Graphs and Groups

Final Degree Dissertation
Degree in Mathematics

Ainize Cidoncha Markiegui

Supervisor:
Gustavo Adolfo Fernández Alcober

Leioa, 1 September 2014

Contents

Introduction

Graph theory has a wide variety of research fields, such as in discrete mathematics, optimization or computer sciences. However, this work will be focused on the algebraic branch of graph theory. Number and group theory are necessary in order to develop this project whose aim is to give enough details and clarifications in order to fully understand the meaning and concept of the automorphism group of a graph. Moreover, the specific automorphism groups of some special families of graphs is developed, Kneser graphs and generalized Petersen graphs, more precisely.

Every chapter in this document is based in a different book or paper. In addition, each chapter is developed around one most relevant reference, but we tried to find and read more related articles in order to combine, use and refer to them for a complete and fully understandable vision of the analyzed topic to the reader.

The first chapter, which is based in the book by C. Godsil and G. Royle [6], contains the most theoretical part, including the definitions, lemmas and theorems necessary for the smooth development of the next chapters. It is used as an introduction in order to show the basic graph and group theory needed.

The second chapter is already focused on a specific family of graphs, Kneser graphs. The last exercise of the previous chapter, which implies finding the automorphism group of a very famous Kneser graph, the so called Petersen graph, gives us the clue of the description of the automorphism groups of all Kneser graphs. Nevertheless, we need a very important result on combinatorics, the Erdős-Ko-Rado theorem, in order to prove the result in all generality. Moreover, the corresponding and complex proof of this famous theorem in this chapter is mostly based in a preprint by P. Cameron [3] although we combine it with the proof in the book by N. Alon and J. Spencer [1, page 13]. In addition, we made some changes in the notation and introduced some more lemmas and pictures in order to make it easier to understand.

In the third chapter we analyze an even more complex family of graphs, the generalized Petersen graphs and their automorphism groups. This whole chapter is related to the paper by R. Frunch, J. E. Graver and M.E. Watkins [5] even if we try to explain everything in a deeper and more understandable way with the aid of some pictures and examples. Although we give the description for almost all generalized Petersen graphs, there are 7 exceptional cases in which the obtained result does not hold. These particular graphs need a ocase-by-case analysis that would exceed the bounds of this project. That is why we refer to the already cited paper [5], in which they give a brief explanation of them and refer to other articles for a complete analysis of each exceptional graph.

The fourth chapter represents my aim of showing an example of what all this theory can be used for. After looking and reading different articles about various applications of graph and group theory I found out the interesting field of chemistry and reaction graphs and I saw it was directly related with the topic. I would have liked to go deeper in this field and prove some very interesting results as they do in [8] and [9], but doing so would have required devoting a whole work only to that. However, I tried to illustrate this kind of application by using an example in which we need the automorphism group of a graph and the final result is a graph that we already analyzed in the previous chapters.

We also include an Appendix with solved exercises. Some of them will help with the development of the chapter while some other will be extra interesting examples related to the topic.

Summarizing, the aim of this project was to learn more about algebraic tools in graph theory analyzing interesting families of graphs with specific properties which can be later on applied in a variety of fields, for instance, the reaction graphs used in chemistry.

Chapter 1

Automorphisms of graphs

We will focus this chapter on the automorphisms of graphs, their definition, properties and some examples.

1.1 Graphs

Definition 1. A *graph* Γ consists of a vertex set $V(\Gamma)$ and an edge set $E(\Gamma)$, where an edge is an unordered pair of distinct vertices of Γ.

It is important to know when two graphs can be considered to be equal. First of all, two vertices are said to be adjacent or neighbours if there exists an edge between them, in addition, the number of adjacent vertices is called the valency of a vertex. Moreover, a graph is said to be regular if all vertices have the same valency. If x and y are two vertices in $V(\Gamma)$ we denote the edge which joins x and y as $\{x, y\}$. Now we can give the definition of two isomorphic graphs.

Definition 2. Two graphs Γ_1 and Γ_2 are *isomorphic* if there is a bijection, say φ, from $V(\Gamma_1)$ to $V(\Gamma_2)$ such that x and y are adjacent in Γ_1 if and only if $\varphi(x)$ and $\varphi(y)$ are adjacent in Γ_2.

If Γ_1 and Γ_2 are isomorphic, then we write $\Gamma_1 \cong \Gamma_2$. Moreover, it is normally appropriate to treat isomorphic graphs as if they were equal.

Example 1. Two isomorphic graphs:

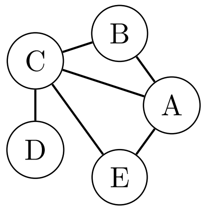
Definition 3. A graph is called *complete* if every pair of vertices are adjacent, and the complete graph on n vertices is denoted by K_n.

Definition 4. A *subgraph* of a graph Γ is a graph Y such that $V(Y) \subseteq V(\Gamma)$ and $E(Y) \subseteq E(\Gamma)$.

Definition 5. A *clique* is a subgraph that is complete. Conversely, an *independent set* is a subgraph such that no two of its vertices are adjacent.

The following are some examples of different kinds of graphs, from some general ones to more specific ones that we are going to use in the next chapters.

Example 2. Consider the following graph:



The set of vertices $V_1 = \{C, A, E\}$ induce a clique and $V_2 = \{B, D, E\}$ an independent set.

Example 3. The *cyclic graph* C_n is a connected graph with n vertices where every vertex has exactly two neighbours.

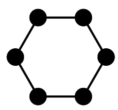


Figure 1.1: The cyclic graph C_6.

Example 4. The *Kneser graph* $KG(4, 2)$ is defined as follows. Fix the set $\Omega = \{1, 2, 3, 4\}$. Then the vertices of $KG(4, 2)$ are the subsets of Ω of size 2, i.e., $V = \{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}, \{2, 4\}, \{3, 4\}\}$, and two subsets are adjacent if their intersection is empty. See Figure 1.2.

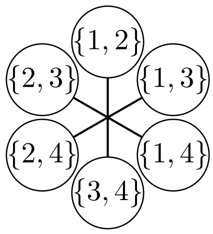


Figure 1.2: Kneser graph $KG(4, 2)$

Example 5. Let Ω be a fixed set of size v, then the Kneser graph $KG(v,k)$ is defined as follows for $1 \leq k \leq \frac{v}{2}$. The vertices of $KG(v,k)$ are the subsets of Ω with size k, where two subsets are adjacent if their intersection is empty. The Kneser graph $KG(5,2)$ is a very famous and important graph and it is known as the *Petersen graph*.

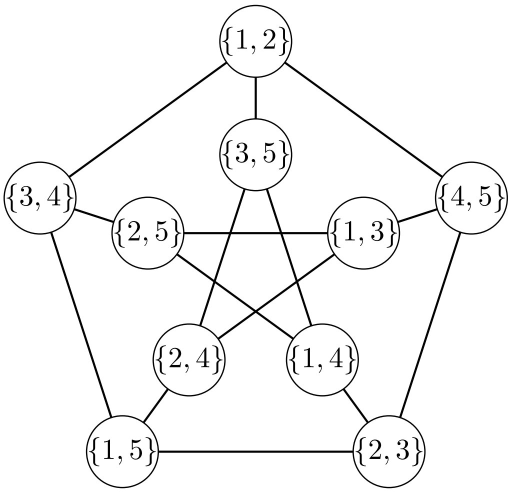


Figure 1.3: Petersen graph $KG(5,2)$.

Definition 6. A *path* of length r from x to y in a graph is a sequence of $r+1$ distinct adjacent vertices starting with x and ending with y. The *distance* $d(x,y)$ between two vertices x and y in a graph is the length of the shortest path from x to y.

1.2 Automorphisms

In this section we are going to define the automorphisms of a graph, analyze their properties and give some interesting examples.

An *automorphism* is an isomorphism from a mathematical object to itself. The exact definition of an automorphism depends on the type of mathematical object in question an we have the following definition when talking about graphs.

Definition 7. An *automorphism* of a graph Γ is a permutation of the vertices of Γ which maintains the adjacency relation between vertices, i.e., two vertices are adjacent if and only if their images are adjacent.

An automorphism permutes the vertices inducing a natural action onto the edges, since they are just unordered pairs of vertices. Then we have the following equivalent definition of an automorphism.

Definition 8. An *automorphism* of a graph Γ is a permutation of the vertices of Γ such that, if we consider the natural action it induces on the unordered pairs of vertices, it maps edges to edges and non-edges to non-edges.

Furthermore, let f be a permutation of the vertices of a graph Γ, then we can define the graph $f(\Gamma)$ induced by f as

$$V(f(\Gamma)) = V(\Gamma),$$

$$E(f(\Gamma)) = \{\{f(x), f(y)\} | \{x, y\} \in E(\Gamma)\}.$$

The description of $f(\Gamma)$ is very useful in order to check when the permutation f induces an automorphism graphically. Actually, we only need to compare the visual representation of both Γ and $f(\Gamma)$. If both graphs have the same visual representation, then f is an automorphism, otherwise, it is not.

Note that we can omit the last part of Definition 8 when talking about finite graphs because mapping non-edges to non-edges would be a consequence of mapping edges to edges. We can justify this using the pigeonhole principle. Suppose that at least one non-edge is mapped to an edge by the automorphism f, then, since f is a permutation, that edge can not be an image of any other element again. As we have a finite amount of edges and there is now one edge less in the possible images than the amount of edges in the first graph, by the pigeonhole principle at least one edge would have more than one preimage, which is a contradiction with f being a permutation.

We refer to the Appendix in order to show an example of an infinite graph in which a permutation of the set of vertices of a graph is not an automorphism even if its natural action maps edges onto edges.

Example 6. The easiest example of an automorphism is the identity.

Example 7. Let Γ be the Petersen graph mentioned before and $f = (13542)$. As f permutes the numbers which form the vertices of Γ, f also induces a permutation of the vertices of Γ, which we still denote by f. It is easy to check that, in the graph $f(\Gamma)$, every vertex is connected to the vertices as in Figure 1.3.

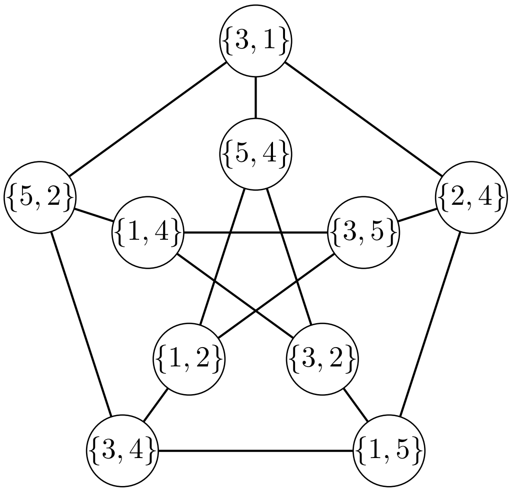


Figure 1.4: After aplying f in Γ, i.e, $f(\Gamma)$.

Example 8. Now let C_5 be the graph with the vertex set $V(\Gamma) = \{1, 2, 3, 4, 5\}$ and the edge set $E(\Gamma) = \{\{1, 2\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{5, 1\}\}$ and let f be the permutation $f = (25)$. Note that f is not an automorphism of Γ since for instance the vertices 2 and 3 are not adjacent any more in $f(\Gamma)$.

Figure 1.5: The graphs Γ and $f(\Gamma)$.

The set of all automorphisms of Γ is denoted by $\operatorname{Aut}\Gamma$.

Proposition 1.2.1. *The set of all automorphisms of* Γ*,* $\operatorname{Aut}\Gamma$*, forms a group under composition.*

Proof. Let S be the group of all the permutations of the set $V(\Gamma)$. We will see that $\operatorname{Aut}\Gamma$ is a subgroup of S. For that we need to prove that if f_1, $f_2 \in \operatorname{Aut}\Gamma$, then $f_1 f_2 \in \operatorname{Aut}\Gamma$ and if $f \in \operatorname{Aut}\Gamma$ then $f^{-1} \in \operatorname{Aut}\Gamma$. For the first statement we need that if x and y are adjacent in Γ, then $f_1 f_2(x)$ and $f_1 f_2(y)$ must be adjacent in Γ and conversely, if x and y are not adjacent in Γ, then $f_1 f_2(x)$ and $f_1 f_2(y)$ must not be adjacent in Γ. That is true since $f_1 f_2(x) = f_2(f_1(x))$ and $f_1 f_2(y) = f_2(f_1(y))$ and as f_1 is an automorphism of Γ, we have that $f_1(x)$ and $f_1(y)$ keep the adjacency relation x and y had before. Moreover, f_2 is an automorphism of Γ as well, so $f_2(f_1(x))$ and $f_2(f_1(y))$ are adjacent in Γ if and only if x and y were adjacent in Γ. Hence if $f_1,\ f_2 \in \operatorname{Aut}\Gamma$, then $f_1 f_2 \in \operatorname{Aut}\Gamma$.

The second statement is also easy to prove. We know that f being an automorphism of Γ means that f is a bijection that keeps the adjacency relation between vertices. Hence there exists f^{-1}. Moreover we have that $f(x)$ and $f(y)$ are adjacent if and only if x and y are adjacent which is the same as saying that $f^{-1}(f(x))$ and $f^{-1}(f(y))$ are adjacent if and only if $f(x)$ and $f(y)$ are. Note that $f(x)$ and $f(y)$ could be any vertex in $f(V(\Gamma)) = V(\Gamma)$ since x and y are any vertex of Γ and f is a bijection. So $f^{-1} \in \operatorname{Aut}\Gamma$. □

From now onwards we are going to use the following notation. The image of an element $x \in V(\Gamma)$ under a permutation $f \in S_{V(\Gamma)}$ will be denoted by x^f. In the same way, if $f \in \operatorname{Aut}\Gamma$ and Y is a subgraph of Γ, then we define Y^f to be the graph with $V(Y^f) = \{x^f : x \in V(Y)\}$ and $E(Y^f) = \{\{x^f, y^f\} : \{x, y\} \in E(Y)\}$. Note that in the particular case $Y = \Gamma$, we recover the definition of $f(\Gamma)$ given before.

Lemma 1.2.2. *If x is a vertex of the graph Γ and f is an automorphism of Γ, then the vertex $y = x^f$ has the same valency as x.*

Proof. Since f is an automorphism, by definition it is a permutation of the vertices of Γ that maps edges to edges and non-edges to non-edges. Thus $y = x^f$ has the same number of incident edges, or which is the same, the same number of adjacent vertices as x. □

Lemma 1.2.3. *If x and y are vertices of Γ and $f \in \operatorname{Aut}\Gamma$, then $d(x, y) = d(x^f, y^f)$.*

Proof. Let $d(x, y) = n$ and let

$$P = \{\{x, v_1\}, \{v_1, v_2\}, ..., \{v_{n-2}, v_{n-1}\}, \{v_{n-1}, y\}\}$$

be a shortest path between them.

Take $P' = \{\{x^f, v_1^f\}, \{v_1^f, v_2^f\}, ..., \{v_{n-2}^f, v_{n-1}^f\}, \{v_{n-1}^f, y^f\}\}$, which is a path from x^f to y^f since f is an automorphism and all the adjacent vertices remain adjacent after applying f. This does not mean that P' is a shortest path between them but we have that $d(x^f, y^f) \leq |P'| = n$.

Now we are going to show by contradiction that $d(x^f, y^f) \geq n$. Suppose that there exists a shortest path

$$Q = \{\{x^f, w_1\}, \{w_1, w_2\}, ..., \{w_{m-2}, w_{m-1}\}, \{w_{m-1}, y^f\}\}$$

form x^f to y^f such that $|Q| = m < |P'| = n$. Then as f is bijective and maintains the adjacent vertices we would have a path Q' from x to y of length m. But that is a contradiction since $d(x, y) = n > m$. So eventually we have $d(x, y) = d(x^f, y^f)$. □

Example 9. $\operatorname{Aut} K_n \cong S_n$. The set of vertices of the graph K_n is the finite set $V(K_n) = \{1, ..., n\}$ and all those vertices are adjacent to each other, so the set of all automorphisms of the graph K_n consists of all the possible permutations of the set $\{1, ..., n\}$, thus $\operatorname{Aut} K_n = S_n$.

1.3 Actions of groups on sets and the Orbit-Stabilizer Theorem

We are going to focus our attention on the Orbit-Stabilizer Theorem now. First of all we need a few more definitions and explanations in order to make the proof of the theorem understandable.

In this section we could explain and state all the theorems and lemmas taking G to be a permutation group, but we are going to generalize a little bit more since in some cases we have to manage with the following situation. Suppose we have a set X and a group G, whose elements permute the ones in X. This means that for each $g \in G$ we have a corresponding permutation in S_X, but the problem arises since we can not assume that different elements in G correspond to different permutations in S_X. Due to this, in general, although the elements of G permute the ones in X we cannot say that G is a permutation group of X.

Example 10. Let G be a group and $X = G$. In this case when we conjugate an element of X by one $g \in G$ we get:

$$\begin{aligned} X = G &\longrightarrow X = G \\ x &\longmapsto x^g = g^{-1}xg \end{aligned}$$

which is a permutation of X. Now suppose that we have $g \in Z(G)$ and $g \neq 1$, let us see which is the permutation we get with this g.

$$\begin{aligned} X = G &\longrightarrow X = G \\ x &\longmapsto x^g = g^{-1}xg = g^{-1}gx = x. \end{aligned}$$

This is the identity permutation so all the elements in the center of G would give us the same permutation. That is the reason why we could not say that G is a permutation group itself by conjugation. Here we introduce a new concept in order to solve this terminology problem.

Definition 9. Let G be a group. A *G-set* is a pair (X, ρ) of a set X and a homomorphism ρ from G into the symmetric group S_X on X.

In this way we match each element of G with its correspondent permutation in S_X through a homomorphism so now we can work with the group G even though it is not a permutation group. We also say that the group G acts on the set X, ρ being the action. Here there are some clarifications about the notation.

When a G-set (X, ρ) is given, the permutation on X that an element g of G determines is $\rho(g)$. For $x \in X$ we write

$$x^g = \rho(g)(x).$$

Moreover, we need to know how the composition works. Since ρ is a homomorphism we have that the composition $x^{gh} = \rho(gh)(x) = \rho(g)\rho(h)(x) = \rho(h)(\rho(g)(x)) = (x^g)^h$ where $g, h \in G$. In addition we need some properties and characteristics of groups acting sets in order to work with them.

Definition 10. Let X be a finite set and G a group acting on X. We say that G is *transitive* on X if given any two points x and y from X there is an element $g \in G$ such that $x^g = y$.

Definition 11. Let X be a finite set and G a group acting on X. We say that G is *faithful* on X if for any two different elements g and h from G there is an element $x \in X$ such that $x^g \neq x^h$.

In other words, G is faithful when the homomorphism ρ is injective. Thus if G is faithful then G is a permutation group on X.

Example 11. Having the set $X = \{\{1, 2\}, \{2, 3\}, \{5, 6\}\}$, the group G representing the natural action of S_6 on X is not faithful since taking g and $e \in G$ where $\rho(e)$ is the identity function and $\rho(g) = (12)(34)(56) \neq 1 \in S_6$ we have that $\{1, 2\}^g = \{1, 2\}^e$, $\{2, 3\}^g = \{2, 3\}^e$ and $\{5, 6\}^g = \{5, 6\}^e$. Thus it is not faithful and so, G is not a permutation group on X.

Definition 12. A non-empty subset S of X is an *orbit* of G if G is transitive on S and S is invariant under the action of G.

It is straightforward to check that for any $x \in X$ the set $x^G = \{x^g : g \in G\}$ is an orbit of G.

Proposition 1.3.1. *Every orbit of G can be described as $x^G = \{x^g : g \in G\}$ for some $x \in X$.*

Proof. As we said it is obvious that the set $x^G = \{x^g : g \in G\}$ is an orbit of G since G is transitive on it and it is invariant under the action of G.
Moreover suppose we have an orbit that can not be described as above. Let us have $S = \{x_1, ..., x_n\}$ where $x_1, ..., x_n \in X$. By definition of an orbit, G must be transitive on it so for any pair of elements $x_i, x_j \in S$ there exist

some element $g \in G$ such that $x_i^g = x_j$. As a consequence we can get any element of S using for instance x_1, since $x_1^r = x_i$ for some $r \in G$. Then $S \subseteq x_1^G$. Moreover, as S is an orbit it must be invariant under the action of G, and consequently $x_1^G \subseteq S$. Thus, we have $x_1^G = S$. □

Proposition 1.3.2. *Let G be a group acting on a set X. Then G is transitive on X if and only if there is only one orbit in which all elements of X are.*

Proof. ⇒ If G is transitive, given any two points from X there is an element in G which maps one point onto the other, hence it is obvious that taking any element $x \in X$ the orbit $x^G = X$ is the only orbit.

⇐ If there is only one orbit in which all elements of X are then $S = X$ is an orbit. By definition S is an orbit of G if S is invariant under the action of G and G is transitive on S. Hence, G is transitive on X. □

Definition 13. Let G be a group acting on a set X. For any $x \in X$ the *stabilizer* G_x of x is the set of all elements $g \in G$ such that $x^g = x$.

