Chapter 2

Group Theory and Symmetry

2.1 The Concept of Groups

A *group* is a collection or *set* of *elements* together with an inner binary operation, conventionally called *multiplication*, satisfying some special rules discussed below. It is not necessary to specify what the elements are in order to discuss the group that they constitute. Of particular interest in the context of this book are groups formed by permutations of sets of small numbers of objects, particularly the roots of algebraic equations; such groups are called *permutation groups*. Frequently the properties of such abstract permutation groups are most readily visualized by considering analogous or *isomorphic* groups formed by sets of symmetry operations on polyhedra or other readily visualized spatial objects. Groups formed by symmetry operations on three-dimensional objects are called *symmetry point groups*. Some features of both of these types of groups will be discussed in this chapter.

A set of elements combined with an binary operation (multiplication) to form a mathematical group must satisfy the following four conditions or rules[1]:

(1) The product of any two elements in the group and the square of each element must be an element of the group. A *product* of two group elements, AB, is obtained by applying the binary operation (multiplication) to them and the *square* of a group element, A^2, is the product of an element with itself. This definition can be extended to higher powers of group elements. The multiplication of two group elements is said to be *commutative* if the order of multiplication is immaterial, i.e., if $AB = BA$. In such a case A is said to *commute* with B. The multiplication of two group elements is *not* necessarily commutative.

(2) One element in the group must commute with all others and leave them unchanged. This element is conventionally called the *identity*

[1]F. J. Budden, *The Fascination of Groups*, Cambridge Univ. Press, London, 1972.

element and often designated as E. This condition may be concisely stated as $EX = XE = X$.

(3) The associative law of multiplication must hold. This condition may be expressed concisely as $A(BC) = (AB)C$, i.e., the result must be the same if C is multiplied by B to give BC followed by multiplication of BC by A to give $A(BC)$ or if B is multiplied by A to give AB followed by multiplication of AB by C to give $(AB)C$.

(4) Every element must have an inverse, which is also an element in the group. The element Z is the *inverse* of the element A if $AZ = ZA = E$. The inverse of an element A is frequently designated by A^{-1}. Note that multiplication of an element by its inverse is always commutative.

These defining characteristics of a group have been summarized concisely[2] by defining a group as "...a mathematical system consisting of elements with *inverses* which can be combined by some operation without going outside the system."

The number of elements in a group is called the *order* of the group. This book will be concerned exclusively with *finite groups*, i.e., groups with finite numbers of elements. Within a given group it may be possible to select various smaller sets of elements, each set including the identity element E, which are themselves groups. Such smaller sets are called *subgroups*. A subgroup of a group G is thus defined as a subset H of the group G which is itself a group under the same multiplication operation of G. The fact that H is a subgroup of G may be written $H \subset G$. The order of a subgroup must be an integral factor of the order of the group. Thus if H is a subgroup of G and $|H|$ and $|G|$ are the orders of H and G, respectively, then the quotient $|G|/|H|$ must be an integer. This quotient is called the *index* of the subgroup H in G.

Let A and X be two elements in a group. Then $X^{-1}AX = B$ will be equal to some element in the group. The element B is called the *similarity transform* of A by X and A and B may be said to be *conjugate*. Conjugate elements have the following properties:

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[2] A. W. Bell and T. J. Fletcher, *Symmetry Groups*, Associated Teachers of Mathematics, 1964.

(1) Every element is conjugate with itself. Thus for any particular element A there must be at least one element X such that $A = X^{-1}AX$.

(2) If A is conjugate with B, then B is conjugate with A. Thus if $A = X^{-1}BX$, then there must be some element, Y, in the group such that $B = Y^{-1}AY$.

(3) If A is conjugate with B and C, then B and C are conjugate with each other.

A complete set of elements of a group which are conjugate to one another is called a *class* (or more specifically a *conjugacy class*) of the group. The number of elements in a conjugacy class is called its *order*; the orders of all conjugacy classes must be integral factors of the order of the group.

An important property of each element of a group is its *period.* In this context the period of an element is the minimum number of times that the element must be multiplied by itself before the identity element E is obtained, i.e., the smallest positive integer n such that $A^n = E$. The period of the identity element E is, of course, 1. The period of an element is sometimes also called its *order* but this is confusing because the term "order" is also used to describe the number of elements in a group or conjugacy class (see above).

Certain elements $g_1, g_2, \ldots, g_m$ of a given finite group G are called a set of *generators* if every element of G can be expressed as a finite product of their powers (including negative powers).[3] A set of generators may be denoted by the symbol $\{g_1, g_2, \ldots g_m\}$. A set of relations satisfied by the generators of a group is called an *abstract definition* or *presentation* of the group if every relation satisfied by the generators is an algebraic consequence of these particular relations. A group with only one generator (i.e., $m = 1$) is a *cyclic group,* $\{g\} \equiv C_n$, whose order n is the period of the single generator g, i.e., $g^n = E$, where E is the identity element. The cyclic group C_1 is the trivial group consisting solely of the identity element.

A group in which every element commutes with every other element is called a *commutative* group or an *Abelian* group after the famous Norwegian mathematician, Abel (1802–1829). In an Abelian group every element is in a

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[3]H. S. M. Coxeter and W. O. J. Moser, *Generators and Relations for Discrete Groups*, Springer-Verlag, Berlin, 1972.

conjugacy class by itself, i.e., all conjugacy classes are of order one. A *normal subgroup* N of G, written $N \lhd G$, is a subgroup which consists only of *entire* conjugacy classes of G.[4] A *normal chain* of a group G is a sequence of normal subgroups $C_1 \lhd N_{a_1} \lhd N_{a_2} \lhd N_{a_3} \lhd \cdots \lhd N_{a_s} \lhd G$, in which s is the number of normal subgroups (besides C_1 and G) in the normal chain. A *simple* group has no normal subgroups other than the identity group C_1. Simple groups are particularly important in the theory of finite groups.[5,6] If a normal chain starts with the identity group C_1 and leads to G and if all of the quotient groups $N_{a_1}/C_1 = C_{a_1}, N_{a_2}/N_{a_1} = C_{a_2}, \ldots, G/N_{a_s} = C_{a_{s+1}}$ are cyclic, then G is a *composite* or *soluble* group.

2.2 Symmetry Groups

Many of the properties of groups are most readily visualized by studying the groups consisting of symmetry operations of polyhedra or other concrete three-dimensional objects. In this context a *symmetry operation* is a movement of an object such that, after completion of the movement, every point of the body coincides with an equivalent point or the same point of the object in its original orientation. The position and orientation of an object before and after carrying out a symmetry operation are indistinguishable. Thus a symmetry operation takes an object into an equivalent configuration.

The symmetry operations for objects in ordinary three-dimensional space can be classified into four fundamental types each of which is defined by a *symmetry element* around which the symmetry operation takes place. The four fundamental types of symmetry operations and their corresponding symmetry elements are listed in Table 2–1.

