to v+2$, where addition is computed mod $(6n+3)$. Each vertex in this digraph has out-degree 2, and so it suffices to prove that $ee(\overrightarrow{G}) \neq eo(\overrightarrow{G})$ for this orientation $\overrightarrow{G}$. Since $\overrightarrow{G}$ is Eulerian and $|E(\overrightarrow{G})| = 12n+6$, $u_k = u_{12n+6-k}$ for $0 \leq k \leq 6n+3$. By inspection, $u_0 = 1$ and $u_{6n+3} = 2$. So let us assume that $1 \leq k \leq 6n+2$.

Let $\overrightarrow{C_k}$ be a connected Eulerian subgraph of $\overrightarrow{G}$ with k edges. We now prove that each $\overrightarrow{C_k}$ must be a directed cycle. Since $\overrightarrow{C_k}$ has k edges, the entire trail $\overrightarrow{C_k}$ consists of $k+1$ vertices, with possibly some vertices overlapping. But $\overrightarrow{C_k}$ is Eulerian, and so the last vertex must coincide with the first vertex v_1, so that v_1 has the same in-degree and out-degree.

If the vertices of $\overrightarrow{C_k}$ are $v_1, v_2, \ldots, v_k, v_1$ (in that order), then we must have $v_{i+1} - v_i = 1$ or $2 \pmod{6n+3}$, for each $1 \leq i \leq k$. Thus, the difference sequence of each $\overrightarrow{C_k}$ must only contain 1's and 2's. Furthermore, its sum must be congruent to 0 (mod $6n+3$), because the trail $\overrightarrow{C_k}$ starts and ends at the same vertex v_1.

Since $1 \leq k \leq 6n+2$, it follows that the sum of these k elements must be at least 1 and at most $12n+4$, since each term is 1 or 2. From the previous paragraph, this sum is congruent to 0 (mod $6n+3$). Thus, this sum must be exactly $6n+3$. In other words, the trail $\overrightarrow{C_k}$ makes exactly one loop around the $6n+3$ vertices of the circulant, before returning to the initial vertex.

Note that every connected Eulerian subgraph on k edges (with $k \leq 6n+2$) must satisfy $k \geq \lceil \frac{6n+3}{2} \rceil = 3n+2$. And so $\overrightarrow{C_k}$ cannot have more than one component. Thus, every Eulerian subgraph $\overrightarrow{C_k}$ (with $1 \leq k \leq 6n+2$) is connected, and hence, is a directed cycle.

To enumerate the number of possible Eulerian subgraphs $\overrightarrow{C_k}$, we will determine the number of k-tuples $(d_1, d_2, \ldots, d_k)$ such that $d_1 + \ldots + d_k = 6n+3$, with each $d_i \in \{1, 2\}$. We then will match up this k-tuple to a directed Eulerian subgraph $\overrightarrow{C_k}$, and check to make sure that each subgraph is counted only once.

Suppose that in a given k-tuple $(d_1, d_2, \ldots, d_k)$, exactly i of the elements are 1 and the other $k-i$ elements are 2. Then we have $i + 2(k-i) = 6n+3$, which gives $i = 2k-6n-3$. So there are $\binom{k}{2k-6n-3}$ k-tuples satisfying the required conditions.

We consider two cases: either $\overrightarrow{C_k}$ includes vertex 0, or it does not. As mentioned earlier, each $\overrightarrow{C_k}$ must be a directed cycle. So in our enumeration of all directed cycles, we will cyclically arrange the vertices of each $\overrightarrow{C_k}$ so that the indices are in increasing order (i.e., the first vertex is either 0 or 1).

If $\overrightarrow{C_k}$ includes vertex 0, then there are $\binom{k}{2k-6n-3}$ possibilities for $\overrightarrow{C_k}$, a unique directed cycle for each of our k-tuples above. If $\overrightarrow{C_k}$ does not include vertex 0, then it must include vertex 1. Hence, in our k-tuple $(d_1, d_2, \ldots, d_k)$ corresponding to the difference sequence of $\overrightarrow{C_k}$, the last entry must be 2 (and not 1). Thus, we need to enumerate the number of k-tuples satisfying this extra condition. In our k-tuple, we can select any $i = 2k-6n-3$ of the first $k-1$ elements to be 1. Thus, there are $\binom{k-1}{2k-6n-3}$ possible choices. Each k-tuple corresponds to a unique $\overrightarrow{C_k}$ that does not include the vertex 0.

We have considered all possible cases, and so we conclude that

$$u_k = \binom{k}{2k-6n-3} + \binom{k-1}{2k-6n-3},$$

for each $1 \leq k \leq 6n+2$.

We now have a formula for u_k for each $1 \leq k \leq 6n+2$. Using this formula, we can determine an expression for $ee(\overrightarrow{G}) - eo(\overrightarrow{G})$ in terms of $S(n)$, as defined in

Lemma 4.12. We have

$$
\begin{aligned}
& ee(\overrightarrow{G}) - eo(\overrightarrow{G}) \\
= \ & \sum_{k=0}^{|E(\overrightarrow{G})|} (-1)^k u_k \\
= \ & \sum_{k=0}^{12n+6} (-1)^k u_k \\
= \ & 2 \cdot \left(\sum_{k=1}^{6n+2} (-1)^k u_k \right) + u_0 - u_{6n+3} + u_{12n+6} \\
= \ & 2 \cdot \left(\sum_{k=1}^{6n+2} (-1)^k u_k \right) + 1 - 2 + 1 \\
= \ & 2 \cdot \sum_{k=1}^{6n+2} (-1)^k \binom{k}{2k-6n-3} + 2 \cdot \sum_{k=1}^{6n+2} (-1)^k \binom{k-1}{2k-6n-3} \\
= \ & 2 \cdot \sum_{k=1}^{6n+2} (-1)^k \binom{k}{2k-6n-3} + 2 \cdot \sum_{k=1}^{6n+1} (-1)^k \binom{k-1}{2k-6n-3} + 2 \cdot (-1)^{6n+2} \cdot 1 \\
= \ & 2 \cdot \sum_{k=1}^{6n+2} (-1)^k \binom{k}{2k-6n-3} + 2 \cdot \sum_{k=1}^{6n+1} (-1)^k \binom{k-1}{2k-6n-3} + 2 \\
= \ & 2 \cdot \sum_{i=0}^{6n+1} (-1)^{6n+2-i} \binom{6n+2-i}{6n+1-2i} + 2 \cdot \sum_{i=0}^{6n} (-1)^{6n+1-i} \binom{6n-i}{6n-1-2i} + 2 \\
= \ & 2 \cdot \sum_{i=0}^{3n} (-1)^{6n+2-i} \binom{6n+2-i}{6n+1-2i} + 2 \cdot \sum_{i=0}^{3n-1} (-1)^{6n+1-i} \binom{6n-i}{6n-1-2i} + 2 \\
= \ & 2 \cdot \sum_{i=0}^{3n} (-1)^{i} \binom{6n+2-i}{6n+1-2i} - 2 \cdot \sum_{i=0}^{3n-1} (-1)^{i} \binom{6n-i}{6n-1-2i} + 2 \\
= \ & 2S(6n+2) - 2S(6n) + 2.
\end{aligned}
$$

By Corollary 4.13, $ee(\overrightarrow{G}) - eo(\overrightarrow{G}) = 2(S(6n+2) - S(6n) + 1) = 2(S(2) - S(6) + 1) = 2(2 - 0 + 1) = 6$. Since this number is not 0, Theorem 4.10 implies that $\chi_l(G) = 3$.

<u>*Case 2:*</u> $m = 2n$ is even.

Note that G is the edge-disjoint union of $C_{3m,\{1\}}$ and $C_{3m,\{2\}}$. The former is a Hamiltonian cycle, and the latter is the union of two disjoint cycles on $3n$ vertices. Orient each of these three cycles clockwise, i.e., $v \to v+1$ and $v \to v+2$, where addition is computed mod $6n$. Each vertex in this digraph has out-degree 2.

By following the exact same technique as Case 1, we see that $u_0 = 1$, $u_{6n} = 2$, and $u_k = u_{12n-k}$ for all $1 \leq k \leq 6n-1$. By the same reasoning as in the previous case, for any Eulerian subgraph $\overrightarrow{C_k}$ with $1 \leq k \leq 6n-1$, $\overrightarrow{C_k}$ must be a directed cycle. By the same combinatorial technique as earlier, we determine that $u_k = \binom{k}{2k-6n} + \binom{k-1}{2k-6n}$, for each $1 \leq k \leq 6n-1$. Using this formula, we now determine an expression for $ee(\overrightarrow{G}) - eo(\overrightarrow{G})$ in terms of $S(n)$. We have

$$\begin{aligned}
& ee(\overrightarrow{G}) - eo(\overrightarrow{G}) \\
= \; & \sum_{k=0}^{|E(\overrightarrow{G})|} (-1)^k u_k \\
= \; & \sum_{k=0}^{12n} (-1)^k u_k \\
= \; & 2 \cdot \left(\sum_{k=1}^{6n-1} (-1)^k u_k \right) + u_0 + u_{6n} + u_{12n} \\
= \; & 2 \cdot \left(\sum_{k=1}^{6n+2} (-1)^k u_k \right) + 1 + 2 + 1 \\
= \; & 2 \cdot \sum_{k=1}^{6n-1} (-1)^k \binom{k}{2k-6n} + 2 \cdot \sum_{k=1}^{6n-1} (-1)^k \binom{k-1}{2k-6n} + 4 \\
= \; & 2 \cdot \sum_{k=1}^{6n-1} (-1)^k \binom{k}{2k-6n} + 2 \cdot \sum_{k=1}^{6n-2} (-1)^k \binom{k-1}{2k-6n} + 2 \cdot (-1)^{6n-1} \binom{6n-2}{6n-2} + 4 \\
= \; & 2 \cdot \sum_{k=1}^{6n-1} (-1)^k \binom{k}{2k-6n} + 2 \cdot \sum_{k=1}^{6n-2} (-1)^k \binom{k-1}{2k-6n} + 2 \\
= \; & 2 \cdot \sum_{i=0}^{6n-2} (-1)^{6n-1-i} \binom{6n-1-i}{6n-2-2i} + 2 \cdot \sum_{i=0}^{6n-3} (-1)^{6n-2-i} \binom{6n-3-i}{6n-4-2i} + 2 \\
= \; & 2 \cdot \sum_{i=0}^{3n-1} (-1)^{6n-1-i} \binom{6n-1-i}{6n-2-2i} + 2 \cdot \sum_{i=0}^{3n-2} (-1)^{6n-2-i} \binom{6n-3-i}{6n-4-2i} + 2 \\
= \; & -2 \cdot \sum_{i=0}^{3n-1} (-1)^{i} \binom{6n-1-i}{6n-2-2i} + 2 \cdot \sum_{i=0}^{3n-2} (-1)^{i} \binom{6n-3-i}{6n-4-2i} + 2 \\
= \; & -2S(6n-1) + 2S(6n-3) + 2.
\end{aligned}$$

Therefore, $ee(\overrightarrow{G}) - eo(\overrightarrow{G}) = 2(S(6n-3) - S(6n-1) + 1)$. By Corollary 4.13, this quantity equals $2(S(3) - S(5) + 1) = 2(2 - 0 + 1) = 6$. Since this number is not 0, Theorem 4.10 implies that $\chi_l(G) = 3$. ∎

This combinatorial argument has some nice ideas, but there is a more elegant proof of Theorem 4.14. For this proof, we incorporate ideas from our earlier work on independence polynomials. We deliberately include both proofs in this section to contrast the different techniques involved, and illustrate the power of connecting our problem to the theory of independence polynomials. First, we require a new definition.

Definition 4.15 *Let $\overrightarrow{G}$ be a digraph. Then, the* **Alon-Tarsi polynomial** *of $\overrightarrow{G}$ is $AT(\overrightarrow{G}, x) = \sum_{k=0}^{|E(\overrightarrow{G})|} u_k \cdot x^k$, where u_k is the number of Eulerian subgraphs of $\overrightarrow{G}$ with k edges.*

For example, in our earlier example for $G = C_{9,\{1,2\}}$, the Alon-Tarsi polynomial is

$$AT(\overrightarrow{G}, x) = 1 + 9x^5 + 30x^6 + 27x^7 + 9x^8 + 2x^9 + 9x^{10} + 27x^{11} + 30x^{12} + 9x^{13} + x^{18}.$$

The following observation is trivial.

Corollary 4.16 *$ee(\overrightarrow{G}) - eo(\overrightarrow{G}) \neq 0$ iff -1 is not a root of $AT(\overrightarrow{G}, x)$.*

There is a significant benefit to combining these values of u_k into one polynomial. As we will see in the following proof, we will now be able to compute the coefficients of the Alon-Tarsi polynomial without actually enumerating any subgraphs (as in the first proof to Theorem 4.14). Once we obtain the polynomial, we just need to check if $x = -1$ is a root. If it is not, then we obtain the desired condition that $ee(\overrightarrow{G}) \neq eo(\overrightarrow{G})$, which enables us to apply Theorem 4.10.

Lemma 4.17 *Define $H_n = C_{n,\{1,2\}}$. Let $\overrightarrow{H_n}$ be the orientation of H_n where $v \to v+1$ and $v \to v+2$ (mod n), for $0 \leq v \leq n-1$. Then,*

$$AT(\overrightarrow{H_n}, x) = x^n \cdot \left[I(C_n, x) + I\left(C_n, \frac{1}{x}\right) \right] + (1 + x^{2n}).$$

Proof: As an example, $1 \to 3 \to 4 \to 6 \to 8 \to 0 \to 1$ is a directed 6-cycle of $\overrightarrow{H_9}$. As discussed in the proof of Theorem 4.14, for each Eulerian subgraph with $n-k$ edges (with $1 \leq k \leq n-1$), the subgraph must be isomorphic to $\overrightarrow{C_{n-k}}$, and hence, there are k isolated vertices. Thus, for each Eulerian subgraph of $\overrightarrow{H_n}$ on $n-k$ vertices, there are k isolated vertices which we will represent by set S. So in the above example of our directed 6-cycle of $\overrightarrow{H_9}$, we have $S = \{2, 5, 7\}$. We claim that these k vertices are independent in C_n. In other words, we prove that each subgraph $\overrightarrow{C_{n-k}}$ of $\overrightarrow{H_n}$ can be mapped to an independent set of C_n by showing that no isolated pair of vertices in $\overrightarrow{C_{n-k}}$ is adjacent in C_n.

On the contrary, suppose that S contains two adjacent vertices t and $t+1$. Then the directed cycle $\overrightarrow{C_{n-k}}$ (formed by the complement of these k vertices) cannot include either of these two vertices. But in this directed cycle $v_1 \to v_2 \to \ldots \to v_{n-k} \to v_1$, each $v_{i+1} - v_i \pmod{n}$ equals 1 or 2. So at least one of t or $t+1$ must appear in the directed cycle, which gives us our desired contradiction. Thus, each of the u_{n-k} possible Eulerian subgraphs maps to a unique independent set of C_n with k vertices. Similarly, for any set of k independent vertices in C_n, its complement will consist of $n-k$ vertices, which can be ordered to form a unique directed cycle in $\overrightarrow{H_n}$. We simply arrange the $n-k$ vertices in increasing order (from 0 to $n-1$), and this will give us the desired directed cycle in $\overrightarrow{H_n}$, since each pair of adjacent vertices has a distance of 1 or 2. Letting i_k be the number of independent sets of cardinality k in C_n, we conclude that $i_k = u_{n-k}$, for each $1 \leq k \leq n-1$.

We observe that $u_0 = 1$, $u_n = 2$, and $u_{2n-k} = u_k$ for each $1 \leq k \leq n-1$. Also, $i_0 = 1$. Therefore,

$$\begin{aligned}
AT(\overrightarrow{H_n}, x) &= \sum_{k=0}^{2n} u_k \cdot x^k \\
&= 1 + \sum_{k=1}^{n-1} u_k \cdot x^k + 2x^n + \sum_{k=n+1}^{2n-1} u_k \cdot x^k + x^{2n} \\
&= \sum_{k=1}^{n-1} u_k \cdot x^k + \sum_{k=n+1}^{2n-1} u_k \cdot x^k + (1 + 2x^n + x^{2n}) \\
&= \sum_{k=1}^{n-1} u_{n-k} \cdot x^{n-k} + \sum_{k=n+1}^{2n-1} u_{2n-k} \cdot x^k + (1 + 2x^n + x^{2n})
\end{aligned}$$

$$
\begin{aligned}
&= x^n \cdot \sum_{k=1}^{n-1} u_{n-k} \cdot x^{-k} + \sum_{k=1}^{n-1} u_{n-k} \cdot x^{n+k} + (1 + 2x^n + x^{2n}) \\
&= x^n \cdot \sum_{k=1}^{n-1} i_k \cdot x^{-k} + x^n \cdot \sum_{k=1}^{n-1} i_k \cdot x^k + (1 + 2x^n + x^{2n}) \\
&= x^n \cdot \left[I\left(C_n, \frac{1}{x}\right) + I(C_n, x) \right] - 2i_0 \cdot x^n + (1 + 2x^n + x^{2n}) \\
&= x^n \cdot \left[I(C_n, x) + I\left(C_n, \frac{1}{x}\right) \right] + (1 + x^{2n}).
\end{aligned}
$$

Thus, we have established the desired identity. ∎

As an immediate corollary, we have a new and elegant proof to Theorem 4.14.

Proof: Let $G = C_{3m,\{1,2\}}$, where $\overrightarrow{G}$ is the same orientation as described in the statement of Lemma 4.17. Then, from Lemma 4.17, we have

$$AT(\overrightarrow{G}, x) = x^{3m} \cdot \left[I(C_{3m}, x) + I\left(C_{3m}, \frac{1}{x}\right) \right] + (1 + x^{6m}).$$

Substituting $x = -1$, we have $AT(\overrightarrow{G}, -1) = (-1)^{3m} \cdot 2 \cdot I(C_{3m}, -1) + 2$. From Lemma 2.2, $I(C_k, x) = I(C_{k-1}, x) + x \cdot I(C_{k-2}, x)$ for all $k \geq 4$. Substituting $x = -1$, $I(C_k, -1) = I(C_{k-1}, -1) - I(C_{k-2}, -1)$. From the initial values $I(C_2, -1) = -1$ and $I(C_3, -1) = -2$, we immediately see that $I(C_{3m}, -1) = 2$ when m is even, and $I(C_{3m}, -1) = -2$ when m is odd. In other words, $I(C_{3m}, -1) = 2 \cdot (-1)^m$.

Therefore, $AT(\overrightarrow{G}, -1) = (-1)^{3m} \cdot 2 \cdot I(C_{3m}, -1) + 2 = (-1)^{3m} \cdot 2 \cdot 2 \cdot (-1)^m + 2 = 4 + 2 = 6$.

Since $x = -1$ is not a root of $AT(\overrightarrow{G}, x)$, Corollary 4.16 implies that $ee(\overrightarrow{G}) - eo(\overrightarrow{G}) \neq 0$. By Theorem 4.10, we conclude that $\chi_l(G) = 3$. ∎

We remark that when $n \not\equiv 0 \pmod 3$, Theorem 4.10 does not help us, since $AT(\overrightarrow{G}, -1) = 2 \cdot (-1)^n \cdot I(C_n, -1) + 2 = 0$. Thus, we need to develop alternative techniques to determine the list-colouring number of $C_{n,\{1,2\}}$, for $n \not\equiv 0 \pmod 3$.

To determine the list-colouring number of $C_{3m,\{1,2\}}$, we developed a bijection between Eulerian subgraphs of $C_{3m,\{1,2\}}$ and independent sets of C_{3m}. This enabled us to apply Theorem 4.10. Naturally, this leads us to ask if there are any other pairs of graph families (G, H) for which we can obtain a simple correspondence between Eulerian subgraphs of G and independent sets of H. We hypothesize that this technique can be applied to calculate the values of $\chi_l(G)$, for other families of graphs G.

4.3 Well-Covered Circulants

Definition 4.18 ([147]) *A graph G is* **well-covered** *if each maximal independent set of vertices has the same cardinality.*

In other words, a graph is well-covered iff every *maximal* independent set is also a *maximum* independent set.

Given a graph G, the problem of determining $\alpha(G)$ is NP-hard [79]. But in a well-covered graph, every independent set can be extended to a maximum independent set, and so $\alpha(G)$ can be trivially computed using the greedy algorithm. In other words, there is a polynomial-time algorithm to compute $\alpha(G)$ for any well-covered graph. Well-covered graphs were first introduced by Plummer in [147], and a detailed survey of properties of well-covered graphs appears in his survey article [148].

As an example, C_7 is well-covered because each maximal independent set has three vertices. However, C_6 is not well-covered because the maximal independent sets are $\{0,3\}$, $\{1,4\}$, $\{2,5\}$, $\{0,2,4\}$, and $\{1,3,5\}$, and these sets do not all have the same cardinality.

In this section, we will classify circulant graphs that are well-covered, by applying our previously-determined formulas for independence polynomials. We characterize the set of all well-covered circulant graphs $C_{n,S}$ for the families $S = \{1, 2, \dots, d\}$ and $S = \{d+1, d+2, \dots, \lfloor \frac{n}{2} \rfloor\}$, as well as for the family of circulants of degree 3. By applying the lexicographic product to these well-covered graphs, we will also generate a larger infinite family of well-covered circulants. Determining whether a graph is well-covered is co-NP-complete [44, 157]. Even when restricted to the family of circulants, we prove that it is *still* co-NP-complete to determine if the graph is well-covered. Thus, there will not exist a nice characterization of well-covered circulants. Nevertheless, we make some progress in characterizing families of well-covered circulants.

To start this section, we first list all connected non-isomorphic well-covered circulants on at most 12 vertices. Table 4.2 was generated via a simple Maple program that enumerated maximum independent sets, and manually checked the well-covered property of each circulant.

$\boldsymbol{n}$	Possible generating sets $\boldsymbol{S}$
6	$\{1,3\}$
7	$\{1\}$
8	$\{1,3\},\{1,4\}$
9	$\{1,3\},\{1,2,4\}$
10	$\{1,4\},\{2,5\},\{1,2,5\},\{1,3,5\}$
11	$\{1,2\},\{1,3\},\{1,2,4\}$
12	$\{1,4\},\{3,4\},\{1,2,6\},\{1,3,5\},\{1,3,6\},\{2,3,4\}$, {2,3,6}, $\{1,4,6\},\{3,4,6\},\{1,2,4,5\},\{1,3,4,6\},\{1,3,5,6\},\{1,2,3,5,6\}$

Table 4.2: Connected well-covered circulants on at most 12 vertices.

A characterization of all well-covered cubic graphs (i.e., graphs of degree 3) is found in [28]. A natural question is to determine which of these graphs are circulants. In this section, we answer this problem in two different ways. Our first proof will follow from the main classification theorem given in [28], while our second proof will follow more elegantly from our work on independence polynomials. In Chapter 3, we introduced the infinite family of circulant graphs $G_{j,k}$. In this chapter, we determine a necessary and sufficient condition for a circulant $G_{j,k}$ to be well-covered.

The independence polynomial of well-covered graphs has been a topic of interest. Brown, Dilcher, and Nowakowski [22] conjectured that if G is well-covered, then $I(G,x)$ is *unimodal* (i.e., the coefficients of $I(G,x)$ are increasing up to a certain term, then decreasing after that term). This was disproved by Michael and Traves in [133], who found counterexamples for $\alpha(G) \in \{4,5,6,7\}$. Matchett [130] extended this result by showing that for all $4 \leq \alpha(G) \leq 11$, there exists a counterexample G to the well-covered unimodality conjecture. Recently in [118], Levit and Mandrescu discovered a general construction for counterexamples for any $\alpha(G) \geq 8$.

Motivated by the literature connecting independence polynomials to well-covered graphs, we investigate well-covered *circulant* graphs, and determine necessary and sufficient conditions for certain circulants to be well-covered. In some of our proofs, we directly apply our earlier theorems on independence polynomials. The basic strategy is as follows: to prove that a graph G is not well-covered, we first list all of its maximum independent sets, and then determine a smaller independent set I' that is not a subset of any of these maximum independent sets. This proves the existence of a maximal independent set that is not maximum, which implies that G is not well-covered.

If we know the exact formula for some $I(C_{n,S}, x)$, we can calculate the $x^{\alpha(C_{n,S})}$ coefficient of the polynomial, giving us the exact number of maximum independent sets. Thus, once our enumeration technique has found $[x^{\alpha(C_{n,S})}]I(C_{n,S}, x)$ independent sets of maximum cardinality, we can immediately stop, because we know that there cannot be any more. This method of extracting the coefficients of our independence polynomials is powerful when proving that a particular circulant is not well-covered. Another technique is to investigate difference sequences; this will be our approach in proving the following two theorems on the well-coveredness of $C_{n,\{1,2,\ldots,d\}}$ and $C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$. After we obtain these two results, we prove our result on the well-coveredness of cubic circulants.

It is well-known [71] that C_n is well-covered iff $n \leq 5$ or $n = 7$. The following theorem generalizes this result.

Theorem 4.19 *Let $d \geq 1$ be fixed. Then, $C_{n,\{1,2,\ldots,d\}}$ is well-covered iff $n \leq 3d + 2$ or $n = 4d + 3$.*

Proof: Let $G = C_{n,\{1,2,\ldots,d\}}$. By Theorem 2.3, $\alpha(G) = \lfloor \frac{n}{d+1} \rfloor = p$, for some integer p. Then, $n = (d+1)p + q$, for some $0 \leq q \leq d$. If $p \leq 2$, then G is trivially well-covered. This is seen by noting that G is a circulant, and hence every vertex of G appears in some maximum independent set, by vertex transitivity. Since the $p \leq 2$ case been dealt with, assume that $p \geq 3$.

Let a and b be the unique pair of integers such that $n = a(p-1) + b$, where $0 \leq b \leq p-2$. Since $n = (d+1)p + q = a(p-1) + b$, it follows that $a \geq d + 1$.

Consider the difference sequence

$$D' = (\underbrace{a,\ a,\ \ldots,\ a}_{p-b-1}, \underbrace{a+1,\ a+1,\ \ldots,\ a+1}_{b}).$$

The sum of the elements of D' is $(p-b-1)a + b(a+1) = n$. Each term in the sequence is at least $d+1$. Thus, D' is a valid difference sequence of G with $|D'| = p-1$. It follows that D' must be the difference sequence of (at least) one independent set $I' = \{v_1, v_2, \ldots, v_{p-1}\}$, with $0 \le v_1 < v_2 < \ldots < v_{p-1} \le n-1$.

If G is well-covered, then there exists an independent set I of cardinality $\alpha(G) = p$ with $I' \subset I$. Let $I = I' \cup \{w\}$, for some $0 \le w \le n-1$. Suppose $1 \le j \le p-1$ is the index for which $v_j < w < v_{j+1}$, where addition is reduced mod $(p-1)$.

Since I is an independent set of G, we require $v_{j+1} - w \ge d+1$ and $w - v_j \ge d+1$. Hence, $v_{j+1} - v_j \ge 2d+2$. In other words, a necessary condition for G to be well-covered is $a+1 \ge v_{j+1} - v_j \ge 2d+2$, which simplifies to

$$\left\lfloor \frac{(d+1)p+q}{p-1} \right\rfloor = a \ge 2d+1.$$

First suppose that $p \ge 4$. Then,

$$\left\lfloor \frac{(d+1)p+q}{p-1} \right\rfloor \le \frac{(d+1)p+d}{p-1} = d+1+\frac{2d+1}{p-1} \le d+1+\frac{2d+1}{3} \le 2d+1,$$

with equality iff $(p,d,q) = (4,1,1)$. This case (which corresponds to $G = C_9$) is not well-covered; this is easily seen by inspection. In all other cases, we have established a contradiction. Thus, G is not well-covered if n and d satisfy $\alpha(G) = p = \lfloor \frac{n}{d+1} \rfloor \ge 4$.

Now suppose $p = 3$. Then if $q \le d-2$, then

$$\left\lfloor \frac{(d+1)p+q}{p-1} \right\rfloor = \left\lfloor \frac{3(d+1)+q}{2} \right\rfloor \le \left\lfloor \frac{3(d+1)+(d-2)}{2} \right\rfloor = \left\lfloor \frac{4d+1}{2} \right\rfloor < 2d+1.$$

Hence, if $p = 3$ and G is well-covered, then we must have $q = d$ or $q = d-1$. Thus, the only two possible well-covered graphs occur in the cases $(p,q) = (3,d)$ and $(p,q) = (3,d-1)$. These pairs correspond to the circulants $G = C_{4d+3,\{1,2,\ldots,d\}}$ and $G = C_{4d+2,\{1,2,\ldots,d\}}$, respectively. We prove that the former is well-covered, while the latter is not.

Consider the graph $G = C_{4d+3,\{1,2,\ldots,d\}}$. By Theorem 2.3, $\alpha(G) = \lfloor \frac{4d+3}{d+1} \rfloor = 3$. We show that every maximal independent set has cardinality 3. Let I' be an independent 2-set. Without loss, let $I' = \{0, x\}$, for some $x \in [d+1, 3d+2]$. If $d+1 \leq x \leq 2d+1$, then $I = \{0, x, x+d+1\}$ is an independent 3-set of G. If $2d+2 \leq x \leq 3d+2$, then $I = \{0, d+1, x\}$ is an independent 3-set of G. In both cases, I' can be extended to a maximum independent set I. Thus, we have shown that every maximal independent set has cardinality $p = 3$, proving that G is well-covered.

Now consider the graph $G = C_{4d+2,\{1,2,\ldots,d\}}$. Assume G is well-covered. By Theorem 2.3, $\alpha(G) = \lfloor \frac{4d+2}{d+1} \rfloor = 3$. Thus, every maximal independent set must have three vertices. Since the set $I' = \{0, 2d+1\}$ is independent in G, there must exist a vertex x such that $I = I' \cup \{x\}$ is independent in G. If $0 \leq x \leq d$ or $3d+2 \leq x \leq 4d+1$, then $|x-0|_{4d+2} \leq d$, and if $d+1 \leq x \leq 3d+1$, then $|x-(2d+1)|_{4d+2} \leq d$. In both cases, we obtain a contradiction. Thus, no such x exists. We have shown that I cannot be an independent set in G, and so I' is a maximal independent set in G (with cardinality 2). Hence, G is not well-covered in this case.