Lemma 1.3.3. *The stabilizer G_x is a subgroup of G.*

Proof. If g_1 and $g_2 \in G_x$ then $g_1g_2 \in G_x$ since $x^{g_1g_2} = x^{g_2} = x$. Moreover, if $g \in G_x$ then $g^{-1} \in G_x$, since we can write $x^{g^{-1}} = (x^g)^{g^{-1}}$ which implies $x^{g^{-1}} = x$, thus $g^{-1} \in G_x$. □

Lemma 1.3.4. *Let G be a group acting on a set X and let S be an orbit of G. If x and y are elements of S, the set of permutations in X that map x to y is a right coset of G_x. Conversely, all elements in a right coset of G_x map x to the same point in S.*

Proof. First of all remember that the right coset G_xg of G_x is defined by $G_xg = \{hg : h \in G_x\}$. Now we must show that all the permutations that map x to y form a right coset of G_x. Since both x and y are in the orbit S there must exist an element, say g, such that $x^g = y$. Now suppose that there is some $h \in G$ that maps x to y as well, i.e., $x^h = y$. Thus $x^g = x^h$, so $(x^g)^{g^{-1}} = (x^h)^{g^{-1}}$, and $x^{hg^{-1}} = x$. Hence $hg^{-1} \in G_x$ and $h \in G_xg$. Consequently, all elements mapping x to y belong to the coset G_xg.

Now we must show that every element of a coset of G_x maps x to the same point. We know by the definition of a coset that every element in G_xg has the form hg where $h \in G_x$. Now as $x^{hg} = (x^h)^g$ and since $h \in G_x$ we have $(x^h)^g = x^g$. Therefore as h could be any element in G_x we conclude that all the elements of G_xg map x to x^g. □

Theorem 1.3.5 (Orbit-Stabilizer Theorem)**.** *Let G be a group acting on the finite set X and let x be a point in X. Then*

$$|G_x||x^G| = |G|.$$

Proof. By the previous lemma we know that each element of the orbit x^G corresponds bijectively to a right coset of G_x and all elements in a right coset of G_x map x to the same point, hence the elements of G can be partitioned into $|x^G|$ cosets. Moreover, we know that the cardinality of a coset of G_x is always $|G_x|$. Therefore, we have $|G| = |x^G||G_x|$. □

1.3.1 Actions on graphs

Note that we defined the action of G for the general case where G acts on a set X, however we should require more conditions when we are talking about actions on a set with some structure, in particular, graphs.

Definition 14. We say that a group G acts on a graph Γ if the group G acts on the set $V(\Gamma)$ and the homomorphism ρ goes from G into the group $\operatorname{Aut}\Gamma$. Thus, the action keeps the adjacency relation between the vertices in the graph.

It is obvious that $\operatorname{Aut}\Gamma$ is a group that acts on the graph Γ. Moreover, all the definitions and propositions above can be formulated for graphs with $X = V(\Gamma)$. However when the object is a graph we distinguish between two different kinds of transitivity, vertex-transitivity and edge-transitivity.

Definition 15. Let Γ be a graph and G a group acting on $V(\Gamma)$. We say that G is *vertex-transitive* if given any two points x and y from $V(\Gamma)$ there is an element $g \in G$ such that $x^g = y$.

The same definition is valid for edge-transitivity if we replace $V(\Gamma)$ by $E(\Gamma)$.

Example 12. Let C_5 be the graph in Example 8 and $G_1 = \{1, (123), (132)\}$, which can be considered as a subgroup of $\operatorname{Aut} C_5$. Then, $1^{G_1} = \{1, 2, 3\} = 2^{G_1} = 3^{G_1}$, $4^{G_1} = \{4\}$ and $5^{G_1} = \{5\}$ are the orbits of G_1. Thus, G_1 is not transitive on C_5.

Example 13. Now let G_2 be the symmetric group S_5 acting on the same graph. Then we have $1^{G_2} = \{1, 2, 3, 4, 5\} = 2^{G_2} = 3^{G_2} = 4^{G_2} = 5^{G_2}$, thus we have only one orbit, i.e., G_2 is transitive on C_5.

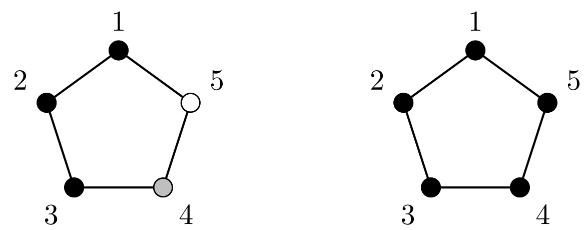


Figure 1.6: The vertices with the same color represent the orbits of G_1 on C_5 and the ones of G_2 on C_5 respectively.

1.4 The automorphism group of a cyclic graph

We are interested in knowing the automorphism groups of different families of graphs. In particular, in this section we are going to discuss the automorphism groups of cyclic graphs. In order to do that we are going to use the theory developed before, showing an application of the Orbit-Stabilizer Theorem.

Example 14. Let C_4 be the cyclic graph with 4 vertices as described in the first section. Then the automorphism group $G \subseteq S_4$ of this graph is $G = \operatorname{Aut} C_4 = \{1, (1234), (13)(24), (1432), (13), (24), (12)(34), (14)(23)\}$. Note that $|\operatorname{Aut} C_4| = 8$.

Theorem 1.4.1. *The automorphism group of a cyclic graph C_n has cardinality $2n$ and $\operatorname{Aut} C_n \cong D_{2n}$, where D_{2n} is the dihedral group of order $2n$.*

Proof. Let us take the cyclic graph C_n with the vertex set $\{1, 2, ..., n\}$ and the edges of the form $\{x, x+1\}$ with $x \in \{1, 2, ..., n\}$, x to be read modulo n. First of all, as every C_n is isomorphic to an n-polygon let us represent the graph C_n graphically projecting it into an n-polygon, each vertex and edge of C_n corresponding to a vertex and edge in the polygon respectively. Therefore, it is obvious that the dihedral group D_{2n}, which by definition is the group of symmetries of a regular polygon, is in $\operatorname{Aut} C_n$.

Then, our aim now is to see that the cardinality of $\operatorname{Aut} C_n$ coincides with that of D_{2n}, i.e., $|\operatorname{Aut} C_n| = 2n$. Let us denote $G = \operatorname{Aut} C_n$. By the previous argument, a rotation $\rho \in D_{2n}$ moving one vertex to the next one is an automorphism of C_n, in addition all the possible rotations in a polygon are in G. This means that we can map every vertex $x \in V(\Gamma)$ to all other vertices in $V(\Gamma)$ by rotations. Therefore we have $|x^G| = n$.

Now we are going to see which is the cardinality of the stabilizer G_x of x. Let x be any vertex in $V(\Gamma)$, let its neighbours be y and z, and take $f \in G_x$. We know from Lemma 1.2.3 that if $f \in G$ then $d(x, y) = d(x^f, y^f)$. Moreover, as $f \in G_x$ and x and y are neighbours we have that $d(x^f, y^f) = d(x, y^f) = 1$, but the only two vertices that are at distance 1 from x are y and z. Thus, we only have two options, either $y^f = y$ or $y^f = z$. Furthermore, we need to see that these two options lead us to two different automorphisms. Obviously the only way of getting $y^f = y$ is by applying the identity function. The second option $y^f = z$, however, leads us to the automorphism that switches the vertices that are at the same distance from x, i.e., a reflection. This is true since if we apply $y^f = z$ and we look at the vertices at distance two from x we will see that the only options for them to remain being neighbors of y and z is to switch and so on with every pair of vertices at the same distance from x. Thus $|G_x| = 2$. Applying now the orbit-stabilizer theorem, $|G| = |G_x||x^G| = 2n$. Hence, as $D_{2n} \subseteq G$ and $|D_{2n}| = |G|$, we conclude that $D_{2n} \cong \operatorname{Aut} C_n$.

□

We refer to the Appendix for the determination of some more automorphism groups of graphs applying the Orbit-Stabilizer Theorem. Starting from the simplest one in Exercise 2 and going through more complex ones in the following chapters, Exercise 3 and Exercise 6.

Chapter 2

Automorphism groups of Kneser graphs

We will focus this section on the Kneser graphs and the determination of the automorphism group of this important family of graphs.

2.1 Kneser graphs

Although we saw some examples in the previous chapter with the construction of Kneser graphs let us define this kind of graph in more detail. Let v and k be fixed positive integers with $k \leq v/2$; let Ω be a fixed set of size v; then, the Kneser graph $KG(v,k)$ has all subsets of Ω of size k as vertices, where two of those subsets are adjacent if their intersection is empty.

Note that when $k > v/2$ the intersection of the k-subsets is always non empty and thus, we do not have any edges and obviously those graphs are not really interesting.

We know that a $KG(v,k)$ has $\binom{v}{k}$ vertices, moreover, it is a regular graph with valency $\binom{v-k}{k}$. This is true since in order to determine all the neighbours of a vertex corresponding to the subset S we need subsets of size k that do not share any of the elements with that vertex. Thus we need all the possible k-subsets of $\Omega \setminus S$. Since $|\Omega \setminus S| = v - k$ we have always $\binom{v-k}{k}$ adjacent vertices.

Moreover, in the special case of $v = 2k$, in which we have $t = \binom{2k}{k}$ vertices, the Kneser graph $KG(2k,2)$ is nothing but the graph that joins any k-subset of $\{1,...,2k\}$ to its complement. This case will be mentioned through the chapter because of its special characteristics.

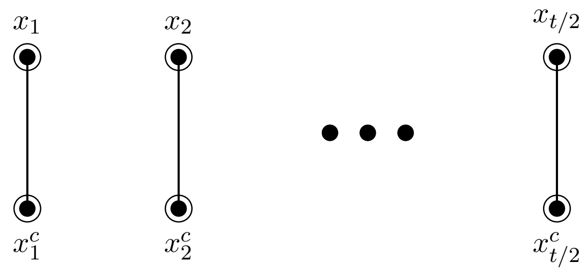


Figure 2.1: The bipartite graph $KG(2k, k)$.

2.2 The automorphism group of all Kneser graphs

First of all, we refer to the first section of the Appendix in which we develop as an exercise the automorphism group of the Petersen graph, without knowing the general result for all Kneser graphs.

However, in this section we want to determine which is the automorphism group of any Kneser graph. Let us take H as the group that the natural action of S_v induces on the vertices of the graph $KG(v, k)$. Note that this a faithful action and $H \subseteq \operatorname{Aut} KG(v, k)$, since the vertices of $KG(v, k)$ are k-sets of the set that S_v permutes, and therefore these sets will be naturally permuted by H. Moreover as the permutations map different elements to different images the intersection between the sets of every pair of vertices is preserved and as a consequence the adjacency relation between vertices as well. Thus, they really provide automorphisms. Our aim is to prove that $\operatorname{Aut} KG(v, k) = H \cong S_v$.

In order to reach that point first of all we need a very important result in extremal combinatorics, the Erdős-Ko-Rado theorem.

2.2.1 The Erdős-Ko-Rado theorem

We have based this section on P. Cameron's proof of the Erdős-Ko-Rado theorem, [3].

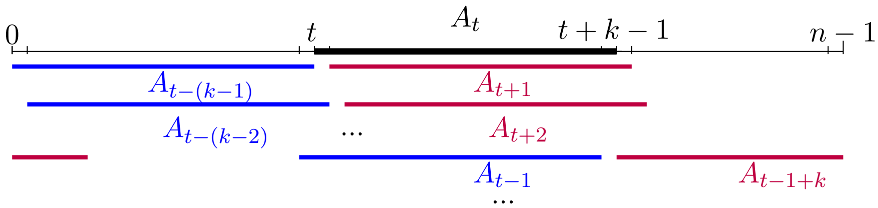
From now onwards we will employ bracketed n to denote the integers 1 through n, i.e., $[n] = \{1, ..., n\}$. In the same way we use $\binom{[n]}{k}$ to denote all k-subsets of $[n]$. Note that $|\binom{[n]}{k}| = \binom{n}{k}$.

Definition 16. A family $\mathcal{F}$ of sets is *intersecting* if any two of its sets have a non-empty intersection, i.e, if for all $A, B \in \mathcal{F}$, we have $A \cap B \neq \emptyset$.

We want to know which is the largest intersecting family of k-subsets of an n-set, $\mathcal{F} \subseteq \dbinom{[n]}{k}$. When $n < 2k$ it is obvious that any two k-sets intersect and so the maximum size is $\binom{n}{k}$. The Erdős-Ko-Rado theorem will give us the answer for the case $n \geq 2k$. We start with the following lemma.

Lemma 2.2.1. *For $n \geq 2k$ and $0 \leq s \leq n-1$ set $A_s = \{s, s+1, ..., s+k-1\}$ where addition is modulo n. Then an intersecting family can contain at most k of the sets A_s.*

Proof. Let $\mathcal{F}$ be an intersecting family. Suppose that for some $t \in \{0, ..., n-1\}$, $A_t \in \mathcal{F}$. Note that after choosing $A_t \in \mathcal{F}$ any other $A_s \in \mathcal{F}$ must intersect with A_t and this is only possible when $s \in \{t-k+1, .., t+k-1\}$. Now we distribute these sets into pairs such that the intersection of each pair is empty. Thus, we get pairs of the form $\{A_{t-i}, A_{t-i+k}\}$ where $1 \leq i \leq k-1$. Let us see that $\mathcal{F}$ contains at most one set of each pair $\{A_{t-i}, A_{t-i+k}\}$. Note that $A_{t-i} = \{t-i, t-i+1, ..., t-i+k-1\}$ and $A_{t-i+k} = \{t-i+k, t-i+k+1, ..., t-i+2k-1\}$ and the last element of A_{t-i} is followed by the first one in A_{t-i+k}. Therefore, as addition is modulo n and $n \geq 2k$ they are disjoint sets, so we can only have one set of each pair in $\mathcal{F}$.



So if we have $A_t \in \mathcal{F}$ then we can only add to $\mathcal{F}$ one set of each pair defined before, moreover, once one of a pair is chosen we must choose the consecutive one in the following pair and so on, since otherwise they will not intersect. Since there are $k-1$ such pairs, we conclude that $\mathcal{F}$ contains at most $1+k-1=k$ of the sets A_s.

□

Now we need to prove a totally different lemma regarding graphs and cliques in order to have the full result we need for proving the Erdős-Ko-Rado Theorem.

Lemma 2.2.2. *Let Γ be a vertex-transitive graph with vertex set V. Let Y be a subset of V with the property that any clique in Y has size at most $|Y|/m$. Then the same proportion holds for V and any clique in the graph has size at most $|V|/m$. Moreover, a clique C meeting the bound satisfies $|C^g \cap Y| = |Y|/m$ for all automorphisms g of Γ.*

Proof. First of all, as we state in Proposition 1.3.2, Γ being vertex-transitive means that there is only one orbit in which all vertices of Γ are. For given $x, y \in V$ the set of automorphisms satisfying $x^g = y$ is a coset of the stabilizer

$(\mathrm{Aut}\,\Gamma)_x$ as we proved in Lemma 1.3.4 and as all the cosets have the same size as the set we can use the Orbit-Stabilizer Theorem, concluding that the number of automorphisms satisfying $x^g = y$ is

$$|(\mathrm{Aut}\,\Gamma)_x| = \frac{|\mathrm{Aut}\,\Gamma|}{|x^{\mathrm{Aut}\,\Gamma}|} = \frac{|\mathrm{Aut}\,\Gamma|}{|V|}.$$

Let C be a clique in Γ. Now we count the pairs x, g where x is a vertex in C and g an automorphism of Γ such that $x^g \in Y$. On the one hand we have $|C|$ choices for x, and $\dfrac{|\mathrm{Aut}\,\Gamma|}{|V|}$ choices of g satisfying $x^g = y$ for each $y \in Y$, as we saw before. Therefore, the number of possible pairs is $\dfrac{|C||Y||\mathrm{Aut}\,\Gamma|}{|V|}$.

On the other hand, as every $g \in \mathrm{Aut}\,\Gamma$ is an automorphism it must maintain the adjacency relations between the vertices and as C is a clique the images of all the points $x^g \in Y$ must continue being parts of a clique. Any clique in Y has size at most $|Y|/m$, thus $|C^g \cap Y| \leq |Y|/m$ and therefore we have at most $\dfrac{|Y|}{m}|\mathrm{Aut}\,\Gamma|$ choices for the pairs we are counting.

Therefore,

$$\frac{|C||Y||\mathrm{Aut}\,\Gamma|}{|V|} \leq \frac{|Y|}{m}|\mathrm{Aut}\,\Gamma|$$

and so

$$|C| \leq \frac{|V|}{m}.$$

Finally $|C^g \cap Y|$ is the number of $x \in C$ satisfying $x^g \in Y$. In the second counting we saw that $|C^g \cap Y| \leq |Y|/m$. Actually, the argument to get the bound $C = \frac{|V|}{m}$ shows that we must have $|C^g \cap Y| = |Y|/m$. □

Theorem 2.2.3 (Erdős-Ko-Rado)**.** *Let* $\mathcal{F} \subseteq \binom{[n]}{k}$ *be an intersecting family and* $n \geq 2k$*. Then* $|\mathcal{F}| \leq \binom{n-1}{k-1}$.

Proof. Consider the graph Γ whose vertices are the k-subsets of an n-set, $V = \binom{[n]}{k}$ and they are joined if and only if their intersection is non-empty. Note that $\mathcal{F} \subseteq V$ is an intersecting family if an only if $\mathcal{F}$ is a clique in Γ. So we want to show that the size of a clique in Γ is at most $\binom{n-1}{k-1}$. Consider the family $Y = \{A_s : 0 \leq s \leq n-1\}$ in which $A_s = \{s, s+1, ..., s+k-1\}$, where addition is modulo n. We have $|Y| = n$ and since $n \geq 2k$ we know from Lemma 2.2.1 that any intersecting family in Y has size at most k. Note that $k = n/(\dfrac{n}{k}) = |Y|/(\dfrac{n}{k})$.

The graph Γ is vertex-transitive since taking all the permutations of the n-set, S_n, which are automorphisms of Γ, we can reach from one vertex any other vertex in the graph. So we can apply Lemma 2.2.2 and conclude that any clique in the graph has size at most

$$|V|/(\frac{n}{k}) = \binom{n}{k}/(\frac{n}{k}) = \frac{k}{n}\binom{n}{k} = \binom{n-1}{k-1}.$$

$\square$

Moreover, in the case of $n = 2k$ the family $\binom{[2k]}{k}$ can be partitioned into $\frac{1}{2}\binom{2k}{k} = \binom{2k-1}{k-1}$ pairs having in each pair a k-subset and its complement. It is obvious that the subsets in the same pair are disjoint and any two k-sets of different pairs have always a non-empty intersection. So every intersecting family will be composed by one set of each k-pair.

Note that every family of sets sharing a fixed point is obviously an intersecting family, since all of them intersect at least in one point. The following theorem will show us that this kind of families are the extremal families if $n > 2k$.

Theorem 2.2.4. *If $n > 2k$, then any intersecting family $\mathcal{F} \subseteq \binom{[n]}{k}$ of cardinality $|\mathcal{F}| = \binom{n-1}{k-1}$ consists of all the k-sets containing some fixed point.*

Proof. Let $\mathcal{F}$ be an intersecting family of cardinality $|\mathcal{F}| = \binom{n-1}{k-1}$. We start with two observations.

First, suppose that there are two points x and y such that every k-set containing x but not y belongs to $\mathcal{F}$, i.e., if $x \in K$ and $y \notin K$, then $K \in \mathcal{F}$. Note also that the case of both x and $y \in K$ does not necessarily imply $K \in \mathcal{F}$. We are going to prove by contradiction that $\mathcal{F}$ consists of all the k-sets containing x.

Suppose that $K \in \mathcal{F}$ is a k-set not containing x. Since $n > 2k$ there are at least $2k$ points different from y. Thus we can choose a k-set L disjoint to K which has the point x but not y, thus by assumption on $\mathcal{F}$, we have $L \in \mathcal{F}$. Since $K \cap L = \emptyset$, and $L \in \mathcal{F}$ and $\mathcal{F}$ is an intersecting family, K can not be in $\mathcal{F}$. Hence, the assumption is false and every set in $\mathcal{F}$ contains x. Moreover, there are $\binom{n-1}{k-1}$ k-sets containing x because we have to choose $k-1$ points from $n-1$ to create the set. Therefore considering that the cardinality of $\mathcal{F}$ is $\binom{n-1}{k-1}$ we must have every such set in $\mathcal{F}$. Hence $\mathcal{F}$ consists of all the k-sets containing x.

Next we show that there are two k-sets, K and K', intersecting in $k-1$ points, such that $K \in \mathcal{F}$ and $K' \notin \mathcal{F}$. We are going to prove this again by contradiction. Suppose that for each $K \in \mathcal{F}$, every k-set meeting K in $k-1$ points is also in $\mathcal{F}$. If we continue choosing K'' such that K' and K'' intersect in $k-1$ points by assumption K'' must be in $\mathcal{F}$, then if we keep applying the same argument to every k-set, by induction every k-set is in $\mathcal{F}$ which is impossible.

Now we are going to prove the theorem by contradiction. Suppose that there exists a counterexample $\mathcal{F}$, then considering our first observation, for every x and y there is a k-set not in $\mathcal{F}$ containing x but not y.

Take K and K' as above and label the points in $K \backslash K'$ and $K' \backslash K$ as 0 and k respectively and all common points from 1 to $k-1$, i.e., $K = \{0, 1, ..., k-1\}$ and $K' = \{1, 2, ..., k-1, k\}$. Note that these two sets can be denoted by A_0 and A_1 respectively as defined in Lemma 2.2.1. Now as we supposed that there exists a counterexample $\mathcal{F}$ such that for every x and y there is a k-set not in $\mathcal{F}$ containing x but not y, we choose the set not in $\mathcal{F}$ containing $x = 0$ and not $y = k$ and we denote it as K''. Moreover, we know K'' and A_0 intersect at least in 0 so let $A_0 \cap K'' = \{0, ..., l-1\}$ where $1 \leq l < k$ and let us label the remaining points of K'' as $\{n-k+l, ..., n-1\}$, this labeling can be safely done, since $n-k+l > k$. Hence we can write this set as $K'' = A_{n-k+l} = \{n-k+l, ..., 0, ..., l-1\}$.