The identity operation, designated as E, leaves the object unchanged. Although this operation may seem trivial, it is mathematically necessary in order

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[4] J. K. G. Watson, On the Symmetry Groups of Non-Rigid Molecules, *Mol. Phys.*, **21**, 577 (1971).

[5] D. Gorenstein, *Finite Groups*, Harper and Row, New York, 1968.

[6] D. Gorenstein, *Finite Simple Groups: An Introduction to their Classification*, Plenum, New York, 1982.

to convey the mathematical properties of a group on the set of all of the symmetry operations applicable to a given object. The reflection operation, designated as σ, involves reflection of the object through a plane, known as a *reflection plane*. For example, in a reflection through the xy-plane (conveniently designated as σ_{xy}) the coordinates of a point (x, y, z) change to $(x, y, -z)$—a reflection operation thus can result in the change of only a single coordinate. A rotation operation, designated as C_n, consists of a 360°/n rotation around a line, known as a *rotation axis*. For example, a C_2 rotation around the z-axis changes the coordinates of a point (x, y, z) to $(-x, -y, z)$—a rotation operation thus can result in a change of only two coordinates. An improper rotation, designated as S_n, consists of a 360°/n rotation around a line followed by a reflection in a plane perpendicular to the rotation axis. An S_2 operation is called an *inversion* and is designated by i; the intersection of the C_2-axis and the perpendicular reflection plane is called an *inversion center*. Inversion through the origin changes the coordinates of a point (x, y, z) to $(-x, -y, -z)$—thus an S_n operation must change the signs of all three coordinates. An S_1 improper rotation in which the C_1 proper rotation component is equivalent to the identity E corresponds to a reflection operation σ. Thus the reflection operation σ is a special type of improper rotation, namely S_1.

Table 2–1: The Four Fundamental Types of Symmetry Operations

Symmetry Operation	Designation	Corresponding Symmetry Element	Dimensions
Identity (no change)	E	The entire object	3
Reflection	σ	Reflection plane	2
Rotation	C_n	Rotation axis	1
Improper rotation	S_n	Improper rotation axis*	0

*Point of intersection of a proper rotation axis and a perpendicular reflection plane

Consider the set of symmetry operations in ordinary three-dimensional space describing the symmetry of an actual object. Such a set of symmetry operations satisfies the properties of a *group* in the mathematical sense and is therefore called a *symmetry point group.* In most cases such a symmetry point group contains a finite number of operations and is therefore a *finite group.*

There is a systematic way to classify objects in three-dimensional space by their symmetry point groups based on the following sequence of questions[7]:

(1) Is the object linear (i.e., only "one-dimensional")?

Linear objects are the only objects having infinite rather than finite symmetry point groups since the linear axis corresponds to an infinite order rotation axis, namely C_∞. If there is a reflection plane perpendicular to the infinite order rotation axis (dividing the object into two equivalent halves), then the symmetry point group is D_∞, if not the symmetry point group is C_∞.

(2) Does the object have multiple "higher-order" rotation axes (i.e., $C_{>2}$ axes)?

Multiple axes in this question refer to noncollinear $C_{>2}$ axes. Such nonlinear objects have the symmetries of well-known regular polyhedra and are generally readily recognizable by containing the regular polyhedra in some manner. Such groups are sometimes called the *polyhedral* point groups. Thus the tetrahedral groups T, T_h, and T_d with 12, 24, and 24 operations, respectively, have four noncollinear C_3 axes and are distinguished by the presence or absence of horizontal (σ_h) or diagonal (σ_d) reflection planes. The octahedral groups O and O_h with 24 and 48 operations, respectively, have not only four noncollinear C_3 axes but also three noncollinear C_4 axes and are distinguished by the presence or absence of reflection planes. Figure 2–1 shows the multiple rotation axes of the regular octahedron and the cube, both of which have the octahedral point group O_h. The icosahedral groups I and I_h with 60 and 120 operations, respectively, have ten noncollinear C_3 axes and six noncollinear C_5 axes and are also distinguished by the presence or absence of reflection planes.

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[7]F. A. Cotton, *Chemical Applications of Group Theory*, Third Edition, Wiley, New York, 1990, Chapter 3.

3. If the object does not belong to either a linear group or a polyhedral group, then does it have proper or improper axes of rotation (i.e. C_n or S_n)?

If no axes of either type are found, the group is either C_s, C_i, or C_1 with 2, 2, and 1 operations, respectively, depending whether the object has a plane of symmetry (σ), and inversion center (i), or neither. The C_1 designation corresponds to an object with no symmetry at all and therefore to a symmetry point group containing only one element, namely the identity element E.

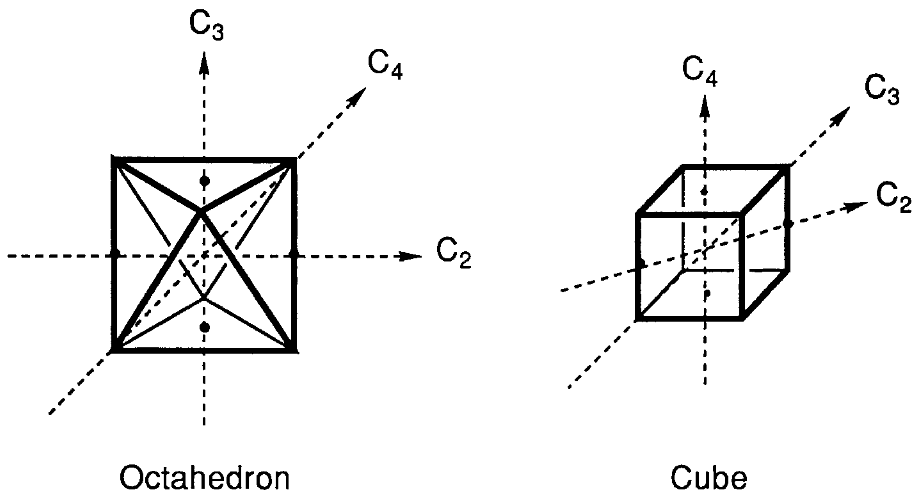

Figure 2–1: The multiple rotation axes in the octahedron and cube, both of which have O_h symmetry. In the octahedron the C_4 axes pass through opposite pairs of vertices, the C_3 axes pass through the midpoints (•) of opposite pairs of faces, and the C_2 axes pass through opposite pairs of edges. In the cube, the C_3 axes pass through opposite pairs of vertices, the C_4 axes pass through midpoints (•) of opposite pairs of faces, and the C_2 axes pass through opposite pairs of edges.

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(4) Does the object have an *even*-order improper rotation axis S_{2n} but no planes of symmetry or any proper rotation axis other than one collinear with the improper rotation axis?

The presence of an even-order improper rotation axis S_{2n} without any noncollinear proper rotation axes or any reflection planes indicates the symmetry point group S_{2n} with $2n$ operations.

(5) **If the object does not belong to the linear point groups, the polyhedral point groups, or the point groups C_s, C_n, C_1, or S_{2n}, then look for the highest order rotation axis.** Call the highest order rotation axis C_n.