We conclude that if $p \geq 3$, then G is well-covered only for the case $(p, q) = (3, d)$, i.e., when $n = 4d+3$. If $p \leq 2$, then $n \leq 3d+2$, and G is trivially well-covered in each of these cases. We conclude that $G = C_{n,\{1,2,\ldots,d\}}$ is well-covered iff $n \leq 3d+2$ or $n = 4d+3$, and this completes the proof. ∎

At the conclusion of this section, we prove that it is co-NP-complete to determine whether an arbitrary circulant G is well-covered. Despite the difficulty of the general problem, we have given a full characterization of well-covered graphs for the family $A_n = C_{n,\{1,2,\ldots,d\}}$. We now determine a full characterization for the complement family $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$.

Theorem 4.20 *Let $d \geq 1$ be fixed. Define $G = B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$ for all $n \geq 2d+2$. Then G is well-covered iff $n > 3d$ or $n = 2d+2$.*

Proof: First note that $G = B_n$ is clearly well-covered if $n = 2d+2$, since G is simply $d+1$ isomorphic copies of K_2. Thus, we can assume that $n > 2d+2$.

By Corollary 2.18, $\alpha(G) = d + 1$. It is easy to see that the difference sequence $(\underbrace{1,\, 1,\, \ldots,\, 1}_{d}, n-d)$ is valid. This gives rise to n independent sets of cardinality $d+1$, namely the sets $\{i, i+1, i+2, \ldots, i+d\}$, for each $i = 0, \ldots, n-1$, where the elements are reduced mod n. By Corollary 2.18, $[x^{d+1}]I(B_n, x) = n$, and so there cannot be any other maximum independent sets. Therefore, if G is well-covered, then every independent set must be a subset of $\{i, i+1, i+2, \ldots, i+d\}$ for some $0 \le i \le n-1$.

First consider the case $2d + 3 \le n \le 3d$. In this case, $d \ge 3$. The set $I' = \{0, d, n-d\}$ is independent in G, since the circular distances are d, $n-d$, and $n - 2d \le d$, none of which appear in the generating set $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. But I' cannot be contained in an independent set of cardinality $d+1 > 3$, since there is no i for which $I' \subseteq \{i, i+1, i+2, \ldots, i+d\}$. Hence, I' cannot be extended to a maximal independent set of cardinality $d+1$, and so G is not well-covered.

Finally, consider the case $n > 3d$. Let I' be any independent set $\{v_1, v_2, \ldots, v_k\}$, with $k < d+1$. Without loss, assume that $v_1 = 0$ and $0 < v_2 < v_3 < \ldots < v_k \le n-1$. Since I' is independent in G, no $v_i \in [d+1, n-d-1]$. So each $v_i \le d$ or $v_i \ge n-d$. If $v_2 \ge n-d$, then $I' \subset \{i, i+1, i+2, \ldots, i+d\}$ where $i = n-d$. If $v_k \le d$, then $I' \subset \{i, i+1, i+2, \ldots, i+d\}$ where $i = 0$. In both cases, I' is contained in a maximal independent set of cardinality $d+1$. So the only other case to consider is when $v_2 \le d$ and $v_k \ge n-d$. Then there is a unique index j such that $v_j \le d$ and $v_{j+1} \ge n-d$. We require $|v_{j+1} - v_j|_n \notin \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$, so $|v_{j+1} - v_j|_n \le d$. Since $0 \le v_j \le d$, this implies that $v_{j+1} \ge n + v_j - d$. Letting $i = n + v_j - d$, we have $I' \subset \{i, i+1, i+2, \ldots, i+d\}$, which shows that I' is contained in a maximal independent set of cardinality $d+1$. This proves that all maximal independent sets have the same cardinality, so G is well-covered.

Thus, we have proven that B_n is well-covered iff $n > 3d$ or $n = 2d+2$. ∎

In Chapter 2, we introduced the graph families A_n and B_n, and examined the class of 3-regular circulants. Having determined the well-coveredness of A_n and B_n, it is a natural question to investigate which 3-regular circulants are well-covered. Our first proof will rely on a known classification of the set of well-covered cubic graphs. Our second proof will be a more elegant proof, which will be a short application of independence polynomials. We provide both proofs as they utilize completely different techniques.

Definition 4.21 *Let X, Y, Z be the graphs defined in Figure 4.8.*

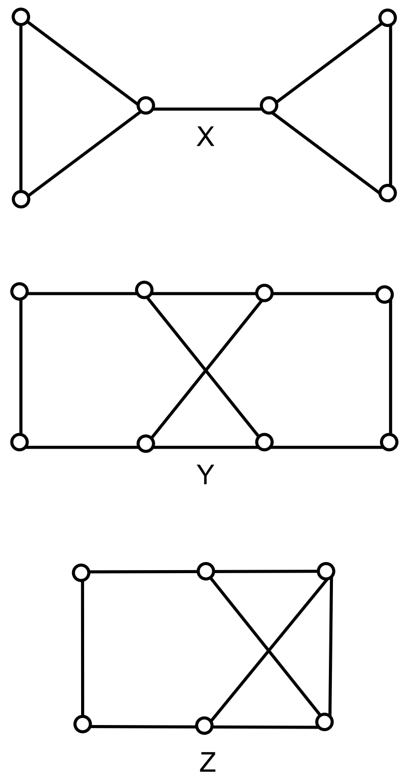

Figure 4.8: Graphs which generate the family of cubic graphs.

Definition 4.22 *A* **terminal pair** *is a pair of adjacent vertices of degree* 2*.*

Thus, X and Y have two terminal pairs while Z has only one.

Theorem 4.23 ([28]) *Let Ψ denote the class of cubic graphs, constructed as follows: given a collection of copies of X, Y, Z, join every terminal pair by two edges to a terminal pair in another (possibly the same) graph, so that the result is cubic. Then every graph in Ψ is well-covered.*

Because X and Y have automorphisms exchanging the two vertices in one terminal pair while fixing the vertices in the other terminal pair, it does not matter how we join up each pair of terminal pairs. Realizing that each X and Y have two terminal pairs and each Z has one, we construct graphs in the family Ψ by stringing together copies of X and Y in cycles, or in paths with a copy of Z at each end. Thus, a connected graph in Ψ can be characterized by giving the sequence in which we join the X's, Y's, and Z's. For example, the graph $ZXYYZ$ is a cubic well-covered graph, as is $-XYYXY-$. In the latter case, the *dashes* indicate that the remaining terminal pairs at the endpoints are to be joined in a cycle.

When we form "cyclic" elements of Ψ, we can use just a single X or Y. Thus, the graphs $-X-$ and $-Y-$ belong to the family Ψ. We can quickly show that the former is isomorphic to $C_{6,\{2,3\}}$ and the latter is isomorphic to $C_{8,\{1,4\}}$. In [28], the following characterization theorem of well-covered connected cubic graphs is presented.

Theorem 4.24 ([28]) *Let G be a connected cubic graph. Then G is well-covered iff $G \in \Psi$, $G = K_{3,3}$, $G = K_4$, or G is one of the four graphs in Figure 4.9.*

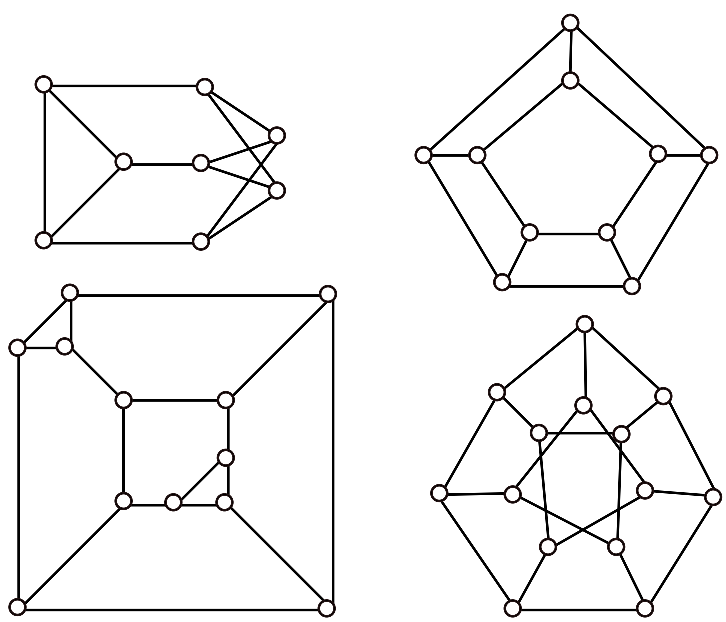

Figure 4.9: Four well-covered cubic graphs.

Using this characterization, we now determine all connected well-covered *circulant* graphs of degree 3.

Theorem 4.25 *Let G be a connected circulant cubic graph. If G is well-covered, then G must be isomorphic to one of the following graphs: $C_{4,\{1,2\}}$, $C_{6,\{1,3\}}$, $C_{6,\{2,3\}}$, $C_{8,\{1,4\}}$, or $C_{10,\{2,5\}}$.*

Proof: As noted earlier, $-X-$ and $-Y-$ are both cubic circulants, corresponding to the graphs $C_{6,\{2,3\}}$ and $C_{8,\{1,4\}}$, respectively. We also note that $K_{3,3} = C_{6,\{1,3\}}$ and $K_4 = C_{4,\{1,2\}}$. Of the four given graphs in the statement of Theorem 4.24, only $C_5 \times K_2$ is a circulant (the top right graph in Figure 4.9), and it is easily seen to be isomorphic to $C_{10,\{2,5\}}$. By Theorem 4.24, it remains to show that other than $-X-$ and $-Y-$, no other graph in Ψ is a circulant. This will complete the proof.

Suppose on the contrary that $G \in \Psi$ is a circulant, where G is not isomorphic to either $-X-$ or $-Y-$. Then G must contain an *induced* subgraph of X, Y, or Z. We show that none of these three cases is possible, completing the proof. Since G is cubic, G must be isomorphic to $C_{2n,\{a,n\}}$, for some $1 \leq a < n$.

Case 1: X is an induced subgraph of G.

Label the vertices of X, as shown in Figure 4.10.

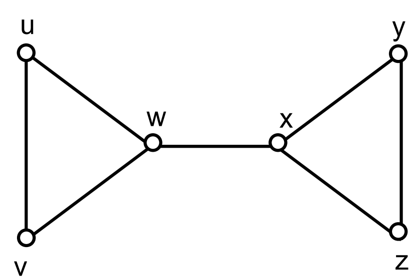

Figure 4.10: Graph X and its vertices labelled.

Without loss, let $w = 0$. Then $\{u, v, x\}$ must be a permutation of $\{a, n, 2n - a\}$. There are six possible triplets (u, v, x) that arise. By isomorphism, we may assume that $u < v$. Furthermore, X is an induced subgraph of G for the case $(u, v, x) =$

$(a, n, 2n - a)$ iff X is an induced subgraph of G for the case $(u, v, x) = (2n - a, n, a)$. This is seen by multiplying the colour assigned to each vertex by -1 and reducing mod $2n$. By this analysis, six cases reduce to four, which then reduce to two.

From the assumption $u < v$, there are only two distinct cases to consider: when $(u, v, x) = (n, 2n - a, a)$ and when $(u, v, x) = (a, 2n - a, n)$. Since $uv \in E(G)$, we must have $|u - v|_{2n} \in \{a, n\}$.

In the first case, we have $|u - v| = n - a \in \{a, n\}$. Since $1 \leq a < n$, it follows that $n - a = a$, or $a = \frac{n}{2}$. But then $v = \frac{3n}{2}$ and $x = \frac{n}{2}$. So $|v - x|_{2n} = n$, which implies that $vx \in E(G)$, a contradiction.

In the second case, $|u - v| = 2n - 2a \in \{a, n\}$. If $2n - 2a = n$, then $a = \frac{n}{2}$, and we get the same contradiction as above. Otherwise, $2n - 2a = a$, so $a = \frac{2n}{3}$. Then $(u, v, w, x) = (\frac{2n}{3}, \frac{4n}{3}, 0, n)$. Since y and z are adjacent to $x = n$, y is either $\frac{5n}{3}$ or $\frac{n}{3}$. But then y is adjacent to u or v (since its circular distance is n), and that is a contradiction because X is an induced subgraph of G.

Case 2: Y is an induced subgraph of G.

Label the vertices of Y, as shown in Figure 4.11.

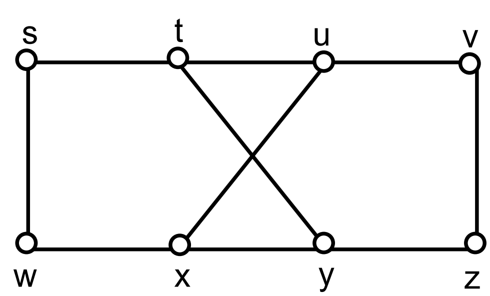

Figure 4.11: Graph Y and its vertices labelled.

Without loss, let $t = 0$. Then $\{s, u, y\}$ is a permutation of $\{a, n, 2n - a\}$. As we did in Case 1, we only need to consider two cases by symmetry: $(s, u, y) = (n, a, 2n - a)$ and $(s, u, y) = (2n - a, a, n)$. In the former case, either x or v must be $n + a$, since it is adjacent to $u = a$. But then this vertex must be adjacent to $s = n$, a contradiction. In the latter case, either $(x, v) = (2a, n + a)$ or $(x, v) = (n + a, 2a)$. But $xy \in E(G)$

and $vy \notin E(G)$, so $x = n + a$ and $v = 2a$. Since $wx \in E(G)$, this forces $w = n + 2a$ (mod $2n$). However, this implies that $vw \in E(G)$, a contradiction.

<u>*Case 3:*</u> Z is an induced subgraph of G.

Label the vertices of Z, as shown in Figure 4.12.

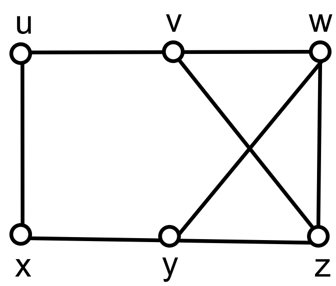

Figure 4.12: Graph Z and its vertices labelled.

Without loss, let $v = 0$. Then $\{u, w, z\}$ is a permutation of $\{a, n, 2n-a\}$. As we did in Case 1, we only need to consider two cases by symmetry: $(u, w, z) = (2n - a, a, n)$ and $(u, w, z) = (n, a, 2n - a)$. In the former case, $zw \in E(G)$ and so $n - a \in \{a, n\}$. Clearly this implies $n - a = a$, or $a = \frac{n}{2}$. But then $|u - z|_{2n} = \frac{n}{2} = a$, which implies $uz \in E(G)$, a contradiction. In the latter case, $|z - w|_{2n} = 2n - 2a \in \{a, n\}$. So $a = \frac{n}{2}$ or $a = \frac{2n}{3}$. If $a = \frac{n}{2}$, then $uw \in E(G)$, a contradiction. And if $a = \frac{2n}{3}$, then $y = w + n = \frac{5n}{3}$. But then $uy \in E(G)$, a contradiction.

This clears all of the cases, and hence, we have established the proof of Theorem 4.25. ∎

In this proof, our solution quotes a known classification of connected well-covered cubic graphs, and then determines which of these graphs are circulants. Although this proof is not complicated, it is somewhat unsatisfying that this proof hinges on a known classification theorem. However, when we use independence polynomials, we can prove our result directly and more elegantly. Here we provide a second proof to Theorem 4.25, using our theorems from Chapter 2.

Proof: Every connected 3-regular circulant G is isomorphic to $C_{2m,\{a,m\}}$, for some $1 \leq a < m$. By Proposition 2.45, G is not connected iff $\gcd(a,m) > 1$. So we must have $\gcd(a,m) = 1$. By Lemma 2.19, every connected 3-regular circulant must be isomorphic to one of the following graphs: $C_{4n,\{1,2n\}}$, $C_{4n+2,\{1,2n+1\}}$, or $C_{4n+2,\{2,2n+1\}}$. Let us consider each of these cases separately.

Case 1: $G = C_{4n,\{1,2n\}}$.

G is well-covered for $n \leq 2$ so suppose $n \geq 3$. By Theorem 2.26, $\alpha(G) = \deg(I(G,x)) = 2n-1$. Let $D = (d_1, d_2, \ldots, d_{2n-1})$ be a valid difference sequence. Then each $d_i \geq 2$ and $\sum d_i = 4n$. The only way this is possible is if some $d_j = 4$ and the rest of the d_i's are 2, or if some $d_j = d_k = 3$ and the rest of the d_i's are 2. In our difference sequence D, we cannot have a subsequence of n consecutive terms equal to 2, or else its total is $2n \in \{1, 2n\}$, a contradiction. Thus, the only valid difference sequence (up to cyclic permutation) is

$$D = (\underbrace{2,\ 2,\ \ldots,\ 2}_{n-1}, 3, \underbrace{2,\ 2,\ \ldots,\ 2}_{n-2}, 3).$$

In other words, every maximum independent set must have the difference sequence D. This difference sequence D gives rise to exactly $4n$ maximum independent sets $\{v_0, v_0+d_1, v_0+d_1+d_2, \ldots, v_0+d_1+d_2+\ldots+d_{2n-2}\}$, by setting each vertex of G as the "initial" vertex v_0 and reducing each element mod $4n$. By the structure of D, these independent sets must all be distinct. We have not missed any maximum independent sets, since $[x^{2n-1}]I(G,x) = [x^{2n-1}]I(C_{4n,\{1,2n\}},x) = [x^{2n-1}]I(C_{4n,\{2n-1,2n\}},x) = 4n$, by Corollary 2.18.

For $n = 3$, consider the independent set $I' = \{0, 4, 8\}$. I' is maximal in $G = C_{12,\{1,6\}}$ because the addition of any vertex to I' will no longer preserve independence. Thus, G is not well-covered in this case, since $|I'| = 3 < 2n-1$. For $n \geq 4$, consider $I' = \{0, 3, 6\}$. Suppose $I' \subset I$ for some maximum independent set $|I| = 2n-1$. If any $v \in \{1, 2, 4, 5\}$ appears in I, then I will no longer be independent. Thus, the difference sequence of I must contain a pair of consecutive elements equal to 3, and thus cannot be a cyclic permutation of D. So I cannot be a superset of $\{0, 3, 6\}$, and we conclude that G is not well-covered in this case. Thus, $G = C_{4n,\{1,2n\}}$ is well-covered iff $n = 1$ or $n = 2$.

Case 2: $G = C_{4n+2,\{1,2n+1\}}$.

G is well-covered for $n = 1$ so suppose $n \geq 2$. By Theorem 2.26, $\alpha(G) = \deg(I(G,x)) = 2n+1$, and the unique difference sequence is $D = (2,2,\ldots,2)$. There are two possible maximum independent sets, the set of even vertices and the set of odd vertices. Now let $I' = \{0,3\}$. Clearly, I' cannot be extended to one of these maximum independent sets. So $G = C_{4n+2,\{1,2n+1\}}$ is well-covered iff $n = 1$.

Case 3: $G = C_{4n+2,\{2,2n+1\}}$.

G is well-covered for $n \leq 2$ so suppose $n \geq 3$. By Theorem 2.26, $\alpha(G) = \deg(I(G,x)) = 2n$. Let $D = (d_1, d_2, \ldots, d_{2n})$ be a valid difference sequence. Then each $d_i \neq 2$ and $\sum d_i = 4n+2$. We cannot have consecutive d_i's being 1, so at most n of the d_i's equal 1. Suppose exactly p of the d_i's equal 1, where $p \leq n$. Then the remaining $(2n-p)$ d_i's sum to $4n+2-p$, each of which is at least 3. Hence, $(4n+2-p) \geq 3(2n-p)$, or $p \geq n-1$.

So we either have $p = n-1$ or $p = n$. In the first case, the remaining $(n+1)$ terms must all equal 3 as its sum is $4n+2-p = 3n+3$. In the second case, the remaining n terms must sum to $3n+2$.

If n is even (let $n = 2t$), a valid difference sequence D occurs when $p = n-1$.

$$D = (1,3,3,\underbrace{1,3,\ \ldots,\ 1,3}_{t-1},1,3,3,\underbrace{1,3,\ \ldots,\ 1,3}_{t-2}).$$

And if n is odd (let $n = 2t-1$), a valid difference sequence D occurs when $p = n$.

$$D = (1,4,\underbrace{1,3,\ \ldots,\ 1,3}_{t-1},1,4,\underbrace{1,3,\ \ldots,\ 1,3}_{t-2}).$$

For example, if $n = 6$, then $D = (1,3,3,1,3,1,3,1,3,3,1,3)$, and if $n = 5$, then $D = (1,4,1,3,1,3,1,4,1,3)$. In both cases, this difference sequence gives rise to $4n+2$ distinct maximum independent sets. By Corollary 2.18, $[x^{2n}]I(G,x) =$

$[x^{2n}]I(C_{4n+2,\{2,2n+1\}},x) = [x^{2n}]I(C_{4n+2,\{2n,2n+1\}},x) = 4n+2$, and so this confirms that there are no other maximum independent sets.

If $n \geq 4$ is even, we let $I' = \{0,5\}$ and if $n \geq 3$ is odd, we let $I' = \{0,3,6\}$. In both cases, I' cannot be a subset of an independent set I with cardinality $2n$, since the difference sequence of I must be a cyclic permutation of D. Therefore, $G = C_{4n+2,\{2,2n+1\}}$ is well-covered iff $n = 1$ or $n = 2$.

We conclude that there are only five connected well-covered circulants of the form $G = C_{2n,\{a,n\}}$, where $\gcd(a,n) = 1$. These circulants are isomorphic to one of the following: $C_{4,\{1,2\}}$, $C_{6,\{1,3\}}$, $C_{6,\{2,3\}}$, $C_{8,\{1,4\}}$, $C_{10,\{2,5\}}$. This completes the proof. ∎

As a corollary, we classify all degree 3 circulants that are well-covered.

Theorem 4.26 *Let $G = C_{2n,\{a,n\}}$, where $1 \leq a < n$. Let $t = \gcd(2n,a)$. Then G is well-covered iff $\frac{2n}{t} \in \{3,4,5,6,8\}$.*

Proof: In Lemma 2.19, we proved that

(a) If $\frac{2n}{t}$ is even, then $G = C_{2n,\{a,n\}}$ is isomorphic to t copies of $C_{\frac{2n}{t},\{1,\frac{n}{t}\}}$.

(b) If $\frac{2n}{t}$ is odd, then $G = C_{2n,\{a,n\}}$ is isomorphic to $\frac{t}{2}$ copies of $C_{\frac{4n}{t},\{2,\frac{2n}{t}\}}$.

By Theorem 4.25, we require $\frac{2n}{t}$ to be 4, 6, or 8 in Case (a), and $\frac{4n}{t}$ to be 6 or 10 in Case (b). This establishes the desired result. ∎

Therefore, we have found necessary and sufficient conditions for a graph $G = C_{n,S}$ to be well-covered, for each of our three families. The following result on the lexicographic product enables us to determine even more families of well-covered circulants.

Theorem 4.27 ([167]) *Let G and H be nonempty graphs. Then $G[H]$ is well-covered iff G and H are both well-covered.*

From Theorems 2.31 and 4.27, if G and H are well-covered circulants, so is its lexicographic product $G[H]$. This gives us infinitely more examples of well-covered circulant graphs. If G and H are any of the well-covered graphs found in Theorems 4.19, 4.20, and 4.26, then $G[H]$ is also well-covered. For example, since $G = C_{15,\{1,2\}}$ and $H = C_{10,\{4,5\}}$ are both well-covered, Theorem 2.31 shows that

$$G[H] = C_{150,\{1,2,13,14,16,17,28,29,31,32,43,44,46,47,58,59,60,61,62,73,74,75\}}$$

is also well-covered.

We have now given a full characterization of all well-covered circulants, for each of the families appearing in Chapter 2. Using the lexicographic product, we have determined infinitely more families of well-covered circulants. We now examine other known families of well-covered graphs and determine which ones are circulants.

At the beginning of Chapter 3, we defined the circulant graph $G_{j,k} = C_{n_k,S_{j,k}}$ for each $1 \leq j \leq k$, where $(a_1, a_2, \ldots, a_k)$ is a k-tuple of integers with each $a_i \geq 3$. We now determine a precise necessary and sufficient condition for $G_{j,k}$ to be well-covered. Before we present our characterization theorem, we require two lemmas.

Lemma 4.28 *Let $1 \leq j \leq k-1$. If $G_{j,k-1}$ is not well-covered, then $G_{j,k}$ is also not well-covered.*

Proof: If $G_{j,k-1}$ is not well-covered, there must exist a maximal independent set $I' = \{v_1, v_2, \ldots, v_m\}$ in $G_{j,k-1}$ that is not a maximum independent set. In other words, $|I'| = m \leq \alpha(G_{j,k-1}) - 1$. Thus, if we add any other vertex $u' \in G_{j,k-1}$ to I', then $|u' - v_i|_{n_{k-1}} \in S_{j,k-1}$ for some index $1 \leq i \leq m$. Using I' as a building block, we will construct a maximal independent set I^* of $G_{j,k}$ for which $|I^*| < \alpha(G_{j,k})$. This will prove that $G_{j,k}$ is not well-covered. Without loss, assume that $0 \leq v_1 < v_2 < \ldots < v_m \leq |G_{j,k-1}| - 1 = n_{k-1} - 1$.

First define the set

$$I = \{pn_{k-1} + v_i : \quad 0 \leq p \leq a_k - 2, \ 1 \leq i \leq m\}.$$

We claim that I is an independent set of $G_{j,k}$. Our proof is similar to that of Lemma 3.16. On the contrary, suppose that I is not independent. Then there exist distinct vertices $x, y \in I$ such that $|x-y|_{n_k} \in S_{j,k}$. Note that $1 \leq |x-y|_{n_k} \leq n_{k-1}-1$, since $\max(S_{j,k}) \leq n_{k-1} - 1$ by Proposition 3.5 (g).

For any $x, y \in I$ with $0 \leq x < y \leq n_{k-1} - 1$, we have $|x - y|_{n_k} = y - x$ or $|x - y|_{n_k} = n_k + x - y$. We now explain why the latter "wraparound" case cannot occur if $|x-y|_{n_k} \leq n_{k-1} - 1$. By definition of the set I, $y \leq (a_k - 2)n_{k-1} + v_m$, where $v_m \in G_{j,k-1}$. Since $G_{j,k-1}$ is a graph on n_{k-1} vertices, labelled $0, 1, 2, \ldots, n_{k-1} - 1$, we have $v_m \leq n_{k-1} - 1$ implying that $y \leq (a_k - 2)n_{k-1} + n_{k-1} - 1$. Therefore,

$$\begin{aligned} n_k + x - y &\geq n_k + 0 - (a_k - 2)n_{k-1} - (n_{k-1} - 1) \\ &= a_k n_{k-1} - 1 - a_k n_{k-1} + 2n_{k-1} - n_{k-1} + 1 \\ &= n_{k-1} \\ &> n_{k-1} - 1. \end{aligned}$$

Since $|x - y|_{n_k} \leq n_{k-1} - 1$, we have shown that $|x - y|_{n_k} = y - x$, for all choices of $x, y \in I$. This implies that $|x - y|_{n_k} = zn_{k-1} + (v_a - v_b)$ for some integer z, and $v_a, v_b \in I'$. By definition, $G_{j,k-1}$ has n_{k-1} vertices, labelled $0, 1, 2, \ldots, n_{k-1} - 1$. Since $0 \leq v_a, v_b \leq n_{k-1} - 1$, the inequality $1 \leq |x - y|_{n_k} \leq n_{k-1} - 1$ implies that $z = 0$ or $z = 1$.

If $z = 0$, then $|x - y|_{n_k} = v_a - v_b$, i.e, $v_a - v_b \in S_{j,k}$. By Proposition 3.5 (a), this implies that $|v_a - v_b|_{n_{k-1}} \in S_{j,k-1}$, contradicting the assumption that v_a and v_b are independent in $G_{j,k-1}$.

If $z = 1$, then $|x-y|_{n_k} = n_{k-1} + v_a - v_b \in S_{j,k}$. By Proposition 3.5 (a), this implies that $v_b - v_a = |v_a - v_b|_{n_{k-1}} \in S_{j,k-1}$, contradicting the assumption that v_a and v_b are independent in $G_{j,k-1}$.

Therefore, I is an independent set of $G_{j,k}$. Essentially, I is created by taking $a_k - 1$ translates of the maximal independent set I', thus constructing an independent set with $m(a_k - 1)$ vertices. We note that every vertex $v \in I$ satisfies the inequality $0 \leq v \leq n_k - n_{k-1}$. The latter inequality follows from the fact that $pn_{k-1} + v_m \leq (a_k - 2)n_{k-1} + (n_{k-1} - 1) = (a_k - 1)n_{k-1} - 1 = a_k n_{k-1} - n_{k-1} - 1 = n_k - n_{k-1}$.

By the maximality of each of the translates of I', any $u \notin I$ with $0 \leq u \leq n_k - n_{k-1}$ cannot be added to I while still preserving independence. Specifically, if $u = pn_{k-1} + u'$ for some $0 \leq p \leq a_k - 2$ and $0 \leq u' \leq n_{k-1} - 1$, then there exists an index $1 \leq i \leq m$ such that $|u' - v_i|_{n_{k-1}} \in S_{j,k-1}$. For this i, let $v = pn_{k-1} + v_i$. Then $v \in I$ satisfies $|u - v|_{n_k} = |u' - v_i|_{n_k} \in S_{j,k}$. Thus, I is maximal when restricted to this subset of

$n_k - n_{k-1} + 1$ vertices.

Now consider the other $n_{k-1} - 1$ vertices of $G_{j,k}$, which appear consecutively in $G_{j,k}$. By Lemma 3.12, any subset of $\Omega(G_{j,k}) = n_{k-1}$ consecutive vertices in $G_{j,k}$ induces a copy of $G_{j,k-1}$. Thus, these remaining $n_{k-1} - 1$ vertices of $G_{j,k}$ induce a proper subgraph of $G_{j,k-1}$, and hence we can select at most $\alpha(G_{j,k-1})$ of these vertices so that they are independent in $G_{j,k}$.