We know that any intersecting family in $Y = \{A_s : 0 \leq s \leq n-1\}$ in which $A_s = \{s, s+1, ..., s+k-1\}$ where addition is modulo n has size at most k from Lemma 2.2.1. Moreover by Lemma 2.2.2, as $\mathcal{F}$ is meeting the bound $|\mathcal{F}| = \binom{n-1}{k-1}$, we have $|\mathcal{F}^g \cap Y| = |Y|/m$ for all $g \in \mathrm{Aut}(\Gamma)$, where $m = n/k$ and Γ are as in the proof of Erdős-Ko-Rado Theorem. Taking the identity automorphism we get $|\mathcal{F} \cap Y| = |Y|/m = k$. So $\mathcal{F}$ contains k of these sets. From the proof of Lemma 2.2.1 $\mathcal{F}$ must contain apart from A_0 one of each pair $\{A_{0-i}, A_{0-i+k}\}$ for all $1 \leq i \leq k-1$. Moreover, from the proof of Lemma 2.2.1, these sets must be consecutive but we said that $A_0 = \{0, ..., k-1\} \in \mathcal{F}$ and $A_1 = \{1, ..., k\} \notin \mathcal{F}$, so the only remaining option is to have $\mathcal{F} = \{A_{n-k+1}, ..., A_{n-k+l}, ..., A_0\}$ but we know that $A_{n-k+l} \notin \mathcal{F}$.

This contradiction proves the theorem. □

We remark again the case of $n = 2k$ for which this last result does not hold. Note that it is true that every intersecting family consisting of all the k-sets containing some fixed point has cardinality $\binom{n-1}{k-1}$. However, there are some other families with this cardinality which are not as described above. We can assure this since we said that we compose the intersecting family chosen one k-set of each pair $\{A, B\}$, in which B is the complement of the k-set A. As we said before that there are $\binom{2k-1}{k-1}$ of this pairs we have $2^{\binom{2k-1}{k-1}}$ intersecting families meeting the bound, while the ones consisting of all the k-sets containing some fixed points are just $n = 2k$. Therefore, as $2^{\binom{2k-1}{k-1}} > 2k$ for $k > 1$ there exists some intersecting family meeting the bound which is not as described in Theorem 2.2.4.

2.2.2 The automorphism group of Kneser graphs

All this combinatorial theory was necessary in order to prove the final result of this chapter, which is summarized in the following theorem. Let us take H as we described at the beginning of Section 2.2, i.e., the group that the natural action of S_v induces on the vertices of the graph $KG(v, k)$.

Theorem 2.2.5. *The automorphism group of any Kneser graph $KG(v, k)$ with $v > 2k$ is equal to the group H and therefore isomorphic to the symmetric group S_v, i.e.,* $\operatorname{Aut} KG(v, k) = H \cong S_v$.

Proof. By Theorem 2.2.4 any intersecting family $\mathcal{F} \subseteq \binom{[n]}{k}$ of maximum cardinality consists of all the k-sets containing some fixed point. In our case $n = v$ and $\Omega = [v]$ and an intersecting family of maximum cardinality corresponds to a maximal independent set of the Kneser graph. Let us denote by α_i the maximal independent set containing some fixed point $i \in \Omega$. Obviously, any automorphism $f \in \operatorname{Aut} KG(v, k)$ permutes the vertices of $KG(v, k)$ and so it must permute the maximal independent sets of $KG(v, k)$ defined before, so we have an action of $\operatorname{Aut} KG(v, k)$ on $\{\alpha_1, ..., \alpha_v\}$. Thus, we have a homomorphism from $\operatorname{Aut} KG(v, k)$ to S_v. Now we need to show that the kernel of this action on $\{\alpha_1, ..., \alpha_v\}$ is trivial. Let us prove this by contradiction. Suppose the kernel is not trivial, then we have $f \in \operatorname{Aut} KG(v, k)$ such that $f(\alpha_i) = \alpha_i$ for all $i \in \{1, ..., v\}$ but $f \neq 1$. Then there exists a vertex x corresponding to a k-set such that $f(x) \neq x$. This implies that there must be an element i in x but not in $f(x)$. However, as $i \in x$ we have $x \in \alpha_i$ and by assumption $f(x) \in \alpha_i$, since $f(\alpha_i) = \alpha_i$. But that means $i \in f(x)$, which is a contradiction. As a consequence of the trivial kernel we know that $|\operatorname{Aut} KG(v, k)| \leq |S_v| = v!$. However, $H \subseteq \operatorname{Aut} KG(v, k)$ and $|H| = v!$ which together with $|\operatorname{Aut} KG(v, k)| \leq |S_v| = v!$ implies $\operatorname{Aut} KG(v, k) = H \cong S_v$.

□

We refer to Exercise 4 in the Appendix in which we give a counterexample to the last theorem for the case $v = 2k$.

Chapter 3

Automorphism groups of generalized Petersen graphs

3.1 The generalized Petersen graphs

For integers $n \geq 3$ and k with $1 \leq k < \frac{n}{2}$, the generalized Petersen graph $G(n,k)$ is defined as follows. The vertex set is divided in two subsets, the outer edges $\{u_0, ..., u_{n-1}\}$ and the inner edges $\{v_0, ..., v_{n-1}\}$, i.e.,

$$V(G(n,k)) = \{u_0, ..., u_{n-1}, v_0, ..., v_{n-1}\}.$$

The edge set $E(G(n,k))$ consists of all edges of the form

$$\{u_i, u_{i+1}\}, \quad \{u_i, v_i\}, \quad \{v_i, v_{i+k}\}$$

where all the indices are to be read modulo n. The set of all the edges of the first form is called Ω and the edges on it are called outer edges. We call Σ the set of edges of the second form and we are going to refer to such edges as spokes. Eventually, the edges of the third form are inner edges and the set of them is I.

This class of graphs was first considered by H. S. M. Coxeter who wrote for instance [4].

Note that one of the properties of this family of graphs is that every graph has $2n$ vertices, and moreover, every vertex has three neighbours, i.e., $G(n,k)$ is always a trivalent graph of order $2n$.

Remark 1. We restrict to the case $k < \frac{n}{2}$ since $G(n,k)$ and $G(n,n-k)$ are the same graph as we prove in Exercise 5 at the Appendix. Moreover we do not take into account the case $k = n/2$ since we always have two edges linking the same two vertices, and we do not get a trivalent graph because of this overlap, see Figure 3.1 and note that there are two edges between every pair of vertices $\{v_i, v_{i+3}\}$.

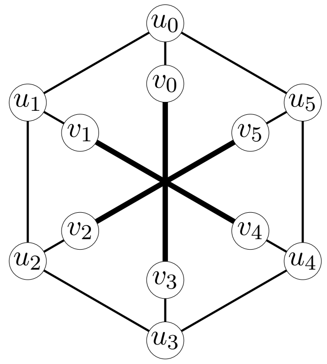


Figure 3.1: The graph $G(6, 3)$.

We can describe $G(n, k)$ as a graph with two linked subgraphs: an outer rim with n vertices and the edge set Ω which is isomorphic to a cyclic graph C_n, and a subgraph generated by I with n vertices matched depending on k. This two subgraphs are always linked naturally by the n-set Σ of edges. From this, we can easily see that $G(n, k)$ is always connected since the connected outer rim's vertices are linked one by one with a different vertex of the interior subgraph generated by I. Thus, we can always find a path from any vertex to another through the outer subgraph. Now that we know that the outer rim and the whole graph $G(n, k)$ are connected let us focus our attention in the subgraph generated by I.

Lemma 3.1.1. *Let d be the greatest common divisor of n and k. Then the subgraph of $G(n, k)$ induced by $\{v_0, ..., v_{n-1}\}$ has d connected components, each of which is a circuit of length $\frac{n}{d}$.*

Proof. Two vertices v_i and v_j of the subgraph are in the same connected component if and only if there exists $l \in \mathbb{Z}$ such that $j = i + kl$. Thus we will have in the same component the vertices with the subindices in the following set $\{\overline{i + kl} \mid l \in \mathbb{Z}\} \subseteq \mathbb{Z}/n\mathbb{Z}$. The set $\mathbb{Z}/n\mathbb{Z}$ together with addition forms a group and $\{\overline{i + kl} \mid l \in \mathbb{Z}\} = \bar{i} + \langle\bar{k}\rangle$ is a coset of $\langle\bar{k}\rangle$. Thus, $|\bar{i} + \langle\bar{k}\rangle| = |\langle\bar{k}\rangle|$. We can calculate the cardinality of the group generated by k using the result $o(g^k) = \frac{o(g)}{\gcd(k, o(g))}$ from group theory.

$$|\langle\bar{k}\rangle| = \frac{o(\bar{1})}{\gcd(k, o(\bar{1}))} = \frac{n}{\gcd(k, n)} = \frac{n}{d}.$$

Therefore the components have $\frac{n}{d}$ vertices, as a consequence we have $\frac{n}{n/d} = d$ connected components. However, we need to know how those vertices are connected in order to conclude that the connected component are circuits. Note that in each component we have the set of vertices with the subindices $\{i, i+k, i+2k, ..., i+(\frac{n}{d}-1)k\}$, let us analyze when two subindices $i+lk$ and $i+mk$ are the same. As all the subindices are to be read modulo n they will be the same if n divides $(i+mk)-(i+lk) = (m-l)k$, or which is the same $\frac{n}{d}|(m-l)\frac{k}{d}$. It follows that as d is the greatest common divisor of n and k this is true when $\frac{n}{d}|m-l$. Looking again at the subindices of the same component we can easily see that this never happens since all the m and l possibles are between 0 and $\frac{n}{d}-1$. Moreover, $i+(\frac{n}{d}-1)k+k = i+(\frac{n}{d})$ and $\frac{n}{d}|\frac{n}{d}-0$, so the subindex that follows the last one is the same as the first one, closing the loop without repetitions. □

Example 15. The Petersen graph $KG(5,2)$ is also the generalized Petersen graph $G(5,2)$. In this case $d=1$ and so we have just one circuit of 5 edges.

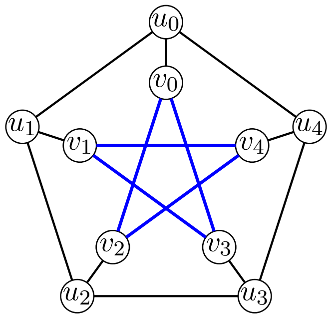


Figure 3.2: Petersen graph $KG(5,2) = G(5,2)$.

Example 16. In the case of the graph $G(6,2)$, we see that $d = \gcd(6,2) = 2$ so we have 2 disjoint 3-circuits which are $\{v_0, v_2, v_4\}$ and $\{v_1, v_3, v_5\}$.

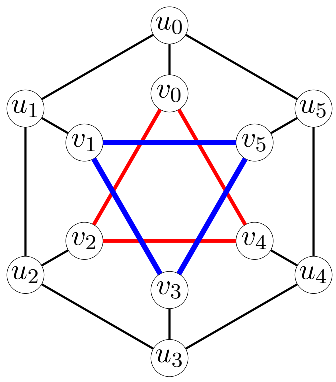


Figure 3.3: The graph $G(6,2)$.

Example 17. In our last example $G(10, 4)$ we have again 2 disjoint circuits but this time they are of length 5.

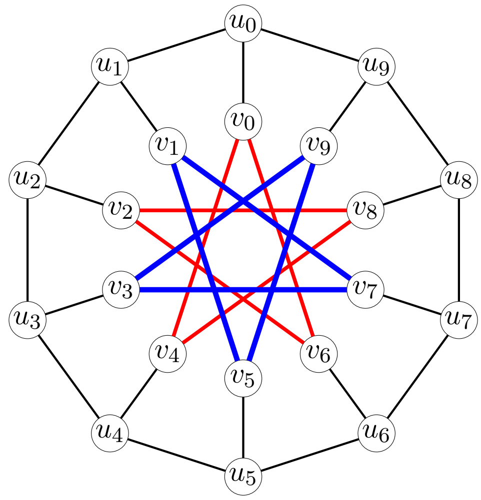


Figure 3.4: The graph $G(10, 4)$.

3.2 Automorphism groups of generalized Petersen graphs

First of all, let us denote the group of automorphisms of $G(n, k)$ by $A(n, k)$. Moreover, let us define an important subgroup of $A(n, k)$, denoted by $B(n, k)$, as the group of automorphisms of $G(n, k)$ that fix Σ set-wise. In this way if $\gamma \in B(n, k)$ and the edge $s_i \in \Sigma$, then $\gamma(s_i) \in \Sigma$, or which is the same, all spokes are mapped onto spokes. The following lemma is going to show us the importance of the subgroup $B(n, k)$.

Lemma 3.2.1. *If $\gamma \in A(n, k)$ fixes set-wise any of the sets Ω, Σ or I, then it either fixes all three sets or fixes Σ set-wise and interchanges Ω and I.*

Proof. First of all let us proof by contradiction that if $\gamma \in A(n, k)$ fixes set-wise any of the sets, it must fix Σ. Suppose that γ fixes set-wise Ω (or I) but it does not fix Σ. Then there must exist a spoke s_i whose image is not in Σ, i.e., $\gamma(s_i) \notin \Sigma$. We know from how we defined the edges of the graph $G(n, k)$ before, that a spoke is an edge that links a vertex in the outer rim generated by Ω with a vertex in the inside subgraph generated by I. Thus one of the vertices that corresponds to an end-point of a spoke is incident only to the spoke and to two outer edges, while the other end-point is incident to the spoke and to two inner edges. It follows that if γ maps a spoke s_i onto an outer (inner) edge, as it must maintain the incident edges, the two incident outer edges must become an outer (inner) edge and a spoke, and the two incident inner edges must become an outer (inner) edge and another spoke. Thus, $\gamma(\{u_i, u_i+1\}) \notin \Omega$ for some i and $\gamma(\{v_j, v_j+k\}) \notin I$ for some j. Hence, none of the sets is preserved, which is a contradiction. Therefore, if γ fixes any of the sets set-wise, it must fix Σ.

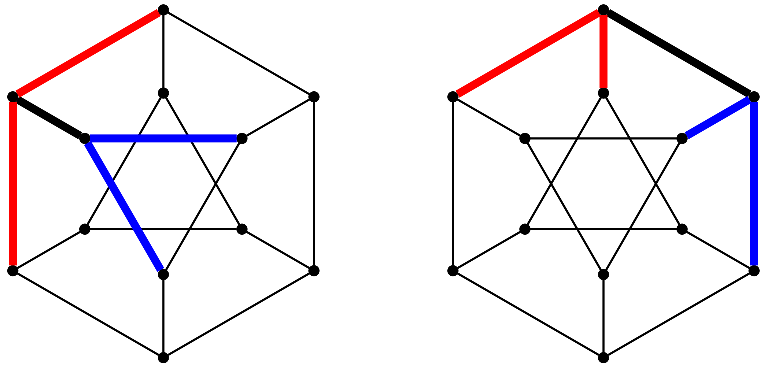


Figure 3.5: Not fixing the set Σ implies the impossibility of fixing any of the other sets Ω and I.

Now let us show that if γ fixes Σ set-wise, then Ω and I are either fixed as well, or they are interchanged. When we remove the spokes the outer edges compose a single connected component, and so as any automorphism must maintain all those connections either it fixes the set Ω or it interchanges the whole set with another one, in this case I. □

Note that we said that if $\gamma \in A(n,k)$ fixes set-wise any of the sets Ω, Σ or I, it must fix Σ, therefore $\gamma \in B(n,k)$. Let us analyze first this special subgroup $B(n,k)$ of $A(n,k)$ and check afterwards which is the exact relation between them.

3.2.1 The subgroup $B(n,k)$

From the previous lemma we know that if $\gamma \in B(n,k)$ there are just two possibilities, fixing all the sets or interchanging Ω and I. Now we are going to analyze each case and try to determine the subgroup $B(n,k)$.

First of all, it is easy to see that the group $\langle \rho, \sigma \rangle$ with

$$\begin{aligned} \rho(u_i) &= u_{i+1}, \qquad \rho(v_i) = v_{i+1} \quad \text{and} \\ \sigma(u_i) &= u_{-i}, \qquad \sigma(v_i) = v_{-i}, \quad \text{for all } i \end{aligned}$$

is a subgroup of $B(n,k)$. This is true since the rotations ρ and the reflections σ are automorphisms of $G(n,k)$ fixing the three edge sets Ω, Σ and I set-wise. Clearly we have $\langle \rho, \sigma \rangle \cong D_{2n}$.

Now we are going to analyze the two cases we mentioned before. In order to do that let us define the subgroup $C(n,k) \subseteq B(n,k)$ to be the set of all automorphisms that fix the three sets. Thus, this subgroup will represent all the automorphisms mentioned as the first case.

$$C(n,k) = \{\gamma \in A(n,k) \mid \gamma(\Omega) = \Omega, \gamma(\Sigma) = \Sigma, \gamma(I) = I\}.$$

Let us prove the following lemma in order to find afterwards the representation of $C(n,k)$.

Lemma 3.2.2. *If $\gamma_1, \gamma_2 \in A(n,k)$ coincide on Ω, then $\gamma_1 = \gamma_2$.*

Proof. If $\gamma_1, \gamma_2 \in A(n,k)$ coincide on Ω, then $\gamma_1(u_i) = \gamma_2(u_i)$ and consequently $\gamma_1^{-1}\gamma_2(u_i) = u_i$ for all i. Since $\gamma_1^{-1}\gamma_2(v_i)$ is linked to $\gamma_1^{-1}\gamma_2(u_i)$ and it can not be a vertex in the outer rim, it follows that $\gamma_1^{-1}\gamma_2(v_i) = v_i$, for all i. Thus, $\gamma_1^{-1}\gamma_2 = 1$ on $G(n,k)$ and moreover, $\gamma_1 = \gamma_2$. □

Theorem 3.2.3. $C(n,k) = \langle \rho, \sigma \rangle$.

Proof. Obviously, $\langle \rho, \sigma \rangle \subseteq C(n,k)$ since we said before that this group fixes Ω, Σ and I set-wise.
By Lemma 3.2.2 every automorphism on $G(n,k)$ is determined by its action on Ω. Moreover, $\{\gamma_{|\Omega} \mid \gamma \in C(n,k)\}$ must belong to the automorphism group of an n-cyclic graph and we saw in Section 1.4 that this group was isomorphic to the dihedral group of order $2n$. It follows that $|C(n,k)| \leq 2n$, and consequently $C(n,k) = \langle \rho, \sigma \rangle$. □

Now our two cases are, either all the sets Ω, I and Σ are fixed for all $\gamma \in B(n,k)$ so $B(n,k) = C(n,k)$, or $B(n,k) \neq C(n,k)$ and so there is some automorphism that interchanges Ω and I.

Let us define the map α on $V(G(n,k))$ by,

$$\alpha(u_i) = v_{ki}, \quad \alpha(v_i) = u_{ki}, \quad \text{for all } i.$$

Note that α sends edges of Ω to I, and viceversa. One can check that α is a bijection if and only if $\gcd(k,n) = 1$. Now we want to see when α is an automorphism of $G(n,k)$. Observe that α maps the spoke $\{u_i, v_i\}$ onto the spoke $\{\alpha(u_i), \alpha(v_i)\} = \{u_{ki}, v_{ki}\}$, the outer edge $\{u_i, u_{i+1}\}$ onto the inner edge $\{v_{ki}, v_{ki+k}\}$, and the inner edge $\{v_i, v_{i+k}\}$ onto the pair $\{u_{ki}, u_{ki+k^2}\}$. We said the pair $\{u_{ki}, u_{ki+k^2}\}$ because it is not always an edge of $G(n,k)$, the outer edges form a rim and two vertices are only adjacent to each other if they are next to each other, $u_{i-1} \sim u_i \sim u_{i+1}$. Therefore, for the pair $\{u_{ki}, u_{ki+k^2}\}$ to be an outer edge we have the necessary and sufficient condition $k^2 \equiv \pm 1 \pmod{n}$. Thus, $\alpha \in A(n,k)$ if and only if $k^2 \equiv \pm 1 \pmod{n}$. Obviously as we said that the spokes are mapped onto spokes when $\alpha \in A(n,k)$ then $\alpha \in B(n,k)$.

Lemma 3.2.4. *If $B(n,k) \neq C(n,k)$, then $B(n,k) = \langle \rho, \sigma, \alpha \rangle$ and this only happens when $k^2 \equiv \pm 1 \pmod{n}$.*

Proof. As $B(n,k) \neq C(n,k)$, then there exists $\gamma \in B(n,k)$ and not in $C(n,k)$ which fixes Σ set-wise and interchanges Ω and I. We are going to compose γ with the appropriate rotations and reflections in order to get the α defined before. First of all, we compose γ with an appropriate power of ρ producing an automorphism which not only interchanges the mentioned sets but interchanges u_0 and v_0 as well. Note that this is always possible since $\gamma \in B(n,k)$, then after applying γ the spoke $\{u_0, v_0\}$ is mapped onto another spoke, say $\{u_t, v_t\}$ where t is an integer modulo n. We can see know that as $\rho \in B(n,k)$, we can always find an appropriate power of ρ that maps that spoke onto the spoke $\{u_0, v_0\}$. Since γ interchanges Ω and I we must have that our composed automorphism maps u_0 onto v_0 and v_0 onto u_0. Furthermore, since we are composing automorphisms u_1 is going to be mapped onto one of the inner neighbours of v_0, i.e., v_k or v_{-k}. Thus, we can force u_1 to be mapped onto v_k by permitting the composition with σ in case u_1 is mapped onto v_{-k}.