(6) **Are there n C_2 axes lying in a plane perpendicular to the C_n axis?** If there are n C_2 axes lying in a plane perpendicular to the C_n axis then the object belongs to one of the symmetry point groups D_n, D_{nh}, or D_{nd} with $2n$, $4n$, and $4n$ operations, respectively, depending on whether there are no planes of symmetry, a horizontal plane of symmetry (σ_h), or n vertical planes of symmetry (σ_v), respectively. If there are no C_2 axes lying in a plane perpendicular to the C_n axis, then the object belongs to one of the symmetry point groups C_n, C_{nv}, C_{nh}, with n, $2n$, and $2n$ operations, respectively, depending upon whether there are no planes of symmetry, n vertical planes of symmetry (σ_v), or a horizontal plane of symmetry (σ_h), respectively. If there are only C_2 axes, then a unique C_2 axis is chosen as the "reference axis" if there is any ambiguity as to which C_2 axis to choose.

2.3 Regular Polyhedra

The symmetries of regular polyhedra are important in the theory of the solution of algebraic equations. The symmetries of the five regular Platonic solids, namely the tetrahedron, octahedron, cube, icosahedron, and dodecahedron (Figures 2–1 and 2–2) were already recognized by the ancient Greeks. The fact that there are only five regular geometric solids in contrast to an infinite number of polygons must have been a major revelation to the ancient thinkers. The reason for only five regular geometric solids can be readily seen by the following arguments.[8,9]

[8]H. S. M. Coxeter, *Regular Polytopes*, Pitman Publishing Corp., New York, 1948.

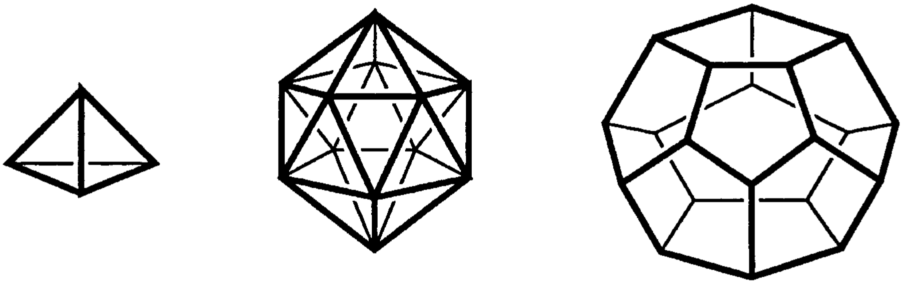

Figure 2–2: The regular tetrahedron, icosahedron, and dodecahedron. The regular octahedron and cube are shown in Figure 2–1.

In order to have the solid angles required for forming closed polyhedra, a minimum of three edges must meet at a vertex. In this connection the number of edges meeting at a vertex is called the *degree* of the vertex. In the case of completely regular polyhedra the configuration of edges meeting at each vertex must be identical. If three equal-length edges meet at every vertex and if they join each other in equilateral triangular faces, the result is a tetrahedron. If instead, four or five equilateral triangles meet at each vertex, the result is an octahedron or an icosahedron, respectively. All of these regular polyhedra with equilateral triangular faces may be considered to have their vertices on finite surfaces with positive curvature such as the sphere. If six equilateral triangles meet at a vertex, an infinite flat two-dimensional lattice is obtained with a familiar hexagon structure with its vertices on an infinite surface with zero curvature. Such planar structures are called *tessellations* (Figure 2–3). More than six equilateral triangles meet at a vertex only with puckering and thus cannot give a regular solid. The vertices of such configurations can only be placed on infinite surfaces with negative curvature. Thus there are only three regular polyhedra with (equilateral) triangular faces, namely the tetrahedron,

[9]O. T. Benfey and L. Fikes, The Chemical Prehistory of the Tetrahedron, Octahedron, Icosahedron, and Hexagon, *Adv. Chem. Ser.*, **61**, 111–128 (1966).

octahedron, and icosahedron. Such polyhedra with triangular faces are called *deltahedra* since their faces are shaped like the Greek letter *delta*, Δ.

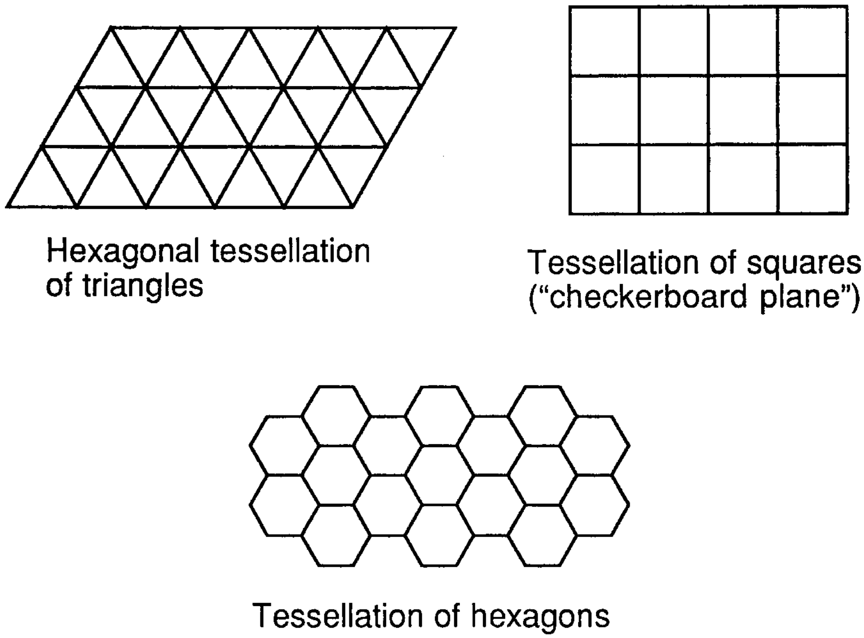

Figure 2–3: Examples of tessellations on a flat plane.

Additional regular solids can be formed from square or regular pentagonal faces. Vertices where three squares meet generate a cube whereas vertices where four squares meet generate a checkerboard plane (Figure 2–3). Vertices where three regular pentagons meet generate a regular dodecahedron; regular pentagons cannot form a tessellation. Regular hexagons with 120° angles can only form a tessellation and regular polygons with more than six sides have angles larger than 120° and thus cannot meet with two other equivalent polygons to form a solid angle at all.

The properties of the regular polyhedra are summarized in Table 2–2.

The regular polyhedra provide examples of pairs of dual polyhedra.[10] In this connection a given polyhedron P can be converted into its dual P^* by locating the centers of the faces of P^* at the vertices of P and the vertices of P^* above the centers of the faces of P. Two vertices in the dual P^* are connected by an edge when the corresponding faces in P share an edge. The process of dualization has the following properties:

(1) The numbers of vertices and edges in a pair of dual polyhedra P and P^* satisfy the relationships $v^* = f$, $e^* = e$, $f^* = v$.

