QUATERNION REPRESENTATION OF CRYSTAL POINT GROUPS

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QUATERNION REPRESENTATION OF CRYSTAL POINT GROUPS

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CHAPTER I

INTRODUCTION

The physical behavior of crystalline solids is very closely related to the internal symmetry of the crystal structure. For this reason it is desirable to represent mathematically this symmetry in such a way that the actual physical problems can be handled as they arise. Such representations are not unknown and the literature is quite extensive. However, there are certain very desirable properties which are not all present in any one of the pre-existing mathematical techniques. For this reason there has been a continuous search for a better method of mathematically representing crystal symmetry. In the case of this thesis the research has been guided by a list of desired properties for such a representation. No claim is made that the list is complete. This list appears later in the chapter.

It was found that the symmetry can be represented by simple operators constructed from the quaternion number system.

It should be noted at the outset that this research is restricted to the type of symmetry used in classifying
crystals into the 32 crystal classes. This is the crystal symmetry most closely related to the observed physical properties of crystals. It is described in terms of rotations, reflections, inversions, etc. Mathematical techniques for representing this symmetry involves the use of symmetry operators.

The set of operators for a particular crystal class form a mathematical group called a crystal point group. Thus there are 32 crystal point groups. The concepts of rotation, reflection, inversion, group, operator, crystal point group, etc. will be explained later in this chapter.

There is a more subtle type of symmetry which leads to a further subdivision of the 32 crystal classes into 230 space groups. Such symmetry is represented mathematically by combining translations with the operations of a crystal point group. In the quaternion representation developed in this paper the translations would be represented by vectors as is done in existing representation. For the point group part of the space group operator the tensor would be replaced by a quaternion operator. The resulting space group operator appears promising, but no investigation in this direction has been made.

A feature of the quaternion system which entered in its being chosen but which is not exploited in this thesis is
that its four-dimensional nature and algebraic structure permit its 'extra' dimension to be used to represent time. This was done by Hamilton, and later others used quaternions for the four-dimensional space of special relativity.

About 1845, Hamilton discovered quaternions as a generalization of the imaginary numbers. This type of system has the unique property that it has one real coordinate and three imaginary coordinates. These are often referred to as the scalar part and the vector part. The scalar part (or the real part) can be reserved as the time coordinate in four-space and the vector part (or imaginary part) is used for the space coordinates of the crystal.

Operations on quaternions are similar to the operations on ordinary complex numbers. Using complex numbers in the two-dimensional space will help one to understand the idea of symmetry operations. The similarity of the operations on the complex numbers to the operations on the quaternions is a desirable property of the system since it aids in obtaining and applying the operator group or groups required in the physical problem.

Crystal Point Groups

Metals, ice, rock salt, and many other solids are composed of small crystals fitted closely together. The macroscopic physical properties of the solid are strongly related to and determined by the microscopic properties of
the particular kind (or kinds) of crystal which constitute the system. These properties are in turn related to the symmetry in the arrangement of the atoms of the crystal. Some properties are present only in crystals having certain types of symmetry.

When conditions are favorable, crystals can grow large enough to be handled with ease, and if the environment does not crowd the crystal during growth, it has a pleasingly symmetrical shape. This shape results from an interior symmetry and repetitivity in the arrangement of the atoms forming the crystal.

A lattice is defined as a repetitive, parallel net-like arrangement of points in space. The environment about any particular point is in every way the same as about any other point. It is essential that a lattice is not confused with the crystal structure. The crystal structure is formed by associating with every lattice point a unit assembly of the atoms making up the crystal. This unit assembly must be identical in composition, arrangement, and orientation. The crystal lattice can then be defined as the symmetrical arrangement in space of the unit assembly. The unit assembly may be a molecule, which in turn is a combination of atoms. It must also be understood that the operations are not to be performed on the crystal structure but upon the crystal lattice points. The point group can now be defined as the collection of symmetry operations which does not change any
of the physical characteristics of the crystal, including the arrangement of the interior structure and orientation of the unit assemblies.

Mathematical Groups

A mathematical group may be defined as a set of elements and a binary operation $O$ which obey the following laws:

(1). For every element $x$ and $y$ in the set, $xOy$ is also an element of the set,

(2). For every element $x$, $y$, and $z$ in the set, $xO(yOz) = (xOy)Oz$,

(3). There exists a unique element $e$, such that $xOe = eOx = x$, and

(4). There exists, for every element $x$ in the set, a unique element $y$ (denoted by $x^{-1}$) such that $xOy = e = yOx$.

A simple example of a mathematical group is the set of all positive integers and the ordinary addition operation. In fact, this is precisely the method of obtaining all of the positive integers. This particular example has an infinite number of elements, but the operation groups that pertain to crystal lattice points are finite in number.

Requirements of the Mathematical Group

The mathematical group must be able to generate the symmetrical arrangement of the crystal lattice points but
leave the physical characteristics invariant, or unchanged. This requirement is better illustrated with the aid of Figure 1. In the figure, the point at the bottom of the v's represents the crystal lattice points, while the v itself represents the unit assembly of atoms. The v's in the figure are assumed to extend indefinitely in any direction in the plane of the paper with the same basic spacing and with the same orientation.

\[
\begin{array}{ccccccccc}
  & & & & & & & & & \\
  & v & v & v & v & v & v & v & v & v \\
  & v & v & v & v & v & v & v & v & v \\
  & v & v & v & v & v & v & v & v & v \\
  & v & v & v & v & v & v & v & v & v \\
  & v & v & v & v & v & v & v & v & v \\
\end{array}
\]

Fig. 1--The translation group

Consider the point A in Figure 1. If this point is moved to the point B, then the structure looks and is physically the same, since all the atoms in this array are bound together to form the whole, every atom will also be moved one v-distance to the right. This simple operation is called a translation and the set of all translations form what is called the translation group. This is not a symmetry operation and is used here to illustrate the idea of changing the points of the system and leaving the physical situation unchanged. The translation can be used to show how the rotations are restricted. The physical situation is unchanged as there is no distinction in the physical
properties of the unit assembly at the point A and the point B. Note there are other directions of translation.

If we now rotate the whole array 180° about the point C with the axis of rotation perpendicular to the plane of the paper in either direction, the point A replaces the point E and the point B replaces the point D. But in the process, the points of the v's are now at the top, or the v's are up-side down. In this case, the physical situation is not the same, thus, a rotation of the points about the axis at C (or any other axis) will not be an operation for this type of array. An array (or structure) such as this is said to have no rotational symmetry, nor does it have reflection symmetry.

If we rotate the array of Figure 2 about the axis at C, perpendicular to the paper, 180° as before, the points at A, B, D, and E are now not distinguishable one from the other, so that the physical situation is invariant.

```
  . . . . . . . . .
  . . . . . D, E . .
  . . . . A, B . . .
  . . . . . . . . .
```

Fig. 2--Rotation group

Figure 2 is an example of a 180° rotation about the point C. It must be noted that the distance from the point A to the axis at C and the distance from the point
E to the axis at C are the same. Likewise, C is the point midway between the points B and D.

If we operate on the point A with the 180° rotation operator, then the result is the point E. In mathematics, if 0 is the operator, the 0A = E. This, then, is the basic idea of the symmetry operators.

The array in Figure 2 has rotation symmetry but it does not have reflection symmetry. If the points are arranged as in Figure 3, then we see that the system of points has both a translation group and a rotation group. All crystal structures must have a translation group.

Consider the plane along the line D and perpendicular to the plane of the paper. This line is equidistant from the nearest points to the plane and on either side of the plane. The points of this figure are assumed to extend indefinitely in both directions of the paper.

```
 o  o  o  o  |  o  o  o  o  E
 o  o  o  Ao  |  oC  o  o  o
 o  o  o  Bo  |  o  o  o  o  D
 o  o  o  o  |  o  o  o  o
```

Fig. 3—Reflection group

The point A is the mirror image of the point B and vice versa. In fact, it is easily seen from Figure 3 that every point above the line D is the mirror image of a point below the line D. A similar situation exists with
the line E. The line D is midway between the points A and B and the line E is midway between the points A and C.