We construct a maximal independent set I^* of $G_{j,k}$ that includes all of the $m(a_k - 1)$ vertices from our set I. From the above paragraph, any extension of I to a maximal independent set I^* of $G_{j,k}$ will add at most $\alpha(G_{j,k-1})$ additional vertices. We now compute the cardinality of I^* and prove that it is not maximum. We have

$$
\begin{aligned}
|I^*| &\leq |I| + \alpha(G_{j,k-1}) \\
&= m(a_k - 1) + \alpha(G_{j,k-1}) \\
&\leq (\alpha(G_{j,k-1}) - 1)(a_k - 1) + \alpha(G_{j,k-1}) \\
&= a_k\alpha(G_{j,k-1}) - (a_k - 1) \\
&< a_k\alpha(G_{j,k-1}) - 1 \quad \text{, since } a_k \geq 3. \\
&= \alpha(G_{j,k}) \quad \text{, by Theorem 3.8.}
\end{aligned}
$$

Hence, I^* is a maximal independent set of $G_{j,k}$ that is not maximum. Thus, we conclude that for any $1 \leq j \leq k-1$, $G_{j,k}$ is not well-covered if $G_{j,k-1}$ is not well-covered. ∎

Lemma 4.29 *Let $k \geq 3$ and let $(a_1, a_2, \ldots, a_k)$ be a k-tuple satisfying the non-decreasing condition $3 \leq a_1 \leq \ldots \leq a_k$. Then $G_{k-1,k} = C_{n_k,\{n_{k-2}, n_{k-2}+1, \ldots, n_{k-1}-n_{k-2}\}}$ is not well-covered.*

Proof: First, we deal with the special case $k = 3$ and $a_1 = a_2 = a_3 = 3$. In this case, we have $n_1 = 2$, $n_2 = 5$, and $n_3 = 14$. Hence, we need to show that $G_{2,3} = C_{14,\{2,3\}}$ is not well-covered. By two applications of Theorem 3.8, $\alpha(G_{2,3}) = a_3\alpha(G_{2,2}) - 1 = a_3 n_1 - 1 = 3 \cdot 2 - 1 = 5$.

For example, the set $I = \{0, 1, 5, 6, 10\}$ is a maximum independent set of $G_{2,3}$. This set I has the difference sequence $(1, 4, 1, 4, 4)$. Note that a valid difference sequence

$D = (d_1, d_2, d_3, d_4, d_5)$ has at most two 1's, or else two vertices in the corresponding independent set will differ by $2 \in S_{2,3}$. Thus, at least three of the d_i's must be at least 4. Since the d_i's sum to 14, it follows that every maximum independent set of $G_{2,3}$ must have a difference sequence that is a cyclic permutation of $D = (1, 4, 1, 4, 4)$.

Thus, the independent 2-set $\{0, 7\}$ cannot be extended to an independent 5-set in $G_{2,3} = C_{14,\{2,3\}}$. Therefore, we have proven the lemma in this special case, and hence we can assume that $k \geq 4$, or that $k = 3$ and $a_3 \geq 4$.

For each $1 \leq i \leq a_k$, define

$$\begin{aligned} T_i &= \{(i-1)n_{k-1} + 1, (i-1)n_{k-1} + 2, \ldots, (i-1)n_{k-1} + n_{k-1}\} \\ &= \{(i-1)n_{k-1} + 1, (i-1)n_{k-1} + 2, \ldots, in_{k-1}\}, \end{aligned}$$

where each element is reduced modulo n_k (if necessary).

For example, $T_1 = \{1, 2, \ldots, n_{k-1}\}$ and $T_2 = \{n_{k-1}+1, n_{k-1}+2, \ldots, 2n_{k-1}\}$. Since $a_k n_{k-1} = n_k + 1$, the case $i = a_k$ corresponds to the set

$$T_{a_k} = \{(a_k - 1)n_{k-1} + 1, (a_k - 1)n_{k-1} + 2, \ldots, n_k - 1, 0, 1\}.$$

Thus, every vertex of $G_{k-1,k}$ is included in exactly one T_i, with the exception of vertex $v = 1$ which appears twice. This separation of the $n_k = a_k n_{k-1} - 1$ vertices into a_k classes is illustrated in Figure 4.13.

By Lemma 3.12, each subgraph H_i of $G_{k-1,k}$ induced by the n_{k-1} vertices of T_i is isomorphic to $G_{k-1,k-1}$. Hence, $\alpha(H_i) = \alpha(G_{k-1,k-1}) = n_{k-2}$, by Theorem 3.8. For any independent set I of $G_{k-1,k}$, we must have $|I \cap T_i| \leq n_{k-2}$. Also by Theorem 3.8, note that $\alpha(G_{k-1,k}) = a_k \alpha(G_{k-1,k-1}) - 1 = a_k n_{k-2} - 1$.

We now explain why every maximum independent set I (containing $v_1 = 1$) must have n_{k-2} elements in common with each T_i. We will then construct an independent set that cannot be extended to satisfy this requirement, thus proving the existence of a maximal non-maximum independent set. This will imply that $G_{k-1,k}$ is not well-covered.

Let I be a maximum independent set of $G_{k-1,k}$. By the vertex transitivity of $G_{k-1,k}$, we assume without loss that $v = 1$ is an element of I. Suppose there exists

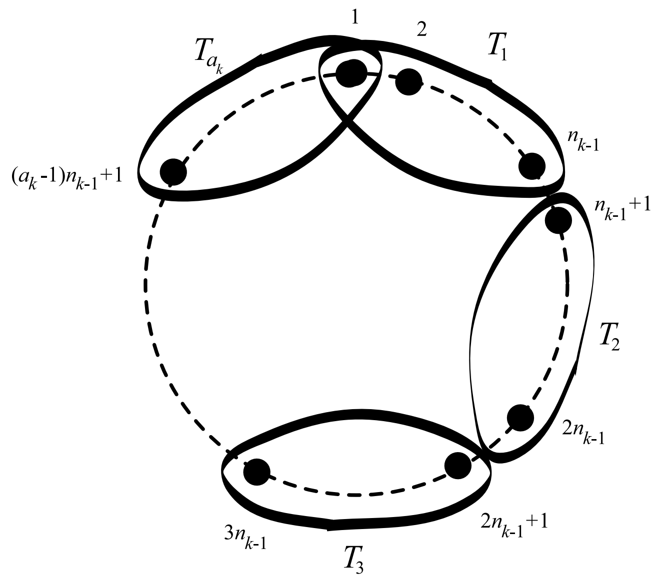

Figure 4.13: Separating $n_k = a_k n_{k-1} - 1$ vertices into a_k classes.

an index $1 \leq i \leq a_k$ for which $|I \cap T_i| < n_{k-2}$. Then,

$$\sum_{i=1}^{a_k} |I \cap T_i| < a_k n_{k-2}.$$

But every vertex of I is included in exactly one T_i, except for $v = 1$ which appears twice. Thus,

$$|I| + 1 = \sum_{i=1}^{a_k} |I \cap T_i| < a_k n_{k-2}.$$

This implies that $|I| < a_k n_{k-2} - 1 = \alpha(G_{k-1,k})$, which contradicts the maximality of I. Hence, in any maximum independent set I containing $v = 1$, we *must* have $|I \cap T_i| = n_{k-2}$ for each $1 \leq i \leq a_k$.

We construct a maximal independent set I^* by first setting four initial vertices: $v_1 = 1$, $v_2 = n_{k-1} - n_{k-2} + 2$, $v_3 = 2(n_{k-1} - n_{k-2}) + 3$, and $v_4 = 3(n_{k-1} - n_{k-2}) + 4$. We will extend this set of 4 vertices to a maximal independent set.

We now justify why these four vertices form an independent set in $G_{k-1,k}$. First note that $v_4 < n_k = a_k n_{k-1} - 1$, since $a_k \geq 3$ and $n_{k-2} \geq n_1 \geq 2$. Furthermore, consecutive vertices are separated by a distance of $n_{k-1} - n_{k-2} + 1$, and so any two vertices from $\{v_1, v_2, v_3, v_4\}$ must be separated by a distance of at least $n_{k-1} - n_{k-2} + 1$.

The only possible exception to this inequality occurs when there is a "wraparound" between v_1 and v_4, namely that $|v_1 - v_4|_{n_k} = n_k - (v_4 - v_1)$. To prove that $n_k + v_1 - v_4 \notin S_{k-1,k}$, it suffices to show that $n_k + v_1 - v_4 > n_{k-1} - n_{k-2}$, i.e., this wraparound difference is greater than the maximum element in $S_{k-1,k}$. This will justify the pairwise independence of these four vertices. We note that the following inequalities are equivalent:

$$\begin{aligned} n_k + v_1 - v_4 &> n_{k-1} - n_{k-2} \\ \Leftrightarrow (a_k n_{k-1} - 1) + 1 - 3(n_{k-1} - n_{k-2}) - 4 &> n_{k-1} - n_{k-2} \\ \Leftrightarrow n_{k-1}(a_k - 4) + 4n_{k-2} &> 4. \end{aligned}$$

If $a_k \geq 4$, the inequality is trivial since $n_{k-1}(a_k - 4) + 4n_{k-2} \geq 4n_{k-2} \geq 4n_1 = 4(a_1 - 1) > 4$. So assume $a_k = 3$. Having dealt with the exceptional case $(k, a_k) = (3, 3)$ in the first paragraph of the proof, we can assume that $k \geq 4$ if $a_k = 3$. By the non-decreasing condition $3 \leq a_1 \leq a_2 \leq \ldots \leq a_k$, we have $a_1 = a_2 = \ldots = a_{k-1} = 3$. Thus, the inequality $n_{k-1} \cdot (3-4) + 4n_{k-2} > 4$ simplifies to $-a_{k-1}n_{k-2} + 1 + 4n_{k-2} > 4$, or $n_{k-2} > 3$. Since $k \geq 4$, we have $n_{k-2} \geq n_2 = a_2 n_1 - 1 = 3 \cdot 2 - 1 = 5 > 3$, as required.

Therefore, the vertices $\{v_1, v_2, v_3, v_4\}$ are independent in $G_{k-1,k}$, and so we include them in I^*. We then add additional vertices (via the greedy algorithm) so that I^* becomes maximal.

Earlier we proved that a maximum independent set I must contain exactly n_{k-2} elements of each T_i. In other words, I intersects each T_i in n_{k-2} places. By our deliberate selection of the v_i's, we will prove that in any extension of this initial 4-set to a maximal independent set I^*, this maximal set can intersect T_2 in at most one vertex. Since $n_{k-2} \geq n_1 > 1$, this will prove that not every maximal independent set is maximum, implying that $G_{k-1,k}$ is not well-covered.

We claim that there are no vertices of I^* between v_2 and v_4, other than v_3. On the contrary, suppose that there exists a vertex v^* in I between v_2 and v_4. First suppose that $v_2 < v^* < v_3$.

If $v_2 < v^* < v_3$, then $v_3 - v_2 = n_{k-1} - n_{k-2} + 1$. Since $S_{k-1,k} = \{n_{k-2}, n_{k-2} + 1, \ldots, n_{k-1} - n_{k-2}\}$, neither $v^* - v_2$ nor $v_3 - v^*$ can be an element of this generating set. It follows that $v^* - v_2 \leq n_{k-2} - 1$ and $v_3 - v^* \leq n_{k-2} - 1$, as otherwise we derive an immediate contradiction.

Adding the two inequalities, we have $n_{k-1} - n_{k-2} + 1 = v_3 - v_2 \leq 2n_{k-2} - 2$, which is equivalent to $n_{k-1} \leq 3n_{k-2} - 3$. Since $n_{k-1} = a_{k-1}n_{k-2} - 1$, we have $(a_{k-1} - 3)n_{k-2} \leq -2$. Since $a_{k-1} \geq 3$, we obtain our contradiction.

If $v_3 < v^* < v_4$, then $v_4 - v_3 = n_{k-1} - n_{k-2} + 1$, and we proceed in the exact same manner as in the previous case, to obtain our contradiction. Therefore, there are no vertices of I^* between v_2 and v_4, other than v_3. Now we go one step further and show that neither v_2 or v_4 belong to the set $T_2 = \{n_{k-1} + 1, n_{k-1} + 2, \ldots, 2n_{k-1}\}$. To do this, we prove that $v_2 \leq n_{k-1}$ and $v_4 \geq 2n_{k-1} + 1$. Recall that $v_2 = n_{k-1} - n_{k-2} + 2$ and $v_4 = 3(n_{k-1} - n_{k-2}) + 4$.

The inequality $v_2 \leq n_{k-1}$ is equivalent to $n_{k-2} \geq 2$, which is trivial since $n_{k-2} \geq n_1 = a_1 - 1 \geq 2$. And the inequality $v_4 \geq 2n_{k-1} + 1$ is equivalent to $3n_{k-1} - 3n_{k-2} + 4 \geq 2n_{k-1} + 1$, which simplifies to $n_{k-1} \geq 3n_{k-2} - 3$. Since $n_{k-1} = a_{k-1}n_{k-2} - 1$, it suffices to establish that $n_{k-2}(a_{k-1} - 3) \geq -2$. But this is trivial, since $n_{k-2} \geq 0$ and $a_{k-1} \geq 3$.

Consider $I^* \cap T_2$. From above, $|I^* \cap T_2| \leq 1$, since the only vertex that can lie in the set $T_2 = \{n_{k-1} + 1, n_{k-1} + 2, \ldots, 2n_{k-1}\}$ is v_3. But this contradicts the requirement that $|I^* \cap T_i| = n_{k-2}$ for all $1 \leq i \leq a_k$.

Hence, I^* is a maximal independent set that is not a maximum independent set. Thus, we conclude that $G_{k-1,k}$ is not well-covered. ∎

We now give a complete characterization of all graphs $G_{j,k}$ that are well-covered.

Theorem 4.30 *Let $(a_1, a_2, \ldots, a_k)$ be a k-tuple of positive integers, with each $a_i \geq 3$. Define $G_{j,k}$ for each k-tuple. Then $G_{j,k}$ is well-covered iff $j = k$, or $(j, k) = (1, 2)$ with $a_2 \leq 4$.*

Proof: First consider the case $j = k$. By Proposition 3.5 (d), $S_{k,k} = \{n_{k-1}, n_{k-1} + 1, \ldots, \lfloor \frac{n_k}{2} \rfloor\}$. By definition, $G_{k,k} = C_{n_k, S_{k,k}}$. If $k = 1$, then $G_{1,1}$ is complete, and thus the circulant is (trivially) well-covered. Thus, let us assume that $k \geq 2$.

By Theorem 4.20, $G_{k,k}$ is well-covered iff $n_k > 3(n_{k-1}-1)$ or $n_k = 2(n_{k-1}-1)+2$. We justify that the former inequality holds. The proof is immediate, since $n_k = a_k n_{k-1} - 1 \geq 3n_{k-1} - 1 > 3(n_{k-1}-1)$. Thus, each $G_{k,k}$ is well-covered, for any k-tuple $(a_1, a_2, \ldots, a_k)$.

Now consider the case $(j,k) = (1,2)$. By Proposition 3.5 (e), we have $G_{1,2} = C_{n_2,\{1,2,\ldots,a_1-2\}}$, where $n_2 = a_2 n_1 - 1 = a_2(a_1-1) - 1$. By Theorem 4.19, $G_{1,2}$ is well-covered iff $n_2 \leq 3(a_1-2)+2$ or $n_2 = 4(a_1-2)+3$.

In the former case, the inequality $a_2(a_1-1)-1 = n_2 \leq 3(a_1-2)+2$ is equivalent to $a_2 \leq 3$. And in the latter case, the equation $a_2(a_1-1)-1 = n_2 = 4(a_1-2)+3$ is equivalent to $a_2 = 4$. Since $a_2 \geq 3$, it follows that $G_{1,2}$ is well-covered iff $a_2 = 3$ or $a_2 = 4$. This clears the case $(j,k) = (1,2)$.

Consider the graph $G_{j,k}$, with $2 \leq j < k$. By Lemma 4.29, the graph $G_{j,j+1}$ is not well-covered. By repeated applications of Lemma 4.28, $G_{j,k}$ is not well-covered (since none of $G_{j,j+2}, G_{j,j+3}, \ldots, G_{j,k-1}$ are either). From the above paragraph, the graph $G_{1,2}$ is not well-covered for $a_2 \geq 5$. By Lemma 4.28, $G_{1,k}$ is not well-covered, whenever $a_2 \geq 5$.

It remains to resolve the well-coveredness of $G_{1,3}$ when $a_2 = 3$ or $a_2 = 4$. In both cases, we will prove that $G_{1,3}$ is not well-covered. By another repeated application of Lemma 4.28, we will conclude that $G_{1,k}$ is not well-covered for $a_2 \leq 4$ and $k \geq 3$. This will establish our claim that $G_{j,k}$ is well-covered iff $j = k$, or $(j,k) = (1,2)$ with $a_2 \leq 4$.

Case 1: The graph $G_{1,3}$ satisfies $a_2 = 3$.

Let $a_1 = a$, $a_2 = 3$, $a_3 = b$. Then $n_1 = a - 1$, $n_2 = 3a - 4$, and $n_3 = b(3a-4) - 1$. By the recursive definition of $S_{1,3}$ as described in Proposition 3.5 (a), we derive

$$G_{1,3} = C_{b(3a-4)-1,\{1,2,\ldots,a-2,2a-2,2a-1,\ldots,3a-5\}}.$$

Also, $G_{1,2} = C_{3a-4,\{1,2,\ldots,a-2\}}$, and $\alpha(G_{1,2}) = \lfloor \frac{3a-4}{a-1} \rfloor = 2$ by Theorem 2.3. By Theorem 3.8, $\alpha(G_{1,3}) = a_3\alpha(G_{1,2}) - 1 = 2b - 1$. We prove the existence of a maximal independent set I with $|I| = 2b - 2 < \alpha(G_{1,3})$. Let D be the following difference sequence, where each of the differences $a-1$ and $2a-3$ appear $(b-2)$ times each.

$$D = (4a-5, \underbrace{a-1, 2a-3,\ a-1, 2a-3,\ \ldots,\ a-1, 2a-3}_{b-2 \text{ copies}}, 2a-4).$$

This difference sequence D contains $1+2(b-2)+1 = 2b-2$ terms, and has sum $\sum D = (4a-5)+(b-2)(3a-4)+(2a-4) = b(3a-4)-1 = n_3$. It is straightforward to check that D is a valid difference sequence of $G_{1,3}$. For notational convenience, we now abbreviate n_3 by n.

Letting the initial vertex be $v_1 = 0$, D corresponds to the following independent set of $G_{1,3}$, with $2b-2$ vertices.

$$I = \{0, 4a-5, 5a-6, 7a-9, 8a-10, \ldots, b(3a-4)-2a+3\}.$$

Let $v_1 = 0$, $v_2 = 4a-5$, $v_3 = 5a-6$, and $v_{2b-2} = b(3a-4)-2a+3 = n-2a+4$. Suppose that a vertex t can be added to I so that $I \cup \{t\}$ is independent. Let $1 \le i \le 2b-2$ be the largest index for which $v_i < t$.

If $2 \le i \le 2b-3$, then $v_{i+1} - v_i \le 2a-3$. Therefore, either $t - v_i \le a-2$ or $v_{i+1} - t \le a-2$, which implies that t must be adjacent to either v_i or v_{i+1}. Thus, we obtain a contradiction. If $i = 2b-2$, then $|v_0 - v_{2b-2}|_n = n - v_{2b-2} = 2a-4$, which implies that either $t - v_{2b-2} \le a-2$ or $|v_0 - t|_n = n-t \le a-2$. So we have a contradiction in this case as well.

It remains to check the case $i = 1$, i.e., $0 < t < 4a-5$. In all cases, we prove the existence of a vertex v_j such that $|t-v_j|_n \in S_{1,3}$, i.e., v_j and t are adjacent in $G_{1,3} = C_{n,\{1,2,\ldots,a-2,2a-2,2a-1,\ldots,3a-5\}}$. This will establish our desired contradiction.

(a) If $1 \le t \le a-2$, then $|t-v_1|_n = t \in S_{1,3}$.

(b) If $t = a-1$, then $|t - v_{2b-2}|_n = t + (2a-4) = 3a-5 \in S_{1,3}$.

(c) If $a \le t \le 2a-3$, then $|t-v_2|_n = (4a-5)-t \in S_{1,3}$.

(d) If $2a-2 \le t \le 3a-5$, then $|t-v_1|_n = t \in S_{1,3}$.

(e) If $t = 3a-4$, then $|t-v_3|_n = (5a-6)-t = 2a-2 \in S_{1,3}$.

(f) If $3a-3 \le t \le 4a-6$, then $|t-v_2|_n = (4a-5)-t \in S_{1,3}$.

This clears all of the cases, and so we conclude that there does not exist a vertex t so that $I \cup \{t\}$ is independent. Since I is a maximal independent set with $|I| < \alpha(G_{1,3})$, we conclude that $G_{1,3}$ is not well-covered.

Case 2: The graph $G_{1,3}$ satisfies $a_2 = 4$.

Let $a_1 = a$, $a_2 = 4$, $a_3 = b$. Then $n_1 = a-1$, $n_2 = 4a-5$, and $n_3 = b(4a-5)-1$. By the recursive definition of $S_{1,3}$ as described in Proposition 3.5 (a), we derive

$$G_{1,3} = C_{b(4a-5)-1,\{1,2,\ldots,a-2,3a-3,3a-2,\ldots,4a-6\}}.$$

Also, $G_{1,2} = C_{4a-5,\{1,2,\ldots,a-2\}}$, and $\alpha(G_{1,2}) = \lfloor \frac{4a-5}{a-1} \rfloor = 3$ by Theorem 2.3. By Theorem 3.8, $\alpha(G_{1,3}) = a_3\alpha(G_{1,2}) - 1 = 3b-1$. We prove the existence of a maximal independent set I with $|I| = 3b-2 < \alpha(G_{1,3})$. Let D be the following difference sequence, where the difference $2a-3$ appears $(b-2)$ times and the difference $a-1$ appears $2(b-2)$ times.

$$D = (3a-4, \underbrace{2a-3, a-1, a-1, \ldots, 2a-3, a-1, a-1}_{b-2 \text{ copies}}, 2a-3, a-1, 2a-3).$$

This difference sequence D contains $1 + 3(b-2) + 3 = 3b-2$ terms, and has sum $\sum D = (3a-4) + (b-2)(4a-5) + (5a-7) = b(4a-5) - 1 = n_3$. It is straightforward to check that D is a valid difference sequence of $G_{1,3}$. For notational convenience, we now abbreviate n_3 by n.

Letting the initial vertex be $v_1 = 0$, D corresponds to the following independent set of $G_{1,3}$.

$$I = \{0, 3a-4, 5a-7, 6a-8, 7a-9, \ldots, b(4a-5)-2a+2\}.$$

Let $v_1 = 0$, $v_2 = 3a-4$, $v_3 = 5a-7$, and $v_{3b-2} = b(4a-5)-2a+2 = n-2a+3$. Suppose that a vertex t can be added to I so that $I \cup \{t\}$ is independent. Let $1 \leq i \leq 3b-2$ be the largest index for which $v_i < t$.

If $2 \leq i \leq 3b-3$, then $v_{i+1} - v_i \leq 2a-3$. Therefore, either $t - v_i \leq a-2$ or $v_{i+1} - t \leq a-2$, which implies that t must be adjacent to either v_i or v_{i+1}. Thus, we obtain a contradiction. If $i = 3b-2$, then $|v_0 - v_{3b-2}|_n = n - v_{3b-2} = 2a-3$, which implies that either $t - v_{3b-2} \le a-2$ or $|v_0 - t|_n = n - t \le a-2$. So we have a contradiction in this case as well.

It remains to check the case $i = 1$, i.e., $0 < t < 3a-4$. In all cases, we prove the existence of a vertex v_j such that $|t - v_j|_n \in S_{1,3}$, i.e., v_j and t are adjacent in $G_{1,3} = C_{n,\{1,2,\ldots,a-2,3a-3,3a-2,\ldots,4a-6\}}$.

(a) If $1 \le t \le a-2$, then $|t - v_1|_n = t \in S_{1,3}$.

(b) If $a-1 \le t \le 2a-4$, then $|t - v_3|_n = (5a-7) - t \in S_{1,3}$.

(c) If $t = 2a-3$, then $|t - v_{3b-2}|_n = t + (2a-3) = 4a-6 \in S_{1,3}$.

(d) If $2a-2 \le t \le 3a-5$, then $|t - v_2|_n = (3a-4) - t \in S_{1,3}$.

This clears all of the cases, and so we conclude that there does not exist a vertex t so that $I \cup \{t\}$ is independent. Since I is a maximal independent set with $|I| < \alpha(G_{1,3})$, we conclude that $G_{1,3}$ is not well-covered.

Therefore, we have proven that $G_{j,k}$ is well-covered iff $j = k$, or $(j,k) = (1,2)$ with $a_2 \le 4$. ∎

Let us now study the well-coveredness of two other families of graphs. This analysis is motivated by some theorems of Finbow, Hartnell, and Nowakowski [71, 72]. Our results will follow immediately from these powerful classification theorems. First, we require several definitions.

Definition 4.31 ([71, 72]) *A* **basic 5-cycle** *of G is any C_5 subgraph that does not contain two adjacent vertices of degree 3 or more in G.*

Definition 4.32 ([71, 72]) *A graph G belongs to the family $\boldsymbol{\mathcal{F}}$ if the vertices of G can be partitioned into two subsets P and C such that P contains all vertices incident with pendant edges (i.e., edges incident to a vertex of degree 1), and C contains all vertices of basic 5-cycles, where the basic 5-cycles form a partition of C.*

In [71], the authors characterize all well-covered graphs of girth at least 5. They define four special graphs P_{10}, P_{13}, P_{14}, and Q_{13}, which are well-covered graphs of girth 5. (For the definitions of these four graphs, we refer the reader to [71]). It is straightforward to prove that none of these graphs are circulants: in fact, three of these graphs are not even regular. Their main result is the following.

Theorem 4.33 ([71]) *Let G be a connected well-covered graph of girth 5 or more. Then G is in the family $\mathcal{F}$, or G is isomorphic to one of K_1, C_7, P_{10}, P_{13}, Q_{13}, or P_{14}.*

From this theorem, we can give a full characterization of all well-covered *circulants* with girth at least 5. We prove that if G is a connected well-covered circulant graph with girth $g \geq 5$, then G must be isomorphic to K_1, K_2, C_5 or C_7.

From Theorem 4.33, either G is one of the six given "special graphs", or $G \in \mathcal{F}$. As discussed, only K_1 and C_7 are circulants, among these six special graphs. We now classify the circulants in $\mathcal{F}$. Let G be a circulant graph in the family $\mathcal{F}$.

If G has a pendant edge, then G contains a vertex of degree 1. Since G is a connected circulant, this implies that $G = K_2 = C_{2,\{1\}}$. If G has no pendant edges, then each vertex of G must belong to a basic 5-cycle. Clearly $G = C_5 \in \mathcal{F}$. Suppose G is not isomorphic to C_5. Then G contains at least two basic 5-cycles, connected by at least one edge. In other words, some vertex of G has degree at least 3. Since G is a circulant, every vertex must have degree $d \geq 3$. But this contradicts the definition of a basic 5-cycle. We have proven that K_2 and C_5 are the only circulant graphs in $\mathcal{F}$, and this establishes our desired result.

We now examine well-covered graphs which contain neither 4-cycles nor 5-cycles. In [72], the authors give a complete characterization of graphs in this family. We determine which of these graphs are also circulants, giving us a complete characterization of all well-covered circulant graphs that contain no C_4 or C_5 subgraph.

Definition 4.34 *A vertex v of G is* **simplicial** *if the subgraph induced by the vertices in the closed neighbourhood $N[v]$ is complete.*

Definition 4.35 ([72]) $\boldsymbol{\mathcal{S}}$ *is the set of graphs G for which there exist a subset of vertices $\{x_1, x_2, \ldots, x_k\} \subseteq V(G)$ such that the following conditions hold:*

1. x_i *is simplicial for each* i.

2. $|N[x_i]| \leq 3$.

3. $\{N[x_i] \mid i = 1, 2, \ldots, k\}$ *is a partition of* $V(G)$.

In [72], the authors define the graph T_{10}, a particular graph on 10 vertices. This graph is irrelevant to our discussion, as T_{10} is not regular, and hence, not a circulant. The following is the characterization theorem of Finbow, Hartnell, and Nowakowski.

Theorem 4.36 ([72]) *Let* G *be a connected well-covered graph containing neither* C_4 *or* C_5 *as a subgraph. Then,* $G \in \mathcal{S}$*, or* G *is isomorphic to* C_7 *or* T_{10}.

As a simple corollary of Theorem 4.36, we now prove that if G is a connected well-covered circulant graph containing neither C_4 or C_5 as a subgraph, then G is isomorphic to K_1, K_2, K_3, or C_7.

Let $G \in \mathcal{S}$. G contains at least one simplicial vertex v. Since $|N[v]| \leq 3$, it follows that $\deg(v) \leq 2$. Since G is a connected circulant, G must be r-regular, for some $r \leq 2$. If $r = 0$ or $r = 1$, then this corresponds to the cases $G = K_1$ and $G = K_2$. If $r = 2$, then G must contain a triangle (since v is simplicial). This implies that $G = C_3 = K_3$, as no other connected 2-regular circulant has a K_3 subgraph.

We know that C_7 is a circulant, while T_{10} is not (it is not regular). Thus, G must be isomorphic to one of K_1, K_2, K_3, or C_7. This establishes the claim.

We have now fully classified all well-covered circulants with girth $g \geq 5$, as well as all well-covered circulants containing no C_4 or C_5 subgraph. However, this analysis does not include many other families of graphs, most notably the set of graphs containing a K_3 (i.e., graphs of girth 3). This is the most difficult case, and there is no known characterization of well-covered graphs of girth 3 or girth 4. Since it is co-NP-complete to decide if an arbitrary graph G is well-covered [44, 157], at least one of these problems is intractable.

To conclude this section, we prove that it is co-NP-complete to decide if an arbitrary circulant graph is well-covered. We first require two lemmas and a definition.