(2) Dual polyhedra have the same symmetry elements and thus belong to the same symmetry point group.

(3) Dualization of the dual of a polyhedron leads to the original polyhedron.

(4) The degree of a vertex in a polyhedron corresponds to the number of edges in the corresponding face in its dual.

Examples of pairs of dual polyhedra among the regular polyhedra are the octahedron/cube dual pair with O_h symmetry (Figure 2–4) and the icosahedron/dodecahedron dual pair with I_h symmetry. The tetrahedron with T_d symmetry is self-dual (i.e., dual to itself). For example, a degree 3 vertex of a polyhedron corresponds to a triangular face in its dual.

Table 2–2: Properties of the Regular Polyhedra

Polyhedron	Face Type	Vertex Degrees	Number of Edges	Number of Faces	Number of Vertices
Tetrahedron	Triangle	3	6	4	4
Octahedron	Triangle	4	12	8	6
Cube	Square	3	12	6	8
Dodecahedron	Pentagon	3	30	12	20
Icosahedron	Triangle	5	30	20	12

[10] B. Grünbaum, *Convex Polytopes*, Interscience, London, 1967, pp. 46–48.

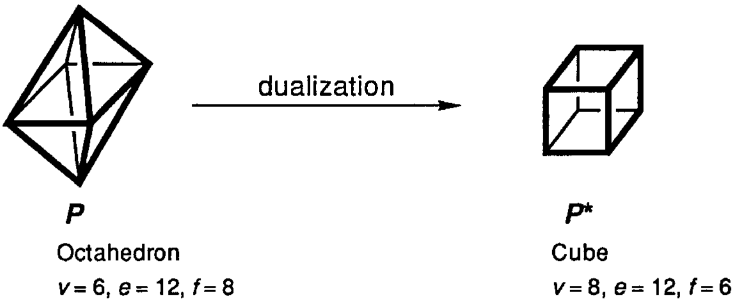

Figure 2–4: The process of dualization to convert an octahedron into a cube.

The regular icosahedron and its dual, the regular dodecahedron, have the I_h symmetry point group with 120 elements. Its pure rotation subgroup, I, with 60 elements is isomorphic with the alternating group A_5. The symmetry point group of the regular tetrahedron, T_d, is a subgroup of I_h of index 5 but *not* a normal subgroup. Nevertheless, the ability to partition an object of icosahedral symmetry into five equivalent objects of tetrahedral or octahedral symmetry ($O_h \approx T_d \times C_2$) is an essential part of the Kiepert algorithm for solution of the general quintic equation (Chapter 6).

There are several ways of visualizing the partition of an object of icosahedral symmetry into five equivalent objects of at least tetrahedral symmetry thereby separating the effect of the fivefold axis of the icosahedron from that of its twofold and threefold symmetry elements. The 20 vertices of the dual of the icosahedron, namely the regular dodecahedron, can be partitioned into five sets of four vertices, each corresponding to a regular tetrahedron. Using the same idea Klein[11] partitions the 30 edges of an icosahedron into five sets of six edges each by the following method (Figure 2–5):

(1) A straight line is drawn from the midpoint of each edge through the center of the icosahedron to the midpoint of the opposite edge;

(2) The resulting 15 straight lines are divided into five sets of three mutually perpendicular straight lines.

[11] F. Klein, *Vorlesungen über das Ikosaeder*, Teubner, Leipzig, 1884, Part I, Chapter I, § 8.

Each of these five sets of three mutually perpendicular straight lines resembles a set of Cartesian coordinates and defines a regular octahedron. The construction is the dual of a construction depicted by Du Val[12] in color in which a regular dodecahedron is partitioned into five equivalent cubes. Alternatively, the 30 edge midpoints of an icosahedron can be used to form an icosidodecahedron having 30 vertices, 60 edges, 32 faces, and retaining icosahedral symmetry. The 30 vertices of this icosidodecahedron can then be partitioned into five sets of six vertices, each corresponding to a regular octahedron (Figure 2–6).

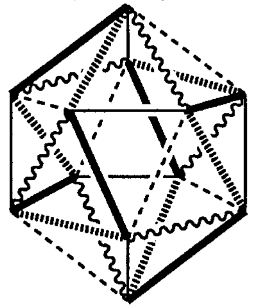

Figure 2–5: A regular icosahedron with its 30 edges partitioned into five sets of six edges each so that the midpoints of the edges in each set form a regular octahedron. The five sets of six edges each are indicated by the following types of lines:

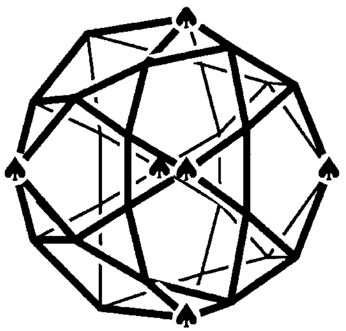

Figure 2–6: The icosidodecahedron formed from the 30 edge-midpoints of a regular icosahedron and the partitioning of its 30 vertices into five sets of six vertices, each corresponding to regular octahedra. The six vertices in one of these sets are indicated by spades (♠).

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[12]P. Du Val, *Homographies, Quaternions, and Rotations*, pp. 27–30 and Figs. 12–15, Oxford University Press, London, 1964.

2.4 Permutation Groups

The previous sections apply the concepts of group theory to symmetry point groups such as those describing the symmetry of readily visualized polyhedra. The concepts of group theory, of course, can be applied to more abstract sets such as the permutations of a set X of n objects, which, for example, may be the n roots of an algebraic equation of degree n. A set of permutations of n objects (including the identity permutation) with the structure of a group is called a *permutation group* of *degree n*.[13] Let G be a permutation group acting on the set X . Let g be any operation in G and x be any object in set X. The subset of X obtained by the action of all operations in G on x is called the *orbit* of x. The operations in G leaving x fixed is called the *stabilizer* of x; it is a subgroup of G and may be abbreviated as G_x. A *transitive* permutation group has only one orbit containing all objects of the set X. Sites permuted by a transitive permutation group are thus equivalent. Transitive permutation groups represent permutation groups of the highest symmetry and thus play a special role in permutation group theory.

The maximum number of distinct permutations of n objects is $n!$. The corresponding group is called the *symmetric* group of degree n and is traditionally designated as S_n (not to be confused with the designation S_n for an improper rotation of order n in Section 2.2). The symmetric group S_n is obviously the highest symmetry permutation group of degree n. All permutation groups of degree n must be a subgroup of the corresponding symmetric group S_n.

Let us now consider the structure of permutation groups. In this connection a permutation P_n of n objects can be described by a $2 \times n$ matrix of the following general type where the top row represents site labels and the bottom row represents object labels:

$$P_n = \begin{pmatrix} 1 & 2 & 3 & \dots & n \\ p_1 & p_2 & p_3 & \dots & p_n \end{pmatrix} \qquad (2.4\text{–}1)$$

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[13] N. L. Biggs, *Finite Groups of Automorphisms*, Cambridge University Press, London, 1971.