Thus, if we use a reflection operator through D on the point A, we obtain the point B. In the language of mathematics, if \( R_d \) is the reflection operator, then \( R_dA = B \). Also for the line E, if \( R_e \) is the reflection operator, then \( R_eA = C \). The set of all reflection operators is called the reflection operator group or the reflection group.

If we operate twice in succession on the same point, then the result must be the same as one operation on the point. This is true by law (1) of the definition of group. Suppose we operate on the point A in Figure 4 with the two-fold rotation operator and without stopping we use the reflection operator on the result of the first operation on A. In Figure 4, the points designated by the dots (.) are above the plane of the paper and the points designated by the circles (o) are below the plane of the paper and at the same distance above and below. This is, therefore, a three-dimensional structure. If \( 0 \) is the two-fold rotation operator about the axis at C and perpendicular to the plane of the paper and \( R \) is the reflection operator through the plane of the paper, then \( R(0A) = (R0)A = B \). It can be seen in Figure 4 that if we first reflect the point A directly below the paper and then rotate that
result 180° about C, we arrive at B once again, or
O(RA) = (OR)A = B. Since B = (RO)A and B = (OR)A,
(RO)A = (OR)A. In this case the two results are the
same and the operators are said to commute, but this is
not generally true.

\[ \ldots \]

\[ \ldots \]

\[ \ldots \]

\[ A \ldots \]

\[ C \]

\[ o \quad o \quad o \quad B o \]

\[ o \quad o \quad o \quad o \]

Fig. 4—Inversion group

The combined operator \((RO) = (OR) = V\) is called the
inversion operator. This operator gives symmetry in three-
space through the origin. The two-dimensional two-fold
rotation operator is sometimes called an inversion operator
but it must be remembered that this interpretation is
necessarily restricted to the two-dimensional case alone.

From the definition of a group, any two operations in
succession is an element, or an operation, of the group,
so that the inversion operation is not the only other
operation that can be obtained in this manner. The others
will be considered as the need arises. The result of
applying twice any one of the operators considered thus
far is to give the original point, or, putting this fact
into the form of a mathematical equation, we have
\[ O(OA) = (00)A = O^2A = A = IA, \]
\[ R(RA) = (RR)A = R^2A = A = IA, \]
and \[ V(VA) = (VV)A = V^2A = A = IA. \]

I is called the identity operator, that is, when I operates on any point, the point is not changed in position at all. I corresponds to \( e \) in law (3) of the definition of a group. Hence I is also an element of the group.

The examples which were given were quite simple and it must be understood that, in general, the reflection can be through any plane whatsoever and the rotation can be about any axis and of any amount. Even though the mathematical operators are not restricted in any manner, the crystal point groups impose certain limitations upon them.

Restrictions Imposed upon the Operators by the Crystal Point Groups

The reflection planes and the rotations are necessarily restricted by the crystal symmetry. Even though it is difficult to state any exact restrictions on the reflection planes (or mirror planes), they generally follow the same pattern as the rotation operators. The reflection planes are found to be at angles of \( 60^\circ \), \( 90^\circ \), and \( 120^\circ \) to each other.

By using the translation operator, it can be shown\(^1\) that the rotation operators are restricted to angles which

are multiples of $2\pi/n$, where $n = 1, 2, 3, 4, \text{ and } 6$. In other words, the rotations are restricted to two-fold, three-fold, four-fold, and six-fold rotations. A one-fold could be included in the above, but this is merely a rotation of $360^\circ$. The n-fold rotation follows the same pattern of the two-fold rotation. Figure 5 shows a six-fold rotation about the axis perpendicular to the plane of the paper and at the center of the hexagon formed by the equivalent points, $o$.

![Six-fold rotation and equivalent points](image)

**Fig. 5—Six-fold rotation and equivalent points**

From Figure 5, the following results of the six-fold rotation operator, $R_6$, are easily seen:

- $R_6(A) = B,$
- $R_6(B) = R_6^2(A) = C,$
- $R_6(C) = R_6^3(A) = D,$
- $R_6(D) = R_6^4(A) = E,$
- $R_6(E) = R_6^5(A) = F,$
- $R_6(F) = R_6^6(A) = A.$
It is also seen from the figure that \( R_6^3(A) = R_2(A) \), where \( R_2 \) is the two-fold rotation operator about the same axis.

Properties Desired of the Symmetry Operators

The use of the symbols \( R_6, R_6^2, \) etc., in the previous discussion are satisfactory for a description of a particular symmetry group. However these give only an abstract description of the group and have no connection with the environment in which the symmetry is found.

In an actual physical situation the symmetry is important because it relates to other features of the situation. For example, a stress may be applied to the crystal. This stress can have an arbitrary orientation with respect to symmetry axes and reflection planes of the crystal. Another example would be a study of the boundary between two crystals having different orientation.

A list of desired properties for operators which are to be used to describe symmetry as encountered in physics follows:

1. Operators can be written which will rotate about an axis of any orientation, and reflect through a plane of any orientation.

2. The points in space must likewise be specifically designated.

3. The mathematical system used to represent the points must be such that its elements can be operated on by
elements of the mathematical system used for the operators. It will be seen that this compatibility is obtained in the two-dimensional case by using the complex number system to represent both the operators and the positions.

4. The operators should "crank". To illustrate, if from the geometry of the situation one obtains the rotation operators $R_1, R_2, \ldots$ and the reflection operators $M_1, M_2, \ldots$ then if $R_1M_1 = M_2$, then there must be a multiplication defined for the system such that when $R_1$ and $M_1$ are multiplied in the order shown the resulting expression is that obtained for $M_2$ from the geometry.

The above explanation is somewhat weak because the symbols are not specific enough. Actual examples will be found in Chapters II and III. The following example will be clarified by Chapter II. Let $e^{i\phi}, e^{i\Theta}, e^{i(\phi + \Theta)}$ be three symmetry operators obtained by a study of the geometry. That $e^{i\phi}e^{i\Theta} = e^{i(\phi + \Theta)}$ is true, follows from the laws of complex numbers and does not need to be postulated from a study of the physical situation.

It is rather difficult to obtain some operators from the geometry, but starting with generating elements for the group the other operators can be cranked out in a simple-minded manner. To sum it up, one wants the operators to be able to operate not just on positions but also on each other.
5. All the 32 macroscopic crystal symmetry groups should be represented within the same mathematical system. This is not just because greater universality has been found to pay off in mathematics and physics but because within a single physical situation there may be two or more things with different symmetry.

6. Since positions and orientations are real physical things, the mathematical quantities which represent positions and operations should be invariant under a change in coordinates, base vectors, or whatever corresponding thing is used with the mathematical system chosen.

All the foregoing requirements are embodied reasonably well in the tensor representations of symmetry. For this, second order tensors are used as operators and first order tensors (vectors) for positions. The second order tensors operate on first order tensors by means of the dot product. This general concept grew through the work of many men. A systematic development of the method is given by Seitz\textsuperscript{2} in a series of papers. Also this is a favorite example in books on group representation\textsuperscript{(3,4)}.

\begin{footnotesize}
\begin{enumerate}
\end{enumerate}
\end{footnotesize}
To illustrate this technique, let $T$ be a tensor giving a reflection and $R$ a rotation tensor. Let $r$ be the radius vector of a point to be operated upon. The image of $r$ is $T \cdot r$. If this reflection is followed by a rotation, the new point is $R \cdot T \cdot r$. This symbolism is obviously compact, neat, and simple. The operators are invariants and the operator multiplication is the common multiplication for tensors.

However it is often required and usually desirable that the representation be more explicit. This can be done with the tensor technique, but one finds that in general the representation is either not specific enough or else is bulky and requires too much time for the mathematical manipulation. As stated previously the purpose of this research is to find a representation which has all the previous properties and is superior to tensors in the following properties.