After fixing those images the images of all u_i are determined since u_2 could only be mapped to v_0 or v_{2k} but as v_0 is the image of u_0 we only have the last option. The same happens if we go on with all the u_i vertices, for instance the image of u_3 can not be v_k so it must be v_{3k} and so on. Thus we have that u_i is mapped onto v_{ki} for all i. Note that the automorphism γ composed with the appropriate power of ρ and perhaps σ coincides with α on Ω and by Lemma 3.2.2 they are the same automorphism. As we said before this can only occur if $k^2 \equiv \pm 1 \pmod{n}$. When this condition holds we can describe every $\gamma \in B(n,k)$ as a combination of ρ, σ and α, hence $B(n,k) = \langle \rho, \sigma, \alpha \rangle$, and $B(n,k) = C(n,k)$ otherwise. □

Lemma 3.2.5. *$B(n,k)$ is vertex-transitive on $G(n,k)$ if and only if there exists α, i.e., $k^2 \equiv \pm 1 \pmod{n}$ and therefore $B(n,k) \neq C(n,k)$.*

Proof. $\Rightarrow$ If $B(n,k)$ is vertex-transitive, for every pair of vertices x and y in $V(G(n,k))$ there exists $\gamma \in B(n,k)$ such that $\gamma(y) = x$. Then there must exist an automorphism that maps some u_i to some v_j and we know there are no such automorphisms in $C(n,k)$. Thus, $B(n,k) \neq C(n,k)$ and by Lemma 3.2.4 $B(n,k) = \langle \rho, \sigma, \alpha \rangle$.

$\Leftarrow$ If there exists α it is obvious that $B(n,k)$ is vertex-transitive on $G(n,k)$ since using the powers of $\rho \in B(n,k)$ we can go from every u_i to every u_j and form every v_i to any other v_j, so as α maps one vertex of the inner subgraph with one of the outer rim, composing α and the appropriate power of ρ we can map any vertex to every vertex in $G(n,k)$. □

Now that we know how $B(n,k)$ can be generated let us analyze its order and presentation. If $k^2 \not\equiv \pm 1 \pmod{n}$, then we have $B(n,k) = C(n,k)$ with order $2n$.

If $k^2 \equiv \pm 1 \pmod{n}$ then $B(n,k) \neq C(n,k)$, and we need to calculate the index of $C(n,k)$ in $B(n,k)$. In order to do that let us apply the Orbit-Stabilizer Theorem again

$$|B(n,k)| = |B(n,k)_\Omega||\Omega^{B(n,k)}|$$

Note that $C(n,k)$ is the stabilizer of Ω, i.e. $B(n,k)_\Omega = C(n,k)$ and then the index:

$$|B(n,k) : C(n,k)| = \frac{|B(n,k)|}{|C(n,k)|} = |\Omega^{B(n,k)}|.$$

But every element in $B(n,k)$ fixes Σ and so it only acts in the sets Ω and I, either fixing them or interchanging them. Therefore, $|B(n,k) : C(n,k)| = |\Omega^{B(n,k)}| \leq 2$. This leads to $|B(n,k) : C(n,k)| = 2$ since otherwise $B(n,k) = C(n,k)$. Hence,

$$|B(n,k)| = |B(n,k) : C(n,k)||C(n,k)| = 4n.$$

It remains to complete the possible exact presentations for $B(n,k)$. For that it is convenient to think of $B(n,k)$ as acting on Σ:

$$\rho(s_i) = s_{i+1}, \quad \sigma(s_i) = s_{-i}, \quad \alpha(s_i) = s_{ki},$$

for all i, where s_i is the spoke $\{u_i, v_i\}$.

Lemma 3.2.6. *If $k > 1$ then $B(n,k)$ acts faithfully on Σ. Thus if $\mu, \phi \in B(n,k)$ and $\mu(s_i) = \phi(s_i)$ for all i, then $\mu = \phi$.*

Proof. The fact of $B(n,k)$ not being faithful means that there exists $\mu \in B(n,k)$ such that $\mu(s_i) = s_i$ for every spoke s_i but that μ is not the identity of $B(n,k)$. Note that from our two options in Lemma 3.2.1 we have to discard the first option, since the only way of fixing Ω and I set-wise and fixing all spokes is applying the identity function. Thus μ must interchange Ω and I while fixing the set Σ point-wise. Therefore, the only option for that μ is to interchange each vertex in the outer rim with its neighbor in the inner rim and thus $\mu(u_i) = v_i$ and $\mu(v_i) = u_i$ which is an automorphism of $G(n,k)$ if and only if $k = 1$. □

Lemma 3.2.7. *If $k = 1$, then $B(n,1) \cong D_{2n} \times C_2$.*

Proof. First of all, from Lemma 3.2.6, $B(n,k)$ is not faithful on Σ and moreover we have the automorphism $\mu(u_i) = v_i$ and $\mu(v_i) = u_i$ which corresponds to the definition of α if and only if $k = 1$. Then in this case $\mu = \alpha$ and it commutes with both ρ and σ:

$$\rho\alpha(s_i) = \rho(s_i) = s_{i+1} = \alpha(s_{i+1}) = \alpha\rho(s_i)$$

$$\sigma\alpha(s_i) = \sigma(s_i) = s_{-i} = \alpha(s_{-i}) = \alpha\sigma(s_i).$$

Due to this, we have that $B(n,1) = \langle \rho, \sigma, \alpha \rangle$ is the internal direct product of $C(n,1)$ and $\langle \alpha \rangle$. First of all, both subgroups are normal subgroups, $C(n,1)$ is normal since it has index 2 and $\langle \alpha \rangle$ is normal since it commutes with every element in $B(n,1)$ and thus it belongs to the center of $B(n,1)$. This implies that $\langle \rho, \sigma, \alpha \rangle = \langle \rho, \sigma \rangle \times \langle \alpha \rangle$. Moreover, their intersection is trivial since $\alpha \notin \langle \rho, \sigma \rangle$. Thus $B(n,1) = \langle \rho, \sigma \rangle \times \langle \alpha \rangle$ and furthermore $B(n,1) \cong D_{2n} \times C_2$.

□

Theorem 3.2.8. *(a) If* $k^2 \not\equiv \pm 1 \pmod{n}$*, then*

$$B(n,k) = \langle \rho, \sigma | \quad \rho^n = \sigma^2 = 1, \quad \rho^\sigma = \rho^{-1} \rangle.$$

(b) If $k^2 \equiv 1 \pmod{n}$*, then*

$$B(n,k) = \langle \rho, \sigma, \alpha | \quad \rho^n = \sigma^2 = \alpha^2 = 1, \quad \rho^\sigma = \rho^{-1}, \quad \alpha\sigma = \sigma\alpha, \quad \rho^\alpha = \rho^k \rangle.$$

(c) If $k^2 \equiv -1 \pmod{n}$*, then*

$$B(n,k) = \langle \rho, \alpha | \quad \rho^n = \alpha^4 = 1, \quad \rho^\alpha = \rho^{-k} \rangle.$$

Proof. We already know generators of $B(n,k)$ in each case and then we will find their order and the conjugation relations between them. This will give us enough information in order to get the presentation.

(a) It is well know that the presentation of the dihedral group is $D_{2n} = \langle \rho, \sigma | \quad \rho^n = \sigma^2 = 1, \quad \rho^\sigma = \rho^{-1} \rangle$.

(b) Let $k^2 \equiv 1 \pmod{n}$. Assume that $k > 1$. Then $B(n,k)$ acts faithfully on Σ. For any $s_i \in \Sigma$,

$$\alpha^2(s_i) = \alpha(s_{ki}) = s_{k^2 i} = s_i \quad \text{thus, } \alpha^2 = 1,$$

$$\sigma^\alpha(s_i) = \alpha\sigma\alpha(s_i) = \alpha\sigma(s_{ki}) = \alpha(s_{-ki}) = s_{-k^2 i} = s_{-i} = \sigma(s_i) \quad \text{thus, } \alpha\sigma = \sigma\alpha,$$

$$\rho^\alpha(s_i) = \alpha\rho\alpha(s_i) = \alpha\rho(s_{ki}) = \alpha(s_{ki+1}) = s_{k^2 i + k} = s_{i+k} = \rho^k(s_i).$$

Note that the special case analyzed before $B(n,1)$ is also of this form. Hence, if $k^2 \equiv 1 \pmod{n}$, then

$$B(n,k) = \langle \rho, \sigma, \alpha | \quad \rho^n = \sigma^2 = \alpha^2 = 1, \quad \rho^\sigma = \rho^{-1}, \quad \alpha\sigma = \sigma\alpha, \quad \rho^\alpha = \rho^k \rangle.$$

(c) Let $k^2 \equiv -1 \pmod{n}$. First of all, note that for any $s_i \in \Sigma$,

$$\alpha^2(s_i) = \alpha(s_{ki}) = s_{k^2 i} = s_{-i} = \sigma(s_i)$$

and this implies $\alpha^2 = \sigma$, so in this case we do not need σ in our description. Moreover it follows that $\alpha^4 = 1$, and $\alpha^{-1}(s_i) = \alpha^3(s_i) = s_{-ki}$ for all i. Then

$$\rho^\alpha(s_i) = \alpha^{-1}\rho\alpha(s_i) = \alpha^{-1}\rho(s_{ki}) = \alpha^{-1}(s_{ki+1}) = s_{-k^2i-k} = s_{i-k} = \rho^{-k}(s_i).$$

Therefore, if $k^2 \equiv -1 \pmod{n}$, then

$$B(n,k) = \langle \rho, \alpha | \quad \rho^n = \alpha^4 = 1, \quad \rho^\alpha = \rho^{-k} \rangle.$$

□

3.2.2 The automorphism group $A(n,k)$

Now that we have the description of the subgroup $B(n,k)$ of the automorphism group $A(n,k)$ let us analyze the complete group and the relation between $B(n,k)$ and $A(n,k)$.

First of all, let us start with the following lemma as a consequence of the previous section.

Lemma 3.2.9. *The following three statements are equivalent:*
(1) $G(n,k)$ is edge-transitive;
(2) There exists $\gamma \in A(n,k)$ which maps some spoke onto an edge which is not a spoke;
(3) $B(n,k)$ is a proper subgroup of $A(n,k)$.

Proof. (1)⇒(2). By definition of transitivity the group $G(n,k)$ is edge-transitive if given any two edges there is an element $\gamma \in A(n,k)$ such that it maps one edge onto the other. Since this is true for any pair of edges (2) is proved.
(2)⇒(3). Since $B(n,k)$ is the group of automorphisms that fix Σ set-wise, the $\gamma \in A(n,k)$ which maps some spoke onto an edge which is not spoke can not be in $B(n,k)$. Hence, $B(n,k)$ is a proper subgroup of $A(n,k)$.
(3)⇒(1). As we stated in Proposition 1.3.2, if $G(n,k)$ is edge-transitive there is only one orbit in which all the edges are. Suppose $G(n,k)$ is not edge-transitive, then $A(n,k)$ must have at least two orbits of edges. Note that $B(n,k)$ has 2 or 3 edge-orbits, since all the edges of Ω, I and Σ are in the same orbit respectively. This is true since we have the rotation $\rho \in B(n,k)$ whose powers allow us to move from any vertex to another if they are in the same set. Then we have 2 orbits when there is $\gamma \in B(n,k)$ that interchanges Ω and I and 3 if not. Moreover, the edge-orbits of $B(n,k)$ are subsets of the edge-orbits of $A(n,k)$ since $B(n,k) \subseteq A(n,k)$. Then $A(n,k)$ must fix Ω, I or Σ. Thus, by Lemma 3.2.1 it must fix Σ and hence $B(n,k) = A(n,k)$, contrary to (3). □

In order to determine when $B(n,k)$ and $A(n,k)$ are equal and when they are not we must introduce some new notation about circuits. Let Z be an arbitrary circuit in $G(n,k)$. Let us denote with $r(Z)$, $s(Z)$ and $t(Z)$ the number of outer edges, spokes and inner edges in Z, respectively. Moreover, for the set Z_j of j-circuits of $G(n,k)$ let

$$R_j = \sum_{Z \in Z_j} r(Z),$$

$$S_j = \sum_{Z \in Z_j} s(Z),$$

$$T_j = \sum_{Z \in Z_j} t(Z).$$

Thus, R_j, S_j and T_j are the sum of all outer edges, spokes and inner edges in all j-circuits, respectively.

Lemma 3.2.10. *If $B(n,k) \neq A(n,k)$, each edge of $G(n,k)$ is contained in the same number of j-circuits.*

Proof. Since if $B(n,k) \neq A(n,k)$, then $B(n,k)$ is a proper subgroup of $A(n,k)$ by the previous lemma $G(n,k)$ is edge-transitive and so for every pair of edges we can find an automorphism that maps one onto another. Thus, if an edge e_i in $G(n,k)$ is contained in c different j-circuits and we apply the automorphism $\gamma(e_i) = e_i'$ as all the relation between vertices remain the same, and the automorphism maps the circuits onto circuits there must be the same number c of j-circuits in which e_i' is contained. As $G(n,k)$ is edge-transitive, we can map e_i onto any other edge, concluding that every edge of $G(n,k)$ is contained in the same number of j-circuits. □

Lemma 3.2.11. *If $B(n,k) \neq A(n,k)$, then $R_j = S_j = T_j$.*

Proof. Note that $R_j = \sum_{Z \in Z_j} r(Z) = \sum_{e \in \Omega} c_j(e)$, where $c_j(e)$ is the number of j-circuits in which e is contained, and similarly for S_j and T_j. By the previous lemma if $B(n,k) \neq A(n,k)$, each edge of $G(n,k)$ is contained in the same number of j-circuits, let us say c, it follows that $R_j = S_j = T_j = nc$. □

Now, let us prove some particular cases using this characterization.

Lemma 3.2.12. *If $n \neq 4$, $B(n,1) = A(n,1)$.*

Proof. Note that if $n \neq 4$, obviously we do not have a 4-circuit only containing outer edges. Moreover, by Lemma 3.1.1 the subgraph containing the inner edges has d circuits of length n/d. In this case $k = 1$, so $d = 1$, thus, we have only 1 n-circuit. Hence, there is no 4-circuit only with inner edges. Therefore the only option is having 2 spokes, 1 inner edge and 1 outer edge in our circuit with the form $\{u_i, u_{i+1}, v_{i+1}, v_i\}$ and obviously we have n of those circuits. It follows that $R_4 = T_4 = n$ while $S_4 = 2n$. By the previous lemma $B(n,1) = A(n,1)$. □

Lemma 3.2.13. *If $n \neq 5$ or 10, then $B(n,2) = A(n,2)$.*

Proof. As we did in the previous lemma note first that we do not have any 5-circuits containing just outer or inner edges since $n \neq 5$ or 10 and $k = 2$ so $d = 1$ or 2 and we can not have $n/d = 5$. Thus, we need again 2 spokes in order to have a 5-circuit. Now we could have two outer edges and one inner edge or two inner and one outer edge, however, the circuit having two inner edges would be $\{u_i, v_i, v_{i+2}, v_{i+4}, u_{i+4}\}$ which is only a circuit if $i+4 \equiv i+1$ or $i+4 \equiv i-1$ modulo n, this is not possible since it means that $4 \equiv \pm 1 \pmod n$ which is only true when $n = 3$ or 5, but $k = 2 > 3/2$ and $n \neq 5$ by hypothesis. Then we only have 5-circuits containing two outer edges, two spokes and on inner edge of the form $\{u_i, u_{i+1}, u_{i+2}, v_{i+2}, v_i\}$, and we have n of these. It follows that $R_5 = S_5 = 2n$ while $T_5 = n$. By Lemma 3.2.11 $B(n,2) = A(n,2)$. □

In order to continue, we need a complete list of the 8-circuits in $G(n,k)$, where $k > 2$. Let us characterize them by saying that two 8-circuits in $G(n,k)$ are of the same type if one is mapped onto the other by some element in the subgroup $C(n,k) = \langle \rho, \sigma \rangle$ of $A(n,k)$. Moreover, we will call a representative Z to any circuit of one of the types after fixing a starting vertex.

Lemma 3.2.14. *If Z and Z' are of the same type, then $r(Z) = r(Z')$, $s(Z) = s(Z')$ and $t(Z) = t(Z')$.*

Proof. If Z and Z' are of the same type, then by definition there exists some element in the subgroup $\langle \rho, \sigma \rangle$ of $A(n,k)$ which maps one onto the other. Since every element in $\langle \rho, \sigma \rangle$ fixes Ω, I and Σ set-wise, i.e., outer edges are mapped onto outer edges, spokes onto spokes and inner edges onto inner edges, the number of each form of edge is going to be preserved. □

Let us show now how can we find all the different types of 8-circuits for $k > 2$. First of all, note that for having an 8-circuit we only have three options when we refer to the number of spokes there are. It is easy to see that the circuit can have either 0, 2 or 4 spokes.

Let us first find the 8-circuits with 2 spokes. In this case we need another 6 edges between outer and inner edges in order to complete the circuit, thus we have 5 options: 1 outer (inner) edge and 5 inner (outer) edges, 2 outer (inner) edge and 4 inner (outer) edges and 3 outer and 3 inner edges.

Type 1. Let $s(Z) = 2$, $r(Z) = 5$ and $t(Z) = 1$. The 8-circuit is then of the form $\{u_i, u_{i+1}, u_{i+2}, u_{i+3}, u_{i+4}, u_{i+5}, v_{i+5}, v_{i+5\pm k}\}$, which only exists if $i + 5 \pm k \equiv i$ modulo n or which is the same $5 \pm k \equiv 0 \pmod n$. Note that if $5 - k \equiv 0 \pmod n$, since $1 \leq k < n/2$ the only options are $k = 5$ and $n = 5 - k$, but the last one only happens with $n = 4$ and $k = 1$ and we said that $k > 2$. Then the remaining option when $5 + k \equiv 0 \pmod n$ for k is

$n = 5 + k$, because when $5 + k = ln$ where $l \in \{2, 3, ...\}$, then $k/2 > n$. By Lemma 3.2.10 every edge in the outer rim is going to have the same number of 8-circuits, moreover, those circuits are going to be of the same type side we can go from one to another by an automorphism, so start from the edge $\{u_0, u_1\}$ in order to give a representative $Z = \{u_0, u_1, u_2, u_3, u_4, u_5, v_5, v_0\}$.

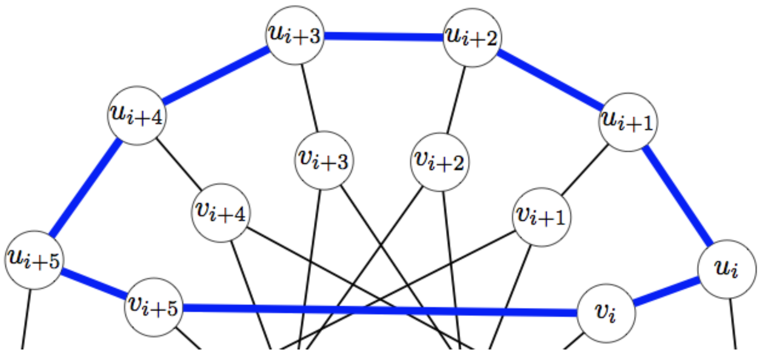


Figure 3.6: An 8-circuit of type 1

Type 2. Let $s(Z) = 2$, $r(Z) = 1$ and $t(Z) = 5$. Let us take u_i as a vertex in the outer rim contained in the 8-circuit. Then as we have only one outer edge, the spoke $\{u_i, v_i\}$ must be in the circuit too. Note that for the 5 inner edges we need them to link the vertices $\{v_i, v_{i+k}, v_{i+2k}, v_{i+3k}, v_{i+4k}, v_{i+5k}\}$ and then we have the spoke $\{v_{i+5k}, u_{i+5k}\}$ linking the inner and outer edges. Since we said that u_i is in the circuit and we only have one outer edge u_{i+5k} must be a neighbor of u_i. Thus $u_{i+5k} = u_{i-1}$ or $u_{i+5k} = u_{i+1}$, which only happens if $5k + 1 \equiv 0 \pmod{n}$ or $5k - 1 \equiv 0 \pmod{n}$, respectively. Therefore, we have two different circuits of type 2. If $5k + 1 = n$ or $2n$ then we have $\{u_1, v_1, v_{1+k}, v_{1+2k}, v_{1+3k}, v_{1+4k}, v_0, u_0\}$ as a representative Z of type 2. If $5k - 1 = n$ or $2n$ then we have $\{u_0, v_0, v_k, v_{2k}, v_{3k}, v_{4k}, v_1, u_1\}$ as a representative Z of type 2'. Note that as in the previous case we only choose equality with n or $2n$ because otherwise $k/2 \geq n$.

Type 3. Let $s(Z) = 2$, $r(Z) = 4$ and $t(Z) = 2$. As in the previous case take the vertex u_i and the spoke $\{u_i, v_i\}$. We only have two inner edges that must link the vertices $\{v_i, v_{i+k}, v_{i+2k}\}$, it follows that the other spoke is $\{v_{i+2k}, u_{i+2k}\}$. As we need to close the circuit and we must have 4 outer edges, the only options are therefore $u_{i+2k} = u_{i-4}$ or $u_{i+2k} = u_{i+4}$. Note that in the second case we need $2k \equiv 4 \pmod{n}$ but if $2k - 4 = 0$ we have $k = 2$ which is not possible and if $2k - 4 = ln$ where $l > 0$ the condition $k < n/2$ does not hold. Then we only have the first option which starting from the vertex u_0 corresponds to $\{u_0, u_1, u_2, u_3, u_4, v_4, v_{4+k}, v_0\}$ as a representative Z of type 3.