Lemma 4.37 ([46]) *For all $n \in \mathbb{N}$, there are non-negative numbers $a_1, a_2, \ldots, a_n$, distinct mod $8^{\lceil \log_2 n \rceil} < 8n^3$, such that all sums $a_i + a_j$ are distinct mod $8^{\lceil \log_2 n \rceil} - 1$, and all sums $a_i + a_j + a_k$ are distinct mod $8^{\lceil \log_2 n \rceil} - 1$. Moreover, the sequence $a_1, a_2, \ldots, a_n$ is computable in time polynomial in n, and the distinctness claims remain true modulo any integer m satisfying $m > 3 \cdot (8^{\lceil \log_2 n \rceil} - 2)$.*

Definition 4.38 *Let G be an arbitrary graph, with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Then* $\boldsymbol{C_{G,A}}$ *is a circulant on $N = 8^{\lceil \log_2 n \rceil} - 1$ vertices, with generating set*

$$S = \{|a_i - a_j|_N : \quad v_i v_j \in E(G)\},$$

where $A = (a_1, a_2, \ldots, a_n)$ is an n-tuple $(a_1, a_2, \ldots, a_n)$ of positive integers satisfying the conditions of Lemma 4.37.

Note that $C_{G,A}$ is not well-defined; but for the purposes of the discussion that follows, any $C_{G,A}$ can be chosen.

Also note that by Lemma 4.37, there is a polynomial-time algorithm to determine an n-tuple $(a_1, a_2, \ldots, a_n)$ satisfying the conditions of this lemma.

As an example, let G be the graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_7\}$ and edge set $E(G) = \{v_1v_2, v_2v_3, v_3v_4, v_4v_5, v_5v_6, v_1v_6, v_1v_7, v_3v_7, v_4v_7\}$. A 7-tuple satisfying the conditions of Lemma 4.37 is

$$A = (a_1, a_2, a_3, a_4, a_5, a_6, a_7) = (54, 113, 14, 27, 85, 92, 36),$$

from which we derive a circulant $C_{G,A}$:

$$C_{G,A} = C_{511,\{7,9,13,18,22,38,58,59,99\}}.$$

Remark that any vertex w of $C_{G,A}$ adjacent to $v = 0$ satisfies $w = a_i - a_j \pmod N$ for some (i, j) with $v_i v_j \in E(G)$. As an example, $w = 412$ is a vertex of $C_{G,A}$ adjacent to $v = 0$, and $w = a_3 - a_2 \pmod{511}$. In this context, we say that the edge $v_i v_j$ of G *corresponds* to the vertex $w = a_i - a_j \pmod N$ in $C_{G,A}$. From now on, we will assume that A is an arbitrarily chosen n-tuple satisfying the conditions of Lemma 4.37, and so we will abbreviate $C_{G,A}$ by C_G.

Lemma 4.39 ([46]) *Let $w_1, w_2, \ldots, w_k$ be a k-clique in C_G, with $w_1 = 0$. Then for all $2 \leq i \leq k$, the edge e_i of G corresponding to w_i in C_G is adjacent to a certain vertex of G independent of i. Moreover, if $w_i = a_p - a_q \pmod N$ and $w_j = a_r - a_s \pmod N$, then $p = r$ or $q = s$.*

As shown in [46], this lemma follows quickly from Lemma 4.37. Let us use our earlier example to illustrate Lemma 4.39. By inspection, $\{0, 13, 22\}$ is a 3-clique in $C_G = C_{511,\{7,9,13,18,22,38,58,59,99\}}$. Notice that $w_2 = 13 = a_4 - a_3$ and $w_3 = 22 = a_7 - a_3$, i.e., e_2 and e_3 share the common vertex v_3 in G.

Since w_2 and w_3 are also adjacent in C_G, it follows that $\{v_3, v_4, v_7\}$ must be a 3-clique in G. In general, if C_G has a k-clique, then this produces a k-clique in G [46]. In the following lemma, we prove that a maximal k-clique of G corresponds to a maximal k-clique of C_G, and vice-versa.

Lemma 4.40 *There exists a maximal k-clique in G iff there exists a maximal k-clique in C_G.*

Proof: Let $W = \{w_1, w_2, w_3, \ldots, w_k\}$ be a maximal k-clique in C_G. By the vertex-transitivity of C_G, we can assume that $w_1 = 0$ without loss of generality. By Lemma 4.39, $w_j = a_m - a_{i_j} \pmod N$ for each $2 \leq j \leq k$ and some fixed index m. This implies that $T = \{v_m, v_{i_2}, v_{i_3}, \ldots, v_{i_k}\}$ is a k-clique in G. Now suppose that this k-clique is not maximal. Then we can add a new vertex v_q that is adjacent to each vertex in T, producing a $(k+1)$-clique in G. Let $w_{k+1} = a_m - a_q \pmod N$. Clearly, w_{k+1} is distinct from the previous k vertices of W. Then $\{w_1, w_2, \ldots, w_k, w_{k+1}\}$ is a $(k+1)$-clique in C_G, contradicting the maximality assumption.

Now we prove the converse. Let $\{v_1, v_2, \ldots, v_k\}$ be a maximal k-clique in G. Let $w_j = a_j - a_1 \pmod N$ for each $1 \leq j \leq k$. Then $S = \{w_1, w_2, w_3, \ldots, w_k\}$ is a k-clique in C_G, with $w_1 = 0$. Suppose that this k-clique is not maximal. Then we can add a new vertex w_{k+1} that is adjacent to each vertex in S, producing a $(k+1)$-clique in C_G. By Lemma 4.39, w_{k+1} must have the vertex label $a_q - a_1 \pmod N$, for some $v_q \in V(G)$, distinct from all of the other v_i's. Then $\{v_1, v_2, \ldots, v_k, v_q\}$ is a $(k+1)$-clique in G, contradicting the maximality assumption.

Therefore, we have proven that there exists a maximal k-clique in G iff there exists a maximal k-clique in C_G. ∎

Theorem 4.41 *Let $G = C_{n,S}$ be an arbitrary circulant graph. Then it is co-NP-complete to determine whether G is well-covered.*

Proof: Say that a graph belongs to the family $\mathcal{F}'$ if it is isomorphic to some $C_{G,A}$, where G is a graph on n vertices and $A = (a_1, a_2, \ldots, a_n)$ is an n-tuple satisfying the conditions of Lemma 4.37. Now let $\mathcal{F}$ be the family of all circulant graphs. Since each $C_{G,A}$ is a circulant, it follows that $\mathcal{F}' \subset \mathcal{F}$.

It is NP-complete to decide if an arbitrary graph G is not well-covered [44, 157]. Thus, it is NP-complete to determine the existence of a maximal k-clique and maximal l-clique in an arbitrary graph G, for some $k \neq l$. By Lemma 4.40, it is NP-complete to determine the existence of a maximal k-clique and maximal l-clique in the corresponding graph C_G, for some $k \neq l$.

Therefore, if we restrict our circulants to just the family $\mathcal{F}'$, it is NP-complete to determine if an arbitrary graph in this family is not well-covered. This implies that the decision problem is co-NP-complete. Since $\mathcal{F}'$ is a subset of the set of all circulants, we conclude that it is co-NP-complete to determine if an arbitrary circulant graph is well-covered. ∎

This proves the main theorem of this section.

4.4 Independence Complexes of Circulant Graphs

We begin by defining the *independence complex* of a graph G, which is a special type of *simplicial complex*.

Definition 4.42 *A* **simplicial complex** *consists of a set V of vertices and a collection Δ of subsets of V called* **faces** *with the following properties:*

1. *If $v \in V$, then $\{v\} \in \Delta$.*

2. *If $F \in \Delta$ and $G \subset F$, then $G \in \Delta$.*

Definition 4.43 *The* **independence complex** $\Delta(G)$ *of a graph* G *is a finite simplicial complex where the faces correspond to independent sets of* G*.*

Note that $\Delta(G)$ must be a simplicial complex since any subset of an independent set is also independent.

We require several more definitions. While we only study independence complexes in this chapter, these terms are defined for all simplicial complexes.

Definition 4.44 *Let* Δ *be a simplicial complex and* F *be a face of* Δ*. The* **dimensions** *of* F *and* Δ *are given by*

$$\dim(F) = |F|, \quad \dim(\Delta) = \max\{\dim(F) \mid F \in \Delta\}.$$

Definition 4.45 *For any face* F *of* Δ*, the* **simplex** *of* F *is*

$$\overline{F} = \{\sigma \in \Delta \mid \sigma \subseteq F\},$$

which is the set of all subsets of F*.*

Definition 4.46 *The faces of maximal dimension are called* **facets**. *A complex* Δ *is* **pure** *if all facets have the same dimension.*

Note that for combinatorists, the dimension is defined as above, but for topologists, $\dim(F)$ is defined as $|F| - 1$. To maintain consistency throughout this chapter, we will use the combinatorial definition of $\dim(F)$. A face with dimension $\dim(F) - 1$ is called a *ridge*.

The *geometric realization* of $\Delta(G)$ illustrates all of the facets belonging to the complex. Figures 4.14 and 4.15 present realizations of the independence complexes of $G = C_6 = C_{6,\{1\}}$ and $G = 3K_2 = C_{6,\{3\}}$.

In $\Delta(C_6)$, the facets are $\{0,3\}$, $\{1,4\}$, $\{2,5\}$, $\{0,2,4\}$, and $\{1,3,5\}$. Hence, this independence complex is not pure. On the other hand, $\Delta(3K_2)$ is pure, since the facets are $\{0,1,2\}$, $\{3,1,2\}$, $\{0,1,5\}$, $\{3,1,5\}$, $\{0,4,2\}$, $\{3,4,2\}$, $\{0,4,5\}$, and $\{3,4,5\}$.

An independent k-set contained in a maximal independent set is equivalent to a k-dimensional face contained in a facet. Therefore, we make the following observation.

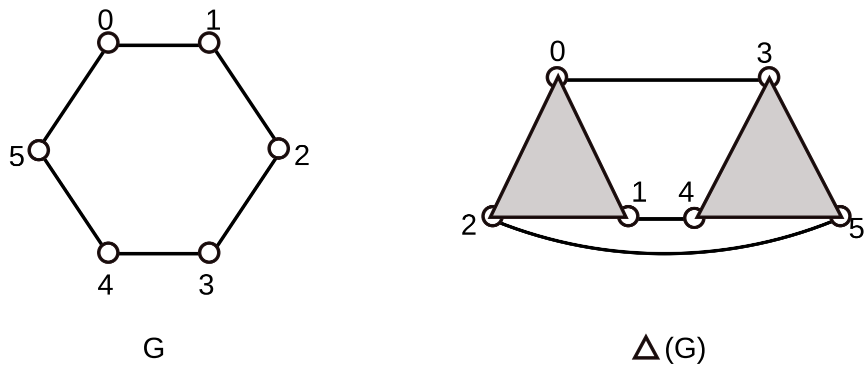

Figure 4.14: The independence complex $\Delta(C_6)$.

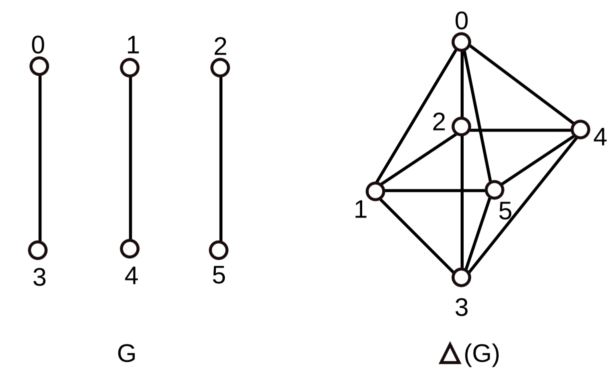

Figure 4.15: The independence complex $\Delta(3K_2)$.

Observation 4.47 *For any graph G, $\Delta(G)$ is pure iff G is well-covered.*

In the previous section, we characterized several families of well-covered circulants. Hence, these circulants correspond *directly* to pure independence complexes. Motivated by these results, we study the properties of these pure complexes. While we can investigate numerous properties of pure independence complexes (such as its homotopy, topology, and Cohen-Macaulayness), the remainder of this section will focus on the *shellability* of these pure independence complexes. We restrict our attention to problems relating to shellability, as we can develop new results on shellability directly from our previous work on independence polynomials.

Definition 4.48 ([27]) *A pure simplicial complex Δ of dimension d is* **shellable** *if* *the facets of* Δ *can be ordered* $F_1, F_2, \ldots, F_t$ *such that*

$$\overline{F_i} \bigcap \left(\bigcup_{j=1}^{i-1} \overline{F_j} \right)$$

is pure of dimension $d-1$ *for all* $i \geq 2$.

In other words, a complex Δ is shellable if its facets can be ordered so that the simplex of each one (other than the first) intersects the union of the simplices of its predecessors in a nonempty union of maximal proper faces. The idea is to build Δ stepwise by introducing the facets one at a time, and attaching each new facet F_i to the complex in the "nicest possible way", i.e., along its ridges.

The 3-dimensional independence complex $\Delta(3K_2)$ is shellable. A possible shelling is $F_1 = \{0,1,2\}$, $F_2 = \{0,4,2\}$, $F_3 = \{0,1,5\}$, $F_4 = \{0,4,5\}$, $F_5 = \{3,1,2\}$, $F_6 = \{3,4,2\}$, $F_7 = \{3,1,5\}$, and $F_8 = \{3,4,5\}$. On the other hand, we justify later in this section that $\Delta(C_7)$ is not shellable.

Shellability is introduced by Bruggesser and Mani in [27], who establish the shellability of boundary complexes of polytopes. Shellability has applications to combinatorial and computational geometry: to cite two examples, shellability is employed for efficient convex hull construction of polytopes [160], and for the proof of the upper bound of the number of faces of polytopes [131]. There is a technical generalization of shellability for non-pure complexes, and we refer the reader to [15, 16] for more information. However, in this section, we will only consider the shellability of pure complexes.

As mentioned by Hachimori in his Ph.D. thesis [89], the decision problems of combinatorial decomposition properties such as shellability are so challenging that almost no result is known currently. One of the few exceptions is a linear time algorithm by Danaraj and Klee [53] that determines if a 3-dimensional pseudomanifold is shellable. A d-dimensional complex is a **pseudomanifold** if any ridge (i.e., a face of dimension $d-1$) is included in at most two facets. For example, $\Delta(3K_2)$ is a 3-dimensional pseudomanifold. Unfortunately in all of our non-trivial examples, our complexes will not be pseudomanifolds. Hence, determining if these pure complexes are shellable is a formidable task.

We mention the following lemma, which provides an equivalent definition of shellability.

Lemma 4.49 ([15, 47]) *An ordering $F_1, F_2, \ldots, F_t$ of the facets of Δ is a shelling iff for every i and k with $1 \leq i < k \leq t$, there exists a j with $1 \leq j < k$ such that $F_i \cap F_k \subseteq F_j \cap F_k = F_k - \{x\}$, for some $x \in F_k$.*

In [15], it is shown that the shellability of independence complexes is closed under disjoint unions. Therefore, $\Delta(G)$ and $\Delta(H)$ are both shellable iff $\Delta(G \cup H)$ is shellable as well. Hence, we will not look at disconnected graphs: for the rest of this section, $\Delta(G)$ will always refer to the independence complex of a *connected* graph.

In the previous section, we gave a partial characterization of connected well-covered circulants. By Observation 4.47, this gives us a partial characterization of pure independence complexes. From Theorems 4.19, 4.20, 4.26, and 4.27, we have the following.

Theorem 4.50 *For each of the following circulants, $\Delta(G)$ is a pure independence complex.*

1. *$G = C_{n,\{1,2,\ldots,d\}}$, where $n \leq 3d+2$ or $n = 4d+3$.*
2. *$G = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$, where $n > 3d$.*
3. *G is one of $C_{4,\{1,2\}}$, $C_{6,\{1,3\}}$, $C_{6,\{2,3\}}$, $C_{8,\{1,4\}}$, or $C_{10,\{2,5\}}$.*
4. *G is the lexicographic product of any two graphs in the above list.*

In this section, we attempt to determine the shellability (or non-shellability) of each of these families of pure complexes. We will use a wide variety of techniques, and apply results found earlier in the thesis. The shellability problem for these four families will be determined in reverse order; starting with the lexicographic product (the easiest case) and working backwards to the family $G = C_{n,\{1,2,\ldots,d\}}$, which is the most difficult. For one particular case in this family, we will explain why the analysis is so challenging. Nevertheless, for every other family of well-covered circulants described in Theorem 4.50, we will determine whether the corresponding independence complex is shellable.

To develop our theorems, we require numerous lemmas and additional definitions.

From Theorem 4.27, G and H are well-covered iff $G[H]$ is well-covered. Therefore, Observation 4.47 tells us that $\Delta(G)$ and $\Delta(H)$ are pure iff $\Delta(G[H])$ is pure. A natural conjecture is that $\Delta(G[H])$ is shellable whenever $\Delta(G)$ and $\Delta(H)$ are both shellable as well. However, the following lemma disproves this conjecture.

Lemma 4.51 *Let G and H be well-covered graphs. If H is not complete, and $\Delta(G)$ has at least two distinct facets, then $\Delta(G[H])$ is not shellable.*

Proof: Let $\{v_1, v_2, \ldots, v_n\}$ be the vertices of G, and let $\{w_1, w_2, \ldots, w_m\}$ be the vertices of H. Every maximum independent set of $G[H]$ has $\alpha(G)\alpha(H)$ vertices, where each vertex is of the form (v_i, w_j), for some $1 \leq i \leq n$ and $1 \leq j \leq m$. By the definition of the lexicographic product, vertices (v_a, w_b) and (v_c, w_d) are adjacent in $G[H]$ iff $(v_a \sim v_c)$ or $(v_a = v_c$ and $w_b \sim w_d)$.

For each maximum independent set I, define $\phi(I)$ to be the set of vertices in G that appear among the elements in I. In other words, $\phi(I)$ is the projection of I onto the first coordinate. Note that each $\phi(I)$ must be a maximum independent set of $\alpha(G)$ vertices in G.

Let $\{F_1, F_2, \ldots, F_t\}$ be a shelling of $\Delta(G[H])$. Then there exists a unique integer $2 \leq k \leq t$ such that $\phi(F_1) = \ldots = \phi(F_{k-1})$ and $\phi(F_1) \neq \phi(F_k)$. Such a k must exist, as otherwise $\phi(F_1)$ is the only maximum independent set of G (i.e., $\phi(F_1)$ is the only facet of $\Delta(G)$), which contradicts our assumption that $\Delta(G)$ has at least two facets.

So consider this unique index k. Since $H \neq K_n$, $\alpha(H) \geq 2$. Also, we have $\phi(F_j) \neq \phi(F_k)$ for all $1 \leq j \leq k-1$. Therefore,

$$|F_j \cap F_k| \leq (\alpha(G) - 1)\alpha(H) < \alpha(G)\alpha(H) - 1 = |F_k| - 1.$$

By Lemma 4.49, if $\Delta(G[H])$ is shellable, then there must exist some index $1 \leq j < k$ such that $F_j \cap F_k = F_k - \{x\}$, for some $x \in F_k$. But this necessitates that

$|F_j \cap F_k| = |F_k| - 1$, a contradiction. Therefore, we conclude that $\Delta(G[H])$ is not shellable whenever H is not complete, and $\Delta(G)$ has at least two distinct facets. ∎

Lemma 4.51 gives us the first main theorem in this section, which examines the shellability of $\Delta(G[H])$.

Theorem 4.52 *Let G and H be connected well-covered circulants with $G \neq K_1$ and $H \neq K_m$. Then $\Delta(G[H])$ is not shellable.*

Proof: Since G and H are both well-covered, so is $G[H]$, implying that $\Delta(G[H])$ is pure. We claim that $\Delta(G)$ has at least two facets.

There are many graphs with a unique maximum independent set; for example, consider any odd path. However, there are no connected circulants with this property. To prove this, assume that $I = \{v_1, v_2, \ldots, v_r\}$ is a maximum independent set of $G = C_{n,S}$. Since G is a circulant, $I' = \{v_1+1, v_2+1, \ldots, v_r+1\}$ is also a maximum independent set, where addition is taken mod n. If $I \equiv I'$ then $I = I' = V(G)$, implying that $G = \overline{K_n}$. This contradicts the assumption that G is connected. Therefore, $I \not\equiv I'$, establishing that any connected circulant graph has at least two maximum independent sets.

Since H is not complete, and $\Delta(G)$ has at least two facets, Lemma 4.51 implies that $\Delta(G[H])$ is not shellable. ∎

This covers the shellablity decision problem for the final case of Theorem 4.50.

Now we consider the well-covered circulants of degree 3. These correspond to five pure complexes, as described in Theorem 4.50. We now determine the shellability of each complex. To do this, we require two results - the first is a characterization of all shellable 2-dimensional complexes, and the second is a powerful theorem of Stanley [164]. In order to establish our result, much work is required to introduce all necessary definitions and theorems. This is done over the next several pages. The following lemma holds for all graphs G (not just circulants).

Lemma 4.53 *If G is a connected graph with $\alpha(G) = 2$, then $\Delta(G)$ is shellable iff $\overline{G}$ is connected.*

Proof: If $\alpha(G) = 2$, the facets of $\Delta(G)$ are precisely the non-edges of G. Suppose there are t non-edges of G. Then $\overline{G}$ contains t edges and $\Delta(G)$ contains t facets.

If $\overline{G}$ is connected, there exists an ordering of edges $e_1, e_2, \ldots, e_t$ so that for any $1 \leq i \leq t$, the subgraph induced by the edges $e_1, e_2, \ldots, e_i$ is connected. One possible ordering is to select any spanning tree of $\overline{G}$, and let the first $|V(\overline{G})| - 1$ edges be the edges of this spanning tree, arranged so that connectedness is preserved at each step. Then the remaining edges can be selected arbitrarily. Letting F_i be the facet consisting of the two vertices of e_i, we see that $F_1, F_2, \ldots, F_t$ is a shelling of $\Delta(G)$.

However, if $\overline{G}$ is not connected, then there is no ordering of edges $e_1, e_2, \ldots, e_t$ with the aforementioned property. Therefore, no shelling $F_1, F_2, \ldots, F_t$ can exist. This completes the proof. ∎

As a corollary, we have a characterization of all shellable independence complexes of dimension 2.

Corollary 4.54 *Let $G = C_{n,S}$ be a connected circulant with $\alpha(G) = 2$. Define $\overline{G} = G_{n,\overline{S}}$, where $\overline{S} = \{t_1, t_2, \ldots, t_k\}$. Then, $\Delta(G)$ is shellable iff* $\gcd(n, t_1, t_2, \ldots, t_k) = 1$.

Proof: By Proposition 2.45, $\overline{G}$ is connected iff $d = \gcd(n, t_1, t_2, \ldots, t_k) = 1$. The conclusion now follows immediately from Lemma 4.53. ∎

The case $\alpha(G) \geq 3$ is significantly harder; in fact, even for $\dim(\Delta) = \alpha(G) = 3$, there is no known classification of the set of shellable complexes. When G is restricted to circulants, virtually nothing is known about $\Delta(G)$. In fact, there is no known example of even one connected circulant $G = C_{n,S}$ for which $\Delta(G)$ is a pure shellable 3-dimensional independence complex. At the end of this chapter, we provide the first such example.

By a remarkable theorem of Stanley [164], there is a simple necessary and sufficient condition to verify that a simplicial complex is shellable. Before stating the theorem, we need to first define the f-vector, h-vector, and M-sequence of a complex Δ.

Definition 4.55 *Let $f_i(\Delta)$ be the number of faces of dimension i. The* **f-vector** *of Δ is the sequence $(f_0(\Delta), f_1(\Delta), \ldots, f_d(\Delta))$, where $\dim(\Delta) = d$.*

Note that the f-vector represents the sequence of coefficients of the independence polynomial $I(G,x)$. In other words, $f_k = [x^k]I(G,x)$ for all $0 \leq k \leq d = \alpha(G)$.

Definition 4.56 *Let $f = (f_0, f_1, f_2, \ldots, f_d)$ be the f-vector of Δ. The* **h − vector** *of Δ (also known as the* **Hilbert-vector***) is $h = (h_0, h_1, h_2, \ldots, h_d)$, where*

$$h_k(\Delta) = \sum_{j=0}^{k} (-1)^{k-j} \binom{d-j}{d-k} f_j(\Delta), \quad 0 \leq k \leq d.$$

Consider the polynomials $F(x) = \sum_{i=0}^{d} f_i x^i$ and $H(x) = \sum_{i=0}^{d} h_i x^i$. Note that $F(x) = I(G,x)$. These two polynomials are related by the identity

$$H(x) = (1-x)^d F\left(\frac{x}{1-x}\right).$$

Later in this section, we introduce Stanley's Theorem, from which it will follow that the h-vector of a shellable complex has no negative terms (see Corollary 4.60). Thus, in a shellable complex $\Delta(G)$, the *real* roots of $H(x)$ must all be negative. For such graphs G, this result implies a simple bound on the real roots of $I(G,x)$.

Corollary 4.57 *Let G be a graph for which $\Delta(G)$ is shellable. Then every real root of $I(G,x)$ lies in the interval $(-1,0)$.*

Proof: Let $r < 0$ be a root of $H(x)$. From above, each root of $I(G,x) = F(x)$ is of the form $\frac{r}{1-r}$, for some $r < 0$. The desired conclusion follows. ∎

In the following chapter, we provide an extensive analysis of the roots of $I(G,x)$, where $G = C_{n,S}$ is an arbitrary circulant graph. We will find that these independence roots are not necessarily restricted to the interval $(-1,0)$; in fact, the set of roots of $I(C_{n,S},x)$ is dense in the entire complex plane!

Definition 4.58 ([13, 163]) *For each pair of positive integers (n,k), there is a unique way of writing*

$$n = \binom{a_k}{k} + \binom{a_{k-1}}{k-1} + \ldots + \binom{a_i}{i}$$

so that $a_k > a_{k-1} > \ldots > a_i \geq i \geq 1$. *Then define*

$$\delta^k(n) = \binom{a_k - 1}{k-1} + \binom{a_{k-1} - 1}{k-2} + \ldots + \binom{a_i - 1}{i-1}.$$

Also, let $\delta^k(0) = 0$.

Then, a sequence of non-negative integers $(n_0, n_1, n_2, \ldots, n_d)$ *is an* **M-sequence** *if* $n_0 = 1$ *and* $\delta^k(n_k) \leq n_{k-1}$ *for each* $2 \leq k \leq d$.

The following result is Stanley's Theorem.

Theorem 4.59 ([164]) *Let* $h = (h_0, h_1, h_2, \ldots, h_d)$ *be a* $(d+1)$*-tuple of integers. Then,* h *is the* h*-vector of a shellable complex of dimension* d *iff* h *is an* M*-sequence.*

Let us briefly explain Theorem 4.59. In any shelling $F_1, F_2, \ldots, F_t$ of $\Delta(G)$, define the restriction $Res(F_j)$ of facet F_j to be the set of vertices v such that $F_j - \{v\}$ is contained in one of the earlier facets. When we build $\Delta(G)$ according to this shelling, the new faces at the j^{th} step are exactly the faces $\{T : \; Res(F_j) \subseteq T \subseteq F_j\}$. This information corresponds to the h-vector of $\Delta(G)$; namely, if we count the number of indices $1 \leq j \leq t$ for which $|Res(F_j)| = i$, then we will find exactly h_i of them. Thus, h_i is non-negative if $\Delta(G)$ is shellable.

Any M-sequence must necessarily be a sequence of non-negative integers. Thus, if the h-vector has a negative term, then h is not an M-sequence. By Theorem 4.59, h cannot be the h-vector of a shellable complex. Therefore, we have the following corollary.

Corollary 4.60 *If the* h*-vector of a simplicial complex has a negative term, then the complex is not shellable.*

We note that the converse to Corollary 4.60 does not hold. As a counterexample, consider the independence complex $\Delta(C_{12,\{1,3,5,6\}})$. There are 16 facets, all of dimension 3. Eight of these facets contain only even vertices (e.g. $\{0, 2, 4\}$ and $\{0, 4, 8\}$), while the other eight contain only odd vertices. Hence, the complex cannot be shellable, since half the facets are completely disjoint from the other half. However, the f-vector is $f = (1, 12, 24, 16)$, from which we derive $h = (1, 9, 3, 3)$. Therefore, a non-shellable independence complex can have an h-vector with all positive terms. By Stanley's Theorem, $h = (1, 9, 3, 3)$ is the h-vector of *some* shellable simplicial complex, not necessarily the independence complex!

Another counterexample is the independence complex of the lexicographic product $G[H] = C_5[C_5]$. By Theorem 4.52, $\Delta(G[H])$ is not shellable. On the other hand, $I(G[H], x) = 1 + 25x + 150x^2 + 250x^3 + 125x^4$ by Theorem 2.33, which implies that $f = (1, 25, 150, 250, 125)$ and $h = (1, 21, 81, 21, 1)$.

We now present our shellability theorem for pure independence complexes of 3-regular circulants. As shown in Theorem 4.26, there are only five pure complexes $\Delta(G)$ for which G is a connected 3-regular circulant. We now determine which of these complexes are shellable.

Proposition 4.61 *The pure complex $\Delta(G)$ is shellable when G is $C_{4,\{1,2\}}$ or $C_{6,\{2,3\}}$, but not when G is $C_{6,\{1,3\}}$, $C_{8,\{1,4\}}$, or $C_{10,\{2,5\}}$.*

Proof: If $G = C_{4,\{1,2\}} = K_4$, then $\Delta(G)$ is trivially shellable. If $G = C_{6,\{2,3\}}$, the desired result follows immediately from Lemma 4.53. Now consider the other three cases.

If $G = C_{6,\{1,3\}}$, then the facets are $\{0, 2, 4\}$ and $\{1, 3, 5\}$, which are disjoint. This implies that $\Delta(G)$ is not shellable. If $G = C_{8,\{1,4\}}$, then $I(G, x) = 1 + 8x + 16x^2 + 8x^3$, which gives us $f(\Delta) = (1, 8, 16, 8)$ and $h(\Delta) = (1, 5, 3, -1)$. If $G = C_{10,\{2,5\}}$, then $I(G, x) = 1 + 10x + 30x^2 + 30x^3 + 10x^4$, which gives us $f(\Delta) = (1, 10, 30, 30, 10)$ and $h(\Delta) = (1, 6, 6, -4, 1)$. In both cases, the h-vector has a negative term. By Corollary 4.60, we conclude that $\Delta(G)$ is not shellable. ∎

Corollary 4.60 is also the key technique required to prove our next result, on the shellability of $\Delta(G) = \Delta(B_n)$, where $G = B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$.