7. For many purposes one desires a symbolism which is independent of any coordinate system and which also has the following properties: (a) it shows the mathematical nature of the quantity; (b) it shows the nature of the mathematical operations; and (c) it shows the nature of the physical thing represented.

The first two are satisfied since bold face type is easily remembered and commonly used as meaning tensor and the $\cdot$ is a common symbol for a basic operation in the
algebra. However the tensor technique is deficient in quality (c). There is nothing in the notation to let one know that \( R \) gives a rotation through the angle \( \Theta \) about an axis with direction given by unit vector \( h \), nor does \( \mathbf{T} \) give the orientation of the reflection plane.

One can use a more descriptive notation such as \( \theta / h \) and \( \mathbf{m} \) where \( \mathbf{m} \) is a unit vector perpendicular to the plane or reflection. Such notation is compact and can be used with a variety of mathematical systems. It has many applications, however it lacks the desirable feature to be stated next.

3. Not only should the base-free notation show the nature of the operator but those parts of the notation which do this should play an essential role in the mathematical structure of the operator. This rather vague statement will be clarified by the following examples.

Using complex numbers for the two-dimensional case, a rotation of \( \phi \) is performed by \( e^{i\phi} \). Note that besides describing the rotation, the \( \phi \) is part of the complex number. In other words the \( \phi \) is not there just to clue the reader, it has a job to do. The \( e^{i\phi} \) is not just symbolism for present purposes, it is the well known function \( e^{iu} \), and \( i \phi \) is the independent variable \( u \).

To further illustrate this rather important and perhaps subtle point, for a rotation in three dimensions the symbolism \( \theta / h \) is introduced in this paper. One of the
results of this paper is the fact that the rotation described by $e^{\frac{\Theta}{h}}$ can be performed by the operator $e^{\frac{\Theta}{2h}}e^{\frac{\Theta}{2}}$. One notes that the last expression is an element in a definite mathematical system and that both $h$ and $\Theta$ enter to form this element in a definite way specified by the notation.

9. Often there are places in the development and application of a mathematical description where the elements of the mathematical system need to be expressed in terms of base elements. For example if the vector $v$ is written as $v = v_1i + v_2j + v_3k$. This gives a more specific description of $v$, provided of course the orientation of the base is known and also the real numbers $v_1$, $v_2$, and $v_3$.

The effectiveness of such a resolution into components can be judged by many considerations; here however, it will be required only to be compact, quickly written, and permit operations to be quickly performed.

10. The last requirement is that it be frequently possible to considerably simplify the mathematical description of the physical situation by choosing an advantageous set of base vectors.

Tensor representation has this property, but it is not very well exploited because of the following situation. If the base vectors are held fixed, the tensors can be set into one to one correspondence with matrices. These matrices together with the usual matrix multiplication and addition
are then used. The attack on a problem or a part of a problem proceeds as follows. From the physical situation, tensors are obtained. From the tensors, matrices are obtained. The mathematical operations are performed using matrices and the result is a scalar or matrix. If the result is a matrix, a tensor is then obtained from this matrix. This technique is preferred by a large majority of workers. A serious disadvantage is that no matter how expertly the base vectors are chosen, the matrix always has the same number of elements. Even though the operations are simplified there is a tedious amount of pen pushing. A mixture of the tensor and the matrix techniques could be used, but this is seldom done. This possibility has not been included in the present research. At this point it might be mentioned that since quaternions are vectors, they can be operated on by tensors. It is thus possible to mix the quaternion and the tensor techniques. This has not been investigated.

The specific problem is, with all the above restrictions, to find the quaternion operators which will give the desired results. Since quaternions are not as generally known as are complex numbers and vectors, the simple two-dimensional point groups will be given first with a brief review of the complex numbers as operators. Then the quaternions themselves will be logically derived from the complex numbers.
We shall see that, while the complex numbers and the operators associated with the complex numbers are commutative and the order of the operators can be reversed without any effect on the result; the quaternions and the operators associated with the quaternions are not necessarily commutative and the order of the operators must in general be preserved.
CHAPTER II

COMPLEX NUMBERS AND THEIR APPLICATION
TO THE TWO-DIMENSIONAL
POINT GROUPS

The purpose of this chapter is to introduce complex numbers and show that they can be used to represent any of the ten two-dimensional point groups. It is assumed that the reader is familiar with the fundamental concepts of complex numbers and vectors.

Complex Numbers and Vectors

Any complex number $z$ may be written in the form of $z = a + bi$. The quantity $a$ is the component of the real part and the quantity $b$ is the component of the imaginary part of the complex number. If $l$ is a unit vector in the direction of the real part and $i$ is a unit vector in the direction of the imaginary part, then the complex number can be interpreted as the vector with components $a$ and $b$ in the directions of $l$ and $i$ respectively. This vector is actually the radius vector terminating at the point whose coordinates are $(a,b)$. The vector $z$ is shown in Figure 6. The complex numbers have an advantage over the ordinary vectors of physics due to the extreme simplicity of the
resulting equations when they are used as operators acting on other complex numbers. But in order to gain this advantage, one must sacrifice a great deal of generality in his choice of coordinates and be quite specific. This may not be a disadvantage in an elementary treatment.

![Diagram of complex number](image)

**Fig. 6—The complex number z**

Another method of writing the complex number $z$ is the exponential form, $z = re^{i\varphi}$, where $r = \sqrt{a^2 + b^2}$ and the angle $\varphi = \tan^{-1}(b/a)$, as shown in Figure 6. In this form, $r$ is the magnitude of the vector and $\varphi$ is the direction of the vector relative to the real direction, $l$.

Addition of the two complex numbers $z_1 = a_1 + b_1i$ and $z_2 = a_2 + b_2i$ gives

$$z_1 + z_2 = (a_1 + a_2) + (b_1 + b_2)i,$$

which is also a complex number.

Multiplication of the two complex numbers gives

$$z_1z_2 = (a_1a_2 - b_1b_2) + (a_1b_2 + b_1a_2)i,$$
\[ = (r_1 e^{i\phi_1}) (r_2 e^{i\phi_2}), \]
\[ = r_1 r_2 e^{i(\phi_1 + \phi_2)}. \]  

(1)

**Rotation Operators**

Complex numbers, as stated before, are useful as the rotation operators. But they must be used in a system of complex numbers, since any number (complex or real) which is operated on by a complex number is a complex number. Multiplication of the two complex numbers \( z_1 \) and \( z_2 \) is a rotation of the first by the direction angle of the second and a multiplication of the magnitude of the first complex number by the real number which is the magnitude of the second. If the magnitude of the second complex number is unity, then the multiplication of the two is merely the rotation of the first complex number by the direction angle of the second. This is readily seen in equation (1).

It should be noted that for \( z_1 z_2 \), \( z_2 \) can be considered as an operator acting on \( z_1 \); or, on the other hand, \( z_1 \) can be considered as an operator acting on \( z_2 \). In the latter case, \( z_2 \) might represent a vector to the point in space and \( z_1 \) a movement of all the points in that space. \( z_1 z_2 \) would then be the new vector to the point which was originally at position \( z_2 \). For \( z_1 = r_1 e^{i\phi_1} \) to produce only a rotation it must, as was previously stated, be of unit length; or, if \( z_1 = e^{i\phi_1} \), then \( z_1 z_2 = r_2 e^{i(\phi_1 + \phi_2)}. \) This is shown at B in Figure 7.
Fig. 7—A rotation through an angle $\varphi_2$

If $r_1 > 1$, then $z_1$ not only rotates all the points through an angle $\varphi_1$, but moves them out from the center of the rotation; this is shown at A in Figure 7. If $r_1 < 1$, then the radial motion is inward as at C in Figure 7.

While such operations are of interest, they are not elements of a crystal point group.