We can keep analyzing all remaining options with 2 spokes and continue with the cases in which there are 4 or 0 spokes in the same way. We summarize those results in the following table from [8]:

Type	A representative Z	Conditions	Number	$r(Z)$	$s(Z)$	$t(Z)$
1	$[u_0, \ldots, u_5, v_5, v_0]$	$k = 5$ or $n-k=5$	n	5	2	1
2	$[u_0, u_1, v_1, v_{k+1}, v_{2k+1}, v_{3k+1}, v_{4k+1}, v_0]$	n or $2n = 5k+1$	n	1	2	5
2′	$[u_1, u_0, v_0, v_k, v_{2k}, v_{3k}, v_{4k}, v_1]$	n or $2n = 5k-1$	n	1	2	5
3	$[u_0, u_1, \ldots, u_4, v_4, v_{\frac{1}{2}(n+4)}, v_0]$	$n = 2k+4$	n	4	2	2
4	$[u_0, u_1, u_2, v_2, v_{2+k}, v_{2+2k}, v_{2+3k}, v_0]$	n or $2n = 4k+2$	n	2	2	4
4′	$[u_2, u_1, u_0, v_0, v_k, v_{2k}, v_{3k}, v_2]$	$n = 4k-2$	n	2	2	4
5	$[u_0, u_1, u_2, u_3, v_3, v_{\frac{1}{3}(n+6)}, v_{\frac{1}{3}(2n+3)}, v_0]$	$n = 3k+3$	n	3	2	3
5′	$[u_3, u_2, u_1, u_0, v_0, v_{\frac{1}{3}(n+3)}, v_{\frac{1}{3}(2n+6)}, v_3]$	$n = 3k-3$	n	3	2	3
6	$[u_0, u_1, v_1, v_{\frac{1}{2}n}, u_{\frac{1}{2}n}, u_{\frac{1}{2}(n+2)}, v_{\frac{1}{2}(n+2)}, v_0]$	$n = 2k+2$	$\frac{1}{2}n$	2	4	2
7	$[v_0, v_k, v_{2k}, \ldots, v_{7k}]$	$n = 8k$	k	0	0	8
7′	$[v_0, v_k, v_{2k}, \ldots, v_{7k}]$	$3n = 8k$	$\frac{1}{8}n$	0	0	8
8	$[u_0, \ldots, u_7]$	$n = 8$	1	8	0	0
9	$[u_0, u_1, v_1, v_{k+1}, u_{k+1}, u_k, v_k, v_0]$	$n \geqslant 4$	n	2	4	2

Figure 3.7: Table 1

Now that we have all the possible 8-circuits and the conditions for them to exist let us proof a more general result.

Lemma 3.2.15. *If* (n, k) *is not the pair* $(8, 3), (10, 3), (12, 5), (13, 5), (24, 5)$ *or* $(26, 5)$*, and if* $k > 2$*, then* $B(n, k) = A(n, k)$*.*

Proof. Since $k > 2$ and we excluded $(8, 3)$ we assume $n \neq 8$. Note that doing this we assure not having an 8-circuit of type 8.

Obviously $G(n, k)$ can not simultaneously contain 8-circuits of types 2 and $2'$, or 4 and $4'$, or 5 and $5'$, or 7 and $7'$. Note that all these pairs have the same number of spokes, inner and outer edges. Then let us define the variable x_i as follows:

$$x_i = 1 \quad \text{if there are circuits of type } i \text{ or } i' \text{ in } G(n, k)$$

$$x_i = 0 \quad \text{otherwise.}$$

Now we can compute R_8, S_8 and T_8 in the following way:

$$R_8 = \sum_{Z \in Z_8} r(Z) = 5nx_1 + nx_2 + 4nx_3 + 2nx_4 + 3nx_5 + nx_6 + 2n,$$

$$S_8 = \sum_{Z \in Z_8} s(Z) = 2nx_1 + 2nx_2 + 2nx_3 + 2nx_4 + 2nx_5 + 2nx_6 + 4n,$$

$$T_8 = \sum_{Z \in Z_8} t(Z) = nx_1 + 5nx_2 + 2nx_3 + 4nx_4 + 3nx_5 + nx_6 + nx_7 + 2n.$$

Observe that we always have $x_9 = 1$ and now let us prove the lemma by contradiction. Suppose $B(n,k) \neq A(n,k)$. Then by Lemma 3.2.11, we have $R_8 = S_8 = T_8$, which implies $R_8 - T_8 = 0$. Hence,

$$(5n-n)x_1 + (n-5n)x_2 + (4n-2n)x_3 + (2n-4n)x_4 + (0-n)x_7 = 0 \Rightarrow$$

$$4x_1 + 2x_3 = 4x_2 + 2x_4 + x_7.$$

Taking into account that $x_i = 0$ or 1 the only possible solutions due to parities would be $x_7 = 0$, $x_1 = x_2$ and $x_3 = x_4$. Now $x_1 = x_2 = 1$ implies that we have circuits of types 1 and 2. Looking at the conditions we need $k = 5$, note that we can not have $n-k = 5$ since then none of the conditions for a circuit of type 2 would hold. Moreover, for $k = 5$, circuits of type 2 exist only for $n = 12, 13, 24$ or 26. All the mentioned pairs are excluded cases.

If $x_3 = x_4 = 1$ the only option for a pair (n,k) satisfying $n = 2k+4$ and one of the conditions for having a circuit of type 4 or $4'$ is $k = 3$ and $n = 10$, which is another excluded case. We may therefore assume that $x_1 = x_2 = x_3 = x_4 = 0$. We know that $R_8 - S_8 = 0$ as well so we have the extra equation

$$3x_1 - x_2 + 2x_3 + x_5 - x_6 - 2 = 0$$

and together with the assumption of $x_1 = x_2 = x_3 = x_4 = 0$ we have the equation $x_5 - x_6 = 2$ which has no solution since x_5 and x_6 can only be 0 or 1. This contradiction proves the lemma. □

There are only two graphs having the automorphism group equal to $B(n,k)$ that we have not already shown to have that property. These are $G(13,5)$ and $G(26,5)$ as we prove in the following lemmas.

Lemma 3.2.16. $B(13,5) = A(13,5)$.

Proof. Let us see how many 7-circuits of different type does $G(n,k)$ have. First of all, it does not have any 7-circuit with only outer or inner edges since $d = 1$ and then, the inner edges are edges of a circuit of length 13. Moreover, note that we can not have a 7-circuit with more than 2 spokes, since even if we can have a path with 4 spokes that will never be a closed circuit and thus, we must have exactly two spokes. It follows that we have to analyze four cases, 4 outer edges and 1 inner edges, 1 outer edge and 4 inner edges, 2 outer and 3 inner edges and 3 outer and 2 inner edges.
The first case, where $r(Z) = 4$ and $t(Z) = 1$, is not possible since starting from the vertex u_i and the spoke $\{u_i, v_i\}$, the only inner edge, say $\{v_i, v_{i+5}\}$ must have its endpoint in either v_{i+4} or v_{i-4} in order to complete a circuit with the four outer edges. This is not possible since $i+5 \not\equiv i+4$ and $i-4$ (mod 13).

In the second case, $r(Z) = 1$ and $t(Z) = 4$, if we start from the vertex u_i and the spoke $\{u_i, v_i\}$ the inner edges must link $\{v_i, v_{i+5}, v_{i+10}, v_{i+15}, v_{i+20}\}$ and $i + 20$ must be $i + 1$ or $i - 1$ modulo 13 which is not possible.

In the third case, $r(Z) = 2$ and $t(Z) = 3$, starting again from u_i and the spoke $\{u_i, v_i\}$ the only option for inner edges is to link the vertex $\{v_i, v_{i+5}, v_{i+10}, v_{i+15}\}$ and since we have two outer edges we need one of the conditions $i + 15 \equiv i + 2 \pmod{13}$ or $i + 15 \equiv i - 2 \pmod{13}$ to hold. Actually, $i + 15 \equiv i + 2 \pmod{13}$ since $15 - 2 = 13$, and thus we have n circuits of the form $\{u_i, v_i, v_{i+5}, v_{i+10}, v_{i+2}, u_{i+2}, u_{i+1}\}$.

For the fourth case, $r(Z) = 3$ and $t(Z) = 2$, we must have a circuit of the form $\{u_i, u_{i+1}, u_{i+2}, u_{i+3}, v_{i+3}, v_{i+8}, v_{i+13}\}$ which is obviously possible since $i + 13 \equiv i \pmod{13}$, and we have again n of these 7-circuits.

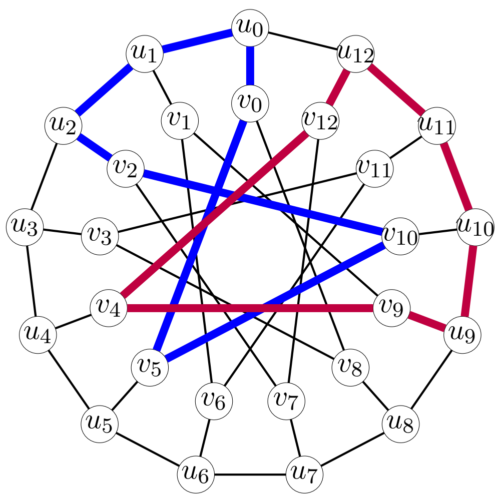


Figure 3.8: $G(13, 5)$ and a representation of each the two different types of 7-circuits.

Thus, as we have the circuits $Z^1 = \{u_i, v_i, v_{i+5}, v_{i+10}, v_{i+2}, u_{i+2}, u_{i+1}\}$ and $Z^2 = \{u_i, u_{i+1}, u_{i+2}, u_{i+3}, v_{i+3}, v_{i+8}, v_{i+13}\}$, counting the outer and inner edges we get

$$R_7 = \sum_{Z \in Z_7} r(Z) = nr(Z^1) + nr(Z^2) = 13(2 + 3) = 65 \quad \text{and}$$

$$S_7 = \sum_{Z \in Z_7} s(Z) = ns(Z^1) + ns(Z^2) = 13(2 + 2) = 52.$$

Hence, it follows from Lemma 3.2.11 that $B(13, 5) = A(13, 5)$. □

Lemma 3.2.17. *$B(26, 5) = A(26, 5)$.*

Proof. We are going to show that any $\gamma \in A(26,5)$ belongs to $B(26,5)$. By Theorem 3.2.8 as we have $k^2 \equiv -1 \pmod{n}$, then $B(26,5) = \langle \rho, \alpha | \quad \rho^{26} = \alpha^4 = 1, \quad \rho^\alpha = \rho^{-5} \rangle$ and by Lemma 3.2.5 $B(26,5)$ is vertex-transitive since $5^2 \equiv 1 \pmod{16}$. Therefore, we can always find an automorphism $\beta \in B(26,5)$ such that $\beta\gamma(u_0) = u_0$. Now let us analyze the vertices that are at distance 4 from u_0. Since each vertex has three neighbors and we do not allow the path to go through the same edge more than once we have $3 \times 2 \times 2 \times 2 = 24$ paths of length 4. However, some of these paths end up in the same vertex. Analyzing these paths and vertices in the graph we get 14 different vertices and they fall into three classes depending on the number of paths existing between u_0 and the vertex under consideration:

(1) $u_{10}, u_{16}, v_7, v_9, v_{17}$ and v_{19} are the vertices that can only be reached through one path.

(2) $u_6, u_{20}, v_3, v_{11}, v_{15}$ and v_{23} are the vertices that can be reached through two different paths.

(3) u_4 and u_{22} are the vertices that can be reached through three different paths.

Since we chose β such that $\beta\gamma$ fixes u_0 and all the vertices must be at the same distance after applying an automorphism, the three groups of vertices are fixed set-wise by $\beta\gamma$. Thus, for the third class we only have two possibilities when we refer to the image of u_4 and u_{22}, either $\beta\gamma(u_4) = u_4$ and $\beta\gamma(u_{22}) = u_{22}$ or $\beta\gamma(u_4) = u_{22}$ and $\beta\gamma(u_{22}) = u_4$. We know that the reflection σ defined before also fixes u_0 and interchanges u_4 and u_{22}, therefore, if $\beta\gamma$ does not fix them, the product $\sigma\beta\gamma$ will fix them.

Thus, we can always find an automorphism of the form $\phi = \sigma^t\beta\gamma$ such that

$$\phi(u_0) = u_0, \quad \phi(u_4) = u_4, \quad \phi(u_{22}) = u_{22}$$

where $t = 0$ or 1 depending on whether $\beta\gamma$ fixes u_4 and u_{22} or not. Note that $\gamma = (\sigma^t\beta)^{-1}\phi$ and $\sigma, \beta \in B(n,k)$. Then, we need to prove that ϕ must be the identity function.

We will see that an automorphism satisfying just $\phi(u_0) = u_0$ and $\phi(u_4) = u_4$ is the identity. In order to do that, consider the two vertices at distance 4 from u_4 that can be reached by three different paths, u_0 and u_8. Since ϕ fixes u_0 it must fix u_8 as well.

Repeating the same argument for u_4 and u_{12}, which are the two vertices that can be reached from u_8 through 3 paths of length 4, we see that $\phi(u_{12}) = u_{12}$ and so on we conclude that in general $\phi(u_i) = u_i$ for i even. But if every vertex with even index is fixed, as the only vertex adjacent to both u_i and u_{i+2} is u_{i+1} it follows that this must be fixed, and by the same argument all the remaining vertices with odd index as well. Hence, $\phi(u_i) = u_i$ for all i, which obviously implies $\phi(v_i) = v_i$ for all i. Thus, ϕ is the identity function and $\gamma = (\sigma^t\beta)^{-1}\phi \in B(26,5)$.

□

Theorem 3.2.18. *$B(n,k) = A(n,k)$ if and only if the ordered pair (n,k) is not one of*

$$(4,1), \quad (5,2), \quad (8,3), \quad (10,2), \quad (10,3), \quad (12,5), \quad (24,5).$$

Proof. The sufficiency of the condition follows from lemmas we already proved. The necessity follows from the study of the 7 exceptional cases, which we are not going to analyze and we refer to the paper by Keith Loyd E. and Gareth A. Jones [8]. However, we are going to develop in the Appendix the exceptional case $G(10,3)$. □

Chapter 4

An application of graphs and groups to reaction graphs

In this chapter we are going to show one example of the applications that group and graph theory can have in real life. This precise case is related to chemistry and more exactly to the rearrangements of chemical compounds, i.e., chemical reactions. At first, all this chemical reactions were only investigated by chemists, without the use of extensive mathematical tools. G.A. Jones and E.K. Lloyd, [7] were the pioneers giving a survey of different investigations of reaction graphs, written in terms of permutation group theory. The paper by M. H. Klin., S. S. Tratch, and N. S. Zefirov [9] goes on with that path of survey applying group theory to the investigation of chemical reactions. However, Jones again together with Keith [8] give a more mathematical view of the problem and that is the reason for the paper [8] being the most useful one in this chapter.

In order to understand how these two fields are related we need an introduction about reaction graphs and some concepts in chemistry.

4.1 Molecular graphs and rearrangements

First of all, let us define two different chemical graphs: molecular and reaction graphs. In chemistry, a compound is a substance formed when two or more chemical elements are chemically bonded together. Moreover isomeric compounds are compound which have the same chemical formula. However, we do not have to confuse with the concept of isomorphic compounds, which means that they have the same structural formula.

Mathematically, a compound can be represented as a molecular graph.

Definition 17. A molecular graph $\Gamma = (V, E)$ represents a compound. Each vertex of the set V corresponds to an atom and they are joined by a multiset E of edges vw $(v, w \in V)$.

In some cases it suffices to label the vertices with the names of the corresponding types of atoms (C,H,O) and add the edges corresponding to the bonds between them in the chemical compound. However, in some other cases, more detailed labeling is necessary and we take into account that molecules have a three-dimensional structure. For a thorough understanding of the theory we distinguish between the sites in which a vertex is and the vertex itself, labeling the sites with the letters $a, b, c, d, ...$ and the vertices with 1,2,3,...(or some other specific names when more convenient).

Let us introduce now the chemical concept of a rearrangement.

Definition 18. A *rearrangement* is a special type of chemical reaction during which a chemical compound transforms into an isomeric compound.

Although the compounds are isomeric, they do not need to be isomorphic. There are, however, cases in which the compounds are isomorphic, i.e., they have the same chemical structure. In these cases the chemical reaction is called a *degenerate rearrangement.* In the simplest case of this form there are just two different labeled forms of the compound, which are isomorphic, and they interconvert by degenerate rearrangements. Besides, there are other cases in which there are three or more differently labeled isomorphic compounds in which conversion between some of them (not necessarily all) is possible by degenerate rearrangements. Then, we have a *highly degenerate rearrangement.*

Example 18. The Beckmann rearrangement in Figure 4.1 is a non-degenerate rearrangement since even if both isomeric compounds have the same chemical formula they do not have the same structural formula, i.e., they are not isomorphic.

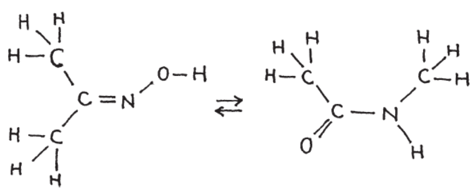


Figure 4.1: The Beckmann rearrangement.

Example 19. Cope rearrangement of cyclohexa-1,5-diene. In this case we have a degenerate rearrangement of the chemical compound since as we see in Figure 4.2 both isomeric compounds have the same structural formula.

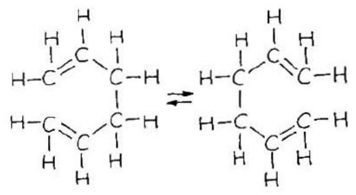


Figure 4.2: Cope rearrangement of cyclohexa-1,5-diene.

Let us show how a degenerate rearrangement ρ acts mathematically in a molecular graph. The degenerate rearrangement ρ maintains the vertices of the molecular graph $\Gamma = (V, E)$ changing the edge set. However, this change leads to a new graph $\Gamma' = (V, E')$ which must be isomorphic to Γ. Thus, one or more edges are removed from Γ and an equal number of edges are added to Γ. As the two graphs are isomorphic we can recover Γ by applying an isomorphism $\pi : \Gamma' \to \Gamma$. Since we have the same structure in both graphs it is enough to use a permutation π of V which takes E' to E.

Example 20. Consider the following carbonium ion.

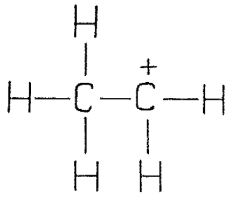


Figure 4.3: Carbonium ion.

Let us denote with a, b, c, d, e, f and g the possible sites in which there is an atom. Now as we can see in Figure 4.4 the rearrangement ρ redefines the edge set replacing the edge $\{a, d\}$ by the new edge $\{a, e\}$. Then we get the new graph $\Gamma' \cong \Gamma$. Now the isomorphism $\pi : \Gamma' \to \Gamma$ defined by the permutation $\pi = (ed)(bf)(cg)$ gives us again the same graph we had before.

Now we define a labeling as $\lambda : \{a, b, c, ..\} \to \{1, 2, 3, ..\}$, where $a, b, c, ...$ are the fixed names of the sites in which there is a vertex and $1, 2, 3, ...$ the number assigned to each vertex that will move due to permutations in the graph. As we require this function to be a bijection we generally have $n!$ labelings, where $n = |V|$. Let us see how a degenerate rearrangement acts on labeled graphs.

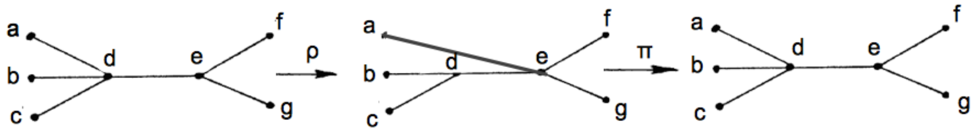


Figure 4.4: The graph Γ, the graph Γ' after the rearrangement and the graph Γ again after applying π.

Example 21. Returning again to Example 20, we now label our graph Γ as follows.

$$\lambda = \begin{pmatrix} abcdefg \\ 3456712 \end{pmatrix}$$

and we see what happens now that our vertices are labeled and they move from one site to another. Let us use the same rearrangement ρ and the same isomorphism $\pi = (ed)(bf)(cg)$ moving each vertex to the corresponding site, for instance vertex 7 which is in site e moves to site d. Then as we see in Figure 4.5 the initial graph specified by λ changes under ρ and π and we get the new labeling

$$\lambda' = \begin{pmatrix} abcdefg \\ 3127645 \end{pmatrix}$$

.

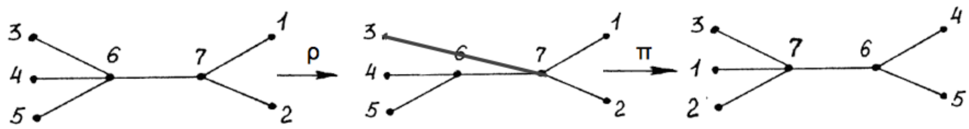


Figure 4.5: The labeling λ of the graph Γ, the graph Γ' and the new labeling λ' of the graph Γ.

Furthermore, note that the vertices have therefore undergone the permutation $r = (14)(25)(67)$.

4.2 Reaction graphs

In order to continue and give the definition of a reaction graph we first need to clarify when two labelings are equivalent. We regard two labelings of a graph Γ as equivalent when they differ by an automophism of Γ of a certain type. Thus, this will depend on the graph Γ and for different cases we will have different equivalent labelings. We therefore choose some fixed subgroup H of the group $\operatorname{Aut}\Gamma$ which will determine when two labelings can be considered as equal.