In Theorem 4.20, we proved that $G = B_n$ is pure iff $n > 3d$. For each ordered pair (n, d) with $n > 3d$, we now determine whether $\Delta(G) = \Delta(B_n)$ is shellable.

We first show that $\Delta(G)$ is shellable for $d \leq 1$. If $d = 0$, then $G = K_n$, and so the result is obvious. If $d = 1$, then $\overline{G} = C_n$, and $\alpha(G) = 2$. The facets of $\Delta(G)$ are precisely the edges of $\overline{G} = C_n$. Since G and $\overline{G}$ are connected and $\alpha(G) = 2$, $\Delta(G)$ is shellable by Lemma 4.53.

The interesting case occurs when $d \geq 2$. We now prove that $\Delta(B_n)$ is never shellable, for any (n, d) with $d \geq 2$. To establish this result, we require the following lemma.

Lemma 4.62 *Let $1 \leq k \leq d+1$. Then*

$$\sum_{j=1}^{k} \binom{d+1-j}{d+1-k}\binom{d}{j-1} x^{k-j} = \binom{d}{k-1}(1+x)^{k-1}.$$

<u>Proof:</u> We have

$$\begin{aligned}
&\sum_{j=1}^{k} \binom{d+1-j}{d+1-k}\binom{d}{j-1} x^{k-j} \\
= \;& \sum_{j=1}^{k} \frac{(d+1-j)!}{(d+1-k)!(k-j)!} \cdot \frac{d!}{(j-1)!(d-j+1)!} x^{k-j} \\
= \;& \sum_{j=1}^{k} \frac{d!}{(d+1-k)!(k-j)!(j-1)!} x^{k-j} \\
= \;& \sum_{j=1}^{k} \frac{d!}{(k-1)!(d+1-k)!} \cdot \frac{(k-1)!}{(k-j)!(j-1)!} x^{k-j}
\end{aligned}$$

$$\begin{aligned}
= \;& \sum_{j=1}^{k} \binom{d}{k-1}\binom{k-1}{k-j} x^{k-j} \\
= \;& \binom{d}{k-1} \sum_{j=1}^{k} \binom{k-1}{k-j} x^{k-j} \\
= \;& \binom{d}{k-1} \sum_{t=0}^{k-1} \binom{k-1}{t} x^{t} \\
= \;& \binom{d}{k-1}(1+x)^{k-1}.
\end{aligned}$$

This concludes the proof. ∎

By substituting $x = -1$ into the above lemma, we have the following.

Corollary 4.63 *Let $1 \leq k \leq d+1$. Then*

$$\sum_{j=1}^{k} \binom{d+1-j}{d+1-k} \binom{d}{j-1} (-1)^{k-j} = 0.$$

Now we prove that $\Delta(B_n)$ is not shellable, for any $d \geq 2$.

Theorem 4.64 *Let $B_n = C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}$, where $n > 3d$ and $d \geq 2$. Then, $\Delta(B_n)$ is not shellable.*

Proof: By Corollary 4.60, it suffices to prove that the h-vector of $\Delta(B_n)$ has a negative term. By Proposition 2.9, $I(B_n, x) = 1 + nx(1+x)^d$. Therefore, $f_0 = 1$ and $f_j = n \cdot \binom{d}{j-1}$, for each $1 \leq j \leq d+1$.

It is straightforward to verify that $h_0 = f_0 = 1$ and $h_1 = f_1 - (d+1)f_0 = n - d - 1$. For $2 \leq k \leq d+1$, we have

$$\begin{aligned}
h_k &= \sum_{j=0}^{k} (-1)^{k-j} \binom{d+1-j}{d+1-k} f_j \\
&= (-1)^k \binom{d+1}{d+1-k} + \sum_{j=1}^{k} (-1)^{k-j} \binom{d+1-j}{d+1-k} \cdot n \cdot \binom{d}{j-1} \\
&= (-1)^k \binom{d+1}{k} + n \sum_{j=1}^{k} \binom{d+1-j}{d+1-k} \binom{d}{j-1} (-1)^{k-j} \\
&= (-1)^k \binom{d+1}{k} \quad \text{, by Corollary 4.63.}
\end{aligned}$$

We have established an explicit formula for the h-vector of $\Delta(B_n)$. Since h_3 is negative, we conclude that $\Delta(B_n)$ is not shellable, for any ordered pair (n, d) with $d \geq 2$. ∎

To conclude our analysis, we now attempt to determine the shellability of $\Delta(A_n)$, where $A_n = C_{n,\{1,2,\ldots,d\}}$. By Theorem 4.19, this complex is pure iff $n \leq 3d+2$ or $n = 4d+3$.

Proposition 4.65 *Let $d \geq 1$ be fixed, and set $A_n = C_{n,\{1,2,\ldots,d\}}$ for all $n \geq 2d$. Then $\Delta(A_n)$ is not shellable for $n = 2d+2$, but is shellable for $n = 2d$, $n = 2d+1$, and all $2d+3 \leq n \leq 3d+2$.*

Proof: If $n = 2d$ or $n = 2d+1$, then $A_n = K_n$, and so $\Delta(A_n)$ is trivially shellable. If $n = 2d+2$, then $\overline{A_n} = C_{2d+2,\{d+1\}}$, which consists of $d+1$ disjoint copies of K_2. Since $\overline{A_n}$ is not connected and $\alpha(A_n) = 2$, Lemma 4.53 shows that $\Delta(A_n)$ is not shellable.

Finally, consider the case $2d + 3 \leq n \leq 3d + 2$. By Theorem 2.3, $\alpha(A_n) = \alpha(C_{n,\{1,2,\ldots,d\}}) = \lfloor \frac{n}{d+1} \rfloor = 2$. By Lemma 4.53, it suffices to show that $\overline{A_n}$ is connected. If $n = 2d+3$, then $\gcd(d,n) = 1$. Hence, $\overline{A_n} = C_{2d+3,\{d+1\}}$ is isomorphic to C_{2d+3}, by Lemma 2.24. And clearly C_{2d+3} is connected.

For $n > 2d+3$, $\overline{A_n}$ connects every pair of vertices that are distance $d+1$ or $d+2$ apart (as well as possibly other pairs of vertices). To prove that $\overline{A_n}$ is connected, it suffices to prove that for each vertex v, there is a path from v to $v+1$. But this is trivial, since $v+d+2$ (reduced modulo n if necessary) is adjacent to both of these vertices. Therefore, $\overline{A_n}$ must be connected. We conclude that $\Delta(A_n)$ is shellable for all $2d \leq n \leq 3d+2$ except in the one case $n = 2d+2$. ∎

We now consider the most difficult case $n = 4d + 3$. For $d = 1$ and $d = 2$, the h-vectors of $\Delta(A_n)$ are $(1, 4, 3, -1)$ and $(1, 8, 14, -1)$. Thus, $\Delta(A_n)$ is not shellable for either of these two cases, by Corollary 4.60. Unfortunately the h-vectors are positive for all $d \geq 3$, and so we cannot apply Corollary 4.60.

A comprehensive study of the shellability of pure 3-dimensional complexes is found in [89], and further work has been done to build upon these results [138, 139]. Unfortunately, all of the known results are either small complexes (less than 7 vertices and 20 facets), pseudomanifolds (where each edge of Δ appears in at most two facets), or complexes where the h-vector satisfies $h_3 = 0$. In each of these three scenarios, much is known, and important results are developed. However, outside of these three scenarios, the analysis becomes extremely complicated, and virtually no techniques have been developed to determine the shellability of these complexes. Unfortunately, our complex $\Delta(G) = \Delta(A_{4d+3})$ is not a pseudomanifold for any $d \geq 2$. Also, $h_3 > 0$ in each case. Finally, the number of facets is too large for us to employ a computer search to find a shellable ordering. Even for the $d = 3$ case, $\Delta(G)$ consists of 50 facets.

Nevertheless, we provide a partial result to the shellability problem. While we cannot verify if $\Delta(G)$ is shellable for $d \geq 3$, we now prove that $\Delta(G)$ is not *extendably* shellable. Before stating our result, we require the following definitions.

Definition 4.66 ([53]) *A* **partial shelling** *of a complex Δ is an ordering of a subset of facets of Δ so that it satisfies the conditions for shellability. The complex Δ is* **extendably shellable** *if every partial shelling of Δ can be extended to a complete shelling.*

Hence, an extendably shellable complex has the property that a shelling can be found using the greedy algorithm; this is analogous to the problem of finding a maximum independent set in a well-covered graph. Clearly, if a complex is extendably shellable, then it is shellable. As shown in [89], the converse holds for particular families of complexes (e.g. 3-dimensional pseudomanifolds), but does not hold in general.

Theorem 4.67 *Let $G = C_{4d+3,\{1,2,\ldots,d\}}$. Then, $\Delta(G)$ is not extendably shellable for any $d \geq 1$.*

<u>Proof:</u> By Theorem 2.3, $\alpha(G) = \alpha(C_{4d+3,\{1,2,\ldots,d\}}) = \lfloor \frac{4d+3}{d+1} \rfloor = 3$. Thus, every facet has dimension 3. For each $1 \leq i \leq 4d+3$, define

$$T_i = \{(i-1)(d+1), i(d+1), (i+1)(d+1)\},$$

where the elements are reduced modulo $4d+3$.

We now claim that each element $0 \leq x \leq 4d+2$ appears exactly three times among the T_i's. Note that $i(d+1) \equiv j(d+1) \pmod{4d+3}$ implies that $(i-j)(d+1) \equiv 0 \pmod{4d+3}$. Since $\gcd(d+1, 4d+3) = 1$ by the Euclidean algorithm, this implies that $i \equiv j \pmod{4d+3}$. By the above analysis, for each $0 \leq x \leq 4d+2$, the congruence equation $m(d+1) \equiv x \pmod{4d+3}$ must have a unique solution m. Furthermore, for this choice of m and x, we have $x \in T_{m-1}$, $x \in T_m$, and $x \in T_{m+1}$, and $x \notin T_i$ for any other i satisfying $1 \leq i \leq 4d+3$. It follows that each x appears exactly three times among the T_i's. Each T_i has a difference sequence of $(d+1, d+1, 2d+1)$, which implies that T_i is a (maximum) independent set in G. In other words, each T_i is a facet of $\Delta(G)$.

Let $F_i = T_i$ for $1 \leq i \leq 4d+1$. Then $\{F_1, F_2, \ldots, F_{4d+1}\}$ is a partial shelling of $\Delta(G)$, and satisfies Lemma 4.49. Note that the F_i's are defined only when $1 \leq i \leq$

$4d{+}1$, and not for $i = 4d{+}2$ or $i = 4d{+}3$. These extra two indices are what distinguish the T_i's from the F_i's. We will show that our partial shelling $\{F_1, F_2, \ldots, F_{4d+1}\}$ cannot be extended by even one more facet F_{4d+2}. We will prove that this facet F_{4d+2} cannot be T_{4d+2}, T_{4d+3}, or any other facet of $\Delta(G)$. All cases will lead to a contradiction.

Since each x satisfying $0 \leq x \leq 4d + 2$ appears in three of the T_i's (where $1 \leq i \leq 4d + 3$), it follows that each of these indices x appears in at least one of the F_i's, where $1 \leq i \leq 4d + 1$.

We now prove that there does not exist a facet F_{4d+2} that can be added to this ordering to preserve the conditions for shellability. Suppose on the contrary that such a facet does exist. By Lemma 4.49, for every $1 \leq i \leq 4d + 1$, there must exist an index j with $1 \leq j \leq 4d + 1$ such that $F_i \cap F_{4d+2} \subseteq F_j \cap F_{4d+2} = F_{4d+2} - \{x\}$, for some $x \in F_{4d+2}$. Suppose that $F_j \cap F_{4d+2} = F_{4d+2} - \{x\} = \{y, z\}$, for some vertices y and z. For each $1 \leq j \leq 4d + 1$, the facet F_j has a difference sequence that is a permutation of $(d + 1, d + 1, 2d + 1)$. Hence, the circular distance $|y - z|_{4d+3}$ must equal $d+1$ or $2d+1$. Thus, the difference sequence of our candidate facet F_{4d+2} must include $d + 1$, or $2d + 1$, or possibly both.

We consider two cases: either $2d + 1$ appears as a difference sequence in our candidate facet F_{4d+2}, or it does not.

<u>*Case 1:*</u> The difference sequence of F_{4d+2} contains the element $2d + 1$.

Since G connects every pair of vertices with distance at most d, every pair of non-adjacent vertices has distance at least $d + 1$. In other words, every term of the difference sequence must be at least $d + 1$, since G has $4d + 3$ total vertices. Hence, if the difference sequence of F_{4d+2} contains the element $2d + 1$, then this difference sequence must be a (cyclic) permutation of $(d + 1, d + 1, 2d + 1)$.

Note that all of the T_i's have the difference sequence $(d{+}1, d{+}1, 2d{+}1)$. Furthermore, the set of T_i's (where $1 \leq i \leq 4d{+}3$) represent *all* of the independent sets with this specific difference sequence. This can be seen by noting that an independent set with this difference sequence must be of the form $\{v, v + d + 1, v + 2d + 2\}$, where the elements are reduced modulo $4d + 3$. There are $4d + 3$ choices for this initial vertex

v: this gives us the set of T_i's.

Thus, there are only two possibilities for this candidate facet F_{4d+2}: as it must be chosen from the remaining two T_i's not already in our partial shelling, either the facet is $T_{4d+2} = \{0, 2d+1, 3d+2\}$ or it is $T_{4d+3} = \{0, d+1, 3d+2\}$. Note that the other $4d+1$ possibilities have already appeared in our partial shelling.

If $F_{4d+2} = T_{4d+2} = \{0, 2d+1, 3d+2\}$, let $i = 1$. Then $F_1 = \{0, d+1, 2d+2\}$, and $F_1 \cap F_{4d+2} = \{0\}$. Hence, there must be some index $1 \leq j \leq 4d+1$ satisfying $F_j \cap F_{4d+2} = \{0, 2d+1\}$ or $\{0, 3d+2\}$. Note that the only T_i's containing the element 0 are $T_1 = F_1 = \{0, d+1, 2d+2\}$, as well as T_{4d+2} and T_{4d+3}. Therefore, the only possible candidate for j is $j = 1$, but then we have $F_1 \cap F_{4d+2} = \{0\}$, a contradiction.

If $F_{4d+2} = T_{4d+3} = \{0, d+1, 3d+2\}$, let $i = 4d+1$. Then $F_{4d+1} = \{d, 2d+1, 3d+2\}$, and $F_{4d+1} \cap F_{4d+2} = \{3d+2\}$. Hence, there must be some index $1 \leq j \leq 4d+1$ satisfying $F_j \cap F_{4d+2} = \{0, 3d+2\}$ or $\{d+1, 3d+2\}$. Note that the only T_i's containing the element $3d+2$ are $T_{4d+1} = F_{4d+1} = \{d, 2d+1, 3d+2\}$, as well as T_{4d+2} and T_{4d+3}. Therefore, the only possible candidate for j is $j = 4d+1$, but then we have $F_{4d+1} \cap F_{4d+2} = \{3d+2\}$, a contradiction.

<u>*Case 2:*</u> The difference sequence of F_{4d+2} contains the element $d+1$, but not $2d+1$.

If F_{4d+2} contains a pair of vertices with distance $d+1$, then it must be of the form $\{x, x+d+1, y\}$ for some pair of integers (x, y), where addition is taken modulo $4d+3$. Recall that every vertex of G is included at least once in our partial shelling $F_1, F_2, \ldots, F_{4d+1}$. Therefore, there exists at least one index i for which $y \in F_i$. Pick any such i for which this is the case. Hence, there must be some index $1 \leq j \leq 4d+1$ satisfying $F_j \cap F_{4d+2} = \{x, y\}$ or $\{x+d+1, y\}$, since $y \in F_i \cap F_{4d+2} \subseteq F_j \cap F_{4d+2}$ and $|F_j \cap F_{4d+2}| = 2$.

By definition, every facet F_j (with $1 \leq j \leq 4d+1$) has a difference sequence of $(d+1, d+1, 2d+1)$. So these two vertices of F_{4d+2} must be separated by a distance of $d+1$, since we are assuming that $2d+1$ does not appear in the difference sequence.

If $\{x, y\} \subset F_{4d+2}$, then $|y - x|_{4d+3} = d+1$, which implies that $y = x+d+1$ or $y = x-d-1$. The former case is impossible, as then F_{4d+2} would only have two distinct elements. The latter case leads to a contradiction since $\{x, x+d+1, y\}$ has a difference sequence of $(d+1, 2d+1, d+1)$.

If $\{x+d+1, y\} \subset F_{4d+2}$, then $|y-(x+d+1)|_{4d+3} = d+1$, which implies that $y = x$ or $y = x+2d+2$. The former case is impossible, as then F_{4d+2} would only have two distinct elements. The latter case leads to a contradiction since $\{x, x+d+1, y\}$ has a difference sequence of $(d+1, d+1, 2d+1)$.

This clears all of the cases, and so the theorem has been proved. ∎

In summary, we have taken all of the families of well-covered circulants from Section 4.4, and determined whether their independence complexes are shellable. We have answered the shellability decision problem for every family of circulants except for $G = C_{4d+3,\{1,2,\ldots,d\}}$, which we showed was not extendably shellable. We make the following conjecture.

Conjecture 4.68 *Let $G = C_{4d+3,\{1,2,\ldots,d\}}$. Then, $\Delta(G)$ is not shellable, for any $d \geq 1$.*

In our results, we found that the majority of independence complexes are not shellable. The only exceptions appeared to be some trivial cases, where $\Delta(G) = \Delta(C_{n,S})$ is a 2-dimensional complex. On the surface, it appears that $\Delta(G) = \Delta(C_{n,S})$ is not shellable for any G satisfying $\alpha(G) \geq 3$. One may conjecture that there exists no circulant for which $\Delta(C_{n,S})$ is a shellable complex of dimension $d \geq 3$. Such is not the case.

Proposition 4.69 *Let $G = C_{12,\{1,3,6\}}$. Then $\Delta(G)$ is pure, and is a shellable independence complex of dimension 3. Moreover, there is no graph on less than 12 vertices with this property.*

Proof: Table 4.2 listed all connected non-isomorphic well-covered circulants on at most 12 vertices. Table 4.3 lists all of the connected well-covered circulants (on at most 12 vertices) with $\alpha(G) \geq 3$. In each case, we compute its independence polynomial, which enables us to compute the h-vector of $\Delta(G)$.

By Corollary 4.60, we can immediately conclude that at most four of these complexes are shellable. The only candidates are $\Delta(G)$, where $G = C_{12,\{1,2,6\}}$, $C_{12,\{2,3,6\}}$, $C_{12,\{1,3,6\}}$, or $C_{12,\{1,3,5,6\}}$,

Using a C-program written by Hachimori [90] based on an algorithm given in [138], $\Delta(G)$ is shown to be non-shellable for $G = C_{12,\{1,2,6\}}$, $C_{12,\{2,3,6\}}$, or $C_{12,\{1,3,5,6\}}$. However, the Hachimori C-program shows that $\Delta(C_{12,\{1,3,6\}})$ is indeed shellable.

While this C-program does not give an actual shelling, we know that at least one shellable ordering of the 28 facets must exist. Table 4.4 presents such an ordering. By inspection, we can verify that this ordering satisfies the conditions for shellability.

Thus, we conclude that $G = C_{12,\{1,3,6\}}$ is the only connected circulant on at most 12 vertices for which $\Delta(G)$ is a pure shellable complex with dimension $d \geq 3$. ∎

The shellability of pure independence complexes is a fascinating area of study. In terms of studying the shellability of $\Delta(C_{n,S})$, we have only scratched the surface. Nevertheless, we did succeed in determining a 3-dimensional shellable independence complex with 28 facets. It remains open to determine the existence of another such independence complex.

n	S	h-vector	Shellablity
6	$\{1,3\}$	$(1,3,-3,1)$	No
7	$\{1\}$	$(1,4,3,-1)$	No
8	$\{1,3\}$	$(1,4,-6,4,-1)$	No
8	$\{1,4\}$	$(1,5,3,-1)$	No
9	$\{1,3\}$	$(1,6,3,-1)$	No
9	$\{1,2,4\}$	$(1,6,-6,2)$	No
10	$\{1,4\}$	$(1,6,1,-4,1)$	No
10	$\{2,5\}$	$(1,6,6,-4,1)$	No
10	$\{1,2,5\}$	$(1,7,3,-1)$	No
10	$\{1,3,5\}$	$(1,5,-10,10,-5,1)$	No
11	$\{1,2\}$	$(1,8,14,-1)$	No
11	$\{1,3\}$	$(1,7,6,-4,1)$	No
11	$\{1,2,4\}$	$(1,8,3,-1)$	No
12	$\{1,4\}$	$(1,8,12,-4,-2)$	No
12	$\{3,4\}$	$(1,8,12,-4,1)$	No
12	$\{1,2,6\}$	$(1,9,15,3)$	No
12	$\{1,3,5\}$	$(1,6,-15,20,-15,6,-1)$	No
12	$\{1,3,6\}$	$(1,9,15,3)$	**YES**
12	$\{2,3,4\}$	$(1,8,0,-4,1)$	No
12	$\{2,3,6\}$	$(1,9,15,3)$	No
12	$\{1,4,6\}$	$(1,8,6,-4,-1)$	No
12	$\{3,4,6\}$	$(1,9,15,-1)$	No
12	$\{1,2,4,5\}$	$(1,8,-12,8,-2)$	No
12	$\{1,3,4,6\}$	$(1,9,3,-1)$	No
12	$\{1,3,5,6\}$	$(1,9,3,3)$	No
12	$\{1,2,3,5,6\}$	$(1,9,-9,3)$	No

Table 4.3: Connected well-covered circulants with $|G| \leq 12$ and $\alpha(G) \geq 3$.

$F_1 = \{1,3,5\}$	$F_8 = \{0,5,7\}$	$F_{15} = \{3,7,11\}$	$F_{22} = \{1,6,8\}$
$F_2 = \{1,3,8\}$	$F_9 = \{0,2,7\}$	$F_{16} = \{0,5,10\}$	$F_{23} = \{1,6,11\}$
$F_3 = \{3,5,10\}$	$F_{10} = \{0,2,4\}$	$F_{17} = \{2,4,9\}$	$F_{24} = \{4,6,11\}$
$F_4 = \{3,8,10\}$	$F_{11} = \{5,7,9\}$	$F_{18} = \{0,8,10\}$	$F_{25} = \{4,9,11\}$
$F_5 = \{1,5,9\}$	$F_{12} = \{2,7,9\}$	$F_{19} = \{0,4,8\}$	$F_{26} = \{0,2,10\}$
$F_6 = \{1,9,11\}$	$F_{13} = \{6,8,10\}$	$F_{20} = \{4,6,8\}$	$F_{27} = \{2,6,10\}$
$F_7 = \{3,5,7\}$	$F_{14} = \{7,9,11\}$	$F_{21} = \{1,3,11\}$	$F_{28} = \{2,4,6\}$

Table 4.4: Shelling of the pure complex $\Delta(C_{12,\{1,3,6\}})$.

Chapter 5

Roots of Independence Polynomials

A great deal of information is represented by the roots of a graph polynomial. To give one example stated in [120], the roots of the characteristic polynomial of a molecular graph are interpreted as energies of the electronic levels of the corresponding molecules. For other graph polynomials, there may not be a direct application to other scientific fields; however, it is natural to investigate the nature and location of the roots of these graph polynomials. As in the case with other graph polynomials, the roots of independence polynomials have been studied extensively [22, 23, 25, 26, 42, 74, 97, 118, 119], and important theories have been developed. In this chapter, we extend the known results and develop new theorems on the roots of $I(G,x)$, when G is a circulant.

We investigate the complete family of circulants on n vertices, i.e., all circulants $C_{n,S}$ where S is an arbitrary subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. For this general family of graphs, we study the roots of $I(C_{n,S}, x)$. We provide conditions for when these roots are real, and in the case when the roots are complex, we determine some requirements for stability. We determine approximations and bounds for the roots of minimum and maximum moduli, and find a new proof that the closure of independence roots is the entire complex plane $\mathbb{C}$. We then characterize circulants for which $I(C_{n,S}, x)$ has at least one rational root, and find conditions for when a rational number r is a root of some independence polynomial $I(C_{n,S}, x)$. We conclude the chapter by determining the closure of the real roots of independence polynomials, answering an open problem from [23]. This result will be applied to determine the closures of the roots of matching polynomials and rook polynomials.

Before we begin our analysis, we briefly describe the special case $G = C_n$, since the roots of $I(C_n, x)$ can actually be determined explicitly.

In [81], Godsil applies *Chebyshev polynomials* to determine formulas for various matching polynomials. While the exact identity for the roots of $I(C_n, x)$ do not formally appear in [81], it can be inferred from his work on matching polynomials. Here we provide the details.

Since $L(C_n) \simeq C_n$, Proposition 1.9 tells us that

$$M(C_n, x) = x^n \cdot I\left(L(C_n), -\frac{1}{x^2}\right) = x^n \cdot I\left(C_n, -\frac{1}{x^2}\right).$$

Therefore, r is a root of $M(C_n, x)$ iff $-\frac{1}{r^2}$ is a root of $I(C_n, x)$. In [81], it is shown that $M(C_n, x) = 2T_n\left(\frac{x}{2}\right)$, where $T_n(x)$ is the n^{th} Chebyshev polynomial. The roots of $T_n(x)$ can be immediately derived from the following well-known formula.

Lemma 5.1 ([155]) $T_n(x) = 2^{n-1}\prod_{k=1}^{n}\left(x - \cos\left(\frac{(2k-1)\pi}{2n}\right)\right)$.

As a direct consequence of these observations, we have our formula for the roots of $I(C_n, x)$.

Theorem 5.2 *For each* $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$, *define* $r_{n,k} = -\frac{1}{4\left[\cos\left(\frac{(2k-1)\pi}{2n}\right)\right]^2}$. *Then* $\{r_{n,1}, r_{n,2}, \ldots, r_{n,\lfloor \frac{n}{2} \rfloor}\}$ *is the set of roots of* $I(C_n, x)$.

By making a connection to Chebyshev polynomials, we are able to determine an explicit formula for the roots of $I(C_n, x)$. Ignoring trivial families of circulants (e.g. $G = K_n$), this is the only known family of circulants whose independence roots can be computed explicitly. Since there is no apparent connection between Chebyshev polynomials (or any other type of orthogonal polynomial) with other families of circulants, it appears unlikely that an explicit formula can be determined for $I(C_{n,S}, x)$, even for the generating sets $S = \{1, 2, \ldots, d\}$ and $S = \{d+1, d+2, \ldots, \lfloor \frac{n}{2} \rfloor\}$.

Let S be an arbitrary subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. We know that there cannot exist a simple formula for the roots of $I(C_{n,S}, x)$, as otherwise we can immediately produce the independence polynomial, contradicting the result that determining $I(C_{n,S}, x)$ is NP-hard [46]. For an arbitrary generating set $S \subseteq \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$, it is very difficult to investigate the roots of $I(C_{n,S}, x)$, especially as we only know the formula for $I(C_{n,S}, x)$ in a handful of cases.

Nevertheless, we make partial progress in answering some of the most important questions on the roots of these polynomials. Specifically, we determine conditions for when $I(C_{n,S},x)$ has all real roots; we find (as a function of n) bounds for the roots of maximum and minimum moduli; we calculate the closure of these roots for certain generating sets S; we provide conditions for when $I(C_{n,S},x)$ has at least one rational root; and finally, we show that the closure of independence roots of circulants is the entire complex plane.

In our analysis, we carefully examine the two families of circulants that have featured prominently throughout the thesis; the families $C_{n,\{1,2,\ldots,d\}}$ and $C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}}$. In the following section, we determine conditions for when $I(C_{n,S},x)$ has only real roots.

5.1 The Real Roots of $I(C_{n,S},x)$

We first mention the following result by Chudnovsky and Seymour [42].

Theorem 5.3 ([42]) *Let G be a claw-free graph, i.e., a graph with no induced $K_{1,3}$ subgraph. Then the roots of $I(G,x)$ are all negative real numbers.*

For any pair (n,d) with $n \geq 2d$, the graph $A_n = C_{n,\{1,2,\ldots,d\}}$ is claw-free. Thus, we have the following corollary.

Corollary 5.4 *Let $d \geq 1$ be a fixed integer, and let $A_n = C_{n,\{1,2,\ldots,d\}}$, where $n \geq 2d$. Then the roots of $I(A_n,x)$ are all negative real numbers.*

Therefore, if $I(C_{n,S},x)$ has a complex root, $C_{n,S}$ must contain a claw. A natural question would be to determine all necessary and sufficient conditions on n and S so that $I(C_{n,S},x)$ has all real roots. It would be ideal if this claw-free condition is also sufficient, i.e., $I(C_{n,S},x)$ has a complex root iff $C_{n,S}$ has a claw. However, we can easily find counterexamples to this claw-free condition. For example, the circulant $G = C_{8,\{1,4\}} \sim C_{8,\{3,4\}}$ has a claw, yet $I(G,x) = 1+8x+16x^2+8x^3 = (1+2x)(1+6x+4x^2)$ has all real roots.

Recall that $I(B_n,x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor\frac{n}{2}\rfloor\}},x)$, since B_n is defined to be the complement of A_n. When we plot the (complex) roots of $I(B_n,x)$, it appears that in almost all cases, each root lies in the left-hand plane, i.e., $Re(r) < 0$ for all roots r. However, in some cases, there exists a pair of roots $r = x \pm yi$ for which $Re(r) = x > 0$. For example, the $I(C_{38,\{16,17,18,19\}}, x)$ includes the roots $0.0001743207895 + 1.732218466i$. This motivates the following well-known definition of *polynomial stability*.

Definition 5.5 ([8]) *A polynomial is* **stable** *if every root has a negative real part.*

An independence polynomial with all real roots is stable, since every real root of $I(G, x)$ is negative. But there are stable independence polynomials with complex roots, such as $I(C_{10,\{4,5\}}, x) = 1 + 10x(1 + x)^3$. Also, some circulants yield non-stable independence polynomials, such as $I(C_{38,\{16,17,18,19\}}, x)$. We would like to determine a precise necessary and sufficient condition on n and S so that $I(C_{n,S}, x)$ is stable, but this problem also appears to be intractable. Nevertheless, we can prove polynomial stability in some cases. First, we require a definition and a theorem.