A simple example of a rotation group is the group of four elements which will perform rotations of $90^\circ$, $180^\circ$, $270^\circ$, and $360^\circ$. If we operate on the vector $z = a + bi$ with the operator $e^{\frac{1}{2}\pi i}$, we obtain the vector to the point at B in Figure 8. Since $e^{\frac{1}{2}\pi i} = i$, $(e^{\frac{1}{2}\pi i})z = i(z = a + bi = -b + ai)$. Let $R_4$ be this rotation operator about the origin, or $R_4$ operating on the point whose coordinates are $(x, y)$ generates the point with coordinates $(-y, x)$. By using the complex numbers as the space coordinates, this becomes $R_4(z) = iz = -b + ai$, if $z = a + bi$. 
Fig. 3—Four-fold rotation axis about the origin

From Figure 3, the following is easily seen, if the point at A has the coordinates of \( z = a + bi \), then:

\[
R_4(A) = B = -b + ai,
\]

\[
R_4(B) = C = -a - bi,
\]

\[
R_4(C) = D = b - ai, \text{ and}
\]

\[
R_4(D) = A = a + bi.
\]

But \( R_4(B) = R_4^2(A) = R_2(A) \), where \( R_2 = -1 \) is the 180° rotation operator about the origin, \( R_4(D) = R_4^4(A) = A \), so that the operator acting four times in succession is the identity operator I. \( R_4(C) = R_4^3(A) = -iA \). The four operators may be written as:

\[
R_4 = i,
\]

\[
R_4^2 = R_2 = -1,
\]
\[ R^3_4 = -i, \]
and
\[ R^4_4 = I = 1. \]

This example is the point group denoted by \( 4 \) in the International short symbol.

**Reflection Operators**

Reflection operators are those which form an "image" of the point. This image is located as the image in a mirror. The mirror need not be a plane mirror but reflection in a plane is much simpler mathematically and this is the type encountered in crystal structures.

The simplest type of reflection is perpendicular to a coordinate axis. This type merely changes the sign of the component of the direction perpendicular to the reflecting plane, or axis in the two-dimensional case.

Consider first a reflection in the \( x \)-axis. For the vector \( z = a + bi \), the image is located by the vector \( a - bi \). But the quantity \( z^* = a - bi \), is the complex conjugate of the vector to the point and is the reflection in the \( x \)-axis as is well known from the theory of complex numbers. The complex conjugate operator is therefore the reflection operator in the \( x \)-axis.

The vector \( w = -a + bi \) is a reflection of the vector \( z = a + bi \) in the \( y \)-axis. This can be written as \( w = -(a - bi) = -z^* \) so that the "negative conjugate" operator is a reflection in the \( y \)-axis.
This "negative conjugate" operator can also be construed to be two distinct operations; that of the conjugate and that of the operator \(-1\). But if \(-1\) is an operator, it must be included in the group. This is indeed the case since the operator \(-1\) was obtained also from the rotational operator \(i\) acting twice upon the point. This operator, \(-1\), is called the inversion operator since it "inverts" the point or reflects it through the origin and consequently the signs of all the components are the negative of those of the original point.

An example of reflections in the two coordinate axes is shown in Figure 9.

![Figure 9: Reflections in the coordinate axes](image)

From Figure 9 we see that:

\[
I(A) = A = 1(\text{re}^1),
\]

\[
C(A) = D = e^{-2\phi}1(\text{re}^1),
\]
\(-I(A) = C = -1(re^{i\phi})\),

\(-C(A) = B = -e^{-2\phi_1}(re^{i\phi})\),

where \(C(A)\) is the conjugate of \(A\) and \(A\) is the point whose coordinates are \((a,b)\), or the complex number \(z = a + bi = re^{i\phi}\). This example is the point group denoted by 2mm (International short symbol) and has the operators:

\[
I = 1,
C = e^{-2\phi_1},
-I = -1,
-C = -e^{-2\phi_1}.
\]

The conjugate operator is seen to be a function of the direction of the vector to the point.

A reflection of the vector \(z = a + bi\) in the line passing through the origin and making an angle \(\phi\) with the positive x-axis is shown in Figure 10.

![Figure 10](image-url)

**Fig. 10**--Reflection at an angle \(\phi\)
The vector to the point in the primed system is \( z' = a' + b'i' \) and the vector to the reflection in the primed system is \( z'^* = a' - b'i' \), which is a reflection of the vector in the \( x' \)-axis. The transformations from the primed system to the unprimed system are:

\[
\begin{align*}
x' &= x \cos \phi + y \sin \phi, \\
y' &= -x \sin \phi + y \cos \phi, \\
l' &= \cos \phi + i \sin \phi, \\
i' &= -\sin \phi + i \cos \phi.
\end{align*}
\]

Substitution of these expressions into the equation \( z'^* = a' - b'i' \) gives

\[
\begin{align*}
z'^* &= (a \cos \phi + b \sin \phi) (\cos \phi + i \sin \phi) \\
&\quad - (-a \sin \phi + b \cos \phi) (-\sin \phi + i \cos \phi), \\
&= (a - bi) (\cos 2\phi + i \sin 2\phi), \\
&= (a - bi)e^{2\phi i} = z^* e^{2\phi i}.
\end{align*}
\]

An example of this is the point group which has the operators

\[
\begin{align*}
i &= 1, \\
R_6 &= e^{i \pi/3}, \\
R_6^2 &= e^{i 2\pi/3}, \\
R_6^3 &= -1, \\
R_6^4 &= -e^{i \pi/3}, \\
R_6^5 &= -e^{i 2\pi/3}, \\
C &= e^{-i 2\phi}, \\
CR_6 &= e^{i (\pi/3 - 2\phi)}.
\end{align*}
\]
\[ CR_6^2 = e^{i(2\pi/3 - 2\varphi)}, \]
\[ CR_6^3 = -e^{i2\varphi}, \]
\[ CR_6^{1/2} = -e^{i(\pi/3 - 2\varphi)}, \]
\[ CR_6^{5} = -e^{i(2\pi/3 - 2\varphi)}. \]

This group is denoted by 6mm and is shown in Figure 11.

![Diagram](image-url)

Fig. 11—Crystallographic point group 6mm

A Representation Theorem for the Ten Two-dimensional Point Groups

By the use of the complex number system, the ten two-dimensional crystal point groups can be represented in a form applicable to physical problems. The positions in space are given as complex numbers and the operators are complex numbers, conjugation, and products of these. The operator multiplication of the complex numbers and conjugation is defined in terms of multiplication of complex numbers.
This last statement may seem obvious, but there are operators used in physics which are simple creatures and the rule for forming their products is rather complicated.

The operators used for the ten two-dimensional crystal point groups form a sub-group of the group derived in this chapter. Hence, the theorem above is actually a summary of the chapter since the "proof" has been given in the development of the operator groups.
CHAPTER III

QUATERNION REPRESENTATION OF CRYSTAL POINT GROUPS

Quaternions

The success of complex numbers for the two-dimensional case suggests that a generalization of complex numbers might serve for three-space. Quaternions are such a generalization. Quaternions are mathematical elements concocted by adjoining to the complex number another element j which is also a square root of \(-1\).

The Algebra of Quaternions

Quaternions can be developed through the following line of thought. Quaternions cannot be a field since in a field the quadratic equation \(x^2 = -1\) can have at most two roots, and we now have at least four such roots. Hence, we shall specify that the multiplication of \(j\) by any complex number is non-commutative, according to the rules:

\[ j^2 = -1, \]

\[ (a + bi)j = j(a - bi). \]

The second rule states that a complex number multiplied by \(j\), in that order, is \(j\) multiplied by the complex conjugate of the number, in that order. Since multiplication by \(j\) is non-commutative, it must be remembered that order of the factors must be preserved. In symbols, if \(z = a + bi\)
and $z^* = a + bi$, the second rule is $zj = jz^*$. In particular, if $z = i$, $ij = -ji$. Using this last relation

$$(ij)^2 = ij(-ji) = -ijji = +ii = -1.$$  

Thus $ij$ is a square root of $-1$. But it cannot be any linear combination of $i$ and $j$ because

$$(ai + bj) (ij) = -aj + bi \neq -1.$$  

Let $ij = k$. $k$ is a new base element and adds another dimension to the space, making four since $1$ is included as a base element.