The numbers $p_1, p_2, p_3, \ldots, p_n$ can be taken to run through the integers 1, 2, 3,...,n in some sequence. For a given n there are $n!$ possible different $\boldsymbol{P_n}$ matrices. The matrix $\boldsymbol{P_n}^0$ in which the bottom row $p_1, p_2, p_3, \ldots, p_n$ has the integers in the natural order 1, 2, 3,...,n (i.e., the bottom row of $\boldsymbol{P_n}^0$ is identical to the top row) can be taken to represent a reference configuration corresponding to the identity element in the corresponding permutation group.

Permutations can be classified as *odd* or *even* permutations based on how many *pairs* of numbers in the bottom row of the matrix $\boldsymbol{P_n}$ are out of their natural order. Alternatively, if the interchange of a single pair of numbers is called a *transposition*, the parity of a permutation corresponds to the parity of the number of transpositions. Thus a permutation which is obtained by an odd number of transpositions from the reference configuration is called an *odd* permutation and a permutation which is obtained by an even number of transpositions from the reference configuration is called an *even* permutation. The identity permutation corresponding to the reference configuration has zero transpositions and is therefore an even permutation by this definition.

A group can be defined relating the $\boldsymbol{P_n}$ matrices for a given n. First redefine the rows of $\boldsymbol{P_n}$ so that the top row represents the reference configuration $\boldsymbol{P_n}^0$ and the bottom row represents the object labels in any of the $n!$ possible permutations of the n objects. These permutations form a group of order $n!$ with the permutation leaving the reference configuration unchanged (i.e., that represented by $\boldsymbol{P_n}^0$ as so redefined) corresponding to the identity element, E. This permutation group is the symmetric group, S_n, of order $n!$ as defined above.

Now consider the nature of the operations in a symmetric permutation group S_n. These operations are permutations of labels which can be written as a product of cycles which operate on mutually exclusive sets of labels, e.g.

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 4 & 5 & 1 & 3 & 6 \end{pmatrix} = (1\ 2\ 4)(3\ 5)(6) \tag{2.4–2}$$

The cycle structure of a given permutation in the symmetric group S_n can be represented by a sequence of indexed variables, i. e., $x_1 x_2 x_3$ for the permutation in equation 2.4–2. A characteristic feature of the symmetric permutation group S_n for all n is that all permutations having the same cycle structure come from the same conjugacy class.[14] Furthermore, no two permutations with different cycle structures can belong to the same conjugacy class. Therefore, for the symmetric permutation group S_n (but not necessarily for any of its subgroups) the cycle structures of permutations are sufficient to define their conjugacy classes. Furthermore, the number of conjugacy classes of the symmetric group S_n corresponds to the number of different partitions of n where a *partition of n* is defined as a set of positive integers $i_1, i_2, \ldots, i_k$ whose sum is n (equation 2.4–3).

$$\sum_{j=1}^{k} i_j = n \tag{2.4–3}$$

An alternative presentation of conjugacy class information for the symmetric groups S_n is given by their cycle indices.[15,16,17] A *cycle index* $Z(S_n)$ for a symmetric permutation group S_n is a polynomial of the following form:

$$Z(S_n) = \sum_{i=1}^{i=c} a_i x_1^{c_{i1}} x_2^{c_{i2}} \ldots x_n^{c_{in}} \tag{2.4–4}$$

In equation 2.4–4 c = number of conjugacy classes (i.e., partitions of n by equation 2.4–3), a_i = number of operations of S_n in conjugacy class i, x_j = dummy variable referring to cycles of length j, and c_{ij} = exponent indicating the number of cycles of length j in class i. These parameters in the cycle indices of the symmetric groups S_n must satisfy the following relationships:

(1) Each of the $n!$ permutations of S_n must be in some class, i.e.,

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[14] C. D. H. Chisholm, *Group Theoretical Techniques in Quantum Chemistry*, Academic Press, New York, 1976, Chapter 6.
[15] G. Pólya, Kombinatorische Anzahlbestimmungen für Gruppen, Graphen, und Chemische Verbindungen, *Acta Math.*, **68**, 145 (1937).
[16] G. Pólya and R. C. Reed, *Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds*, Springer Verlag, New York, 1987.
[17] N. G. Debruin in *Applied Combinatorial Mathematics*, E. F. Beckenbach, Ed., Wiley, New York, 1964, Chapter 5.

$$\sum_{i=1}^{i=c} a_i = n! \tag{2.4–5}$$

(2) Each of the n objects being permuted must be in some cycle of each permutation in S_n (counting, of course, fixed points of cycles of length 1 represented by $x_1^{c_1}$), i.e.,

$$\sum_{j=1}^{j=n} j c_{ij} = n \text{ for } 1 \le i \le c \tag{2.4–6}$$

The relationship between symmetry point groups and permutation groups as well as some important concepts can be illustrated by the symmetry point groups of the tetrahedron and trigonal bipyramid and the corresponding permutation groups on their vertices (Figure 2.7). The permutation group of the tetrahedron vertices is a transitive group since all four vertices are equivalent. However, the permutation group of the trigonal bipyramid vertices is an intransitive group partitioning its five vertices into two orbits, namely the two axial vertices (A in Figure 2.7) and the three equatorial vertices (E in Figure 2.7).

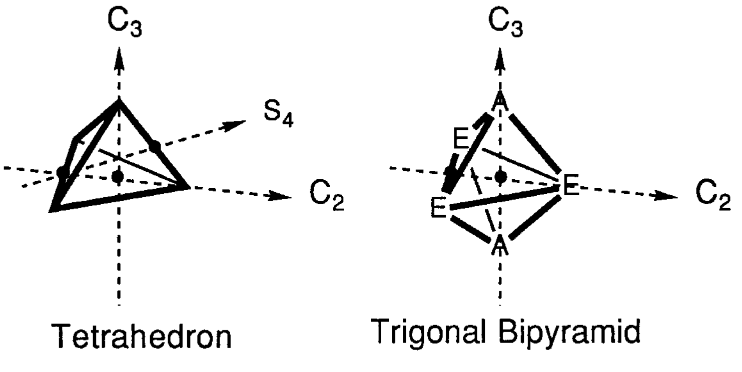

Figure 2.7: The tetrahedron and the trigonal bipyramid showing the proper and improper rotation axes (Note that S_4 refers to an improper rotation axis of order 4 rather than the symmetric permutation group on four objects). The axial (A) and equatorial vertices (E) of the trigonal bipyramid are also shown.