Definition 5.6 ([62]) *Let $v \geq 2$ be an integer. The* **complex symmetric Newton polynomial** *of order v is*

$$(v - 1)z^v - vz_0z^{v-1} + 1,$$

where $z_0 \in \mathbb{C}$.

Theorem 5.7 ([62]) *For any value of z_0, the complex symmetric Newton polynomial $(v - 1)z^v - vz_0z^{v-1} + 1$ has at least $v - 1$ roots inside the unit circle $|z| = 1$.*

As an example, we establish the following result on the family of circulants $\{B_n\}$.

Proposition 5.8 *Fix $d \geq 1$ and let $n > 3d$. Then the polynomial $I(B_n, x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}, x)$ is stable.*

Proof: We prove a stronger result by establishing that all roots of $I(B_n, x)$ lie in the disk $|x + 1| < 1$. This implies that every root x of $I(B_n, x)$ has real part in $(-2, 0)$, thus establishing the stability of $I(B_n, x)$.

Since $n > 3d$, $I(B_n, x) = 1+nx(1+x)^d$, by Theorem 2.10. Making the substitution $y = x + 1$, we have $f(y) = I(B_n, y - 1) = 1 + ny^d(y - 1)$. We now prove that each solution to the equation $y^d(y - 1) + \frac{1}{n} = 0$ lies in the disk $|y| = |x + 1| < 1$.

By Theorem 5.7, $(v-1)z^v - vz_0z^{v-1} + 1$ has at least $v-1$ roots inside the unit circle $|z| = 1$, regardless of the value of z_0. Now make the substitutions $v = d+1$, $z = cy$, and $z_0 = \frac{dc}{d+1}$, where c is some positive constant to be determined. Then, our equation becomes

$$y^{d+1} - y^d + \frac{1}{dc^{d+1}} = 0.$$

Now select the unique c so that $dc^{d+1} = n$. Since $n > 3d$, c is some positive constant satisfying $c^{d+1} > 3$, which shows that $c > 1$. By Theorem 5.7, our transformed polynomial must have at least d roots inside the disk $|cy| = 1$, i.e., the disk $|y| = \frac{1}{c} < 1$. This proves that, with at most one exception, every root of $y^d(y-1) + \frac{1}{n}$ must satisfy $|y| < \frac{1}{c}$.

Consider this possible exception, y^*, and suppose that $|y^*| > \frac{1}{c}$. We know that y^* must be real, since all complex roots occur as conjugate pairs. Therefore, we only need to concern ourselves with the case when y^* is real.

If $y^* \geq 1$, then $0 = (y^*)^d(y^*-1) + \frac{1}{n} \geq 0 + \frac{1}{n} > 0$, which is a contradiction. And if $y^* \leq -1$, then $|(y^*)^d(y^*-1)| \geq |y^*-1| \geq 2$, and so $(y^*)^d(y^*-1) + \frac{1}{n} \neq 0$. Therefore, y^* must satisfy $\frac{1}{c} < |y^*| < 1$, i.e., $|y^*| < 1$.

We conclude that all $d+1$ roots of $y^d(y-1) + \frac{1}{n}$ satisfy $|y| < 1$. Hence, all $d+1$ roots of $I(B_n, x)$ satisfy $|x+1| < 1$, implying that the real part of each root lies in $(-2, 0)$. This establishes the stability of $I(B_n, x)$. ∎

As we see from Corollary 2.11, the simplified formula for $I(B_n, x)$ depends on the value of $\frac{n}{d}$. For $\frac{n}{d} > 3$, we just established the stability of $I(B_n, x)$. However, in all other cases, there is at least one ordered pair (n, d) for which $I(B_n, x) = I(C_{n,\{d+1,d+2,\ldots,\lfloor \frac{n}{2} \rfloor\}}, x)$ is not stable. From some computations on Maple, it appears that the polynomial $I(C_{10k+5,\{5k+1,5k+2\}}, x)$ is not stable for any $k \geq 4$. Table 5.1 lists some ordered pairs (n, d) for which $I(B_n, x)$ is not stable.

Let $f(x) = \sum a_i x^i$ and $g(x) = \sum b_i x^i$. Then the *Hadamard product* is defined to be $f \cdot g(x) = \sum a_i b_i x^i$. In [80], it is shown that $f \cdot g(x)$ is stable whenever $f(x)$ and $g(x)$ are both stable. Naturally, we may ask if stability is also preserved under other products.

Value of $\frac{n}{d}$	**Example of Pair** (n,d)
$\frac{5}{2} < \frac{n}{d} \leq 3$	$(48,19)$
$\frac{7}{3} < \frac{n}{d} \leq \frac{5}{2}$	$(38,16)$
$\frac{9}{4} < \frac{n}{d} \leq \frac{7}{3}$	$(50,22)$
$\frac{11}{5} < \frac{n}{d} \leq \frac{9}{4}$	$(45,20)$
$\frac{13}{6} < \frac{n}{d} \leq \frac{11}{5}$	$(55,25)$
$\frac{15}{7} < \frac{n}{d} \leq \frac{13}{6}$	$(65,30)$
$\frac{17}{8} < \frac{n}{d} \leq \frac{15}{7}$	$(75,35)$
$\frac{19}{9} < \frac{n}{d} \leq \frac{17}{8}$	$(85,40)$
$\frac{21}{10} < \frac{n}{d} \leq \frac{19}{9}$	$(95,45)$

Table 5.1: Examples of graphs for which $I(B_n, x)$ is not stable.

In Chapter 2, we examined the lexicographic product $G[H]$, and showed that $G[H]$ is a circulant whenever G and H are. Based on the result for Hadamard products, we may conjecture that $I(G[H], x)$ is stable whenever $I(G, x)$ and $I(H, x)$ are. However, we find that there are infinitely many counterexamples to this conjecture.

Proposition 5.9 *Let* $G = C_n$ *and* $H = \overline{K_3}$*. Then* $I(G[H], x)$ *is not stable for any* $n \geq 18$*.*

Proof: Clearly, $I(H, x) = (1 + x)^3$ is stable. Also, by Theorem 5.2, the roots of $I(C_n, x)$ are all negative real numbers, and so $I(C_n, x)$ is stable for all n. We now prove that $I(G[H], x)$ is not stable, for any $n \geq 18$. By Theorem 2.33, $I(G[H], x) = I(C_n, (1 + x)^3 - 1)$.

Let u be any root of $I(C_n, x)$. Then three of the roots of $I(G[H], x)$ are given by the solutions to $(1 + r)^3 - 1 = u$. Let $v = \sqrt[3]{-u-1}$. If $u < -1$, these three roots of $I(G[H], x)$ are $-1 + v \cdot \mathrm{cis}\frac{\pi}{3}$, $-1 + v \cdot \mathrm{cis}\frac{3\pi}{3}$, and $-1 + v \cdot \mathrm{cis}\frac{5\pi}{3}$. Specifically, two of these three roots have a real part of $-1 + v \cos\frac{\pi}{3} = -1 + \frac{v}{2}$.

In other words, if $v > 2$ (i.e., $u < -9$), then $I(G[H], x)$ is not stable. To conclude the proof, it suffices to show that $I(C_n, x)$ has a root u with $u < -9$ for each $n \geq 18$. This will complete the proof. By Theorem 5.2, $r_{2n,n} = -\frac{1}{4\left[\cos\left(\frac{(2n-1)\pi}{4n}\right)\right]^2}$ and $r_{2n+1,n} = -\frac{1}{4\left[\cos\left(\frac{(2n-1)\pi}{4n+2}\right)\right]^2}$. Both sequences $r_{2n,n}$ and $r_{2n+1,n}$ are decreasing.

Since $r_{10,5} < -9$ and $r_{19,9} < -9$, this implies that $r_{2n,n} < -9$ for $n \geq 5$ and $r_{2n+1,n} < -9$ for $n \geq 9$. Therefore, it follows that $I(G[H], x) = I(C_n[\overline{K_3}], x)$ is not stable for any $n \geq 18$, as well as for $n = 10, 12, 14,$ and 16. $\blacksquare$

Later in this chapter, we prove the surprising result that the roots of $I(C_n[\overline{K_m}], x)$ are dense in the entire complex plane $\mathbb{C}$. In other words, these roots don't just sporadically appear on the right-half of the plane, they actually fill out the entire complex plane.

5.2 The Root of Minimum Modulus of $I(C_{n,S}, x)$

Now we examine the roots of maximum and minimum moduli in $I(C_{n,S}, x)$, and determine bounds for these roots as a function of n. We first establish our bound for the root r_{min} of minimum modulus. In [22], it is shown that for every well-covered graph G, the root of minimum modulus of $I(G, x)$ satisfies $|r_{min}| \geq \frac{1}{n}$, with equality occurring iff G is the complete graph K_n. In [119], it is shown that in a general independence polynomial $I(G, x)$, $|r_{min}| > \frac{1}{2n-1}$ for an arbitrary graph G. While Levit and Mandrescu [119] mention that "it is pretty amusing that one cannot improve this bound using only simple algebraic transformations", we now show that this bound indeed *can* be improved using a very simple pairing argument. We prove that the optimal bound for well-covered graphs [22] is also the optimal bound for an arbitrary graph G. First we cite an important result from Fisher [74].

Theorem 5.10 ([74]) *Let $D(G, x)$ be the* dependence polynomial *of G, as defined in Chapter 1. For any polynomial $D(G, x)$, the root of minimum modulus is real.*

Since $I(G, x) = D(\overline{G}, x)$ for all graphs G, we have the following corollary.

Corollary 5.11 *Let r_{min} be the root of minimum modulus of $I(G, x)$. Then, r_{min} is real.*

Theorem 5.12 *Let G be any graph of order n. Then the root r_{min} of minimum modulus of $I(G, x)$ satisfies $|r_{min}| \geq \frac{1}{n}$, with equality occurring iff G is the complete graph K_n.*

Proof: Let $I(G, x) = i_0 + i_1 x + i_2 x^2 + \ldots + i_k x^k$, where $k = \alpha(G)$. By Corollary 5.11, r_{min} is always real, and so we only need to focus our attention on the real roots of $I(G,x)$. We will show that for all integers $0 \le l \le \frac{k}{2}$, the function $g_l(x) = i_{2l}x^{2l} + i_{2l+1}x^{2l+1}$ is non-negative at $x = -\frac{1}{n}$, and positive for all $x > -\frac{1}{n}$.

Consider the i_{2l+1} independent sets of cardinality $2l+1$. Each of these sets is formed by taking an independent set of cardinality $2l$ and adding one of the other $(n-2l)$ vertices so that the resulting set remains independent. Thus, the number of independent sets of cardinality $2l+1$ is at most $\frac{i_{2l}(n-2l)}{2l+1}$. (This bound is known as *Sperner's Lemma* [47]). Note that we must divide this product by $2l+1$ since each of our independent sets will appear $2l+1$ times by our construction.

It follows that $i_{2l+1} \le \frac{i_{2l}(n-2l)}{2l+1}$, which implies that $\frac{i_{2l+1}}{i_{2l}} \le \frac{n-2l}{1+2l} \le n$, with equality iff $l = 0$. Therefore, if $g_l(x) = x^{2l}(i_{2l} + i_{2l+1}x)$, then $g_l(-\frac{1}{n}) \ge 0$. Also, for $x > -\frac{1}{n}$, $g_l(x) > 0$ since $i_{2l} + i_{2l+1}x > i_{2l} - \frac{i_{2l+1}}{n} \ge 0$. Since $I(G,x) = \sum_{l \ge 0} g_l(x)$, we have $I(G,x) \ge 0$ for all $x \ge -\frac{1}{n}$, with equality iff $x = -\frac{1}{n}$ and $\alpha(G) = k = 1$. In other words, equality occurs iff $I(G,x) = 1 + nx$, i.e., $G = K_n$. In all other cases, $I(G,x) > 0$ for $x \ge -\frac{1}{n}$, implying that $|r_{min}| > \frac{1}{n}$. ∎

As an immediate corollary, we have answered the minimum modulus problem for circulants.

Corollary 5.13 *Let n be fixed, and let S be an arbitrary subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. Then the root r_{min} of minimum modulus of $I(C_{n,S}, x)$ satisfies $|r_{min}| \ge \frac{1}{n}$, with equality iff $S = \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ (i.e., the circulant is the complete graph).*

For some specific families of circulants $G = C_{n,S}$, we can improve this bound considerably. As an example, consider the easiest case $G = C_n$. Since $|\cos(\theta)| \le 1$ for any θ, Theorem 5.2 shows that the roots of $I(C_n, x)$ are bounded below by $|r_{min}| \ge \frac{1}{4}$, a constant independent of n.

We now generalize this bound by proving that for the family $G = A_n = C_{n,\{1,2,\ldots,d\}}$, the roots of $I(G,x)$ are bounded below by $|r_{min}| \ge \frac{d^d}{(d+1)^{d+1}}$. To prove this, we establish a stronger result that the *closure* of roots of $I(A_n, x)$ is the interval $(-\infty, -\frac{d^d}{(d+1)^{d+1}}]$. To prove this, we state some analytical results on recursive families of graphs. This collection of definitions and theorems is taken from [23].

Definition 5.14 *If $\{f_n(x)\}$ is a family of (complex) polynomials, a number $z \in \mathbb{C}$ is a* **limit of roots** *of $\{f_n(x)\}$ if either $f_n(z) = 0$ for all sufficiently large n, or z is a* *limit point of the set* $\mathcal{R}(\{f_n(x)\})$*, where* $\mathcal{R}(\{f_n(x)\})$ *is the union of the roots of the* $f_n(x)$*.*

By Corollary 5.4, each root of $f_n(x) = I(A_n, x)$ is a negative real number. We will show that $z \in \mathbb{C}$ is a limit of roots of $\{f_n(x)\}$ iff $z \leq -\frac{d^d}{(d+1)^{d+1}}$. By definition, this will imply that the closure of roots of $I(A_n, x)$ is $(-\infty, -\frac{d^d}{(d+1)^{d+1}}]$.

Definition 5.15 *A family* $\{f_n(x)\}$ *of polynomials is a* **recursive family of polynomials** *if the polynomials satisfy a homogeneous linear recurrence relation*

$$f_n(x) = \sum_{i=1}^{k} g_i(x) f_{n-i}(x),$$

where the $g_i(x)$ *are fixed polynomials with* $g_k(x) \not\equiv 0$*. The index* k *is the* **order** *of the recurrence.*

Specifically, if $f_n(x) = I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$, then $\{f_n(x)\}$ is a recursive family of polynomials of order $d+1$ since

$$f_n(x) = f_{n-1}(x) + x f_{n-d-1}(x),$$

by Lemma 2.2.

We now form the *characteristic equation* of this recurrence relation, namely

$$\lambda^{d+1} - \lambda^d - x = 0,$$

whose roots $\lambda_i(x)$ are algebraic functions. There are $(d+1)$ such roots, counting multiplicity.

If these roots are distinct, the general solution to this recurrence [8] is

$$f_n(x) = \sum_{i=1}^{d+1} \alpha_i(x) \lambda_i(x)^n, \tag{*}$$

where the $\alpha_i(x)$'s are determined uniquely from the given initial conditions.

The following result of Beraha, Kahane, and Weiss is the key theorem we need to prove our formula on the closure of the roots of $I(A_n, x)$.

Theorem 5.16 ([23]) *Consider the identity for $f_n(x)$ given in (*). Under the non-degeneracy requirements that no $\alpha_i(x)$ is identically zero and that for no pair $i \neq j$ is $\lambda_i(x) \equiv \omega\lambda_j(x)$ for some $\omega \in \mathbb{C}$ of unit modulus, then $z \in \mathbb{C}$ is a limit of roots of $\{f_n(x)\}$ if and only if either*

1. *two or more of the $\lambda_i(z)$ are of equal modulus, and strictly greater (in modulus) than the others; or*
2. *for some j, $\lambda_j(z)$ has modulus strictly greater than all the other $\lambda_i(z)$'s, and $\alpha_j(z) = 0$.*

To apply Theorem 5.16, we first need to verify the non-degeneracy requirements. In the following proposition and two lemmas, we establish non-degeneracy.

Proposition 5.17 *Let $r_1, r_2, \ldots, r_k \in \mathbb{C}$ be a set of distinct non-zero numbers, and $a_1, a_2, \ldots, a_k \in \mathbb{R}$ satisfy $\sum_{i=1}^{k} a_i \cdot r_i^n = 0$ for each $1 \leq n \leq k$. Then $a_i = 0$, for all $1 \leq i \leq k$.*

Proof: We have k equations and k unknowns. This system has a unique solution $(a_1, a_2, \ldots, a_k)$ iff the matrix

$$M = \begin{pmatrix} r_1 & r_2 & \cdots & r_n \\ r_1^2 & r_2^2 & \cdots & r_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ r_1^n & r_2^n & \cdots & r_n^n \end{pmatrix}$$

has a non-zero determinant.

By elementary operations, $\det(M) = r_1 r_2 \cdots r_n \cdot \det(M')$, where

$$M' = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ r_1 & r_2 & \cdots & r_n \\ \vdots & \vdots & \ddots & \vdots \\ r_1^{n-1} & r_2^{n-1} & \cdots & r_n^{n-1} \end{pmatrix}.$$

Since all the r_i's are distinct, M' is a *Vandermonde* matrix with $\det(M') \neq 0$. Therefore, $\det(M) \neq 0$ and the system has a unique solution. Since $a_1 = a_2 = \ldots = a_k = 0$ satisfies the system, the proof is complete. ∎

Lemma 5.18 *Consider the identity for $f_n(x)$ given in (*), where $f_n(x) = I(A_n, x)$. Then $\alpha_i(x) \equiv 1$ for all i. In other words, no $\alpha_i(x)$ is identically zero, and we have $f_n(x) = \sum_{i=1}^{d+1} \lambda_i(x)^n$, for all x.*

Proof: Fix x, and let $g(\lambda) = \lambda^{d+1} - \lambda^d - x$. First, we find all values of x for which $g(\lambda)$ has a root r of multiplicity greater than 1. Clearly, such an r must satisfy $g(r) = g'(r) = 0$. Since $g'(\lambda) = (d+1)\lambda^d - d\lambda^{d-1}$, r must be 0 or $\frac{d}{d+1}$, from which $g(r) = 0$ implies that $r = 0$ or $r = -\frac{d^d}{(d+1)^{d+1}}$, respectively. For now, let us assume that x does not take either of these values, and we will consider these two exceptional cases at the end.

Since $x \neq 0$ and $x \neq -\frac{d^d}{(d+1)^{d+1}}$, $g(\lambda)$ has $d+1$ *distinct* roots. The general solution to $f_n(x)$ is given in (*). We know that

$$f_n(x) = \sum_{i=1}^{d+1} \alpha_i(x)\lambda_i(x)^n,$$

for some constants $\alpha_i(x)$. We now prove that each $\alpha_i(x) = 1$. Since x is assumed to be some fixed number, let us define $\alpha_i(x) = c_i$ and $\lambda_i(x) = r_i$, for notational simplicity.

Let σ_k denote the k^{th} *elementary symmetric polynomial* on $\{r_1, r_2, \ldots, r_{d+1}\}$. For example, $\sigma_2 = \sum_{1\leq i<j\leq d+1} r_i r_j$ and $\sigma_3 = \sum_{1\leq i<j<k\leq d+1} r_i r_j r_k$.

A *symmetric polynomial* is any polynomial that is invariant under any permutation of its variables. Each of the power sums $S_n = \sum_{i=1}^{d+1} r_i^n$ is symmetric, and hence, can be expressed as a polynomial function of the σ_k's (c.f. [8]). For example,

$$\begin{aligned}
S_1 &= \sigma_1 \\
S_2 &= \sigma_1^2 - 2\sigma_2 \\
S_3 &= \sigma_1^3 - 3\sigma_1\sigma_2 + 3\sigma_3 \\
S_4 &= \sigma_1^4 - 4\sigma_1^2\sigma_2 + 4\sigma_1\sigma_3 + 2\sigma_2^2 - 4\sigma_4
\end{aligned}$$

Since $\{r_1, r_2, \ldots, r_{d+1}\}$ are the roots of the equation $\lambda^{d+1} - \lambda^d - x = 0$, the sequence $S_n = \sum_{i=1}^{d+1} r_i^n$ must satisfy a recurrence relation, whose characteristic equation is precisely $\lambda^{d+1} - \lambda^d - x = 0$. This unique recurrence relation is $S_n(x) = S_{n-1}(x) + xS_{n-d-1}(x)$, for all $n \geq d+1$. Observe that this recurrence relation has the exact same form as the recurrence for $f(x) = I(A_n, x)$.

There is a well-known relationship between the roots of a given polynomial. Since $\{r_1, r_2, \ldots, r_{d+1}\}$ are the roots of $\lambda^{d+1} - \lambda^d - x = 0$, we have $\sigma_1 = 1$, $\sigma_{d+1} = (-1)^d x$, and $\sigma_i = 0$ for all $2 \le i \le d$. For each $1 \le i \le d$, when S_i is written as a polynomial function of the σ_k's, the first term is $(\sigma_1)^i$, and every other term must be 0 since it contains at least one factor from the set $\{\sigma_2, \sigma_3, \ldots, \sigma_i\}$. Therefore, $S_i = (\sigma_1)^i = 1$ for each $1 \le i \le d$. The function $S_n = \sum_{i=1}^{d+1} r_i^n$ satisfies $S_0 = d+1$ and $S_i = 1$ for all $1 \le i \le d$.

In our proof to Theorem 2.3, we proved that $f_n(x) = I(A_n, x)$ satisfies the recurrence relation $f_n(x) = f_{n-1}(x) + x f_{n-d-1}(x)$, with initial values $f_0(x) = d+1$ and $f_i(x) = 1$ for all $1 \le i \le d$. Since S_n and $f_n(x)$ are defined by the exact same recurrence relation of order $d+1$, it follows that $S_n = f_n(x)$ since their initial $d+1$ values are identical.

Therefore $\sum_{i=1}^{d+1} r_i^n = S_n = f_n(x) = \sum_{i=1}^{d+1} c_i r_i^n$ for some constants $c_1, c_2, \ldots, c_{d+1}$. We can rewrite this as $\sum_{i=1}^{d+1} (c_i - 1) r_i^n = 0$, and this identity holds for all n, but specifically for $1 \le n \le d+1$. By Proposition 5.17, we must have $\alpha_i(x) = c_i = 1$ for each i.

To conclude the proof, we examine the exceptional cases $x = 0$ and $x = -\frac{d^d}{(d+1)^{d+1}}$, and show that $\alpha_i(x) = 1$ for each of these cases too. For $x = 0$, the roots of $g(\lambda)$ are 0 and 1, with the root $r = 0$ having multiplicity d. Since each $f_n(0) = I(A_n, 0) = 1$, we have

$$f_n(0) = \sum_{i=1}^{d+1} \lambda_i(0)^n = 1^n + 0^n + 0^n + \ldots + 0^n = 1.$$

Finally, let us consider the case $x = -\frac{d^d}{(d+1)^{d+1}}$. Let $r_1 = r_2 = \frac{d}{d+1}$. Then in the case of a double root, our function $f_n(x)$ must be of the form

$$f_n(x) = (c_1 + c_2 n) r_1^n + \sum_{i=3}^{d+1} c_i r_i^n.$$

This is a standard result (c.f. [8]). From the same analysis as before, $f_n(x) = S_n$ for all $n \ge 1$, from which we quickly conclude that $c_1 = 2$, $c_2 = 0$, and $c_i = 1$ for all $3 \le i \le d+1$. Therefore,

$$f_n(x) = 2r_1^n + \sum_{i=3}^{d+1} r_i^n = \sum_{i=1}^{d+1} r_i^n,$$

and the conclusion follows.

For all x, we have shown that $f_n(x) = \sum_{i=1}^{d+1} \lambda_i(x)^n$, where $\{\lambda_1(x), \ldots, \lambda_{d+1}(x)\}$ are the roots of $\lambda^{d+1} - \lambda^d - x = 0$. Therefore, $\alpha_i(x) \equiv 1$ for all $1 \le i \le d+1$, and hence, no $\alpha_i(x)$ is identically zero. $\blacksquare$

Lemma 5.19 *Consider the identity for $f_n(x)$ given in (*). There do not exist indices i and j for which $\lambda_i(x) \equiv \omega\lambda_j(x)$ for some $|\omega| = 1$.*

Proof: Let $x \neq 0$ be a fixed real number, and let $\{\lambda_1(x), \lambda_2(x), \ldots, \lambda_{d+1}(x)\}$ be the roots of the characteristic equation $\lambda^{d+1} - \lambda^d - x = 0$. Suppose there exist i and j so that $\lambda_i(x) = \omega\lambda_j(x)$ for some $|\omega| = 1$. Then, $\lambda_i(x) = a + bi$ for some a and b, and $|\lambda_i(x)| = |\lambda_j(x)|$ for some $i \neq j$.

We prove that $\lambda_j(x) = a - bi$. Earlier, we showed that $g(\lambda) = \lambda^{d+1} - \lambda^d - x$ can only have a multiple root at $r = 0$ or $r = \frac{d}{d+1}$. In other words, $\lambda_i(x) = \lambda_j(x)$ implies that $(a, b) = (0, 0)$ or $(\frac{d}{d+1}, 0)$.

Let $\lambda_j(x) = p + qi$. Then by our assumption, $a^2 + b^2 = p^2 + q^2$. Since $\lambda^{d+1} - \lambda^d = x$, we have $x = |x| = |\lambda^d(\lambda - 1)| = |\lambda|^d \cdot |\lambda - 1|$. Therefore,

$$\begin{aligned} |\lambda_i(x)|^d \cdot |\lambda_i(x) - 1| &= |\lambda_j(x)|^d \cdot |\lambda_j(x) - 1| \\ |\lambda_i(x) - 1| &= |\lambda_j(x) - 1| \\ |(a-1) + bi| &= |(p-1) + qi| \\ (a-1)^2 + b^2 &= (p-1)^2 + q^2 \\ (a^2 + b^2) - 2a + 1 &= (p^2 + q^2) - 2p + 1 \\ -2a + 1 &= -2p + 1 \\ p &= a. \end{aligned}$$

We have shown that $p = a$. Since $a^2 + b^2 = p^2 + q^2$, it follows that $q = \pm b$. If $q = -b$, then $\lambda_j(x) = a - bi$. If $q = b$, then $\lambda_i(x) = \lambda_j(x)$, implying that $b = q = 0$. Hence, $\lambda_j(x) = a + bi = a - bi$ in this case as well.

Therefore, if $|\lambda_i(x)| = |\lambda_j(x)|$, then $\lambda_i(x)$ and $\lambda_j(x)$ must be complex conjugates, with the exception of the cases when the roots are 0 or $\frac{d}{d+1}$. We now prove that there does not exist ω with $|\omega| = 1$ such that $\lambda_i(x) \equiv \omega\lambda_j(x)$, i.e., we show that this identity cannot hold for all x.

Suppose on the contrary that such a ω does exist. Then for any constants c_1 and c_2,

$$\frac{\lambda_i(c_1)}{\lambda_j(c_1)} = \frac{\lambda_i(c_2)}{\lambda_j(c_2)} = \omega.$$

Since this identity holds for all pairs of constants (c_1, c_2), let us assume that neither c_1 nor c_2 equals 0 or $-\frac{d^d}{(d+1)^{d+1}}$, and that $c_1 \neq c_2$. Thus, $\lambda_i(c_t)$ and $\lambda_j(c_t)$ must be distinct complex conjugates for $t = 1, 2$.

So if $\lambda_i(c_1) = a + bi$ and $\lambda_i(c_2) = c + di$, then $\frac{a+bi}{a-bi} = \frac{c+di}{c-di}$, implying that $ad = bc$, or $\lambda_i(c_2) = \frac{c}{a}(a + bi) = k\lambda_i(c_1)$ for the real constant $k = \frac{c}{a}$. In other words, $a + bi$ is a root of $\lambda^{d+1} - \lambda^d = c_1$ and $k(a + bi)$ is a root of $\lambda^{d+1} - \lambda^d = c_2$. Hence, we have

$$\begin{aligned} (a+bi)^d((a+bi)-1) &= c_1 \\ k^d(a+bi)^d(k(a+bi)-1) &= c_2. \end{aligned}$$

Therefore, $\frac{k(a+bi)-1}{(a+bi)-1} = \frac{c_2}{c_1k^d}$. Comparing the complex parts of both sides, we have $\frac{b(1-k)}{(a-1)^2+b^2} = 0$, implying that $b(1 - k) = 0$. Thus, we must have $b = 0$ or $k = 1$. The former implies that $\lambda_i(c_1) = \lambda_j(c_1) = a$, contradicting the fact that $\lambda_i(c_1)$ and $\lambda_j(c_1)$ are distinct complex numbers that are pairwise conjugate. The latter implies that $c_1 = c_2$, which contradicts the given assumption.

We conclude that no such ω exists, and we are done. ∎

Now we prove our theorem on the closure of roots of $I(A_n, x)$.

Theorem 5.20 *Let $d \geq 1$ be fixed, and set $f_n(x) = I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$. Then, the roots of $f_n(x)$ are real, and the closure of roots is* $\left(-\infty, -\dfrac{d^d}{(d+1)^{d+1}}\right]$.

Proof: By Lemmas 5.18 and 5.19, the family $\{f_n(x)\}$ satisfies the non-degeneracy requirements that enables us to apply Theorem 5.16.

Since each root of $f_n(x) = I(A_n, x)$ is real and negative by Corollary 5.4, the closure of roots of $\{f_n(x)\}$ is some subset of $(-\infty, 0]$. In particular, if $z \in \mathbb{C}$ is a limit of roots of $\{f_n(x)\}$, then z is a non-positive real number. We consider three separate cases.

<u>*Case 1:*</u> $\quad -\dfrac{d^d}{(d+1)^{d+1}} < z \leq 0.$

The characteristic equation of $f_n(z) = I(A_n, z)$ is $g(\lambda) = \lambda^{d+1} - \lambda^d - z = 0$, which has $d+1$ roots, namely $\{\lambda_1(z), \lambda_2(z), \ldots, \lambda_{d+1}(z)\}$.