The rules and the definition of $k$ gives the following multiplication table for $1$, $i$, $j$, and $k$:

\[ i^2 = j^2 = k^2 = -1, \]
\[ ij = -ji = k, \]
\[ jk = -kj = i, \]
and
\[ ki = -ik = j. \]

The similarity of the multiplication table for the dot and cross products of the unit vectors $i$, $j$, and $k$ is readily apparent.

Quaternions are quantities of the form:

$$q = u_1 + u_2j,$$

where $u_1$ and $u_2$ are ordinary complex numbers. If we expand this, we get

$$q = a_1 + b_1i + a_2j + b_2ij,$$

where $u_1 = a_1 + b_1i$ and $u_2 = a_2 + b_2i$. Since $ij = k$, we have

$$q = a_1 + b_1i + a_2j + b_2k.$$
This is the usual way of writing a quaternion. For some purposes the method of equation (2) has some advantages over the method of equation (3); one is that it is more compact, but it must be remembered that the quantity of equation (2) is a quaternion and not a complex number. This will not be confusing since the imaginary number \( i \) will always be used for complex numbers and the imaginary number \( j \) will always be used for quaternions.

Two quaternions are equal if and only if each of the components are equal, as in vectors and complex numbers. The algebraic operations on quaternions are similar to the operations on complex numbers. If \( q = a_1 + b_1 i + c_1 j + d_1 k \) and \( p = a_2 + b_2 i + c_2 j + d_2 k \), then
\[
q + p = (a_1 + a_2) + (b_1 + b_2)i + (c_1 + c_2)j + (d_1 + d_2)k.
\]
This result is a quaternion so that quaternions are closed with respect to addition.

If \( q = u_1 + u_2 j = (a_1 + b_1 i) + (c_1 + d_1 i)j \) and \( p = v_1 + v_2 j = (a_2 + b_2 i) + (c_2 + d_2 i)j \), then the product of \( q \) and \( p \) is formed by multiplying out the two expressions, remembering to preserve the order of the factors \( i, j, \) and \( k \), as in ordinary complex numbers. This gives
\[
qp = u_1 v_1 + u_1 v_2 j + u_2 j v_1 + u_2 j^2 v_2 j,
\]
but \( j v_1 = v_1^* j \) and \( v_2 j = j v_2^* \), so that
\[
qp = u_1 v_1 + u_1 v_2 j + u_2 v_1^* j + u_2 j^2 v_2^*.
\]
But, since \( j^2 = -1 \), we have

\[
qp = (u_1^* v_1 - u_2^* v_2) + (u_1^* v_2 + u_2^* v_1) j.
\]

This result is a quaternion so that quaternions are closed with respect to multiplication.

Equation (4) can be expanded further to give,

\[
qp = (a_1 a_2 - b_1 b_2 - c_1 c_2 - d_1 d_2) \\
+ (a_1 b_2 + b_1 a_2 + c_1 d_2 - d_1 c_2) i \\
+ (a_1 c_2 - b_1 d_2 + c_1 a_2 + d_1 b_2) j \\
+ (a_1 d_2 + b_1 c_2 - c_1 b_2 + d_1 a_2) k.
\]

If \( b_1 = c_1 = d_1 = 0 \), then \( q \) is the real number \( a \) and is then called a scalar to distinguish it from a quaternion. Actually all real numbers are quaternions since complex numbers are special quaternions. The product \( ap \) is called the scalar product, or scalar multiplication. The real part of the quaternion is sometimes called the scalar part and the imaginary part is sometimes called the vector part.

If \( q, p, \) and \( r \) are quaternions, then the following relations are easily verified by direct computation:

1. \( (p + q) + r = p + (q + r) \);
2. \( p + q = q + p \);
3. There is a unique element \( 0 \), namely \( 0 + 0i + 0j + 0k \), such that \( p + 0 = p \);
4. For each element \( p \), there is a unique element \( q \) (denoted by \(-p\)), such that \( p + q = 0 \);
5. \( (pq)r = p(qr) \);
6. In general, \( pq \neq qp \).
(7). There is a unique element $l$, namely $i = 0i + 0j + 0k$, such that $lp = p = pl$;

(8). For each $p \neq 0$, there is a unique element $q$ (denoted by $p^{-1}$), such that $pq = 1 = qp$; and

(9). $p(q + r) = pq + pr$, and 

$(p + r)p = qp + rp$.

Any system which obeys the nine rules given above is said to form a non-commutative division ring.

The method of finding the multiplication inverse for quaternions is quite similar to finding the inverse for complex numbers. If $q = a + bi + cj + dk$, then let $a - bi - cj - dk$ be defined as the conjugate of $q$ and represented by $q^\ast$. Multiplication of $q$ by $q^\ast$ gives $qq^\ast = a^2 + b^2 + c^2 + d^2 = r^2$. Division of the quaternion $p$ by the quaternion $q$ is defined as $p/q = pq^{-1} = \frac{1}{r^2} q^\ast p$.

**Geometry of Quaternions**

The geometry of quaternion space is closely related to the algebra and it is of course this property which permits quaternions to algebraically represent geometrical operations and properties.

Quaternion space is a four-dimensional vector space since $l, i, j, k$ are linearly independent and the algebra meets the requirements for addition of vectors and scalar multiplication.

For many purposes it is convenient to write quaternions in the following two forms.
\[ q = q_o + q_1 i + q_2 j + q_3 k \]
\[ q = q_o + q_v \]
\[ q_v = q_1 i + q_2 j + q_3 k. \]

The \( q_o \) is called the real part and \( q_v \) is called the vector or the vector part. Although quaternions are vectors it is customary to refer to \( q \) as a quaternion and \( q_v \) as a vector.

It is convenient to consider \( 1, i, j, \) and \( k \) as mutually orthogonal and to use the usual metric. This works in well with the algebra since, as with complex numbers, the scalar product can be defined in terms of the algebra.

\[ p \cdot q = \frac{p^*q + q^*p}{2} = \frac{pq^* + qp^*}{2} \]

\[ = p_o q_o + p_1 q_1 + p_2 q_2 + p_3 q_3 \]
\[ = p_o q_o + p_v q_v. \]

The above is not the scalar product associated with the generalized metric used in special relativity. This latter product is

\[ p \cdot q = (pq)_o = \frac{pq + (pq)^*}{2} = \frac{pq + q^*p^*}{2} \]

\[ = p_o q_o - p \cdot q. \]

One notes that the sign of the second term differs from that of the scalar product which will be used in this paper.

Let \( Q \) be quaternion space; i.e., \( Q \) is the set of all quaternions. Let \( V \) be the set of all vectors. It will now be shown that \( V \) is isotropic. Since \( q \) is a vector
it is possible to take any triple of mutually orthogonal unit vectors in \( V \), label them \( i', j', k' \) in right-handed order and write \( q = q_o + q_v = q_o + q_1' i' + q_2' j' + q_3' k' \).

To show that \( V \) is isotropic, \( p q \) can be multiplied out by using components, and the result arranged to give

\[
pq = p_0 q_0 + p_v q_v + p_0 q_v + p_v q_0 + p_v \wedge q_v.
\]

In the above (\( \ast \)) is the ordinary scalar product and (\( \wedge \)) is the ordinary vector product (sometimes written as \( \times \)). It is well known that each of the products in this sum has a multiplication law which is invariant for such a change in coordinates. Thus \( pq \) must have such a law. This completes the proof.

To illustrate, let \( p = j' \) and \( q = k' \), then all the terms in the sum are zero except \( p \wedge q \). Here \( p \wedge q = j' \wedge k' \). The vector \( j' \wedge k' \) is perpendicular to \( j' \) and \( k' \) and using right hand rule it can be none other than \( i' \).

The principal source of difficulty in the manipulation of quaternions comes from the fact that in general \( pq \neq qp \). Also \( pq \neq -qp \) in general.