Definition 19. Two labelings of Γ are *equivalent*, with respect to H, if some element of H converts one labeling into the other.

Remark 2. Note that the choice of H usually depends on chemical, rather than mathematical criteria; we will often take $H = \mathrm{Aut}\,\Gamma$, but it is sometimes more appropriate to choose a proper subgroup such as the isometry group or the rotation group of Γ.

We said before we have $n!$ labelings of a molecular graph. Now that we determined which of them are equivalent we conclude that we have $\frac{n!}{|H|}$ different labelings of Γ. Let us define the set Ω as the set of equivalence classes

$$\Omega = \{\alpha_i = [\lambda_i] : i = 1, ..., \frac{n!}{|H|}\}.$$

Definition 20. A *reaction graph* R is a directed graph with the vertex-set Ω and with an arc (directed edge) from a vertex α_i to a vertex α_j if and only if some labeling in the class α_j can be obtained from a labeling in the class α_i by a single application of a rearrangement.

Remark 3. In the cases in which each arc from α_i to α_j is paired with an arc from α_j to α_i, we replace each such pair with a single undirected edge between α_i and α_j. In this way we get an indirect graph which simplifies R without changing such properties as automorphisms and connectivity.

However, usually the reaction graph is not connected, so it can be represented as the union of its connected components $\overline{R}$. As we can see in both papers [8] and [9] the two most intriguing questions related to this are :

(1) How large is the number of vertices in any connected component $\overline{R}$ of a reaction graph R?

(2) What is the full automorphism group $\mathrm{Aut}\,\overline{R}$ of the connected component $\overline{R}$?

It is not easy to answer and prove the general solutions to these questions, that is why we are going to analyze these questions in a specific example in order to see how graph and group theory are related to this issue.

4.2.1 1,2-shift in the carbonium ion

As in Examples 20 and 21, let Γ be the carbonium ion. In this case we want to analyze the reaction graph of the 1,2-shifts in the carbonium atom. This rearrangement was first considered by A. T. Balaban [2].

In chemistry a 1,2-shift is an organic reaction in which one atom migrates to the adjacent atom in a chemical compound, as in Figure 4.6.

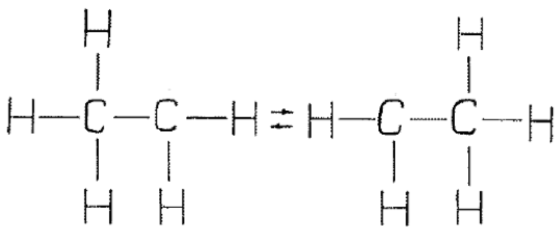


Figure 4.6: 1,2-shift in carbonium ion.

Let Γ be again the representation of the the carbonic ion. The carbon atoms are the interior atoms while the hydrogen atoms are in the boundary. We are going to determine how the 1,2-shift rearrangement acts on the graph.

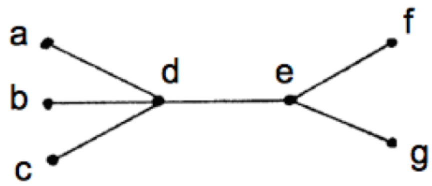


Figure 4.7: The representation graph Γ of the carbonium ion.

First of all, let us take H as the automorphism group of the graph $\mathrm{Aut}\,\Gamma$, which is isomorphic to $S_3 \times S_2$ as calculated in Exercise 2 in the Appendix. Note that under the action of H the vertices of Γ are divided into four orbits, $\{a, b, c\}, \{d\}, \{e\}$ and $\{f, g\}$, which are indicated in Figure 4.8 by the symbols 1, 2, 3 and 4 referring to the orbit in which each vertex is.

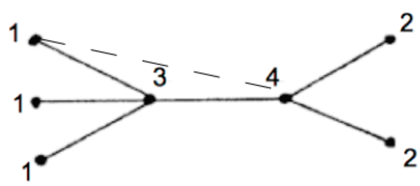


Figure 4.8: Γ and the orbits that H induces indicated with numbers. The broken edge indicates the resulting edge after the rearrangement.

In a 1,2-shift one vertex of type 1 exchanges roles with a vertex of type

2. One way to envisage this mechanism is that an edge joining a type 1 vertex to a type 3 vertex pivots about its end of type 1 so as to join it to the type 4 vertex, see Figure 4.8.

If we take the labeling

$$\lambda_1 = \begin{pmatrix} abcdefg \\ 3456712 \end{pmatrix}$$

which correspond to a vertex α_1 of the reaction graph, and we apply all possible rearrangements ρ corresponding to a 1,2-shift, it is easy to see that we get these three different labelings of the carbonium ion, each of them representing a vertex α_i in the reaction graph.

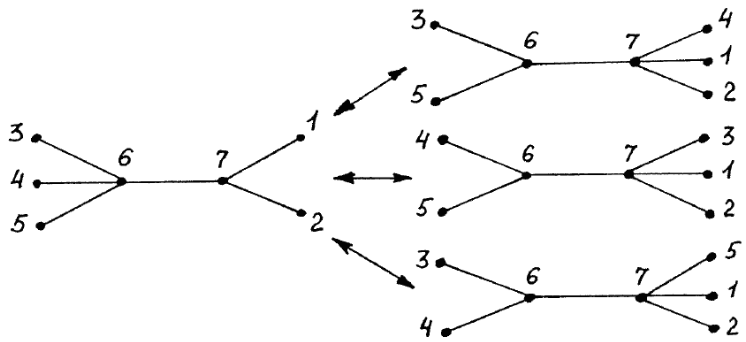


Figure 4.9: λ_1 and the three resulting different labelings λ_2, λ_3 and λ_4 of Γ.

Taking $H = \operatorname{Aut}\Gamma$ means that two labelings are regarded as the same if they differ by an automorphism of Γ. Thus, as $|H| = 12$ we consider $\frac{7!}{12}$ different labelings of Γ. Then, the reaction graph R is the graph with the vertex set $\Omega = \{\alpha_i = [\lambda_i] : i = 1, ..., 420\}$ each of the elements corresponding to a different labeling of Γ. Note that in each $\alpha_i = [\lambda_i]$ there are all the labelings which correspond to the graph with exactly the same adjacency relations, thus, the same graph. For simplicity of notation, when we refer to the labeling of a vertex, we mean one of the equivalent labelings in α_i.

It is obvious that R is not connected, for instance, we can not start from the vertex α_1 and reach the vertex α_k with a labeling

$$\lambda_k = \begin{pmatrix} abcdefg \\ 6453712 \end{pmatrix}$$

since we can only apply 1,2-shifts and these never interchange the boundary atoms and the interior atoms.

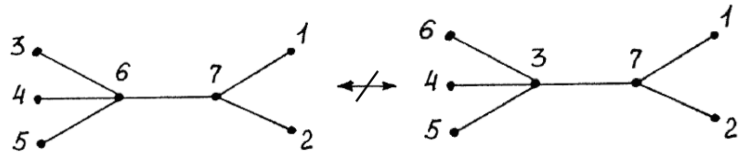


Figure 4.10: The labelings λ_1 and λ_k, we can not get one from another by a 1,2-shift.

Thus, we are interested in the connected components of R. Let us analyze the connected component $\overline{R}$ which includes the vertex α_1. As we said in the previous paragraph, for this specific numbering we see that the carbon atoms have a restricted set of numbers, they can only be 6 or 7, because a 1,2-shift does not interchange the interior atoms (carbon) with any boundary atoms (hydrogen). Thus the vertices of $\overline{R}$ will be different labelings in which all hydrogen atoms have numbers from the set $\{1, 2, 3, 4, 5\}$, so using combinatorics we know that there are $2\frac{5!}{12} = 20$ vertices in $\overline{R}$.

Moreover, fixing for instance the carbon atom with number six, note that every class of labelings α_i can be determined by the subset of numbers of hydrogen atoms which are adjacent to the the carbon atom having that number. If we know this subset, which can be either of 2 or 3 hydrogen atoms, we know the subset which is adjacent to the carbon atom having the number seven, that is why the labeling is totally determined. Obviously, as all the labelings in the same α_i are isomorphic, they have the same subset of numbers adjacent to 6. For instance, the class of labelings that correspond to numberings in Figure 4.9 are determined by:

$$\alpha_1 \equiv \{3, 4, 5\},$$

$$\alpha_2 \equiv \{3, 5\},$$
$$\alpha_3 \equiv \{4, 5\},$$
$$\alpha_4 \equiv \{3, 4\}.$$

Then as we said we only need to fix the subset of $\{1, 2, 3, 4, 5\}$ that corresponds to the hydrogen atoms adjacent to the carbon atom with the number 6. These are 2 or 3 element subsets of $\{1, 2, 3, 4, 5\}$ and so we have $\binom{5}{3} + \binom{5}{2} = 20$ such subsets, which implies again that $\overline{R}$ has 20 vertices.

Let us now analyze the adjacency relations between these vertices. Observing Figure 4.9 we see that $\{3, 4, 5\}$ is only adjacent to $\{3, 5\}$, $\{4, 5\}$ and $\{3, 4\}$, which are the only vertices whose set is a proper subgroup of $\{3, 4, 5\}$. Let us see that this holds for every vertex.

First of all, in a 1,2-shift one of the atoms in the 3-element orbit moves to the 2-element orbit, which means that if the carbon atom with number 6 has 3 adjacent atoms by the 1,2-shift it will end up having just two adjacent atoms. Thus,a 3-element subset can only be adjacent to a 2-element one. Moreover, as we said that one atom from the 3-element subset moves, the remaining 2-element subset must be part of it. Summarizing, a 3-element subset A is adjacent to a 2-element subset B if and only if $B \subset A$. This means that an hydrogen atom adjacent to the carbon atom having number 6 becomes adjacent of the carbon atom having number 7. The result is the Desargues graph $KG(10, 3)$.

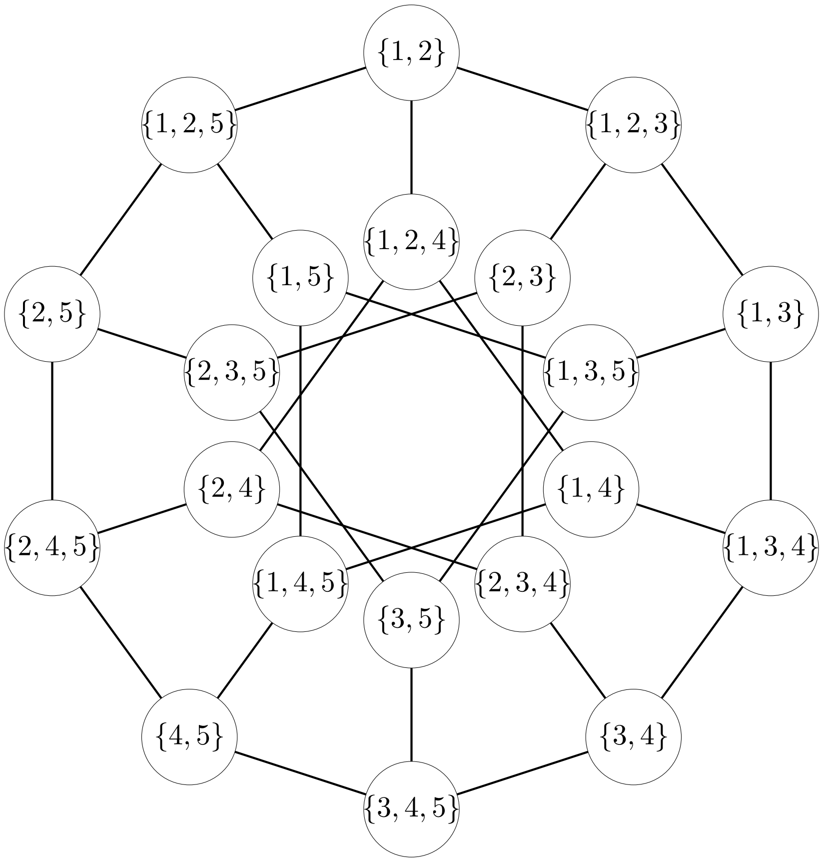


Figure 4.11: The connected component $\overline{R}$ of the reaction of of the 1,2-shift of the carbonioum ion can be represented as the Desargues graph $G(10, 3)$.

Therefore, we found a representation for the connected component $\overline{R}$. Moreover we know that its automorphisms group is isomorphic to $S_5 \times C_2$, since it is a exceptional case of the generalized Petersen graphs analyzed in exercise 5 in the Appendix.

This subsection and exercise 8 developed in the Appendix are just simple examples in order to illustrate how theoretical mathematics can help understanding and investigating different fields as chemistry. We refer to the paper written by G.A. Jones and E.K. Lloyd, Reaction Graphs [8] in order to see deeper and more complex results from group and graph theory applied in reaction graphs.

Appendix A

Solved exercises

A.1 Chapter 1

Exercise 1.

Definition 21. An *automorphism* of a graph Γ is a permutation of the vertices of Γ such that, if we consider the natural action it induces on the unordered pairs of vertices, it maps edges to edges and non-edges to non-edges.

Show using an example that the definition above is not correct for all graphs.

Solution. We are going to see an example that shows why the last part of the definition is necessary if we refer to all kind of graphs. There is no problem with the definition above when restricting our graphs to finite graphs, but let us see what happens when the graph is infinite. Let Γ be the infinite graph in Figure A.1 with the vertex set $V(\Gamma) = \mathbb{Z}$ and the edge set $E(\Gamma) = \{\{i, i+1\} \mid i \in \mathbb{N}\}$. Moreover, let the permutation f be $f(i) = i+1$. Then, f induces the following action on edges:

$$f(\{i, i+1\}) = \{i+1, i+2\}, \quad \text{for all } i \in \mathbb{Z}.$$

Note that all edges are mapped onto edges since for all $i > 0$ we have the images $\{i+1, i+2\}$ where $i+1 \in \mathbb{N}$ therefore they belong to $E(\Gamma)$. However, the non-edge $\{0, 1\}$ has the image $f(\{0, 1\}) = \{1, 2\} \in E(\Gamma)$. Therefore, in infinite graphs the fact that all edges are mapped onto edges does not imply that all non-edges are mapped onto non-edges. This makes sense since after mapping all the edges to edges as our graph is infinite we can always find one more edge so that we can map a non-edge onto that edge. Moreover, we can see in Figure A.1 and A.2 using the visual representation of Γ and $f(\Gamma)$ that they do not represent the same graph and hence f is not an automorphism. □

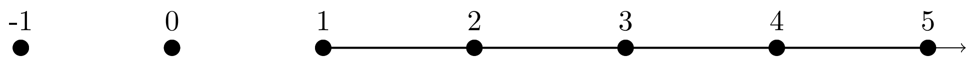


Figure A.1: Infinite graph Γ.

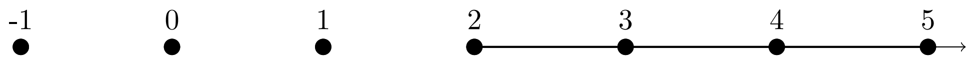


Figure A.2: Infinite graph $f(\Gamma)$.

Exercise 2. Let Γ be the graph in Figure A.3. Prove using the Orbit Stabilizer Theorem that $\operatorname{Aut}\Gamma \cong S_3 \times S_2$.

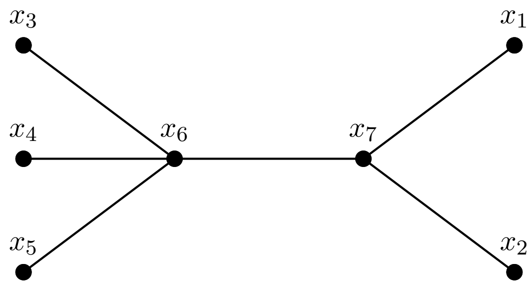


Figure A.3: Γ.

Solution. First of all, note that the vertices x_6 and x_7 must be fixed by any automorphism since they are the only vertices with 3 and 4 neighbours respectively. Then, we can see that x_3, x_4, x_5 are only adjacent to x_6 and so if we permute them we will keep the adjacency relations. Thus we have that the permutations $(x_3x_4), (x_3x_5), (x_4x_5), (x_3x_4x_5), (x_3x_5x_4) \in \operatorname{Aut}\Gamma$. We can describe these permutations as the permutations in $\langle (x_3x_4), (x_3x_4x_5)\rangle = H$ obviously isomorphic to $S_3 = \langle (12), (123)\rangle$. Moreover, if we look now at the vertices adjacent to x_7 we can see that the only permutation, besides the identity, we can apply in order to maintain the adjacency relations is (x_1x_2), and obviously $K = \langle (x_1x_2)\rangle \cong S_2$. Hence, as K and H are subgroups of $\operatorname{Aut}\Gamma$, we know that $\langle H, K\rangle \subseteq \operatorname{Aut}\Gamma$, since it is the smallest subgroup containing H and K. It is obvious that $H \cap K = \{1\}$ simply because $(x_1x_2) \notin H$. Since $(x_3x_4)(x_1x_2)(x_3x_4) = (x_1x_2)$ and $(x_3x_5x_4)(x_1x_2)(x_3x_4x_5) = (x_1x_2)$, we have that $K \trianglelefteq H$ and $H \trianglelefteq K$. This implies that $HK = KH$ and and HK is a subgroup of $\operatorname{Aut}\Gamma$. Moreover, $|\langle H, K\rangle| = |HK| = \frac{|H||K|}{|H\cap K|} = 6 \times 2 = 12$.

Now, if we prove that $G = \operatorname{Aut}\Gamma$ has at most the same cardinality as the subgroup $\langle H, K\rangle$ we will complete the proof. In order to do that we are going to use the Orbit-Stabilizer Theorem, which states $|G| = |G_x||x^G|$. Let us start from the vertex x_3. It is easy to see that $|x_3^G| \leq 3$ since it can only be mapped either to itself or x_4 or x_5. Then,

$$|G| = |G_{x_3}||x_3^G| \leq 3|G_{x_3}|$$

Taking now the vertex x_1 and the x_3-stabilizer, we see in the same way that the orbit $x_1^{G_{x_3}}$ can only contain x_1 and x_2, note that in this case it does not affect fixing x_3 or not, thus

$$|G_{x_3}| = |G_{x_3x_1}||x_1^{G_{x_3}}| \leq 2|G_{x_3x_1}| \Rightarrow |G| \leq 6|G_{x_3x_1}|.$$

Now, the orbit of x_4 under the stabilizer of x_1 and x_3 is contained in $\{x_4, x_5\}$ and thus, applying the Orbit Stabilizer Theorem again,

$$|G_{x_3x_1}| = |G_{x_3x_1x_4}||x_4^{G_{x_3x_1}}| \leq 2|G_{x_3x_1x_4}| \Rightarrow |G| \leq 12|G_{x_3x_1x_4}|$$

Finally, note that $|G_{x_3x_1x_4}| = 1$, since when we fix x_1, also x_2 is fixed and when we fix x_3 and x_4 the same happens with x_5 that must remain in the same place. Hence,

$$|G| \leq 12|G_{x_3x_1x_4}| \leq 12,$$

and that together with $\langle H, K\rangle \subseteq G$ and $|\langle H, K\rangle| = 12$ is enough to conclude that

$$\operatorname{Aut}\Gamma = \langle (x_3x_4), (x_3x_4x_5)\rangle \times \langle (x_1x_2)\rangle \cong S_3 \times S_2.$$

□

A.2 Chapter 2

Exercise 3. Find the automorphism group of the Petersen graph $KG(5, 2)$ without applying the result for all Kneser graphs proved on Chapter 2.

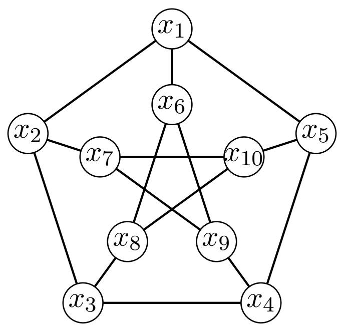


Figure A.4: Petersen graph $KG(5, 2)$

Solution. As we saw in Example 5 in the first chapter the Petersen graph is the Kneser graph $KG(5,2)$. Thus, it is a graph with the vertex set $\binom{\{1,2,3,4,5\}}{2}$, where two vertices are adjacent if and only if their intersection is empty.
Let us show that the permutation group S_5 induces all the automorphisms of $\operatorname{Aut} KG(5,2)$. We said that two vertices are adjacent if their intersection is empty, as the elements of S_5 are permutations of the set $\{1,2,3,4,5\}$, two elements can not have the same image because different elements have different images. Thus, after applying any permutation the vertices would intersect in the same amount of elements as before. Therefore, an empty intersection will remain empty and conversely. Summarizing, being $\{x,y\}$ and $\{z,w\}$ any two vertices of $KG(5,2)$, if $\sigma \in S_5$:

$$\{x,y\} \sim \{z,w\} \iff \{x,y\} \cap \{z,w\} = \emptyset \iff \{\sigma(x),\sigma(y)\} \cap \{\sigma(z),w\} = \emptyset$$

$$\iff \{\sigma(x),\sigma(y)\} \sim \{\sigma(z),\sigma(w)\}.$$

Thus, $S_5 \subseteq \operatorname{Aut} KG(5,2)$ and so $|\operatorname{Aut} KG(5,2)| \geq 120$. What we want to prove now is that actually $|\operatorname{Aut} KG(5,2)| = 5! = 120$ and that S_5 is the full automorphism group of $KG(5,2)$.
For simplicity of notation, let us denote $G = \operatorname{Aut} KG(5,2)$. Consider the vertex $x_1 = \{1,2\}$ of the graph. As we said that $S_5 \subseteq G$ and S_5 is obviously a transitive subgroup, in particular we know that we can find an automorphism that moves x_1 to any other vertex of the graph. Thus $|x_1^G| = 10$.