Let us now consider some of the properties of the symmetric permutation groups, S_n. Any symmetric permutation group S_n has a normal subgroup of index 2 (and thus of order $n!/2$) consisting of only the permutations of even parity (which necessarily includes the identity permutation). This special subgroup of S_n is called the *alternating group* and is designated as A_n. The symmetric permutation group S_4 is isomorphic with the full tetrahedron symmetry point group of order $4! = 24$, T_d, (Figure 2.7) whereas the alternating permutation group A_4 is isomorphic with the tetrahedral proper rotation subgroup T of order $4!/2 = 12$. The corresponding chain of normal subgroups for S_4 is $C_1 \lhd C_2 \lhd D_2 \lhd A_4 \equiv T \lhd S_4 \equiv T_d$ with the quotient groups $C_2/C_1 = C_2$; $D_2/C_2 = C_2$; $A_4/D_2 = C_3$; $S_4/A_4 = C_2$.

The problem of solving the general quintic equation relates to the fact that the alternating group A_5 is a simple group. This can be proved by showing that A_5 has no normal subgroups and that A_5 is the only normal subgroup of S_5. The proof of this fact can be related to the symmetries of the icosahedron (e.g., Figure 2.5). Thus the 60 permutations of A_5 can be partitioned into the following classes:

(1) The identity;

(2) 24 cycles of period 5 such as (12345), each of these corresponding to a rotation through $2\pi k/5$ ($k = 1, 2, 3, 4$) around a diameter passing through opposite vertices of the icosahedron;

(3) 20 cycles of period 3 such as (123), each of these corresponding to a rotation through $\pm 2\pi/3$ around a diameter passing through midpoints of opposite faces of the icosahedron;

(4) 15 double transpositions of period 2 such as (12)(34) corresponding to half turns around a diameter passing through midpoints of opposite edges of the icosahedron.

A normal subgroup of a group G consists of *entire* conjugacy classes of G. For this reason the order of a *normal* subgroup of A_5 must be of the form $1 + 24n_5 + 20n_3 + 15n_2$ where n_5, n_3, and n_2 are each 0 or 1 (but not all 0 nor all 1). But this number must be a factor of 60 and thus must be 30, 20, or 15, which is clearly impossible. Thus the alternating group A_5 cannot have any normal subgroups.

A similar argument can be used to show that A_5 is the only normal subgroup of S_5. Furthermore all A_n ($n \geq 6$) can also be shown to be simple groups.

The transitive groups of low degrees are particularly significant in the theory of permutation groups and the theory of solution of algebraic equations. The transitive groups of degrees up to eleven have been tabulated and their properties are given in detail.[18] All of the transitive permutation groups of degree ≤ 7 are listed in Table 2–3.

The following points about Table 2–3 are of interest:

(1) In the groups C_n the order is the same as the number of classes; therefore these groups are Abelian.

(2) The groups $C_3, C_4, A_4 \equiv T, C_5, A_5 \equiv I$, and A_6 contain only even operations.

(3) The groups M_5 and M_7 are *metacyclic* groups of degrees 5 and 7, respectively. For prime n, metacyclic groups of order $n(n + 1)$ are the largest permutation groups of degree n which are soluble groups. A metacyclic group is defined in terms of two generators s and t and the relationships $s^p = t^{p-1} = E$ and $t^{-1}st = s^r$ where p is a prime (5 in the case of M_5) and r is a primitive root (mod p) which is 2 when $p = 5$.[3]

(4) The dihedral group D_3 can be a transitive permutation group of either degree 3 or 6. Similarly, the tetrahedral rotation group T of order 24 can be a transitive permutation group of either degree 4 (e.g., the faces of a tetrahedron) where it is the alternating group A_4 or degree 6 (e.g., the edges of a tetrahedron). In addition, the icosahedral rotation group I of order 60 can be a transitive permutation group of either degree 5 where it is the alternating group A_5 (see Section 2.3 and Figures 2–5 and 2–6 for more details) or degree 6 permuting the six diameters of the icosahedron connecting pairs of antipodal vertices.

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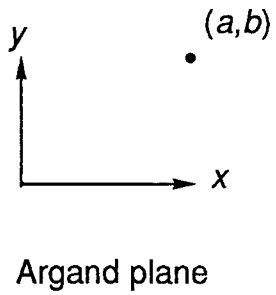
[18] G. Butler and J. McKay, The Transitive Groups of Degree up to Eleven, *Communications in Algebra*, 11, 863–911 (1983).

Table 2–3: Transitive Permutation Groups of Degrees Less than Eight

Group	Degree	Order	Number of Classes	Special Properties
C_3	3	3	3	Even, Abelian
$D_3 \equiv S_3$	3	6	3	Dihedral, Symmetric
C_4	4	4	4	Abelian
D_2	4	4	4	Even, Abelian
D_{2d}	4	8	5	
$A_4 \equiv T$	4	12	4	Even
$S_4 \equiv T_d$	4	24	5	Symmetric
C_5	5	5	5	Even, Abelian
D_5	5	10	4	Dihedral
M_5	5	20	5	Metacyclic
$A_5 \equiv I$	5	60	5	Even, Simple
S_5	5	120	7	Symmetric,**Not I_h!**
C_6	6	6	6	Abelian
D_3	6	6	3	
D_6	6	12	3	Dihedral
$A_4 \equiv T$	6	12	4	Even
	6	18	9	
	6	24	8	
	6	24	5	Even
	6	24	5	Isomorphic to T_d
	6	36	9	
	6	36	6	
	6	48	10	
$L(2,5) \equiv I$	6	60	5	
	6	72	9	
	6	120	7	Isomorphic to S_5
A_6	6	360	7	Even, Simple
S_6	6	720	11	Symmetric
C_7	7	7	7	Even, Abelian
D_7	7	14	5	Dihedral
	7	21	5	Even
M_7	7	42	7	Metacyclic
$L(3,2)$	7	168	6	Even, Simple
A_7	7	2520	9	Even, Simple
S_7	7	5040	15	Symmetric

2.5 Polyhedral Polynomials

The usual type of convex polyhedra, including the regular polyhedra discussed in Section 2.3, can be represented as points on the surface of a sphere. The same sphere, taken as a special unit sphere called the *Riemann sphere*, can also be used to represent the complex numbers $z = a + bi$ thereby providing a method for generating special polynomials associated with a given polyhedron. First represent the complex numbers $z = a + bi$ by points on the (x,y) plane with the x-coordinate corresponding to a and the y-coordinate corresponding to b; such a plane is called an *Argand plane* (Figure 2–8a). The Argand plane can correspond to the equatorial plane of the *Riemann sphere*, (Figure 2–8b) in which the north pole is ∞ and the south pole is 0; the 0–∞ axis can be called the *polar axis*.[19] The equation of the Riemann sphere is taken to be $p^2 + q^2 + r^2 = 1$.



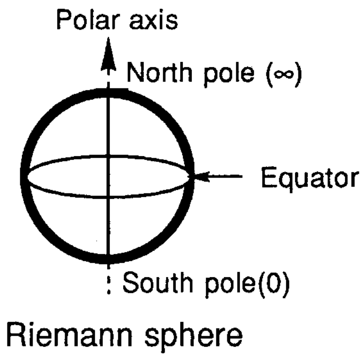


Figure 2–8: (a) The Argand plane indicating the point for $z = a + bi$; (b) The Riemann sphere.