However, for any \( pq \) it is possible to split one of the quaternions into two parts, such that one part commutes and the other does not commute. This technique is related to the geometry in the following way. Place \( k \), say, in the direction of \( p \). Then \( l \) and \( k \) are base elements for a complex number system. Designate this space by \( Q_k \) (or \( Q_p \)).
The i and j are base elements for a two dimensional space which is perpendicular to \( Q_k \). Designate this space by \( k Q \). Then any \( q \) can be separated into two parts: \( q = q_k + k q \) where \( q_k \) is in \( Q_k \) and \( k q \) is in \( k Q \).

Since complex numbers commute, \( pq_k = q_k p \) where \( p \) is in its complex space; \( Q_p = Q_k \). The \( p k q \) part of the product follows the law \( p k q = k q p^* \) since the real part of \( p \) commutes but the \( k \)-part anticommutes. Combining the two operations gives

\[
pq = p(q_p + p q) = q_p p + pq_p^* .
\]

For the case where \( p \) is a vector

\[
pq = q_p p - p q_p .
\]

Although not so neat, it is possible and often desirable to use a complex space which contains neither \( p \) nor \( q \). Let \( i, j, k \) be base vectors and use say \( Q_i \).

Each quaternion is then divided into two parts and multiplication order can be reversed as follows:

\[
pq = (p_k + p) (q_k + k q)
= q_k p_k + (k q p)^* + k q p_k^* + q_k^* k p .
\]

In the above expansion the first two terms are in \( Q_k \) and the last two terms are in \( k Q \). Let the notation \( Q_k Q_k \) mean the set formed by multiplying every element of \( Q_k \) by every element of \( k Q \) in that order.

The nature of the four terms can now be clarified by the following laws for multiplication of the subspaces:
\[ Q_k Q_k = Q_k \]
\[ Q_{kk} Q = Q_k \]
\[ k Q_k Q = Q_k \]
\[ k Q_k Q = Q_k \]

Later when rotations are developed it will be shown that if a unit vector from the complex space \( Q_k \) is multiplied by a vector in \( Q \) the product which, by the above, lies in \( Q \) is none other than a rotation of the original vector. More explicit, the unit vector may be written as \( e^k \theta \) and it will be found that \( e^k \theta \) rotates \( Q \) about \( k \) through an angle \( \theta \).

One notes that this line of argument has returned to the original concept given in the introduction to the algebra. Replacing \( j \) by \( k \) one writes \( q = v_1 + v_2 i \) where \( v_1 \) and \( v_2 \) are elements from the complex space belonging to \( k \), and \( i \) is used since, using the positive order, \( i \) follows \( k \).

One may obtain the expression used to introduce quaternions by separating the space into \( Q = i Q + Q_i \) and writing \( q = u_1 + u_2 j \) where \( u_1 \) and \( u_2 \) are from \( Q_i \).

**Quaternions as Rotation Operators in Three-dimensions**

Quaternions as rotation operators are similar to complex numbers as rotation operators. One exception to this is the fact that quaternions do not commute so that all the quaternion operations in this paper shall be on
the left. The choice is arbitrary, but in order to be less confusing, this order shall be used.

A rotation of angle $\theta$ about the $z$-axis is shown in Figure 12. The $z$-axis is perpendicular to the plane of the paper and the points considered are all at the same perpendicular distance $d$ from the plane of the paper and all of the points are on the same side of the paper.

![Diagram of rotation about the z-axis]

**Fig. 12—Rotation about the z-axis**

It can be seen in Figure 12 that the following relations are true:

\[
\begin{align*}
b &= r \cos \phi, \\
c &= r \sin \phi, \\
b' &= r \cos(\phi + \theta), \\
c' &= r \sin(\phi + \theta), \\
r &= \sqrt{b^2 + c^2} = \sqrt{b'^2 + c'^2}.
\end{align*}
\]

If $q_A = a + bi + cj + dk$ and $q_B = a + b'i + c'j + d'k$ are the quaternion representation of the coordinates of the point $A$ and $B$ respectively and $a$ is a constant, then
substitution for the values of $b'$ and $c'$ gives:

\[ q_B = a + r \cos(\phi + \theta)i + r \sin(\phi + \theta)j + dk \]
\[ = a + r(\cos\phi\cos\theta - \sin\phi\sin\theta)i + r(\sin\phi\cos\theta + \cos\phi\sin\theta)j + dk. \]

But $r \cos \phi = b$ and $r \sin \phi = c$, so that

\[ q_B = a + (b \cos \theta - c \sin \theta)i + (c \cos \theta + b \sin \theta)j + dk, \]
\[ = a + b (\cos \theta i + \sin \theta j) + c (\cos \theta j + \sin \theta i) + dk, \]
\[ = a + b (\cos \theta + k \sin \theta)i + c (\cos \theta + k \sin \theta)j + dk, \]
\[ = a + (\cos \theta + k \sin \theta) (bi + cj) + dk. \]

But $\cos \theta + k \sin \theta = e^{k\theta}$ and we have

\[ q_B = a + e^{k\theta} (bi + cj) + dk. \]

Similar arguments give similar results for rotations about the $x$- and $y$-axis. These results are given as the following definitions for a rotation of angle $\theta$ about the:

- $x$-axis is $R_{\phi x}(A)$,
- $y$-axis is $R_{\phi y}(A)$,
- and $z$-axis is $R_{\phi z}(A)$.

One may also use the unit vectors in the notation in place of the coordinates, and with reasonable care the two notations can be used together. The notation would then be

\[ R_{\phi i} q \quad R_{\phi j} q \quad R_{\phi k} q \quad R_{\phi h} q. \]
In the latter expression $R_{\theta h}$ is a rotation about an axis in the direction of the vector $h$. Another notation for such a rotation could be $\theta/h$. This last is easier to form, especially on a typewriter, but it has no $h$ to suggest rotation.

If $q = a + bi + cj + dk$ is the quaternion representation of the point $A$, they the definitions become

$R_{\theta x}q = a + bi + e^{i\theta}(cj + dk),$
$R_{\theta y}q = a + cj + e^{j\theta}(bi + dk),$
and $R_{\theta z}q = a + dk + e^{k\theta}(bi + cj).$

The above operator is defined in terms of both addition and multiplication. Although it is desirable to have an operator involve only one of the operations defined for the mathematical system chosen, it is sometimes found convenient to do otherwise.

A search will now be made for a definition of $R_{\theta k}$ using only quaternion multiplication. From the derivation of $R_{\theta k} = R_{\theta z}$ it is seen that a unit vector in the complex space belonging to $k$ can be written as $e^{k\theta}$. Then

$e^{k\theta}q = e^{k\theta}(q_k + q) = e^{k\theta}q_k + e^{k\theta}q.$

The first term is simply the complex number $q_k$ rotated through an angle $\theta$. The second term is a vector in the space perpendicular to the complex space, and as was shown in the derivation of $R_{\theta k}$ that this was $q_k$ rotated $+\theta$ about the $k$-axis.
Clearly \( e^{k\theta} \) is not the desired rotation because the coordinate is changed. Trying \( q e^{-k\theta} \) the following expression is obtained:

\[
q e^{-k\theta} = (q_k + kq)e^{-k\theta} = e^{-k\theta} q_k + (e^{-k\theta})^* kq = e^{-k\theta} q_k + e^{+k\theta} kq.
\]

One sees that this last operator rotates \( kq \) through \(+\theta\), but through a negative \( \theta \). Thus it would seem that the two operators could be combined to cancel out the unwanted rotation. Attempting this one finds

\[
e^{k\theta} q e^{-k\theta} = e^{k\theta} (q_k + kq)e^{-k\theta} = e^{k\theta} (e^{-k\theta} q_k + e^{k\theta} kq) = q_k + e^{k2\theta} kq.
\]

This operator thus gives a rotation of \( 2\theta \) about the \( k \)-axis. Thus \( R_{k\theta} \) can be defined as \( R_{k\theta} = e^{k\theta/2} q e^{-k\theta/2} \).