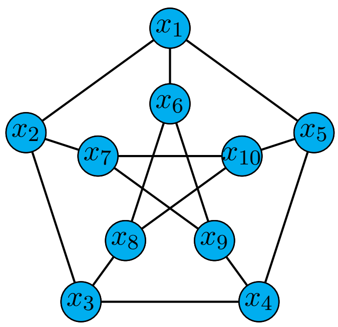


Figure A.5: We see that the size of the orbit of x_1 (in blue) is 10 since G is transitive.

Using the Orbit-Stabilizer Theorem, in which we state that $|G_x||x^G| = |G|$:

$$|G| = |G_{x_1}||x_1^G| = 10|G_{x_1}|.$$

Let us continue now by fixing x_1 in order to find the order of G_{x_1}. Consider now an adjacent vertex to x_1, for instance $x_2 = \{3, 4\}$. Now that we have x_1 fixed the only options for the image of x_2 are x_6 and x_7 or x_2 itself since it must remain being a neighbor of x_1. Thus, $x_2^{G_{x_1}} \subseteq \{x_2, x_6, x_5\}$.

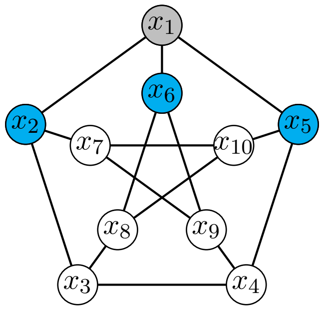


Figure A.6: x_1 fixed and the orbit of x_2 under G_{x_1} is contained in $\{x_2, x_6, x_5\}$ (in blue).

Applying the Orbit-Stabilizer Theorem again:

$$|G_{x_1}| = |G_{x_1x_2}||x_2^{G_{x_1}}| \Rightarrow |G| = 10|G_{x_1}| = 10|G_{x_1x_2}||x_2^{G_{x_1}}| \leq 30|G_{x_1x_2}|.$$

In order to continue with the same procedure we fix x_2 as well and we see which options we have for the image of $x_6 = \{3, 5\} \sim x_1$ under $G_{x_1x_2}$. Now $x_6^{G_{x_1}G_{x_2}} \subseteq \{x_6, x_5\}$ since x_1 and x_2 are fixed and moreover any element in $x_6^{G_{x_1}G_{x_2}}$ must remain being a neighbor of x_1.

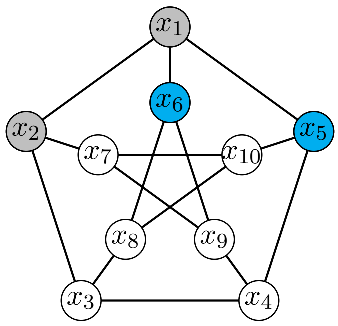


Figure A.7: x_1 and x_2 fixed and the orbit of x_6 under $G_{x_1x_2}$ is contained in $\{x_6, x_5\}$ (in blue).

Thus,

$$|G_{x_1x_2}| = |G_{x_1x_2x_6}||x_6^{G_{x_1x_2}}| \Rightarrow |G| \leq 30|G_{x_1x_2}| =$$

$$= 30|G_{x_1x_2x_6}||x_6^{G_{x_1x_2}}| \leq 60|G_{x_1x_2x_6}|.$$

Finally consider the vertex $x_3 = \{1,5\} \sim x_2$. Using the same procedure as before we get $x_3^{G_{x_1x_2x_6}} \subseteq \{x_3, x_7\}$.

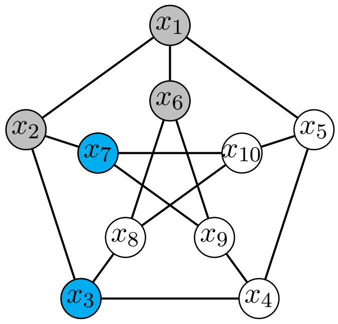


Figure A.8: x_1, x_2 and x_6 fixed and the orbit of x_3 under $G_{x_1x_2x_6}$ is contained in $\{x_3, x_7\}$ (in blue).

Therefore,

$$|G_{x_1x_2x_6}| = |G_{x_1x_2x_6x_3}||x_3^{G_{x_1x_2x_6}}| \Rightarrow |G| \leq 60|G_{x_1x_2x_6}| =$$

$$= 60|G_{x_1x_2x_6x_3}||x_3^{G_{x_1x_2x_6}}| \leq 120|G_{x_1x_2x_6x_3}|.$$

Now we only need to know $|G_{x_1x_2x_6x_3}|$. Let us show that $|G_{x_1x_2x_6x_3}| = 1$ since all the remaining vertices are fixed under $G_{x_1x_2x_6x_3}$.
First of all, x_8 is fixed since it is the only neighbour of both x_6 and x_3 which are already fixed.

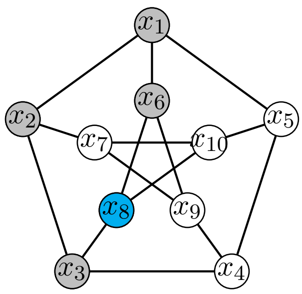


Figure A.9: x_6 and x_3 fixed and so x_8 fixed.

Moreover x_5 is fixed because all the other neighbours of x_1 are fixed. By the same argument we used for x_8 we see that x_{10} and x_4 are fixed.

From there the only two remaining vertices x_7 and x_9 are fixed as well, we can argue in the same way we did for x_8, x_4 and x_{10}.

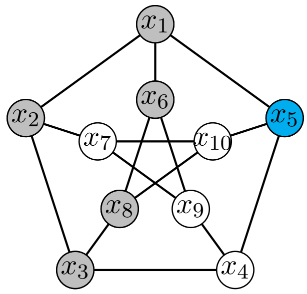


Figure A.10: x_5 if fixed because the other two neighbors of x_1 are fixed.

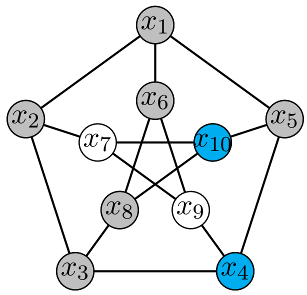


Figure A.11: x_{10} and x_4 are fixed because they are common neighbors of the pairs x_5 and x_8 and x_5 and x_3 respectively.

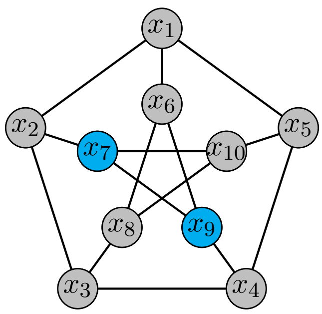


Figure A.12: x_7 and x_9 are fixed because they are common neighbors of the pairs x_2 and x_{10} and x_6 and x_4 respectively

Therefore, $|G| \leq 120$ and since $S_3 \subseteq G$ and $|S_5| = 120$, it follows that $G = S_5$. □

Exercise 4. Find a counterexample in order to prove that Theorem 2.2.5 is not true when $v = 2k$.

Solution. Take $t = \binom{v}{v/2}$. Note that when $v = 2k$ the Kneser graph $KG(v, v/2)$ corresponds to a bipartite graph in which the vertices are linked in pairs, see Figure A.13.

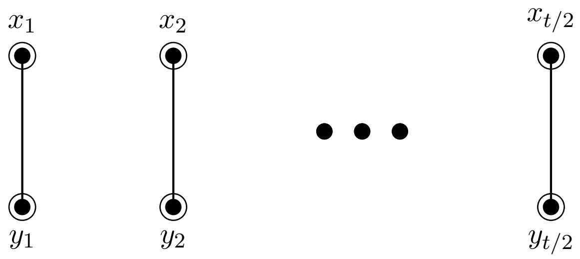


Figure A.13: The bipartite graph $KG(v, v/2)$.

It is obvious that any automorphism $f \in \operatorname{Aut} KG(v, v/2)$ is totally determined by its action on x_i for all $i \in \{1, .., t/2\}$, since the image of the y_i to which x_i is linked is going to be the only adjacent vertex of $f(x_i)$. Let us count how many options we have for choosing the images of each x_i.
For x_1 we have t options since it can be mapped to any other vertex. However, after the image of x_1 is determined we only have $t-2$ options for x_2 since it can be mapped neither to the image of x_1 nor to the adjacent vertex of $f(x_1)$. So on x_3 has $t-4$ options and the last point $x_{t/2}$ will have just two options. Therefore we have

$$t(t-2)(t-4)...4 \cdot 2$$

automorphisms. Now note that

$$t = \binom{v}{v/2} = \frac{v!}{(v/2)!(v/2)!}.$$

Let us show by induction $t(t-2)(t-4)...4 \cdot 2 > v!$ for $v > 2$. When $v = 4$ we have $t = \binom{4}{2} = 6$ and $6 \cdot 4 \cdot 2 = 48 > 4! = 26$.
Suppose that it is true for $v-2$ and $t' = \binom{v-2}{(v-2)/2}$, and let us prove it for v and $t = \binom{v}{v/2}$. We have

$$t(t-2)...2 = \binom{v}{v/2}\left[\binom{v}{v/2} - 2\right]...2$$

Note that this product is divisible by $t'(t'-2)...2 = \binom{v-2}{(v-2)/2}\left[\binom{v-2}{(v-2)/2} - 2\right]...2$, since all the factors in the latter appear in the former. More precisely,

$$t(t-2)...2 = \binom{v}{v/2}\left[\binom{v}{v/2} - 2\right]...2 =$$

$$= \binom{v}{v/2}\left[\binom{v}{v/2} - 2\right]...\left[\binom{v-2}{(v-2)/2} + 2\right]\binom{v-2}{(v-2)/2}\left[\binom{v-2}{(v-2)/2} - 2\right]...2 >$$

$$> \binom{v}{v/2}\left[\binom{v}{v/2}-2\right]...t'(t'-2)...2 >$$

$$> \binom{v}{v/2}\left[\binom{v}{v/2}-2\right]...\left[\binom{v-2}{(v-2)/2}+2\right](v-2)!,$$

by using the induction hypothesis. Now, taking into account that every factor is even and $\frac{(v-2)!}{(v/2)!(v/2)!} \geq 1/2$ for $v > 2$ we have

$$\binom{v}{v/2}\left[\binom{v}{v/2}-2\right]...\left[\binom{v-2}{(v-2)/2}+2\right] =$$

$$= v(v-1)\frac{(v-2)!}{(v/2)!(v/2)!}\left[\binom{v}{v/2}-2\right]...\left[\binom{v-2}{(v-2)/2}+2\right] > v\cdot(v-1).$$

This leads us to

$$t(t-2)...2 = \binom{v}{v/2}\left[\binom{v}{v/2}-2\right]...2 > v!,$$

which completes the induction. Thus, except for $v = 2$, when we obtain that $v! = 2$, for the case $v = 2k$ we obtain that the cardinalities of $\text{Aut}\,KG(v, v/2)$ and H or S_v differ and so they are not isomorphic. □

A.3 Chapter 3

Exercise 5. Prove that $G(n,k) = G(n,n-k)$.

Solution. Using the definition of the generalized Petersen graph we have the vertex set

$$V(G(n,k)) = \{u_0,...,u_{n-1},v_0,...,v_{n-1}\}$$

for both graphs since it only depends on n. Let us see if the edge sets coincide as well. Note that the edge set of $G(n,k)$ consists of all edges of the form

$$\{u_i,u_{i+1}\},\quad \{u_i,v_i\},\quad \{v_i,v_{i+k}\}$$

where all the indices are to be read modulo n, and the one for $G(n,n-k)$:

$$\{u_i,u_{i+1}\},\quad \{u_i,v_i\},\quad \{v_i,v_{i+n-k}\}.$$

Obviously the outer edges and the spokes are the same in both cases. Note that it is the same having edges of the form $\{v_i,v_{i+k}\}$ or $\{v_i,v_{i-k}\}$ and therefore, as the indices are to be read modulo n we have that $i-k \equiv i+n-k \mod n$ and then we have the same inner edges for both graphs. We conclude that $G(n,k) = G(n,n-k)$. □

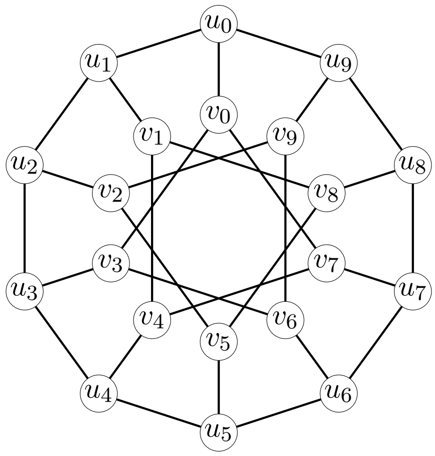


Figure A.14: Desargues graph.

Exercise 6. (a) Prove that the automorphism group of the Desargues graph is isomorphic to $S_5 \times C_2$.

(b) Write $B(n, k)$ as a direct product of the corresponding subgroups of H and K where $A(n, k) = H \times K$.

Solution. The so-called Desargues graph is the generalized Petersen graph $G(10, 3)$. Thus we have an outer rim with 10 vertices and an inner subgraph inducing a 10-circuit. In addition to this definition, we can describe the Desargues graph using algebraic combinatorics as the graph with vertex set $\binom{\{1,2,3,4,5\}}{2} \cup \binom{\{1,2,3,4,5\}}{3}$ and having an edge between them if and only if one vertex is a subset of the other.

We want to prove that the automorphism group of the Desargues graph is isomorphic to $S_5 \times C_2$. First of all, note that the natural action of S_5 on the set $\{1, 2, 3, 4, 5\}$ induces an action of S_5 on the graph $G(10, 3)$ by applying permutations to the elements that constitute each of the vertices. Moreover, this action is faithful and preserves the link between vertices. Thus, we obtain a subgroup H of $\operatorname{Aut} G(n, k)$ which is isomorphic to S_5.

In addition, let us take $K = \langle \rho^5 \rangle$, where ρ is the map defined in Chapter 3, i.e. $\rho(u_i) = u_{i+1}$ and $\rho(v_i) = v_{i+1}$ for all i. Observe that ρ^5 maps every vertex onto the one just opposite to it, one vertex corresponding to the complement of the other one,

$$\rho^5(u_i) = u_{i+5} \quad \text{and} \quad \rho^5(v_i) = v_{i+5} \quad \text{for every } i.$$

Note that $\rho^5 \neq 1$ and $(\rho^5)^2 = 1$ and so, $K \cong C_2$. Moreover, $\rho^5 \in \operatorname{Aut} G(10, 3)$ since all rotations maintain the links between vertices.
For simplicity, let us use G again in order to refer to the automorphism group of $G(10, 3)$, i.e., $G = \operatorname{Aut} G(10, 3)$.

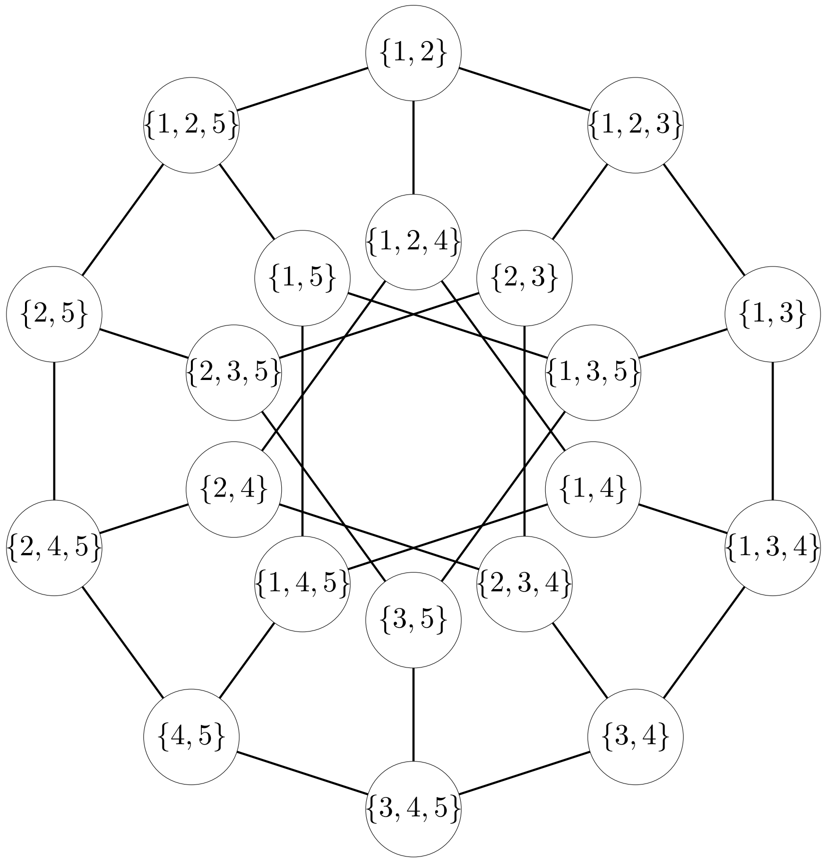


Figure A.15: Desargues graph.

The intersection of the two subgroups H and K is trivial because $\rho^5 \notin H$ since it maps a vertex representing a two element subset onto one representing a three element subset, and that does not happen with any of the permutations in H.

First of all we want to see that ρ^5 commutes with every element in H. Take any 2-element subset $X = \{i, j\} \in V(G(10,3))$, and take any element $\mu \in H$. Then

$$\rho^5\mu(\{i,j\}) = \rho^5(\{\mu(i), \mu(j)\}) = \{1,2,3,4,5\}\backslash\{\mu(i), \mu(j)\} \quad \text{and,}$$

$$\mu\rho^5(\{i,j\}) = \mu(\{1,2,3,4,5\}\backslash\{i,j\}) =$$
$$= \{\mu(1), \mu(2), \mu(3), \mu(4), \mu(5)\}\backslash\{\mu(i), \mu(j)\} = \{1,2,3,4,5\}\backslash\{\mu(i), \mu(j)\}.$$

Exactly the same happens when we choose a 3-element subset. Thus, $\rho^5\mu = \mu\rho^5$ for all $\mu \in H$.

Hence, $K \trianglelefteq \langle H, K\rangle$ and as ρ^5 is the only generator of K and all the elements of H commute with it, $H \trianglelefteq \langle H, K\rangle$ as well. This implies that $KH = HK$ and HK is a subgroup of G. In addition as $\langle H, K\rangle$ is the smallest subgroup of G which contains both H and K, we have $\langle H, K\rangle = HK$. Thus, $|\langle H, K\rangle| = |HK| = \frac{|H||K|}{|H\cap K|} = 120 \times 2 = 240$, and $\langle H, K\rangle \cong H \times K \cong S_5 \times C_2$.

Note that H induces two orbits in $G(10, 3)$: one with the 2-element subset vertices, and another one with the 3-element subset vertices. Moreover, $\langle\rho^5\rangle$ induces for each 2-element subset vertex the orbit with the vertex itself and the 3-element subset vertex with the subset such that their intersection is empty, and conversely. Therefore, $G(10, 3)$ is vertex-transitive since S_5 allows us to map any vertex with any other vertex corresponding to a subset of the same size and ρ^5 maps a 2-element subset vertex into a 3-element subset vertex. Hence, we start in the same way as in the previous case, applying the Orbit-Stabilizer Theorem and taking into account that the orbit of u_0 is at most of size 20.

$$|G| = |G_{u_0}||u_0^G| \leq 20|G_{u_0}|.$$

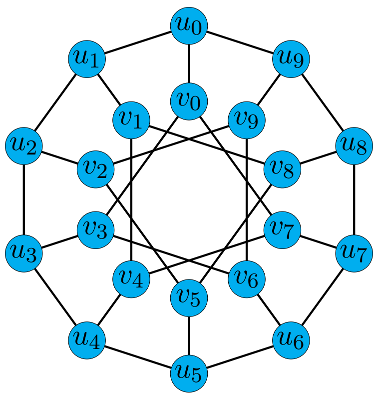


Figure A.16: All the vertices can be in the orbit of u_0.

Moreover if we do as we did before and we fix u_0 in order to see the possible orbits of u_1 under G_{u_0}, we get,

$$|G_{u_0}| = |G_{u_0u_1}||u_1^{G_{u_0}}| \Rightarrow |G| \leq 20|G_{u_0}| = 20|G_{u_0u_1}||u_1^{G_{u_0}}| \leq 60|G_{u_0u_1}|.$$

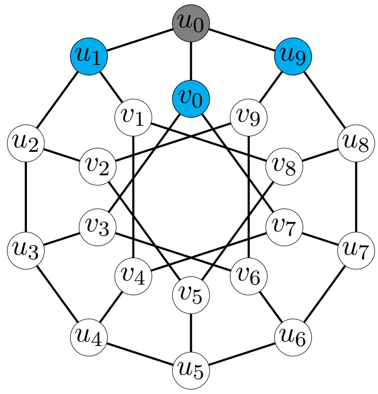


Figure A.17: As u_0 is fixed the orbit of u_1 is contained in$\{u_1, v_0, u_9\}$.