The polyhedral polynomials are polynomials whose roots correspond to the locations of the polyhedral vertices, the midpoints of the polyhedral edges, or the midpoints of the polyhedral faces on the surface of the Riemann sphere.

[19]F. Klein, *Vorlesungen über das Ikosaeder*, Teubner, Leipzig, 1884, Part I, Chapter II.

Polyhedral polynomials are frequently expressed in terms of *homogeneous variables* so that all terms are the same combined degree in two variables, i.e.,

$$\sum_{i=1}^{n} a_{n-i}x^i = \sum_{i=1}^{n} a_{n-i}u^i v^{n-i} \tag{2.5–1}$$

The use of homogeneous variables corresponds to the substitution $x = u/v$. The special symmetry of the regular polyhedra corresponds to the vanishing of some special functions of these polyhedral polynomials known as *transvectants* (Section 2.6).

Now consider the projection of points on the Riemann sphere onto its equatorial plane, taken as an Argand plane as noted above (Figure 2–8). A complex number $z = a + bi$ gives

$$a = \frac{p}{1-r}\ ,\ b = \frac{q}{1-r}\ ,\ a + bi = \frac{p+iq}{1-r} \tag{2.5–2}$$

Solving for p, q, and r gives

$$p = \frac{2a}{1+a^2+b^2}\ ,\ q = \frac{2b}{1+a^2+b^2}\ ,\ r = \frac{-1+a^2+b^2}{1+a^2+b^2} \tag{2.5–3}$$

Every rotation of the Riemann sphere around its center corresponds to a linear substitution

$$z' = \frac{\alpha z + \beta}{\gamma z + \delta} \tag{2.5–4}$$

For a rotation of the sphere by an angle θ where p, q, r and $-p, -q, -r$ remain constant,

$$z' = \frac{(v+iu)z - (t-is)}{(t+is)z + (v-iu)} \tag{2.5–5}$$

where $s = p\sin(\theta/2)$, $t = q\sin(\theta/2)$, $u = r\sin(\theta/2)$, and $v = \cos(\theta/2)$ so that

$$s^2 + t^2 + u^2 + v^2 = 1 \tag{2.5–6}$$

For a rotation about the polar axis this reduces to

$$z' = e^{i\theta}z \tag{2.5–7}$$

Now consider the vertices of a regular octahedron and a regular icosahedron as points on the surface of such a Riemann sphere oriented such that the north pole ($z = \infty$) is one of the vertices in each case. This leads to the following homogeneous polynomials for these regular polyhedra in these orientations where z is taken to be u/v.[20]

(a) Octahedron (O_h symmetry):

Vertices: $\tau = uv(u^4 - v^4)$ (2.5–8a)

Edges: $\chi = u^{12} - 33u^8v^4 - 33u^4v^8 + v^{12}$ (2.5–8b)

Faces: $W = u^8 + 14u^4v^4 + v^8$ (2.5–8c)

(b) Icosahedron (I_h symmetry):

Vertices: $f = uv(u^{10} + 11u^5v^5 - v^{10})$ (2.5–9a)

Edges: $T = u^{30} + 522u^{25}v^5 - 10{,}005\, u^{20}v^{10} - 10{,}005\, u^{10}v^{20} - 522\, u^5v^{25} + v^{30}$ (2.5–9b)

Faces: $H = -u^{20} + 228\, u^{15}v^5 - 494\, u^{10}v^{10} - 228\, u^5v^{15} - v^{20}$ (2.5–9c)

The roots of these polyhedral polynomials correspond to the locations of the vertices, edge midpoints, and face midpoints on the Riemann sphere. Their degrees are equal to the numbers of corresponding elements (vertices, edges, or faces).

The following features are of interest concerning the polyhedral polynomials such as those in equations 2.5–8 and 2.5–9:

(1) The vertices of a regular polygon with n vertices in the equatorial plane with one vertex at $z = 1$ correspond to the n roots of unity.

(2) Derivation of the vertex polynomial of the octahedron, $\tau(u,v)$, is particularly obvious. Orientation of an octahedron so that two of the vertices are at the poles ($z = 0,\infty$) and one vertex is at $z = 1$ (Figure 2–9) forces the other three vertices to be at $z = -1$, i, and $-i$ so that

$$\tau = z(z-1)(z+1)(z-i)(z+i) = z(z^4-1) = uv(u^4 - v^4) \tag{2.5–10}$$

after converting to homogeneous variables by $z = u/v$.

[20]L. E. Dickson, *Modern Algebraic Theories*, Sanborn, Chicago, 1930, Chapter 13.

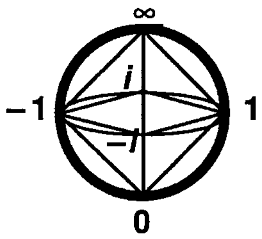


Figure 2–9: Orientation of the regular octahedron inside the Riemann sphere.

(3) The vertex and face polynomials of a polyhedron correspond to the face and vertex polynomials, respectively, of its dual. Thus the vertex polynomial τ (equation 2.5–8a) and face polynomial W (equation 2.5–8c) of the octahedron corresponds to the face polynomial and vertex polynomial, respectively, of its dual, namely the cube.

(4) A cube can be composed of two mutually dual tetrahedra, whose edges correspond to face diagonals of the cube (Figure 2–10). A single tetrahedron in this orientation has the following polynomial functions:

Vertices: $\Phi = u^4 + 2\sqrt{-3}\,u^2v^2 + v^4$ (2.5–11a)

Edges: $\tau = uv(u^4 - v^4)$ (2.5–11b)

Faces: $\Psi = u^4 - 2\sqrt{-3}\,u^2v^2 + v^4$ (2.5–11c)

Note that the tetrahedron edge polynomial (equation 2.5–11b) is the same as the octahedron vertex polynomial (equation 2.5–8a) since the midpoints of the six edges of the tetrahedron in this orientation are in the same locations ($z = 0, \infty, \pm 1, \pm i$) as the six vertices of the standard octahedron. Furthermore, the face polynomial Ψ of the tetrahedron is the same as the vertex polynomial of its dual. Since the four vertices of the tetrahedron and the four vertices of its dual together make the eight vertices of a cube, the product of the vertex functions of the two tetrahedra equals the vertex function of the cube made by the two tetrahedra $\Phi\Psi = W$.

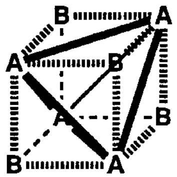


Figure 2–10: Decomposition of a cube into two tetrahedra, whose vertices are indicated by **A** and **B**. The edges of the **A** tetrahedron are shown to the extent that they are visible.