Notationwise this might be improved in the following ways:

\[
2\theta/k = e^{k\theta}(q)e^{-k\theta}
\]

On the left, half angles are used for measuring the angles. The use of half angles is fairly common in physics and should not be too confusing. On the right, operator notation a notational convention is adopted. It is simply that when \( e^{k\theta} \) appears as an operator it is understood that the actual operation involves an \( e^{-k\theta} \) as specified.

Actually performing the indicated operations has been found to be somewhat laborious and ends with an expression
about as in the original definition of \( R_\theta k \) which uses both addition and multiplication. Thus a further search is indicated, this time for an operator which lies entirely to the left of the position quaternion. Such is obtained by the following manipulation.

\[
R_\theta k q = e^k q e^{-k} = e^k \theta(q e^{-\theta})^{**} = e^k \theta(e^k \theta q)^{**} = e^k \theta q e^k \theta q.
\]

In this last expression the \( * \) on the same level as the symbols means that the conjugate is to be taken of everything to the right of the symbol.

It is notationally convenient to replace \( * \) with the symbol \( e \) or \( c \) since later related symbols such as \( q_1 \) will be introduced. Using this last convention, the rotation operator is written as

\[
R_2 \theta k = e^k \theta e^k \theta c \text{ OR } (e^k \theta c)^2.
\]

This last operator is a left handed operator and specifically describes what is to be done to \( q \) and does so in terms of quaternion algebra. However this operator involves both multiplication and conjugation and actual calculations make it look rather doubtful that this can be used as effectively as the original definition of \( R_\theta k \).

As a final attempt one may define \( R_\theta k \) as a quaternion which is a function of the quaternion operated upon. This quaternion then operates by ordinary quaternion multiplication.

The result of \( R_\theta z(A) \) can be verified by direct multiplication of the quaternion \( q = a + bi + cj + dk \)
as $R_{\theta z}q$, where $R_{\theta z}$ is the quaternion
\[
\frac{1}{r^2} \left\{ \left[ a^2 + (b^2 + c^2) \cos \theta + d^2 \right] \\
+ \left[ (ab - cd) \cos \theta - (ac + bd) \sin \theta - ab + cd \right] i \\
+ \left[ (ac + bd) \cos \theta + (ab - cd) \sin \theta - ac - bd \right] j \\
+ \left[ (c^2 + b^2) \sin \theta \right] k \right\},
\]
where $r^2 = a^2 + b^2 + c^2 + d^2$. The reason for the definition of the short-hand operation $R_{\theta z}(q) = a + dk + e^{\theta k}(bi + cj)$ is obvious.

As an example of the application of rotation operators, consider a four-fold rotation axis coinciding with the $z$-axis. This has a crystal point group denoted by $4$. This group is shown in Figure 13. The points are all the same distance from the paper and are all on the same side of the paper.

![Figure 13](image)

**Fig. 13**—Four-fold rotation axis about $z$

Since this is a four-fold rotation axis, $\theta = \pi/2$ and the operation becomes
\[ R_{4z} q = a + dk + e^{k \pi/2} (bi + cj), \]
\[ = a + dk + k(bi + cj), \]
where \( q = a + bi + cj + dk \). Since \( e^{k \pi/2} = k \), then
\[ R_{4z} q = a + dk + bki + ckj, \]
\[ = a - ci + bj + dk. \]

This result is readily verified by the point B in Figure 13.

Hence,
\[ R_{4z} (A) = R \pi/2 (A) = B, \]
\[ R_{4z} (B) = a + dk + k(-ci + bj), \]
\[ = a + dk - cki + bki, \]
\[ = a - bi - cj + dk, \]
or
\[ R_{4z} (B) = C. \]

This also is readily verified by the figure.
\[ R_{4z} (C) = a + dk + k(-bi - cj), \]
\[ = a + dk - bki - ckj, \]
\[ = a + ci - bj + dk, \]
which corresponds to the point at D.
\[ R_{4z} (D) = a + dk + k(ci - bj), \]
\[ = a + dk + cki - bkj, \]
\[ = a + bi + cj + dk, \]
and we are now back at the point which we started. The operators for this group are:

\[ I, \]
\[ R_{4z}. \]
\[ R_{4z}^2 = R_{2z}, \]
and
\[ R_{4z}^3, \]
where \[ R_{4z}^3 (A) = R_{4z} \left\{ R_{4z} \left[ R_{4z}(A) \right] \right\}. \]

**Quaternion Conjugates**

If the quaternion \( q = a + bi + cj + dk \), then the conjugate of \( q \) is \( q^* = a - bi - cj - dk \). This is comparable to the complex conjugate and it is obvious that if \( q \) is the quaternion of the point \( A \) then \( q^* \) is the quaternion of the inversion of the point \( A \).

The inversion operator can also be obtained by a reflection through each of the perpendicular planes.

In view of this interpretation, three more conjugate operators are defined such that \( C_x \left\{ C_y \left[ C_z(A) \right] \right\} = C(A) \) and the order need not be preserved. The conjugates are defined separately as follows:

\[ C_x q = a - bi + cj + dk, \]
\[ C_y q = a + bi - cj + dk, \]
and
\[ C_z q = a + bi + cj - dk, \]

where \( q = a + bi + cj + dk \). It must be remembered that the \( C \)'s can also be quaternions. In fact, they are

\[ C_x = \frac{1}{r^2} \left[ (a^2 - b^2 + c^2 + d^2) - 2b(ai + dj - ck) \right], \]
\[ C_y = \frac{1}{r^2} \left[ (a^2 + b^2 - c^2 + d^2) - 2c(-di + aj + bk) \right], \]
\[ C_z = \frac{1}{r^2} \left[ (a^2 + b^2 + c^2 - d^2) - 2d(ci - bj + dk) \right]. \]
Quaternions as Reflection Operators in Three-dimensions

The various conjugate operators were found to change the sign of only one of the components of the vector part of the quaternion. These conjugate operators then are merely the reflection operators in the various planes formed by the coordinate axes. A simple example of this is the group denoted by \( \text{mmm} \). This is shown in Figure 14. The points denoted by the dots (\( \circ \)) are above the paper and the points denoted by the circles (\( \odot \)) are below the paper and at the same distance.

\[
\begin{array}{c|c}
\circ & \odot \\
B, B^1 & A, A^1 \\
\odot & \\
C, C^1 & D, D^1 \\
\end{array}
\]

**Fig. 14**—Three perpendicular reflection planes

Let the unprimed letters represent the points above the plane and the primed letters represent the points below the plane. The following are easily seen:

\[
\begin{align*}
I(A) &= A, \\
C_z(A) &= A^1, \\
C_x(A) &= B,
\end{align*}
\]
\[ c_z[c_x(A)] = b^1, \]
\[ c_y[c_x(A)] = c, \]
\[ c_z[c_y[c_x(A)]] = c(A) = c^1, \]
\[ c_y(A) = d, \]
\[ c_z[c_y(A)] = d^1. \]

The eight operators associated with this group are found from the preceding equations.

The problem of finding the operators for a reflecting plane containing the z-axis and making an angle \( \theta \) with the positive x-axis is similar to the two-dimensional problem. This is shown in Figure 15.

![Diagram of reflection at angle \( \theta \)](image)

**Fig. 15**--Reflection at angle \( \theta \)

The transformation equations from the primed system to the unprimed system are:
\[ x' = x \cos \theta + y \sin \theta, \]
\[ y' = -x \sin \theta + y \cos \theta, \]
\[ z' = z, \]
\[ i' = i \cos \theta + j \sin \theta, \]
\[ j' = -i \sin \theta + j \cos \theta, \]
and \[ k' = k. \]

Let \( q = a + bi + cj + dk \) and \( q' = a + b'i' + c'j' + dk \) be the quaternions of the point \( A \) in the unprimed and primed systems respectively. Then \( \overline{q} \) is the conjugate in the \( y' \) direction and is given by \( C_{y'}(q) = a + b'i' - c'j' + dk \).