By Theorem 5.7, the equation $(v-1)x^v - vx_0x^{v-1} + 1 = 0$ has at least $v-1$ roots inside the unit circle $|x| = 1$ regardless of the value of x_0. Let c be the unique positive (real) constant satisfying $\frac{1}{dc^{d+1}} = -z$.

Substituting $v = d+1$, $x = c\lambda$ and $x_0 = \frac{cd}{d+1}$ into the above equation, we see that the resulting equation $\lambda^{d+1} - \lambda^d + \frac{1}{dc^{d+1}} = 0$ must have at least d roots inside the disk $|c\lambda| = 1$, or $|\lambda| = \frac{1}{c}$.

Since $\frac{1}{dc^{d+1}} = -z$, we have $\left(\frac{1}{c}\right)^{d+1} = -zd < \frac{d^{d+1}}{(d+1)^{d+1}}$, implying that $\frac{1}{c} < \frac{d}{d+1}$. Therefore, $\lambda^{d+1} - \lambda^d - z = 0$ has at least d roots on or inside the disk $|\lambda| = \frac{1}{c} < \frac{d}{d+1}$. We now show that there must exist a real root in $(\frac{d}{d+1}, 1)$, i.e., there is exactly one root outside of this disk.

We have $g(\frac{d}{d+1}) = -\frac{d^d}{(d+1)^{d+1}} - z < 0$ and $g(1) = -z \geq 0$. By the Intermediate Value Theorem, there is a real root in $(\frac{d}{d+1}, 1]$. Hence, if $\{\lambda_1(z), \lambda_2(z), \ldots, \lambda_{d+1}(z)\}$ is the set of roots of $g(\lambda)$ arranged in order of increasing magnitude, then $|\lambda_{d+1}(z)| > \frac{d}{d+1}$, while $|\lambda_i(z)| \leq \frac{d}{d+1}$ for all $1 \leq i \leq d$. By Theorem 5.16, z cannot be a limit of roots since there is only one root of maximum modulus.

<u>*Case 2:*</u> $\quad z = -\dfrac{d^d}{(d+1)^{d+1}}.$

We apply Theorem 5.7 as in the previous case, and let $\frac{1}{dc^{d+1}} = -z = \frac{d^d}{(d+1)^{d+1}}$. Then $c = \frac{d+1}{d}$, and so $g(\lambda) = \lambda^{d+1} - \lambda^d - z = 0$ has at least d roots on or inside the disk $|\lambda| = \frac{1}{c} = \frac{d}{d+1}$. In other words, there is at most one root outside this disk. This one root must be real, as complex roots occur as conjugate pairs.

However, $g(\lambda) = 0$ has a double root at $\lambda = \frac{d}{d+1}$, and no other positive real roots. It follows that $g(\lambda) = 0$ has all of its roots inside $|\lambda| = \frac{d}{d+1}$, with the exception of the two roots on the boundary. Therefore, the roots $\lambda_d(z) = \lambda_{d+1}(z) = \frac{d}{d+1}$ are the roots of maximum modulus. By Theorem 5.16, $z = -\frac{d^d}{(d+1)^{d+1}}$ is a limit of roots of $\{f_n(x)\}$.

<u>*Case 3:*</u> $\quad z < -\dfrac{d^d}{(d+1)^{d+1}}$.

If $g(\lambda) = \lambda^{d+1} - \lambda^d - z$, then $g'(\lambda) = 0$ has solutions $\lambda = 0$ and $\lambda = \frac{d}{d+1}$. So these are the only two critical points of $g(\lambda)$. Since $g(0) = -z > 0$ and $g(\frac{d}{d+1}) = -\frac{d^d}{(d+1)^{d+1}} - z > 0$, the equation $g(\lambda) = 0$ has at most one real root c, depending on the parity of d.

If d is odd, then $g(\lambda)$ has no real roots and so all of its roots must occur as conjugate pairs. Thus, if $\lambda_i(z) = a + bi$ is a root of maximum modulus, then there exists a root $\lambda_j(z) = a - bi$, so that two (or more) of the $\lambda_i(z)$'s are of equal modulus and strictly greater than the others. By Theorem 5.16, z is a limit of roots.

If d is even, then $g(\lambda)$ has a real root $c < 0$. We claim that c must be the root of minimum modulus, and that the other d roots occur as conjugate pairs. To prove this, suppose there exists a root $r \in \mathbb{C}$ such that $|r| < |c| = -c$. Then $g(r) = g(c) = 0$, implying that $r^d(r-1) = c^d(c-1)$, or $|r|^d(|r-1|) = |c|^d(|c-1|) = c^d(1-c)$. Hence, $\frac{1-c}{|r-1|} = \left(\frac{|r|}{-c}\right)^d < 1^d = 1$. It follows that $1 - c < |r-1| \leq |r| + 1$, by the Triangle Inequality. This simplifies to $|r| \geq -c$, which establishes our desired contradiction. Therefore, all complex roots $\lambda_i(z)$ must satisfy $|\lambda_i(z)| \geq -c$, proving that the root of largest modulus cannot be real. Hence, the maximum roots are complex and appear as conjugate pairs, establishing the desired conclusion that z is a limit of roots.

We conclude that $z \in \mathbb{C}$ is a limit of roots iff z is a real number satisfying $z \leq -\frac{d^d}{(d+1)^{d+1}}$. This completes the proof. ∎

We have shown that the closure of roots of $f_n(x) = I(A_n, x)$ is $(-\infty, -\frac{d^d}{(d+1)^{d+1}}]$. We proved this by considering limit points, and showing that z is a limit point iff z lies in the aforementioned interval. Thus, we conclude that $|r_{min}| \geq \frac{d^d}{(d+1)^{d+1}}$.

In Theorem 2.3, we proved that

$$I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x) = \sum_{k=0}^{\lfloor \frac{n}{d+1} \rfloor} \frac{n}{n-dk}\binom{n-dk}{k} x^k.$$

We have proven that this independence polynomial $I(C_{n,\{1,2,\ldots,d\}}, x)$ has all negative real roots, and that the root r_{min} of minimum modulus satisfies $|r_{min}| \geq \frac{d^d}{(d+1)^{d+1}}$.

Furthermore, our analysis proves that this lower bound is optimal.

5.3 The Root of Maximum Modulus of $I(C_{n,S}, x)$

Having determined the optimal bound for the root r_{min} of minimum modulus of $I(C_{n,S}, x)$, we now turn our attention to the root r_{max} of maximum modulus. We derive an optimal bound on $|r_{max}|$ when G is a circulant. In [25], it is shown that for any graph G, the root r_{max} of $I(G, x)$ satisfies

$$|r_{max}| \leq \left(\frac{n}{\alpha(G) - 1}\right)^{\alpha(G)-1} + O(n^{\alpha(G)-2}).$$

In other words, $|r_{max}|$ is at most $O(n^{\alpha(G)-1})$, and in [25], Brown and Nowakowski construct graphs for which this upper bound is attained. We now answer the equivalent problem where G is restricted to circulants. We prove that $|r_{max}|$ is bounded above by $\Theta(n^{\alpha(G)-2})$, i.e., the exponent reduces by 1. Furthermore, we prove the existence of infinitely many circulants achieving this upper bound. To prove our result, we introduce the *Enestrom-Kakeya Theorem.*

Theorem 5.21 ([22, 25]) *Let $f(x) = i_0 + i_1 x + \ldots + i_k x^k$ be a polynomial with positive real coefficients. Then the roots of $f(x)$ lie in the annulus*

$$\min\left\{\frac{i_{t-1}}{i_t}, t = 1, \ldots, k\right\} \leq |z| \leq \max\left\{\frac{i_{t-1}}{i_t}, t = 1, \ldots, k\right\}.$$

Using Theorem 5.21, we prove our bound for $|r_{max}|$. Before we prove our bound, we require several results. Our first result is a theorem of Newton, which produces an important corollary.

Theorem 5.22 ([49]) *Let $P(x) = \sum a_k x^k$ be a polynomial with each $a_k > 0$. If the roots of $P(x)$ are all (negative) real numbers, then $P(x)$ is* **log-concave***. In other words,*

$$\frac{a_0}{a_1} \leq \frac{a_1}{a_2} \leq \frac{a_2}{a_3} \leq \ldots \leq \frac{a_{n-1}}{a_n}.$$

The following corollary is an immediate consequence of Corollary 5.4.

Corollary 5.23 *For a fixed $d \geq 1$, define $A_n = C_{n,\{1,2,\ldots,d\}}$, for each n. Then $I(A_n, x)$ is log-concave.*

We present another key result. While this lemma appears contrived, this is a key inequality that will enable us to prove our desired bound for $|r_{max}|$.

Lemma 5.24 *For any pair of integers (n, k) with $n \equiv 0 \pmod{k}$ and $n > k \geq 2$, define $i_k = \frac{n}{k}$, $i_{k-1} = \frac{n}{\frac{n}{k}+k-1}\binom{\frac{n}{k}+k-1}{k-1} = \frac{n}{k-1}\binom{\frac{n}{k}+k-2}{k-2}$, and $i_{k-2} = \frac{n}{\frac{2n}{k}+k-2}\binom{\frac{2n}{k}+k-2}{k-2}$. Then, $i_{k-1}^2 > 4i_k i_{k-2}$.*

Proof: Let $d = \frac{n}{k}$ and $f(d,k) = \frac{i_{k-1}^2}{i_k i_{k-2}}$. Then the inequality $i_{k-1}^2 > 4i_k i_{k-2}$ is equivalent to $f(d,k) > 4$, where $f(d,k)$ simplifies to

$$f(d,k) = \binom{2d}{d} \cdot \frac{k}{k-1} \cdot \frac{((d+k-2)!)^2}{(k-1)!(2d+k-3)!}.$$

We have $\frac{f(d+1,k)}{f(d,k)} = \frac{2(2d+1)(d+k-1)^2}{(d+1)(2d+k-1)(2d+k-2)}$. Then the condition $f(d+1,k) > f(d,k)$ is equivalent to $d^2(4k-4)+d(3k^2-5k+4)+(k^2-k) > 0$, which is true since $d, k \geq 1$. Therefore, $f(d+1,k) > f(d,k)$. Also, $f(2,k) = \frac{6k^2}{k^2-1} > 4$ for all $k \geq 2$. Therefore, $f(d,k) > 4$ for all $d, k \geq 2$. ∎

We are now ready to prove our bound on r_{max}.

Theorem 5.25 *Let $G = C_{n,S}$ be a circulant graph with $k = \alpha(G)$. Consider the roots of $I(C_{n,S}, x)$. Then the root r_{max} of maximum modulus satisfies*

$$|r_{max}| < \frac{k}{(k-1)!} n^{k-2}.$$

Furthermore, the optimal upper bound must be some $\Theta(n^{k-2})$ function, as there are infinitely many independence polynomials $I(C_{n,\{1,2,\ldots,d\}}, x)$ satisfying $|r_{max}| = \Theta(n^{k-2})$.

Proof: Let $I(G,x) = 1 + nx + i_2x^2 + \ldots + i_{k-1}x^{k-1} + i_kx^k$, where $k = \alpha(G) = \alpha(C_{n,S})$. Consider the ratio $\frac{i_{k-1}}{i_k}$. By definition, $i_{k-1} \leq \binom{n}{k-1}$. Now consider i_k. Since $i_k > 0$, there exists at least one independent set I with k vertices. We prove that in a circulant, $i_k \geq 1$ implies that $i_k \geq \frac{n}{k}$. Letting $D = (d_1, d_2, \ldots, d_k)$ be the difference sequence corresponding to I, we can form n independent sets with a difference sequence of D. Specifically, each set will be of the form

$$V_j = \{j, j+d_1, j+d_1+d_2, \ldots, j+d_1+d_2+\ldots+d_{k-1}\},$$

where $0 \leq j \leq n-1$, and the indices are reduced mod n, and arranged in increasing order.

Note that each V_j is an independent set of cardinality k in $C_{n,S}$. However, it is possible that some of the k-sets overlap, i.e., $V_j \equiv V_{j'}$ for some $j \neq j'$. For any given V_j, we can have at most k overlaps, one for each cyclic permutation of V_j. Therefore, $i_k \geq \frac{n}{k}$. Equality occurs iff $n \equiv 0 \pmod{k}$, and $D = \left(\frac{n}{k}, \frac{n}{k}, \ldots, \frac{n}{k}\right)$. We have

$$\frac{i_{k-1}}{i_k} \leq \frac{\binom{n}{k-1}}{\frac{n}{k}} < \frac{k}{n}\binom{n}{k-1} < \frac{k}{(k-1)!}n^{k-2}.$$

Let $1 \leq t \leq k-1$. Since $n \geq k \geq t$, the exact same analysis shows that $\frac{i_{t-1}}{i_t} \leq \frac{\binom{n}{t-1}}{\frac{n}{t}} < \frac{t}{(t-1)!}n^{t-2}$.

To justify why $\frac{t}{(t-1)!}n^{t-2} < \frac{k}{(k-1)!}n^{k-2}$ for $t < k$, note that this inequality is equivalent to $n^{k-t} > \frac{(k-1)!}{(t-1)!} \cdot \frac{t}{k} = \frac{t}{k} \cdot (k-1)(k-2)\cdots(k-(k-t))$. This latter inequality is true, since $t < k$ and the right side has $k-t$ factors, all of which are less than $k \leq n$. Therefore, by Theorem 5.21, we have

$$|r_{max}| \leq \max\left\{\frac{i_{t-1}}{i_t}, t = 1, \ldots, k\right\} < \frac{k}{(k-1)!}n^{k-2}.$$

To conclude our proof, we now prove the existence of infinitely many circulants for which $|r_{max}| = \Theta(n^{k-2}) = \Theta(n^{\alpha(G)-2})$, for each possible value of $\alpha(G)$. This establishes that the optimal upper bound is a polynomial function of order $n^{\alpha(G)-2}$.

If $\alpha(G) = 1$, then $G = K_n$, and so $I(K_n, x) = 1 + nx$, which implies that $|r_{max}| = \frac{1}{n} = O(n^{-1})$.

Consider the case $\alpha(G) \geq 2$. For each (n,k) with $\alpha(G) = k$ and $k|n$ (with $n \geq 2k$), define $H_{n,k} = C_{n,\left\{1,2,\ldots,\frac{n}{k}-1\right\}}$. By Theorem 2.3, $\alpha(G_k) = \left\lfloor \frac{n}{\frac{n}{k}} \right\rfloor = k$, and

$$I(H_{n,k}, x) = \sum_{i=0}^{k} \frac{n}{n - i\left(\frac{n}{k}-1\right)} \binom{n - i\left(\frac{n}{k}-1\right)}{i} x^i.$$

By Corollary 5.4, the roots of $I(H_{n,k}, x)$ are all real. Letting $i_t = [x^t]I(H_{n,k}, x)$, we have $i_k = \frac{n}{k}$, $i_{k-1} = \frac{n}{\frac{n}{k}+k-1}\binom{\frac{n}{k}+k-1}{k-1} = \frac{n}{k-1}\binom{\frac{n}{k}+k-2}{k-2}$, and $i_{k-2} = \frac{n}{\frac{2n}{k}+k-2}\binom{\frac{2n}{k}+k-2}{k-2}$. This enables us to apply Lemma 5.24.

We now prove that for this polynomial,

$$-\frac{k}{k-1}\binom{\frac{n}{k}+k-2}{k-2} \le r_{max} \le -\frac{k}{2(k-1)}\binom{\frac{n}{k}+k-2}{k-2},$$

which will imply that $|r_{max}|$ is $\Theta(n^{k-2})$ since

$$\begin{aligned}
\frac{k}{(k-1)}\binom{\frac{n}{k}+k-2}{k-2} &= \frac{1}{(k-1)!k^{k-3}}n^{k-2}+O(n^{k-3}) \\
\frac{k}{2(k-1)}\binom{\frac{n}{k}+k-2}{k-2} &= \frac{1}{2(k-1)!k^{k-3}}n^{k-2}+O(n^{k-3})
\end{aligned}$$

For each $0 \le l \le \frac{k}{2}$, let $g_l(x) = i_{k-2l}x^{k-2l} + i_{k-2l-1}x^{k-2l-1}$. Then, $I(G,x) = \sum_{l\ge 0} g_l(x)$. By Corollary 5.23, $I(G,x)$ is log-concave. Therefore,

$$\frac{i_{k-2l-1}}{i_{k-2l}} \le \frac{i_{k-2l}}{i_{k-2l+1}} \le \dots \le \frac{i_{k-3}}{i_{k-2}} \le \frac{i_{k-2}}{i_{k-1}}.$$

Specifically, $\frac{i_{k-2l-1}}{i_{k-2l}} \le \frac{i_{k-2}}{i_{k-1}}$. By Lemma 5.24, $\frac{i_{k-2}}{i_{k-1}} < \frac{i_{k-1}}{i_k}$. It follows that $i_{k-2l-1} < i_{k-2l}\cdot\frac{i_{k-1}}{i_k}$, which is equivalent to $i_{k-2l}r + i_{k-2l-1} < 0$, where $r = -\frac{i_{k-1}}{i_k}$.

For this r, we have $g_0(r) = 0$, and for $l \ge 1$, $g_l(r) = r^{k-2l-1}(i_{k-2l}r + i_{k-2l-1})$, which has the same sign as $(-1)^{k-2l-1}\cdot(-1) = (-1)^k$. Therefore, $\text{sign}(I(H_{n,k},r)) = (-1)^k$. The same argument shows that $\text{sign}(I(H_{n,k},x)) = (-1)^k$, for all $x < r = -\frac{i_{k-1}}{i_k}$.

Now we prove that for $r' = \frac{r}{2}$, $\text{sign}(I(H_{n,k},r')) = (-1)^{k-1}$. This enables us to apply the Intermediate Value Theorem, and conclude the existence of a root in (r,r'). For each $1 \le l < \frac{k}{2}$, let $h_l(x) = i_{k-2l-1}x^{k-2l-1} + i_{k-2l-2}x^{k-2l-2}$. Then,

$$I(H_{n,k},x) = i_kx^k + i_{k-1}x^{k-1} + i_{k-2}x^{k-2} + \sum_{l\ge 1} h_l(x).$$

Let $r' = \frac{r}{2} = -\frac{i_{k-1}}{2i_k}$. By Lemma 5.24,

$$i_kr' + i_{k-1} + \frac{i_{k-2}}{r'} = -\frac{i_{k-1}}{2} + i_{k-1} - \frac{2i_ki_{k-2}}{i_{k-1}} = \frac{i_{k-1}^2 - 4i_ki_{k-2}}{2i_{k-1}} > 0.$$

Therefore, $i_k(r')^k + i_{k-1}(r')^{k-1} + i_{k-2}(r')^{k-2} = (r')^{k-1}(i_kr' + i_{k-1} + \frac{i_{k-2}}{r'})$ has the same sign as $(-1)^{k-1}$. Now we prove that $\text{sign}(h_l(r')) = (-1)^{k-1}$ for each $l \ge 1$.

Since $h_l(r') = (r')^{k-2l-1}(i_{k-2l-1} + \frac{i_{k-2l-2}}{r'})$, it suffices to prove that $i_{k-2l-1} + \frac{i_{k-2l-2}}{r'} > 0$. By Corollary 5.23, $\frac{i_{k-2l-2}}{i_{k-2l-1}} \le \frac{i_{k-2}}{i_{k-1}}$, which implies that $\frac{i_{k-2l-2}}{i_{k-2l-1}} + r' \le \frac{i_{k-2}}{i_{k-1}} + r' =$

$\frac{i_{k-2}}{i_{k-1}} - \frac{i_{k-1}}{2i_k} < 0$, by Lemma 5.24. It follows that $\frac{i_{k-2l-2}}{i_{k-2l-1}} + r' < 0$, implying that $i_{k-2l-1} + \frac{i_{k-2l-2}}{r'} > 0$, as required. Thus, $\text{sign}(I(H_{n,k}, r')) = (-1)^{k-1}$.

Therefore, we have proven that $\text{sign}(I(H_{n,k}, r)) \cdot \text{sign}(I(H_{n,k}, r')) = -1$, where $r = -\frac{i_{k-1}}{i_k}$ and $r' = \frac{r}{2} = -\frac{i_{k-1}}{2i_k}$. By the Intermediate Value Theorem, there must exist a root r^* in the interval (r, r'). Furthermore, $I(H_{n,k}, x)$ has the same sign as $(-1)^k$ for all $x < -\frac{i_{k-1}}{i_k}$, and so it follows that this root r^* is the root of maximum modulus. Therefore, the root r_{max} of $I(H_{n,k}, x)$ satisfies

$$|r_{max}| \geq \frac{i_{k-1}}{2i_k} = \frac{k}{2(k-1)}\binom{\frac{n}{k}+k-2}{k-2} = \frac{1}{2(k-1)! \cdot k^{k-3}}n^{k-2} + O(n^{k-3}).$$

We have proven that for any fixed $k \geq 1$, the largest root of $I(H_{n,k}, x)$ has a modulus of order $\Theta(n^{k-2})$, for all $n \equiv 0 \pmod{k}$. We have thus established the desired optimal bound. ∎

Therefore, we have proven that among all circulant graphs with $\alpha(G) = k$, the root r_{max} of maximum modulus satisfies

$$\frac{1}{2(k-1)! \cdot k^{k-3}}n^{k-2} < |r_{max}| < \frac{k}{k-1}n^{k-2}.$$

It would be interesting to find the optimal constant c (as a function of k) for which $|r_{max}| \leq cn^{k-2} + O(n^{k-3})$ for all independence polynomials $I(C_{n,S}, x)$ with $\alpha(C_{n,S}) = k$. We leave this as an open problem.

5.4 The Rational Roots of $I(C_{n,S}, x)$

For certain circulant graphs, the roots of $I(C_{n,S}, x)$ can take rational values. An example of this is $I(C_6, x)$, since the independence polynomial $I(C_6, x) = 1 + 6x + 9x^2 + 2x^3 = (1 + 2x)(1 + 4x + x^2)$ has the root $r = -\frac{1}{2}$.

Let us begin our analysis by considering the simplest case $I(C_n, x)$. We determine all values of n for which $I(C_n, x)$ has a rational root r. Let $g_0 = 2$, $g_1 = 1$, $g_2 = 1+2x$, and $g_n = I(C_n, x)$ for all $n \geq 3$. So each g_n is a polynomial in x. By Corollary 2.4,

$$g_n = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n}{n-k}\binom{n-k}{k}x^k,$$

for all $n \geq 2$.

We obtain a simple recurrence relation for g_n, and use this to derive properties of the roots of $g_n = I(C_n, x)$.

Lemma 5.26 *Let* $0 \leq a \leq \lfloor \frac{n}{2} \rfloor$. *Then,*

$$g_n = g_a g_{n-a} + (-1)^{a+1} x^a g_{n-2a}.$$

Proof: We proceed by strong induction on n. By inspection, the lemma is verified for $n \leq 2$, so assume $n \geq 3$. By the induction hypothesis and two applications of Lemma 2.2, we have

$$\begin{aligned} g_n &= g_{n-1} + x g_{n-2} \\ &= [g_{a-1} g_{n-a} + (-1)^a x^{a-1} g_{n-2a+1}] + x[g_{a-2} g_{n-a} + (-1)^{a-1} x^{a-2} g_{n-2a+2}] \\ &= g_{n-a}[g_{a-1} + x g_{a-2}] + (-1)^a x^{a-1} [g_{n-2a+1} - g_{n-2a+2}] \\ &= g_{n-a} g_a + (-1)^a x^{a-1} (-x g_{n-2a}) \\ &= g_a g_{n-a} + (-1)^{a+1} x^a g_{n-2a}. \end{aligned}$$

This completes the induction, and we are done. ∎

Corollary 5.27 *Let* $I(C_n, x)$ *be the independence polynomial of* C_n. *Then,*

(a) $r = -\frac{1}{2}$ *is a root of* $I(C_n, x)$ *iff* $n \equiv 2 \pmod 4$.

(b) $r = -\frac{1}{3}$ *is a root of* $I(C_n, x)$ *iff* $n \equiv 3 \pmod 6$.

Proof: From Lemma 5.26, $g_n = g_2 g_{n-2} - x^2 g_{n-4} = (1+2x) g_{n-2} - x^2 g_{n-4}$. Therefore, $r = -\frac{1}{2}$ is a root of g_n iff it is also a root of g_{n-4}. Since $r = -\frac{1}{2}$ is a root of $g_2 = 1+2x$, but not g_1, g_3, or g_4, the result follows. Similarly, $r = -\frac{1}{3}$ is a root of g_n iff it is also a root of g_{n-6}. One can quickly verify that $r = -\frac{1}{3}$ is a root of $g_3 = 1 + 3x$, but not a root of g_1, g_2, g_4, g_5, or g_6. This completes the proof. ∎

Lemma 5.26 also yields the following result.

Proposition 5.28 *Let* (m, n) *be an ordered pair of positive integers. If* $\frac{m}{n}$ *is an odd number, then* g_n *divides* g_m.

Proof: Let $\frac{m}{n} = p$. We proceed by induction on p, and prove that the result holds for all pairs of positive integers (m, n) satisfying $m = pn$, where p is odd.

The claim is trivial for $p = 1$. Suppose the result is true for $p = 2k - 1$, where $k \geq 1$. Then for $p = 2k+1$, Lemma 5.26 gives us $g_{2kn+n} = g_n g_{2kn} + (-1)^{n+1} x^n g_{2kn-n}$. By the induction hypothesis, g_n divides g_{2kn-n}, and so

$$g_m = g_{pn} = g_{2kn+n} \equiv 0 \pmod{g_n}.$$

This completes the induction, and so we conclude that g_n divides g_m whenever $\frac{m}{n}$ is odd. ∎

By the Rational Root Theorem, any rational root of $I(G, x)$ must be of the form $r = -\frac{1}{d}$, where d is a divisor of n. For the specific case $G = C_n$, we now prove that the only possible rational roots of $I(G, x)$ are $r = -\frac{1}{2}$ and $r = -\frac{1}{3}$.

Theorem 5.29 *Let $n \geq 2$. Then r is a rational root of $I(C_n, x)$ iff $r = -\frac{1}{2}$ or $r = -\frac{1}{3}$.*

Proof: From Theorem 5.2, $r_{n,k} = -\frac{1}{4\left[\cos\left(\frac{(2k-1)\pi}{2n}\right)\right]^2}$ is a root of $I(C_n, x)$ for each $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. Moreover, this is the set of roots of $I(C_n, x)$. Suppose $r_{n,k} = -\frac{1}{d}$, for some integers d, n, and k. Then by Theorem 5.2, $u_{n,k} = \pm\frac{\sqrt{d}}{2}$, where $u_{n,k} = \cos(\frac{(2k-1)\pi}{2n})$.

If $d = 4$, then $|u_{n,k}| = 1$, which can only occur if $2n$ divides $2k - 1$. Clearly this is impossible. If $d > 4$, then $|u_{n,k}| > 1$, which is also a contradiction. If $d = 1$, then $|u_{n,k}| = \frac{1}{2}$, which can only occur if $\frac{(2k-1)}{2n} = 2\pi \pm \frac{\pi}{3}$. But $\frac{(2k-1)}{2n}$ has an odd numerator, while the denominator is even. Thus, when this fraction is reduced to lowest terms, the denominator must remain even. Specifically, this fraction cannot have a denominator of 3, and so this case also leads to a contradiction.

Therefore, we require $d = 2$ or $d = 3$. Now the conclusion follows immediately from Corollary 5.27. ∎

From Corollary 5.27 and Theorem 5.29, we have determined our necessary and sufficient condition for $I(C_n, x)$ to have a rational root.

Corollary 5.30 *The polynomial $I(C_n, x)$ has a rational root iff n is congruent to* 2*,* 3*,* 6*,* 9*, or* 10 $\pmod{12}$.

Proof: By Corollary 5.27, $I(C_n, x)$ has a rational root iff $n \equiv 2 \pmod 4$ or $n \equiv 3 \pmod 6$. Considering each equivalence class of $\mathbb{Z}_{12}$ separately, we obtain the desired conclusion. ∎

We now examine the possible rational roots of $I(C_{n,S}, x)$, when S is an arbitrary subset of $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$. The problem of determining rational roots of independence polynomials is investigated in [119], where it is shown that for any rational number $r = -\frac{1}{d}$, there exists a well-covered tree T so that r is a root of $I(T, x)$. Let us investigate the equivalent problem for circulants.

By the Rational Root Theorem, every rational root of $I(G, x)$ must be of the form $r = -\frac{1}{d}$, for some integer $d \geq 1$. If G is not required to be connected, then there are infinitely many circulants for which $r = -\frac{1}{d}$ is a root of its independence polynomial. This is easily seen by taking the disjoint union of k isomorphic copies of K_d, which corresponds to the circulant $C_{dk,\{k,2k,\ldots,\lfloor \frac{dk}{2} \rfloor\}}$ and has independence polynomial $I(G, x) = (1 + dx)^k$.

So we will phrase the problem as follows: for which integers $d \geq 1$ is $r = -\frac{1}{d}$ a root of infinitely many *connected* circulant graphs G? While this is a tantalizing problem, we will only make partial progress in answering this question. Nevertheless, we include our results in this section, and conclude by providing various conjectures and ideas for further research. For notational convenience, we introduce the following definition.

Definition 5.31 *A rational number r is* **CC-infinite** *if there exist infinitely many connected circulant graphs $G = C_{n,S}$ for which $I(C_{n,S}, r) = 0$.*

For example, Corollary 5.27 shows that $r = -\frac{1}{2}$ and $r = -\frac{1}{3}$ are CC-infinite, since every cycle is a connected circulant. To prove our partial result, we first require the following lemma.

Lemma 5.32 *If p is a positive integer such that $r = -\frac{1}{p}$ is CC-infinite, then $r = -\frac{1}{mp}$ is CC-infinite for all $m \geq 1$.*

Proof: Fix $m \geq 1$. Suppose that there exist graphs $G_1, G_2, G_3, \ldots$ for which $I(G_i, -\frac{1}{p}) = 0$ for all $i \geq 1$. Now define $H_i = G_i[K_m]$ for each i. By Theorem 2.31, each H_i is a connected circulant. Then $I(H_i, x) = I(G_i[K_m], x) = I(G_i, I(K_m, x) - 1) = I(G_i, mx)$, by Theorem 2.33. Therefore, $I(H_i, -\frac{1}{mp}) = I(G_i, -\frac{1}{p}) = 0$, for all $i \geq 1$. We conclude that $r = -\frac{1}{mp}$ is CC-infinite, for all $m \geq 1$. ∎

We state the following simple result.