Continuing in the same way, we fix u_1 and we see that the orbit of v_0 under $G_{u_0u_1}$ is contained in $\{v_0, u_9\}$, so:

$$|G| \leq 60|G_{u_0u_1}| \leq 120|G_{u_0u_1v_0}|.$$

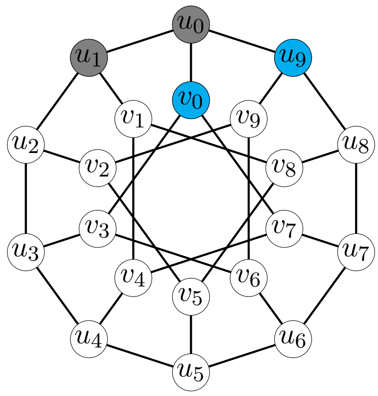


Figure A.18: The orbit of v_0 under $G_{u_ou_1}$ is contained in $\{v_0, u_9\}$.

Now fixing v_0 as well we get that the orbit of u_2 is a subset of $\{u_2, v_1\}$ and from the Orbit-Stabilizer Theorem again:

$$|G| \leq 120|G_{u_0u_1v_0}| \leq 240|G_{u_0u_1v_0u_2}|.$$

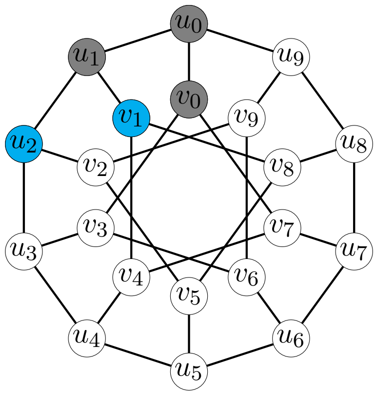


Figure A.19: The orbit $u_2^{G_{u_0u_1v_0}} \subseteq \{u_2, v_1\}$.

Let us show now that $|G_{u_0u_1v_0u_2}| = 1$, or which is the same, that all the remaining vertices are fixed.

Note that v_1 and u_9 are fixed since they are the only remaining neighbours of u_1 and u_0 respectively. In addition, v_9 is fixed because it is the only vertex at distance 1 from u_9 and 2 from u_2, which are fixed, and distances must remain the same. The same argument is valid for v_2. Now, u_8 and u_3 are fixed because they are the only neighbors of u_9 and u_2 respectively that are not already fixed. Moreover, v_8 is fixed for being the only common neighbor of u_8 and v_1, and the same for v_3. If we continue like this we can see that u_7 and u_4 are fixed because all the other neighbors of u_8 and u_3 are fixed, which implies that v_7 is fixed since it is the only common neighbor of u_7 and v_0. We can apply the same for v_4. We can continue with the same arguments until we conclude that all the vertices are fixed, after checking that u_0, u_1, v_0 and u_2 are fixed.

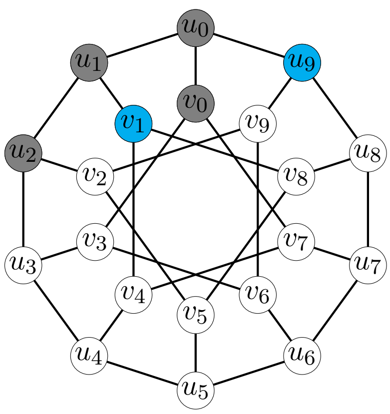


Figure A.20: v_1 and u_9 are fixed.

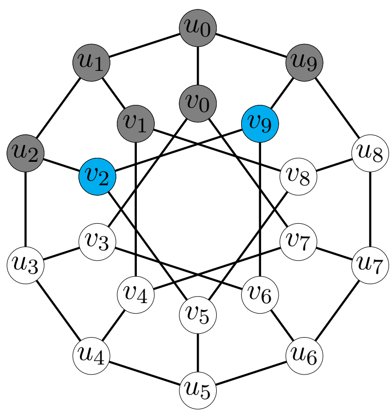


Figure A.21: v_9 and v_2 are fixed.

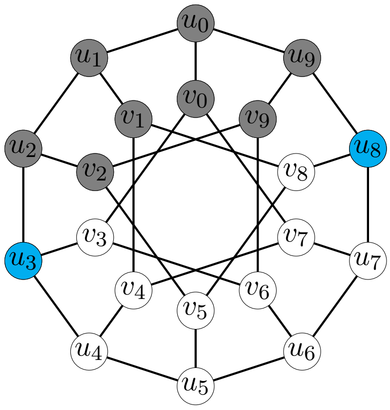


Figure A.22: u_8 and u_3 are fixed.

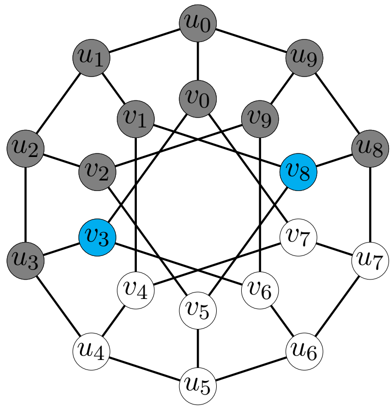


Figure A.23: v_8 and v_3 are fixed.

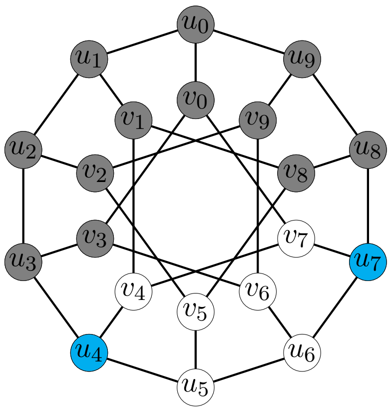


Figure A.24: u_7 and u_4 are fixed.

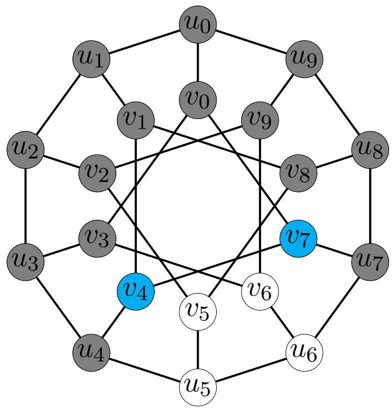


Figure A.25: v_7 and v_4 are fixed.

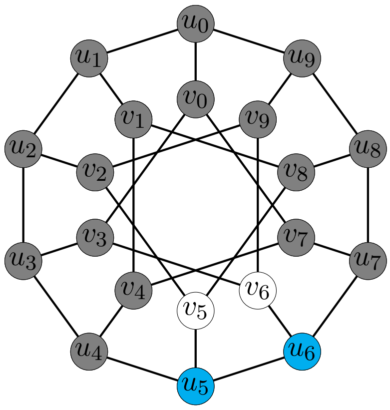


Figure A.26: u_5 and u_6 are fixed.

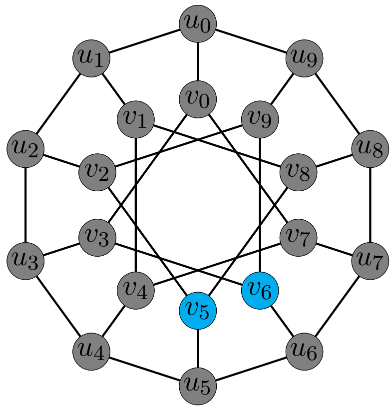


Figure A.27: v_5 and v_6 are fixed.

Therefore, $|G| \leq 240 = |HK|$ and thus $G = \langle H, K \rangle \cong H \times K \cong S_5 \times C_2$.

Now recall from Chapter 3 we defined $B(n,k)$ for $k^2 \equiv -1 \pmod n$ as $B(n,k) = \langle \rho, \alpha | \quad \rho^n = \alpha^4 = 1, \quad \rho^\alpha = \rho^k \rangle$, which in our case is

$$B(10,3) = \langle \rho, \alpha | \quad \rho^{10} = \alpha^4 = 1, \quad \rho^\alpha = \rho^{-3} \rangle.$$

Note that, as we said in Chapter 3, $G(10,3)$ is one of the 7 exceptional cases in which $A(n,k) \neq B(n,k)$, since $|B(10,3)| = 40$ is not equal to $|A(10,3)| = 240$.

(b) Let us find the corresponding elements of the subgroup $B(10,3)$ in the representation $G = H \times K$. In order to do that, let us see what parts of our normal subgroups H and K lie in $B(10,3)$.

On the one hand, it is obvious that $\rho^5 \in B(10,3)$ and therefore K is fully contained in $B(10,3)$, i.e., $K \subseteq B(10,3)$. Due to this $B(10,3) = (H \cap B(10,3)) \times K$ so we only have to determine the intersection of H with $B(10,3)$. Observe that since $|B(10,3)| = 40$ and $|K| = 2$, we have $|H \cap B(10,3)| = 20$, remember that $H \cap K = \{1\}$.

Let us analyze then the intersection $H \cap B(10,3)$. Note that $\rho \notin H$ since it maps a vertex of a 2-element subset onto a a vertex of a 3-element subset and none of the elements in H can do that. However we can recognize the element ρ^2 in $B(10,3)$ as the automorphism of H induced by the permutation $(12543) \in S_5$.

We have a similar situation with α, it is not in H since it maps vertices of some size to vertices of different size. Note that $A(10,3) = H \times \langle \rho^5 \rangle$ and $|A(10,3) : H| = \frac{|A(10,3)|}{|H|} = \frac{240}{120} = 2$. Since the index is 2 we only have two right (left) cosets and moreover, $A(10,3) = H \cup Hg$ for some $g \notin H$. Since ρ^5 and $\alpha \notin H$, we have

$$A(10,3) = H \cup H\rho^5,$$

$$A(10,3) = H \cup H\alpha,$$

from which we conclude that $H\rho^5 = H\alpha$ and this only happens when $\alpha\rho^{-5} \in H$ or which is the same $\alpha\rho^5 \in H$. This gives us the clue of the element that will complete our description of $H \cap B(10,3)$. Looking at the graph we can identify $(1325) \in S_5$ as the permutation that induces the element $\alpha\rho^5$, whose order is 4 since $(\alpha\rho^5)^2 = \alpha^2 \neq 1$, $(\alpha\rho^5)^3 = \alpha^3\rho^5 \neq 1$ and $(\alpha\rho^5)^4 = \alpha^4 = 1$. Hence $\langle \rho^2, \alpha\rho^5 \rangle \subseteq H \cap B(10,3)$. Moreover, $\langle \rho^2 \rangle \cap \langle \alpha\rho^5 \rangle = 1$ and therefore we have $|\langle \rho^2, \alpha\rho^5 \rangle| \geq |\langle \rho^2 \rangle||\langle \alpha\rho^5 \rangle| = 5 \times 4 = 20$. Since $|H \cap B(10,3)| = 20$ we can conclude that $H \cap B(10,3) = \langle \rho^2, \alpha\rho^5 \rangle$. Therefore,

$$B(10,3) = \langle \rho^2, \alpha\rho^5 \rangle \times \langle \rho^5 \rangle \cong \langle (12543), (1325) \rangle \times \langle \rho^5 \rangle.$$

$\square$

A.4 Chapter 4

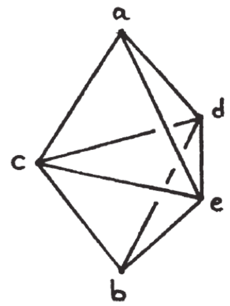


Figure A.28: Γ

Exercise 7. Let us have the following molecular graph Γ. And let us have the rearrangement ρ which redefines the edge set by replacing the edge joining the vertices in sites d and e with a new edge joining the vertices in sites a and b. Give the resulting graph Γ' and see if ρ is a degenerate rearrangement. If so, give the the permutation describing the isomorphism $\pi : \Gamma' \to \Gamma$.

Solution. Let us show graphically how ρ acts on Γ.

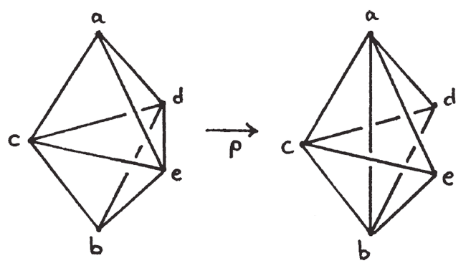


Figure A.29: Γ and Γ'.

First of all, note that in both graphs all the vertices are connected to each other except for one pair of vertices, thus they are isomorphic to a complete graph K_5 without an edge, and so $\Gamma \equiv \Gamma'$. This implies that ρ is a degenerate rearrangement.
Now as they are isomorphic there must exist $\pi : \Gamma' \to \Gamma$ such that we get again the same representation as before. In this case this is given by the permutation $\pi = (aebd)$ as we can see in Figure A.30, in which, for example $a = d\pi$ means that the vertex in site a is moved by π to the site d. $\square$

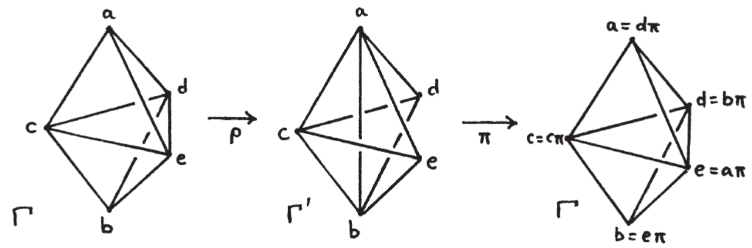


Figure A.30: We get Γ again after applying π on Γ'.

Exercise 8. *The Berry mechanism.* Consider a molecule with a central atom M linked to five atoms called *ligands* forming a triagonal bipyramid with M at the center. Moreover, let us call the ligands on the top and bottom, in Figure A.31 L_1 and L_2, *axials* and the other three forming the triangle in the middle, L_3, L_4 and L_5 in Figure A.31, *equatorial.* In the *Berry mechanism*, one of the equatorial ligands is fixed, while all the other ligands move. In order to illustrate it let us take for instance that L_3 is the fixed ligand. Then in the *Berry mechanism* L_4 and L_5 will move closer to L_3 while L_1 and L_2 will move further. Moreover, this happens in a way such that the angles that each pair of ligands form with M changes always in the same way. Each pairs of ligands, the one aproximating and the one going further remain planar with L_3 but the angle that L_4 and L_5 form with M changes from 120° to 180° and conversely the angle that L_1 and L_2 form with M changes from 180° to 120°. Note that the result is again a triagonal bypiramid, but now with L_4 and L_5 as axial and L_1, L_2 and L_3 as equatorial.

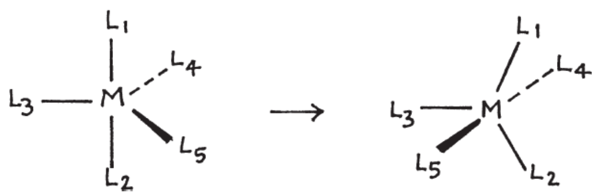


Figure A.31: In these molecules with a central atom M the broken edges represent edges that should be visualized behind the plan of the page, and the thick edges in front of it.

(a) Find the graph representing the molecular graph and describe the Berry mechanism on it using labelings.

(b) Find the reaction graph of the Berry mechanism and its automorphism group.

Solution. (a) First of all, let us choose a graph Γ that can be labelled in a way that represents our molecule and all its possible labelings. Note in Figure A.31 that the bonds do not change, and M remains always in the middle and with the same connections. Then, let us take Γ to be the graph consisting of the vertices and edges of a triangular bipyramid. Then we refer to Figure A.28 in Exercise 7 and choose the labeling

$$\lambda = \begin{pmatrix} abcde \\ 12345 \end{pmatrix},$$

each of the numbers representing one atom L_i where $i \in \{1, ..., 5\}$. In this way, keeping the natural edges of a triangular bipyramid we have that the vertices i and j are adjacent if and only if the angle L_iML_j is $90°$ or $120°$. See the first graph in Figure A.32, which represents the first molecule in Figure A.31. Note that in the previous Exercise 7 we have analyzed exactly the same rearrangement ρ replacing the edge joining the vertices in sites c and d by a new edge joining the vertices in sites a and b.

This last Figure A.32 represents the example of the Berry mechanism described before, with the rearrangement ρ replacing the edge $\{4, 5\}$ by the edge $\{1, 2\}$ and in order to have the same structure as before if we move our labeled vertices applying $\pi = (aebd)$, we get the last labelled graph in Figure A.32 which corresponds to the labeling

$$\lambda' = \begin{pmatrix} abcde \\ 45321 \end{pmatrix}.$$

By comparing the first and the third graph in that figure, we se how the Berry mechanism has transformed one labeling of Γ into another, to indicate how the ligands have changed roles. Note also that the last graph represents the second molecule in Figure A.31 if we look at the triangular bipyramid from the bottom.

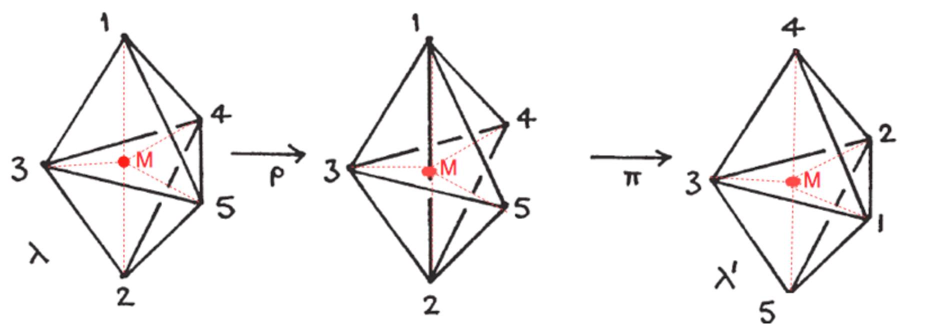


Figure A.32: The red broken edges represent the links with M and we can see how those change under the rearrangement ρ and the permutation π.

(b) Let as take as H the automorphism group of the triagonal bipyramid, in fact $S_2 \times S_3$. This is true since it is easy to see that for the graph labelled

with λ we have $\operatorname{Aut}\Gamma = \langle(34),(345)\rangle \times \langle(12)\rangle$ (we can prove this in the same way we did for the graph in Exercise 2 since we have the same group G and normal subgroups). Then, since H contains 12 elements we have that our reaction graph has $5!/12 = 10$ vertices.
Now we need to find a good notation for the vertices in the vertex set $\Omega = \{\alpha_i = [\lambda_i] : i \in 1, ..., 12\}$ in order to determine the edges of the reaction graph. Note that the automorphism group of the triangular bipyramid determines when two labelings are the same. Actually, looking at the graph, all the graphs with the same axial ligands are isomorphic, thus, the set of axial ligands completely defines the class of labeling and in consequence, the vertex. Hence, a vertex α_k of R corresponds to an unordered pair of labels $\{i, j\}$ indicating that the axial ligands are L_i and L_j.

Figure A.32 shows that there is an edge between the vertex $\{1, 2\}$ and $\{4, 5\}$. In general, when applying the rearrangement of the Berry mechanism two of the equatorial ligands take the role of the two axial ligands, which end up being equatorial ligands. Then, a rearrangement ρ of this type is only going to occur between two labelings if and only if their pair of axial ligands are completely different, thus their intersection is empty. Going back to our reaction graph, each of our vertices is denoted by a 2-subset representing the axial ligands, taking into account what we just said, two of this subsets will be adjacent to each other if and only if their intersection is empty. This leads to a reaction graph R with 10 vertices, which are subgroups of size 2 from the set $\{1, 2, 3, 4, 5\}$ adjacent to each other when their intersection is empty, thus $KG(5, 2)$, the Petersen graph.

Hence we have found that our reaction graph $R \cong KG(5, 2)$ and from Exercise 3 we know that the automorphism group of the Petersen graph is isomorphic to S_5, therefore $\operatorname{Aut} R \cong S_5$. □

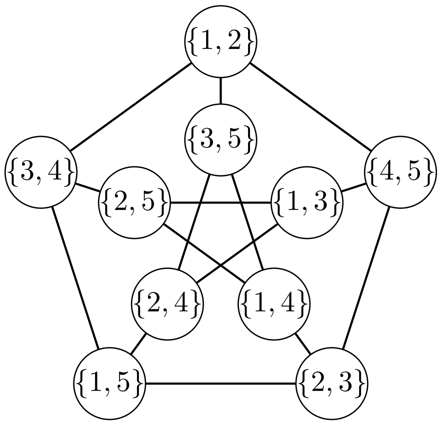


Figure A.33: Petersen graph $KG(5, 2) \cong R$.

Bibliography

[1] N. Alon and J. Spencer, *The probabilistic method.* Wiley, (1992), 13.

[2] A. T. Balaban, D. Fărcaşiu, and R. Bănică, Chemical graphs II. Graphs of multiple 1,2-shifts in carbonium ions, *Rev. Roumaine Chim.* 11 (1966), 1205-1227.

[3] P. Cameron, The Erdős-Ko-Rado Theorem, preprint.

[4] H. S. M. Coxeter, Self-dual configurations and regular graphs. *Bull. Amer. Math. Soc.* 56, (1950), 413-455.

[5] R. Frucht, J. E. Graver and M. E. Watkins. The groups of the generalized Petersen graphs. *Mathematical Proceedings of the Cambridge Philosophical Society*, 70 (1971), 211-218.

[6] C. Godsil and G. Royle, *Algebraic Graph Theory*, Graduate Texts in Mathematics, Springer, (2001).

[7] G.A. Jones and E.K. Lloyd, Chemical Applications of Topology and Graph Theory, ed. R.B. King, *Studies in Physics and Theoretical Chemistry*, Vol. 28 (Elsevier, 1983).

[8] G.A. Jones and E.K. Lloyd, Reaction Graphs, *Acta Appliandae Mathematicae* 52(1-3), (1998), 121-147.

[9] M. H. Klin, S. S. Tratch, and N. S. Zefirov. Group-theoretical approach to the investigation of reaction graphs for highly degenerate rearrangements of chemical compounds. I. Criterion of the connectivity of a graph, *J. Math. Chem.* 7 (1991), 135-151.