Substitution for the primed numbers yields

\[ p = a + b'i' - c'j' + dk \]
\[-= a + (b \cos \theta + c \sin \theta) (i \cos \theta + j \sin \theta) \]
\[-(-b \sin \theta + c \cos \theta) (-i \sin \theta + j \cos \theta) + dk, \]
\[-= a + bi \cos^2 \theta - sin^2 \theta + cj \sin^2 \theta - \cos^2 \theta + 2b \sin \theta \cos \theta + 2ci \sin \theta \cos \theta + dk, \]
\[-= a + (bi - cj) \cos^2 \theta - \sin^2 \theta \]
\[-+(b \overline{j} + ci) 2 \sin \theta \cos \theta + dk, \]
\[-= a + (bi - cj) \cos 2\theta + (bj + ci) \sin 2\theta + dk, \]
\[-= a + (bi - cj) \cos 2\theta + (b ki - ckj) \sin 2\theta + dk, \]
\[-= a + (\cos 2 \theta + k \sin 2\theta) (bi - cj) + dk, \]
\[-= a + e^{2\theta} k (bi - cj) + dk, \]
\[-= R_{2\theta}(a + bi - cj + dk), \]
\[-= R_{2\theta} [ C_{y}(A)]. \]
TABLE I

FUNDAMENTAL OPERATORS

<table>
<thead>
<tr>
<th></th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identity</td>
<td>$I(q) = a + bi + cj + dk$</td>
</tr>
<tr>
<td>Inversion</td>
<td>$C(q) = a - bi - cj - dk$</td>
</tr>
</tbody>
</table>

Reflection parallel to:

<table>
<thead>
<tr>
<th>Axis</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x-axis</td>
<td>$C_x(q) = a - bi + cj + dk$</td>
</tr>
<tr>
<td>y-axis</td>
<td>$C_y(q) = a + bi - cj + dk$</td>
</tr>
<tr>
<td>z-axis</td>
<td>$C_z(q) = a + bi + cj - dk$</td>
</tr>
</tbody>
</table>

Rotation about:

<table>
<thead>
<tr>
<th>Axis</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x-axis</td>
<td>$R_{\theta x}(q) = a + bi + e^{i\theta}(cj + dk)$</td>
</tr>
<tr>
<td>y-axis</td>
<td>$R_{\theta y}(q) = a + cj + e^{j\theta}(bi + dk)$</td>
</tr>
<tr>
<td>z-axis</td>
<td>$R_{\theta z}(q) = a + dk + e^{k\theta}(bi + cj)$</td>
</tr>
</tbody>
</table>

Two-fold rotation axis about:

<table>
<thead>
<tr>
<th>Axis</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x-axis</td>
<td>$R_{2x}(q) = a + bi - (cj + dk) = a + bi - cj - dk$</td>
</tr>
<tr>
<td>y-axis</td>
<td>$R_{2y}(q) = a + cj - (bi + dk) = a - bi + cj - dk$</td>
</tr>
<tr>
<td>z-axis</td>
<td>$R_{2z}(q) = a + dk - (bi + cj) = a - bi - cj + dk$</td>
</tr>
</tbody>
</table>

Four-fold rotation axis about:

<table>
<thead>
<tr>
<th>Axis</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>x-axis</td>
<td>$R_{4x}(q) = a + bi + i(cj + dk) = a + bi - dj + dk$</td>
</tr>
<tr>
<td>y-axis</td>
<td>$R_{4y}(q) = a + cj + j(bi + dk) = a + di + cj - bk$</td>
</tr>
<tr>
<td>z-axis</td>
<td>$R_{4z}(q) = a + dk + k(bi + cj) = a - ci + bj + dk$</td>
</tr>
</tbody>
</table>

Reflection in the plane containing the z-axis and at an angle $\theta$ with the positive x-axis is

$$R_{2\theta z}[C_y(q)] = a + dk + e^{2\theta k}(bi - cj).$$
Since the order is preserved, it is easily seen that the point A is first reflected in the xz-plane and then that result is rotated by an angle of $2\pi$. This is the same as for complex numbers but is more clearly seen with quaternions.

A table of the fundamental operators is given in Table I. Other operators can be obtained by using two or more operators in succession. Table II gives a few of the more important relationships of the combination of pairs of operators.

**TABLE II**

**FUNDAMENTAL RELATIONS OF THE OPERATORS**

\[
\begin{align*}
C_y \left[ C_x(q) \right] &= C_x \left[ C_y(q) \right] = R_{4z}(q) = R_{2z}(q) \\
C_z \left[ C_x(q) \right] &= C_x \left[ C_z(q) \right] = R_{4y}(q) = R_{2y}(q) \\
C_z \left[ C_y(q) \right] &= C_y \left[ C_z(q) \right] = R_{4x}(q) = R_{2x}(q) \\
C_x \left\{ C_y \left[ C_z(q) \right] \right\} &= C_y \left\{ C_x \left[ C_z(q) \right] \right\} = C_z \left\{ C_x \left[ C_y(q) \right] \right\} = C(q) \\
R_{4h} \left[ C_h(q) \right] &= C_h \left[ R_{4h}(q) \right], \quad h = x, y, \text{ or } z. \\
R_{4f} \left[ C_g(q) \right] &= C_h \left[ R_{4f}(q) \right], \quad f, g, \text{ and } h \text{ are all different.} \\
R_{4x} \left[ R_{4y}(q) \right] &= R_{4y} \left[ R_{4x}(q) \right] = R_{4z} \left[ R_{4x}(q) \right].
\end{align*}
\]

It is seen in Table II that the operators will in general not commute. The rotation and conjugate operators commute if the axis of the rotation coincides with the axis perpendicular to the plane of the reflection.
As a final example of the operators, consider the cubic structure of Figure 16.

Fig. 16--Illustration of rotation axis
The unprimed characters in Figure 16 are near the observer and the primed characters are away from the observer. The three-fold rotation axes A-A', B-B', C-C', D-D' have the following operations on the quaternion \( a + bi + cj + dk \):

\[
R_{3A}(q) = R_{4x} \left[ R_{4z}(q) \right] = a - ci - dj + bk,
\]

\[
R_{3B}(q) = R_{4y} \left[ R_{4x}(q) \right] = a + ci - dj - bk,
\]

\[
R_{3C}(q) = R_{4z} \left[ R_{4y}(q) \right] = a - ci + dj - bk,
\]

and \( R_{3D}(q) = R_{4x} \left[ R_{4y}(q) \right] = a + di + bj + ck. \)

The two-fold rotation axes E-E', F-F', G-G', H-H', I-I', and J-J' have the following operators on the quaternion \( a + bi + cj + dk \):

\[
R_{2E}(q) = R_{2x} \left[ R_{4z}(q) \right] = a - ci - bj - dk,
\]

\[
R_{2F}(q) = R_{2y} \left[ R_{4z}(q) \right] = a + ci + bj - dk,
\]

\[
R_{2G}(q) = R_{2z} \left[ R_{4x}(q) \right] = a - bi + dj + ck,
\]

\[
R_{2H}(q) = R_{2z} \left[ R_{4y}(q) \right] = a - di - cj - bk,
\]

\[
R_{2I}(q) = R_{2y} \left[ R_{4x}(q) \right] = a - bi - dj - ck,
\]

and \( R_{2J}(q) = R_{2x} \left[ R_{4y}(q) \right] = a + di - cj + bk. \)

There are more operators, but the others are the same which were given in previous examples.

**A Representative Theorem for the Thirty-two Three-dimensional Point Groups**

By the use of quaternions, the thirty-two three-dimensional point groups can be represented in a form
applicable to physical problems. The positions in space are given by the vector part of the quaternions and the operators are quaternions. The quaternion operators are multiplied as ordinary quaternions.

The quaternion multiplication was in general rather complicated so that this method seemed to be hopeless until the special conjugates were introduced and the short-hand multiplication was defined. This made the operations much easier.

Solving physical problems was not actually considered in this thesis but it seems to be a promising field for further study.
BIBLIOGRAPHY

Books


Articles