Proposition 5.33 *If* $\gcd(d, 6) > 1$, *then* $r = -\frac{1}{d}$ *is CC-infinite.*

Proof: By Corollary 5.27, $r = -\frac{1}{2}$ and $r = -\frac{1}{3}$ appear as roots of infinitely many circulants. By Lemma 5.32, the same is true for all rational numbers of the form $r = -\frac{1}{2m}$ or $r = -\frac{1}{3m}$, for any $m \geq 1$. The conclusion follows. ∎

We conjecture that $r = -\frac{1}{p}$ is CC-infinite for every prime p. This will imply that $r = -\frac{1}{d}$ is CC-infinite for all $d \geq 2$. While we believe that each $r = -\frac{1}{p}$ is CC-infinite, we have only been able to find several instances where $r = -\frac{1}{p}$ is a root of some $I(C_{n,S}, x)$ for primes $p \geq 5$. Of course, the difficulty lies in not knowing a formula for $I(C_{n,S}, x)$, except for a handful of families.

Let us consider one of these known families. Set $(n, d) = (p^3, \frac{(p^2-1)(p-1)}{3})$, where $G = A_n = C_{n,\{1,2,\ldots,d\}}$. By Theorem 2.3,

$$
\begin{aligned}
I(G, x) &= \sum_{k=0}^{\lfloor \frac{n}{d+1} \rfloor} \frac{n}{n-dk} \binom{n-dk}{k} x^k \\
&= 1 + nx + \frac{n(n-2d-1)}{2} x^2 + \frac{n(n-3d-1)(n-3d-2)}{6} x^3 \\
&= 1 + p^3 x + \frac{p^3(p^3+2p^2+2p-5)}{6} x^2 + \frac{p^3(p^2+p-2)(p^2+p-3)}{6} x^3 \\
&= (1+px)\left(1 + (p^3-p)x + \frac{p^2(p^2+p-2)(p^2+p-3)}{6} x^2\right).
\end{aligned}
$$

Therefore, $r = -\frac{1}{p}$ is a root of this circulant on p^3 vertices. Naturally we may conjecture that for some $d \geq 1$, $r = -\frac{1}{p}$ is also a root of $I(A_n, x) = I(C_{n,\{1,2,\ldots,d\}}, x)$ for $n = p^4$. However, a Maple analysis shows that this is not the case. The same appears to be true for any $n = p^d$, with $d \geq 4$. Thus, if $I(C_{p^4,S}, -\frac{1}{p}) = 0$, then S

cannot be of the form $\{1,2,\ldots,d\}$. In order to find such a set S, we will need to develop new formulas for $I(C_{n,S},x)$ for other families of generating sets.

Let p be a prime. If $x=-\frac{1}{p}$ is a root of $I(C_{n,S},x)$, then what are all possible values of n, expressed as a function of p? By answering this question, we can simplify the task of determining circulants $C_{n,S}$ for which $x=-\frac{1}{p}$ is a root of its independence polynomial. While the general problem is extremely difficult, we now give a complete answer to this problem for the case $\alpha(G)\leq 2$.

Proposition 5.34 *Let $G=C_{n,S}$ be a connected circulant with $\alpha(G)\leq 2$. Let $p\geq 3$ be prime. If $r=-\frac{1}{p}$ is a root of $I(G,x)$, then n equals p, p^2, or $2p^2$.*

Proof: Let G be a circulant with $I(G,-\frac{1}{p})=0$. Trivially, if $\alpha(G)=1$, then $G=K_p$. So assume $\alpha(G)=2$.

Let $C_{n,S}$ be k-regular. Then $I(G,x)=1+nx+mx^2$, where $m=\binom{n}{2}-\frac{nk}{2}$ is the number of non-edges in G. If $r=-\frac{1}{p}$ is a root of $I(G,x)$, then we require that $I(G,x)=(1+px)(1+(n-p)x)$, implying that $m=p(n-p)$. From $p(n-p)=\binom{n}{2}-\frac{nk}{2}$, we simplify and find that $k=n-1-2p+\frac{2p^2}{n}$.

Since p is prime, n must be one of: 1, 2, p, $2p$, p^2, or $2p^2$. We can trivially reject the first two cases, and note that the $n=p$ case corresponds to $G=K_p$ above (i.e., $\alpha(G)=1$). Thus, we have three cases to consider.

If $n=2p$, then $k=n-1-2p+p=p-1$, and $I(G,x)=1+2px+p^2x^2=(1+px)^2$. We require our S to be chosen so that $C_{2p,S}$ has degree $p-1$, and satisfies $\alpha(C_{2p,S})=2$. Using the Pigeonhole Principle, a detailed case analysis shows that S must be $\{2,4,\ldots,p-1\}$, i.e., G is the disjoint union of two K_p's. Since G is required to be connected, we may disregard this case.

If $n=p^2$, then $k=n-1-2p+2=(p-1)^2$, and so $I(G,x)=1+p^2x+p(p^2-p)x^2=(1+px)(1+(p^2-p)x)$. There exist graphs G satisfying the required conditions, depending on the value of p. For example, if G is of the form $A_n=C_{n,\{1,2,\ldots,d\}}$, then $(n,d)=(p^2,\frac{(p-1)^2}{2})$ satisfies $I(G,x)=(1+px)(1+(p^2-p)x)$.

If $n=2p^2$, then $k=n-1-2p+1=2p^2-2p$, and so $I(G,x)=1+2p^2x+p(2p^2-p)x^2=(1+px)(1+(2p^2-p)x)$. There exist graphs G satisfying the required conditions, depending on the value of p. For example, if G is of the form $A_n = C_{n,\{1,2,\ldots,d\}}$, then $(n,d) = (2p^2, p^2 - p)$ satisfies $I(G,x) = (1+px)(1+(2p^2-p)x)$.

Therefore, if $I(C_{n,S}, -\frac{1}{p}) = 0$, then n must equal p, p^2, or $2p^2$. ∎

If $\alpha(C_{n,S}) = 2$, then clearly $I(C_{n,S}, x)$ has either none or both of its roots being rational. However, this is usually not the case when $\alpha(C_{n,S}) \geq 3$, as often only one root is rational. A fascinating question is to classify the circulants $C_{n,S}$ for which its independence polynomial has *all* rational roots.

The proof of Proposition 5.34 describes infinitely many circulants satisfying this property for $\alpha(C_{n,S}) = 2$. For $\alpha(C_{n,S}) \geq 3$, we have found two such circulants using Maple. Both circulants have independence number 3.

$$\begin{aligned} I(C_{1681,\{1,2,\ldots,464\}}, x) &= (1-41x)(1-492x)(1-1148x). \\ I(C_{6859,\{1,2,\ldots,2160\}}, x) &= (1-19x)(1-1653x)(1-5187x). \end{aligned}$$

Note that in our above examples for $\alpha(C_{n,S}) = 3$, n is either a perfect square $(1681 = 41^2)$ or a perfect cube $(6859 = 19^3)$. If $I(C_{n,S}, x)$ is a degree 3 polynomial with all rational roots, must n be a perfect square or a perfect cube? Of course, we can further the analysis for $\alpha(C_{n,S}) = 4$ and beyond. Here is the broad formulation of our general question.

Problem 5.35 *Determine all necessary and sufficient conditions on n and S such that every root of $I(C_{n,S}, x)$ is rational.*

When examining the roots of graph polynomials, it is often interesting to verify whether $r = -1$ can be a root. For example, we defined the Alon-Tarsi polynomial $AT(\overrightarrow{G}, x)$ in Chapter 4. By Corollary 4.16, the number of even Eulerian subgraphs differs from the number of odd Eulerian subgraphs iff $r = -1$ is not a root of $AT(\overrightarrow{G}, x)$. For independence polynomials, $I(G, -1) = 0$ iff the number of independent sets with odd cardinality equals the number of independent sets with even cardinality.

We do not know whether $r = -1$ is a root of infinitely many circulants $I(G,x)$; in fact, we could not even find *one* circulant for which $I(C_{n,S}, -1) = 0$, despite extensive computations on Maple. This leads us to conjecture the following theorem.

Conjecture 5.36 *There does not exist a circulant $G = C_{n,S}$ for which $I(G,-1) = 0$.*

Definition 5.37 *The* **Euler characteristic** *of a simplicial complex Δ is the alternating sum*

$$EC(\Delta) = f_1 - f_2 + f_3 - \ldots,$$

where f_k represents the number of faces of dimension k in Δ.

In Chapter 4, we introduced the **f-vector** of the independence complex $\Delta(G)$. By definition, $I(G,x) = \sum_{k\geq 0} f_k x^k$, and so the Euler characteristic of G is simply the value of $1 - I(G,-1)$, since $f_0 = 1$. Therefore, we restate the conjecture as follows.

Conjecture 5.38 *There does not exist a circulant $G = C_{n,S}$ for which the Euler characteristic of its independence complex is* 1*.*

If G is an arbitrary graph, then there are infinitely many instances where $r = -1$ is a root of $I(G,x)$, i.e., $EC(\Delta(G)) = 1$. For example, consider the complement of any tree T of order n. Then $I(\overline{T}, x) = 1 + nx + (n-1)x^2 = (1+x)(1+(n-1)x)$. However, when the graphs are restricted to being circulants, it appears that $I(G,-1) \neq 0$.

If Conjecture 5.36 holds, then this implies that for every circulant graph G, the total number of independent sets with odd cardinality differs from the total number of independent sets with even cardinality. That would be a surprising result.

5.5 The Roots of Independence Polynomials and their Closures

Earlier in this chapter, we investigated the closure of the roots of a family of polynomials. By applying Theorem 5.16, we proved that the closure of roots of $I(A_n, x)$ is $(-\infty, -\frac{d^d}{(d+1)^{d+1}}]$. To do this, we considered the set of limit points, and showed that the roots are fully dense in this interval. Let us explore the concept of closure further in this section.

We first prove that the closure of roots of $I(C_{n,S}, x)$ is the entire complex plane $\mathbb{C}$, even when G is restricted to one family of circulants. In other words, given any $z \in \mathbb{C}$ and $\varepsilon > 0$, there is a circulant graph $C_{n,S}$ such that $|r - z| < \varepsilon$, where r is a root of $I(C_{n,S}, x)$.

In Corollary 2.32, we showed that $C_n[\overline{K_m}]$ is a circulant for all ordered pairs (n, m). We now determine an explicit formula for these roots.

Lemma 5.39 *There are $m\lfloor \frac{n}{2} \rfloor$ roots of $I(C_n[\overline{K_m}], x)$, where each root z satisfies the equation $(z+1)^m = 1 + r_{n,k}$, for some root $r_{n,k}$ of $I(C_n, x)$, where $1 \le k \le \lfloor \frac{n}{2} \rfloor$.*

Proof: By Theorem 5.2, the roots of $I(C_n, x)$ are $r_{n,k} = -\frac{1}{4u_{n,k}^2}$, where $u_{n,k} = \cos(\frac{(2k-1)\pi}{2n})$ for $1 \le k \le \lfloor \frac{n}{2} \rfloor$. Since $I(\overline{K_m}, x) - 1 = (1+x)^m - 1$, Theorem 2.33 implies that the roots of $I(C_n[\overline{K_m}], x) = I(C_n, I(\overline{K_m}, x) - 1)$ are the $m\lfloor \frac{n}{2} \rfloor$ values of z for which $z = \sqrt[m]{1 + r_{n,k}} - 1$. This completes the proof. ∎

The roots of $I(G, x)$ are known to be dense in $\mathbb{C}$. Brown and Hickman [23] proved this by showing that the independence roots are dense in $\mathbb{C}$ when G is restricted to the family of well-covered graphs, or when G is restricted to the family of comparability graphs. In the following theorem, we go even further and show that the closure of independence roots is $\mathbb{C}$, even when G is restricted to this one specific family of circulant graphs.

Theorem 5.40 *The closure of roots of $I(C_n[\overline{K_m}], x)$ is the entire complex plane $\mathbb{C}$.*

Proof: Our analysis follows the same lines as a proof given in [23]. We select any $z \in \mathbb{C}$, and show that for any $\varepsilon > 0$, there exists a root r of some $I(C_n[\overline{K_m}], x)$ such that $|z - r| < \varepsilon$.

We may assume that $z \neq -1$, so $|z+1| > 0$. Select an odd integer m large enough so that some m^{th} root of $-|z+1|^m$ lies within an $\frac{\varepsilon}{2}$-ball of $z+1$. In other words, select m (and the corresponding k) such that $|w - (z+1)| < \frac{\varepsilon}{2}$, where $w = |z+1|e^{\frac{(2k-1)\pi i}{m}}$.

Since $(z+1)^m$ is continuous and the roots of $I(C_n, x)$ are dense in the interval $(-\infty, -\frac{1}{4}]$, there must exist a positive integer n and a constant $0 \le \delta < \frac{\varepsilon}{2}$ such that $r' = (-|z+1| + \delta)^m - 1$, for some root r' of $I(C_n, x)$. Let w' be the corresponding m^{th}

root of $r'+1$, i.e., $w' = (|z+1|-\delta)e^{\frac{(2k-1)\pi i}{m}}$. Then, $w'-1$ is a root of $I(C_n[\overline{K_m}], x)$, from Lemma 5.39.

Then $|(w'-1)-z| \leq |w'-w| + |w-(z+1)| < |\delta e^{\frac{(2k-1)\pi i}{m}}| + \frac{\varepsilon}{2} = \delta + \frac{\varepsilon}{2} < \varepsilon$. Letting $r = w'-1$, we have proven that $|z-r| < \varepsilon$. ∎

In [23], Brown and Hickman examine the roots of $I(L(G), x)$, where $L(G)$ is the line graph of G. They prove that the roots of $I(L(G), x)$ are dense in at least $(-\infty, -\frac{1}{4}]$, and it is left as an open problem to determine if the closure of these roots is the entire negative real axis. In this section, we resolve the question by showing that this is indeed the case. Our proof will involve an analysis of $I(L(G), x)$, where G is the family of complete bipartite graphs $K_{a,b}$.

There is a natural connection between $I(L(G), x)$ and the *matching polynomial* $M(G, x)$, which was defined in Chapter 1. By Proposition 1.9, $M(G, x) = x^n \cdot I(L(G), -\frac{1}{x^2})$, and so r is a root of $M(G, x)$ iff $-\frac{1}{r^2}$ is a root of $I(L(G), x)$. It is known [96] that each root of $M(G, x)$ must be a positive real number, hence each root of $I(L(G), x)$ must be a negative real number. Based on our proof that $I(L(G), x)$ has its roots being dense in $(-\infty, 0]$, it will immediately follow that the closure of roots of $M(G, x)$ is the entire positive real axis. This answers another open problem posed in [23]. Also in this section, we study the roots of *rook polynomials*, and show that the closure of its roots is $(-\infty, 0]$. This generalizes some theorems given in [145].

We now prove that the closure of roots of $I(L(K_{n,n}), x)$ is $(-\infty, 0]$, which immediately implies that the closure of roots of $I(L(G), x)$ is also $(-\infty, 0]$. First, we quote a result that relates $I(L(K_{n,n}), x)$ to *Legendre polynomials*.

Definition 5.41 *For each integer $k \geq 1$, the k^{th}* **Legendre polynomial** *is*

$$P_k(x) = \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{x^j}{j!}.$$

Lemma 5.42 ([22]) $I(L(K_{n,n}), x) = n! x^n P_n(-\frac{1}{x})$*, for all $n \geq 1$.*

By Lemma 5.42, r is a root of $I(L(K_{n,n}), x)$ iff $-\frac{1}{r}$ is a root of $P_n(x)$. This motivates us to look at the roots of $P_n(x)$. If we can prove that the roots of $P_n(x)$

are dense in $[0, \infty)$, then this will immediately imply that the roots of $I(L(K_{n,n}), x)$ are dense in $(-\infty, 0]$. Note that $I(L(K_{n,n}), x) = \sum_{k=0}^{n} k! \binom{n}{k}^2 x^k$, by Theorem 4.4.

Like the Chebyshev polynomials earlier in this chapter, the Legendre polynomials $(P_n(x))_{n\geq 0}$ are orthogonal. Much is known about the roots of orthogonal polynomials. Here we quote two results by Chihara that establishes our closure result.

Theorem 5.43 ([39]) *Consider a sequence of monic polynomials $(P_n(x))_{n\geq 0}$ defined by a recurrence relation of the form*

$$P_n(x) = (x - c_n)P_{n-1}(x) - \lambda_n P_{n-2}(x),$$

where $P_{-1}(x) = 0$ and $P_0(x) = 1$. Then $(P_n(x))_{n\geq 0}$ is an orthogonal sequence iff each c_n is real and $\lambda_{n+1} > 0$ for all $n \geq 1$.

Theorem 5.44 ([39]) *In an orthogonal sequence $(P_n(x))_{n\geq 0}$ with*

$$P_n(x) = (x - c_n)P_{n-1}(x) - \lambda_n P_{n-2}(x),$$

suppose that

$$c_n = an + b \quad (\text{where } a > 0)$$

and

$$\lambda_n = dn^2 + fn + g > 0 \quad \text{for all } n > 1.$$

Let X be the union of roots of $(P_n(x))_{n\geq 0}$. If $4d = a^2$, then X is dense in $[\sigma, \infty)$, where

$$\sigma = b - \sqrt{d} - \frac{f}{\sqrt{d}}.$$

As discussed earlier, $(P_n(x))_{n\geq 0}$ is orthogonal, after we normalize each polynomial so that it is monic. Thus, we know that there exist functions c_n and λ_n satisfying the conditions of the recurrence relation. The following lemma establishes these two functions.

Lemma 5.45 *For each $n \geq 0$, define $Q_n(x) = (-1)^n n! P_n(x)$, which makes each $Q_n(x)$ monic. Then, $\{Q_n(x)\}$ satisfies the recurrence relation*

$$Q_n(x) = (x - c_n)Q_{n-1}(x) - \lambda_n Q_{n-2}(x),$$

where $c_n = 2n - 1$ and $\lambda_n = (n - 1)^2$.

<u>Proof:</u> By the definition of $P_n(x)$, we have

$$Q_n(x) = \sum_{j=0}^{n} (-1)^{n+j} \binom{n}{j}^2 (n-j)! x^j.$$

Now we compare the x^k coefficients in our desired identity, and show that for all $k \geq 0$, both sides are equal. This will prove that

$$Q_n(x) = (x - 2n + 1)Q_{n-1}(x) - (n-1)^2 Q_{n-2}(x).$$

Since $[x^k]Q_n(x) = (-1)^{n+k}\binom{n}{k}^2(n-k)!$, we have

$$\begin{aligned}
& [x^k]Q_n(x) \\
= \;& (-1)^{n+k}\binom{n}{k}^2 (n-k)! \\
= \;& (-1)^{n+k}\frac{n^2}{k^2}\binom{n-1}{k-1}^2 (n-k)! \\
= \;& (-1)^{n+k}\binom{n-1}{k-1}^2 (n-k)! \left[1 + \frac{n^2-k^2}{k^2}\right] \\
= \;& (-1)^{n+k}\binom{n-1}{k-1}^2 (n-k)! \left[1 + \frac{(2n-1)(n-k)}{k^2} - \frac{(n-k)(n-k-1)}{k^2}\right] \\
= \;& (-1)^{n+k}\binom{n-1}{k-1}^2 (n-k)! \\
& \quad - (2n-1)(-1)^{n-1+k}\binom{n-1}{k}^2 (n-k-1)! \\
& \quad - (n-1)^2(-1)^{n+k-2}\binom{n-2}{k}^2 (n-k-2)! \\
= \;& [x^{k-1}]P_{n-1}(x) - [x^k](2n-1)P_{n-1}(x) - [x^k](n-1)^2 P_{n-2}(x) \\
= \;& [x^k](x-2n+1)P_{n-1}(x) - (n-1)^2 P_{n-2}(x).
\end{aligned}$$

Therefore, $Q_n(x) = (x - 2n + 1)Q_{n-1}(x) - (n-1)^2 Q_{n-2}(x)$, and our proof is complete. ∎

We now have all of the necessary results to prove our theorem on the roots of $I(L(K_{n,n}), x)$.

Theorem 5.46 *The closure of roots of* $I(L(K_{n,n}), x)$ *is* $(-\infty, 0]$.

Proof: Let $\{P_n(x)\}$ be the sequence of Legendre polynomials. We defined the normalized sequence $\{Q_n(x)\}$, which clearly has the same roots as $\{P_n(x)\}$. By Lemma 5.45, this sequence is orthogonal, and satisfies the recurrence relation $Q_n(x) = (x - c_n)Q_{n-1}(x) - \lambda_n Q_{n-2}(x)$, with $c_n = 2n - 1$ and $\lambda_n = (n-1)^2$. By Theorem 5.44, the roots of $\{Q_n(x)\}$ (equivalently the roots of $\{P_n(x)\}$) are dense in $[\sigma, \infty)$, where $\sigma = -1 - \sqrt{1} + \frac{2}{\sqrt{1}} = 0$.

By Lemma 5.42, r is a root of $I(L(K_{n,n}), x)$ iff $-\frac{1}{r}$ is a root of the Legendre polynomial $P_n(x)$. Since the closure of roots of $\{P_n(x)\}$ is $[0, \infty)$, we conclude that the closure of roots of $I(L(K_{n,n}), x)$ is $(-\infty, 0]$. ■

Corollary 5.47 *The closure of roots of $I(L(G), x)$ is $(-\infty, 0]$.*

As discussed earlier, $r > 0$ is a root of $M(G, x)$ iff $-\frac{1}{r^2}$ is a root of $I(L(G), x)$. As a result, the next corollary follows immediately from the observation that every root of $M(G, x)$ is a positive real number.

Corollary 5.48 *The closure of roots of the matching polynomial $M(G, x)$ is $[0, \infty)$.*

We now define the *rook polynomial* $R_n(x)$, and determine the closure of its roots.

Definition 5.49 *Let B_n denote the chessboard with n rows and n columns. Then, the* **rook polynomial** *is $R_n(x) = \sum_{k=0}^{n} r_k x^k$, where r_k is the number of ways that k rooks can be placed on B_n so that no two rooks lie on the same row or column.*

The rook polynomial was first introduced in [106] with applications to card-matching problems. Since then, various researchers have applied rook polynomials to make important connections to Fibonacci theory [70], group theory [129], hypergeometric series summation [93], and the computation of the permanents of various matrices [36, 91, 92]. A comprehensive analysis of rook polynomials can be found in [154]. There are several papers [96, 142, 145] on the roots of rook polynomials. It was shown in [142] that each root of $R_n(x)$ is a negative real number, but there has been no result describing the closure of its roots. Based on the work in this section, we can now answer this problem.

Theorem 5.50 *The roots of the rook polynomial $R_n(x)$ are real and the closure of its roots is* $(-\infty, 0]$.

Proof: It is well-known [81, 154] and straightforward to show that in an n by n chessboard, there are $m_k = k!\binom{n}{k}^2$ ways of placing k rooks so that they are non-attacking, for each $1 \leq k \leq n$. This can also be seen by observing the bijection between the set of k-matchings of $K_{n,n}$ and placements of k non-attacking rooks on the n by n chessboard. In other words,

$$R_n(x) = \sum_{k=0}^{n} k!\binom{n}{k}^2 x^k = I(L(K_{n,n}), x).$$

Our result now follows immediately from Theorem 5.46. ∎

We summarize these results by displaying a table of the closures of the roots of various graph polynomials. We separate our analysis into two categories: the closure of the real roots, and the closure of the complex roots. In addition to our theorems in this section, we also mention that the equivalent problem has been solved for chromatic polynomials [101, 162, 166] and partially solved for reliability polynomials [21]. Thus, we include these results as well. The results in bold highlight our results.

Polynomial	**Real Closure**	**Complex Closure**
Independence	$\mathbf{(-\infty, 0]}$	$\mathbb{C}$
Matching	$\mathbf{[0, \infty)}$	$\mathbf{[0, \infty)}$
Rook	$\mathbf{(-\infty, 0]}$	$\mathbf{(-\infty, 0]}$
Chromatic	$\{0\} \cup \{1\} \cup [\frac{32}{27}, \infty)$	$\mathbb{C}$
Reliability	$\{0\} \cup (1, 2]$	some unknown superset of $\lvert z - 1\rvert \leq 1$

Table 5.2: The closures of the roots of graph polynomials.

Chapter 6

Conclusion

We conclude the thesis by providing a hodgepodge of interesting open problems. Many of these problems ask for a full generalization of our results. For some of these questions, we ask if a full characterization theorem can be found, knowing that a simple characterization theorem will not exist if the decision problem is NP-complete.

Chapter 2:

1. We determined an explicit formula for $I(C_{n,S}, x)$, for an arbitrary circulant of degree $r \leq 3$. Is it possible to determine a general formula for the independence polynomials of circulants of degree $r = 4$?

2. It is NP-hard to determine $\alpha(G)$ for an arbitrary graph G [79]. Even when G is restricted to the family of $K_{1,4}$-free graphs, the problem is still NP-hard [29]. Thus, it is NP-hard to compute $I(G, x)$ when G is restricted to $K_{1,4}$-free graphs. It is known [135] that if G is restricted to claw-free graphs, there is a polynomial-time algorithm to compute $\alpha(G)$. This motivates the following question: determine the complexity of determining the independence polynomial $I(G, x)$, when G is restricted to the family of claw-free graphs.

3. In [3], the following (still open) conjecture is made: if F is a forest, then $I(F, x)$ is unimodal. Motivated by this, let us ask the same question for circulants: if $G = C_{n,S}$ is a circulant, prove or disprove that $I(G, x)$ must be unimodal. Must $I(G, x)$ also be log-concave?

4. We gave a full characterization theorem of circulant graphs that are independence unique. Generalize this theorem to all graphs: determine a simple characterization theorem for the set of all independence unique graphs.

Chapter 3:

5. There are infinitely many star extremal graphs, and infinitely many non star extremal graphs. For a given n, are there more star extremal circulant graphs on n vertices than non star extremal circulant graphs?

   Let $c(n)$ be the number of non-isomorphic circulants on n vertices, and let $s(n)$ be the number of distinct circulants on n vertices that are star extremal. As an example, $\frac{s(10)}{c(10)} = \frac{19}{20}$, with the lone exception being $C_{10,\{1,3,4,5\}}$.

   Define $X = \left\{ \dfrac{s(n)}{c(n)} \ : \ n \in \mathbb{N} \right\}$. Determine the values of $\limsup X$ and $\liminf X$.

6. We determined a formula for the fractional Ramsey number and the circular chromatic Ramsey number. However, these formulas are only defined in the case where all the a_i's are positive integers. If each $a_i \geq 2$ is an arbitrary *real* number, determine a formula for $r_{\omega_f}(a_1, a_2, \ldots, a_k)$ and $r_{\chi_c}(a_1, a_2, \ldots, a_k)$.

7. We determined the optimal Nordhaus-Gaddum inequalities for the fractional and circular chromatic numbers. To establish optimality, we constructed an extremal graph for each of our four bounds. Characterize the set of *all* extremal graphs for these Nordhaus-Gaddum inequalities.

Chapter 4:

8. We introduced the Alon-Tarsi polynomial $AP(G, x)$, and applied our formula for $I(C_n, x)$ to provide a proof that $\chi_l(C_{3n,\{1,2\}}) = 3$. Determine other families of circulants for which $\chi_l(G)$ can be easily calculated by relating independence polynomials to the Alon-Tarsi polynomial.

9. We determined the existence of a connected circulant $G = C_{n,S}$ for which $\Delta(G)$ is a pure 3-dimensional shellable complex. For each $k > 3$, determine whether there exists a connected circulant $G = C_{n,S}$ so that $\Delta(G)$ is a pure k-dimensional shellable complex.

Chapter 5:

10. Determine all necessary and sufficient conditions on n and S so that $I(C_{n,S}, x)$ has all real roots.

11. Recall that a polynomial is *stable* if every root has a negative real part. Determine all necessary and sufficient conditions on n and S so that $I(C_{n,S}, x)$ is stable.

12. Among all circulant graphs with $\alpha(G) = k$, we proved that the root r_{max} of maximum modulus satisfies

$$\frac{1}{2(k-1)! \cdot k^{k-3}} n^{k-2} < |r_{max}| < \frac{k}{k-1} n^{k-2}.$$

For each k, determine the optimal constant $c(k)$ for which $|r_{max}| \leq c(k)n^{k-2} + O(n^{k-3})$ for all independence polynomials $I(C_{n,S}, x)$ with $\alpha(C_{n,S}) = k$.

13. We note that $r = -1$ is a root of infinitely many independence polynomials. For example, consider the complement of any tree T of order n. As discussed in Chapter 5, we have $I(\overline{T}, x) = 1 + nx + (n-1)x^2 = (1+x)(1+(n-1)x)$. Motivated by this, we ask whether $r = -1$ can be a root of an independence polynomial $I(C_{n,S}, x)$. Also, do there exist circulants for which $r = -1$ is the only rational root of $I(C_{n,S}, x)$?

14. Let $r \geq 1$ be a fixed integer. As a function of n, determine bounds for the roots of $I(C_{n,S}, x)$, where $C_{n,S}$ is an r-regular circulant. If $r = 2$, our analysis from Chapter 5 proves that $\frac{n^2}{4\pi^2} \leq |r| \leq \frac{1}{4}$. Determine bounds for each $r \geq 3$.

Additional Problems:

15. Determine all necessary and sufficient conditions on the i_k's so that $\sum_{k=0} i_k x^k$ is the independence polynomial of some circulant graph.

16. For each n, define $c(n)$ to be the number of non-isomorphic circulants on n vertices. Define $d(n)$ to be the sum of the independence numbers of each of

these $c(n)$ circulants. Then, the ratio $\frac{d(n)}{c(n)}$ is the *average* independence number of a circulant on n vertices. To give some small examples, $\frac{d(6)}{c(6)} = \frac{22}{8}$, $\frac{d(7)}{c(7)} = \frac{14}{4}$, and $\frac{d(8)}{c(8)} = \frac{38}{12}$. Determine a formula for $c(n)$ and $d(n)$.

Define $X = \left\{ \dfrac{d(n)}{c(n)} \ : \ n \in \mathbb{N} \right\}$. Determine the values of $\limsup X$ and $\liminf X$.

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