---

(5) The special symmetries of the regular deltahedra lead to the following identities:

Tetrahedron: $12\sqrt{-3}\,\tau^2 - \Phi^3 + \Psi^3 \equiv 0$ (degree 12) (2.5–12a)

Octahedron: $108\,\tau^4 - W^3 + \chi^2 \equiv 0$ (degree 24) (2.5–12b)

Icosahedron: $1728 f^5 - H^3 - T^2 \equiv 0$ (degree 60) (2.5–12c)

Note that the degrees of the left side of the identities (2.5–12) in (u,v) correspond to the orders of the pure rotation groups of the corresponding deltahedra, which are isomorphic to the permutation groups relevant to the solution of algebraic equations, i.e., $\mathrm{O} \approx S_4$ for the quartic equation and $\mathrm{I} \approx A_5$ for solution of the quintic equation. In this connection the icosahedral identity (equation 2.5–12c) will be seen to be important for the solution of the quintic equation.

2.6 Transvectants of Polyhedral Polynomials

The polyhedral polynomials in homogeneous form can be related by their transvectants derived from their partial derivatives by means of invariant theory.[21,22] In this connection the nth transvectant of two homogeneous polynomials $f(x,y)$ and $g(x,y)$, designated as $(f,g)^n$ is defined by the equation

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[21] J. H. Grace and A. Young, *The Algebra of Invariants*, Cambridge, 1903.

[22] O. E. Glenn, *A Treatise on the Theory of Invariants*, Ginn and Co., Boston, 1915.

$$(f,g)^n = \sum_{k=1}^{n} (-1)^k \left(\frac{n!}{k!(n-k)!}\right)\left(\frac{\partial^n f(x,y)}{\partial x^{n-k}\partial y^k}\right)\left(\frac{\partial^n g(x,y)}{\partial x^k \partial y^{n-k}}\right) \qquad (2.6\text{–}1)$$

Of particular interest are the transvectants of a polynomial with itself, i.e., $(f,f)^n$.

Odd transvectants of the type $(f,f)^n$ (n = 1, 3, 5, 7,...) vanish since they have *even* numbers of terms of alternating sign which cancel out completely corresponding to the $(-1)^k$ factor in equation (2.6–1). The first transvectant $(f,g)^1$ is also known as the *functional determinant* of f and g, since it can be expressed by the determinant

$$(f,g)^1 = \begin{vmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{vmatrix} \qquad (2.6\text{–}2).$$

The second transvectants $(f,g)^2$ are also known as *Hessians* and can also be expressed by the determinant

$$(f,g)^2 = \begin{vmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 g}{\partial y \partial x} & \frac{\partial^2 g}{\partial y^2} \end{vmatrix} \qquad (2.6\text{–}3).$$

Let v, e, and f, be the number of vertices, edges, and faces of regular deltahedra, namely the tetrahedron, octahedron, and icosahedron. The functional determinants and Hessians relate the vertex ($\mathcal{V}(u,v)$ of degree v), edge ($\mathcal{E}(u,v)$ of degree e), and face ($\mathcal{F}(u,v)$ of degree f) functions by the following relationships where $k_{v,v}$ and $k_{v,f}$ are integers:

$$(\mathcal{V},\mathcal{V})^2 = k_{v,v}\,\mathcal{F} \qquad (2.6\text{–}4a)$$

$$(\mathcal{V},\mathcal{F})^1 = k_{v,f}\,\mathcal{E} \qquad (2.6\text{–}4b)$$

The fact that each differentiation step lowers the degree of the polynomial by 1 can be used to relate equation (2.6–4b) to Euler's theorem[23] as follows:

$$\deg(\mathcal{V},\mathcal{F})^1 = (v-1)+(f-1) = \deg(\mathcal{E}) = e$$

$$\Rightarrow v+f-2 = e \text{ corresponding to Euler's theorem.} \qquad (2.6\text{–}5)$$

Similarly from equation (2.6–4a)

$$\deg\,(\mathcal{V},\mathcal{V})^2 = 2(v-2) = 2v-4 = f. \qquad (2.6\text{–}6).$$

For a deltahedron in which all faces are triangles

$$3f = 2e \Rightarrow e = {}^3/_2 f \qquad (2.6\text{–}7)$$

so that Euler's theorem becomes

$$v+f-2 = {}^3/_2 f \Rightarrow 2v-4 = f \qquad (2.6\text{–}8)$$

Note the resemblance of equations (2.6–6) and (2.6–8).

A special feature of the vertex polynomials for regular deltahedra, namely τ of equation (2.5–8a) for the octahedron, f of equation (2.5–9a) for the icosahedron, and Φ of equation (2.5–11a) for the tetrahedron is the identical vanishing of their fourth transvectants, i.e., $(\tau,\tau)^4 \equiv 0$, $(f,f)^4 \equiv 0$, and $(\Phi,\Phi)^4 \equiv 0$, respectively. This is a special indication of the symmetry of the regular deltahedra.

Figure 2–11 illustrates the procedure for calculating the second and fourth transvectants $(\tau,\tau)^2$ and $(\tau,\tau)^4$ of the octahedral vertex function $\tau = uv(u^4-v^4)$. Note that the Hessian $(\tau,\tau)^2$ is a multiple of the corresponding face function, namely $-25W$ whereas the fourth transvectant $(\tau,\tau)^4$ vanishes identically.

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[23]B. Grünbaum, *Convex Polytopes*, Interscience Publishers, New York, New York, 1967, pp 130–142.

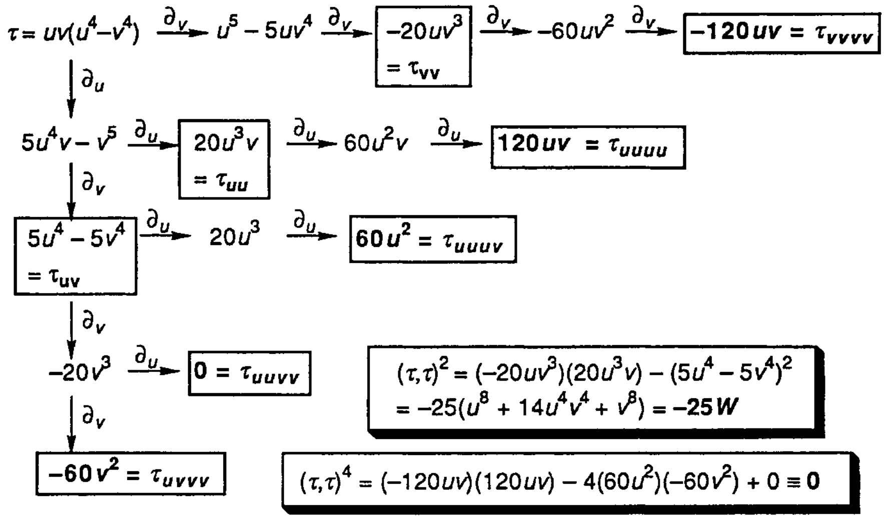

Figure 2–11: Illustration of the calculation of the second transvectant $(\tau,\tau)^2$ and the fourth transvectant $(\tau,\tau)^4$ of the octahedral vertex function $\tau = uv(u^4-v^4)$. Subscripts indicate differentiation variables and ∂_u and ∂_v indicate differentiation with respect to u and v, respectively.

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