CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 17: Matrix Representations of Rotation Operation

I will be continuing the discussion on two-dimensional point groups, and in this lecture, we will look at how matrices can be used to represent symmetry operations. We will begin with matrix representation, so this becomes the matrix representation of symmetry operations.

Consider the xy plane, and imagine the z-axis is normal to this plane. We work in Cartesian coordinates. Take a point (x, y), and since we are restricting ourselves to the xy plane, we do not write the z coordinate. After a rotation by an angle θ, this point (x, y) moves to a new point (x', y'). The distance of both points from the origin is r, and the rotation is counterclockwise by θ.

The new coordinates can be written as

$$x' = rcos(\alpha + \theta)$$

and

$$y' = rsin(\alpha + \theta).$$

Expanding these expressions gives

$x' = rcos\alpha cos\theta - rsin\alpha sin\theta,$

$y' = rsin\alpha cos\theta + rcos\alpha sin\theta.$

From the geometry, $rcos\alpha = x$ and $rsin\alpha = y$.

Substituting these into the expressions above gives

$x' = xcos\theta - ysin\theta,$

$y' = xsin\theta + ycos\theta.$

Since the motion is entirely in the xy plane, the z coordinate does not change, so $z' = z$.

To write all three components in a uniform form, we add the terms

$x' = x\cos\theta - y\sin\theta + 0 \cdot z,$

$y' = x\sin\theta + y\cos\theta + 0 \cdot z,$

$z' = 0 \cdot x + 0 \cdot y + 1 \cdot z.$

These three equations can be written in matrix form:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

This becomes the rotation matrix about the z-axis, denoted $R_z(\theta)$. Similarly, we can write rotation matrices about the x- and y-axes.

Rotation about the x-axis:

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}.$$

Rotation about the y-axis:

$$R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}.$$

Knowing these three basic rotation matrices allows us to construct rotations about any arbitrary axis. For example, suppose in three dimensions the rotation axis lies in the xy plane and makes an angle α with the x-axis. To compute a rotation of θ around this axis:

1. First rotate the coordinate system so that the axis aligns with the x-axis.
   This is achieved by a rotation of $-\alpha$ about the z-axis:
   $R_z(-\alpha)$.

2. Then perform the required rotation θ about the x-axis:

   $R_x(\theta)$.

3. Finally rotate back to the original orientation using

   $R_z(+\ \alpha)$.

Thus, the full rotation matrix is: $R = R_z(\alpha)\, R_x(\theta)\, R_z(-\ \alpha)$.

Now let us see how this representation helps with point groups. Consider the group 2 discussed earlier. Group 2 consists of the identity operation and a 180° rotation.

The identity operation corresponds to the identity matrix:

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The identity matrix, when multiplied with the vector (x, y, z), simply gives back the same vector. Matrix multiplication proceeds in the usual way.

When multiplying matrices, the standard procedure is to take a row from the first matrix and a column from the second matrix, multiply the corresponding elements, and then sum the products. For example, multiplying the first row with the first column gives x because the other elements contribute zero. Thus, the result is $x + 0 \cdot y + 0 \cdot z = x$.

Repeating this for the second row gives y, and for the third row gives z. Therefore, the coordinates x, y, and z remain unchanged when multiplied by the identity matrix, exactly as expected.

The first element of the group is the identity I. For the second operation, which is a rotation about the z-axis, we use the standard rotation matrix $R_z(\theta)$. Considering the specific operation A_π, we write it as $R_z(\pi)$ and insert π into the sine and cosine terms.

This yields the matrix $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. If we now perform two such operations in succession, i.e., $R_z(\pi)$ followed by another $R_z(\pi)$, the product trivially gives the identity matrix.

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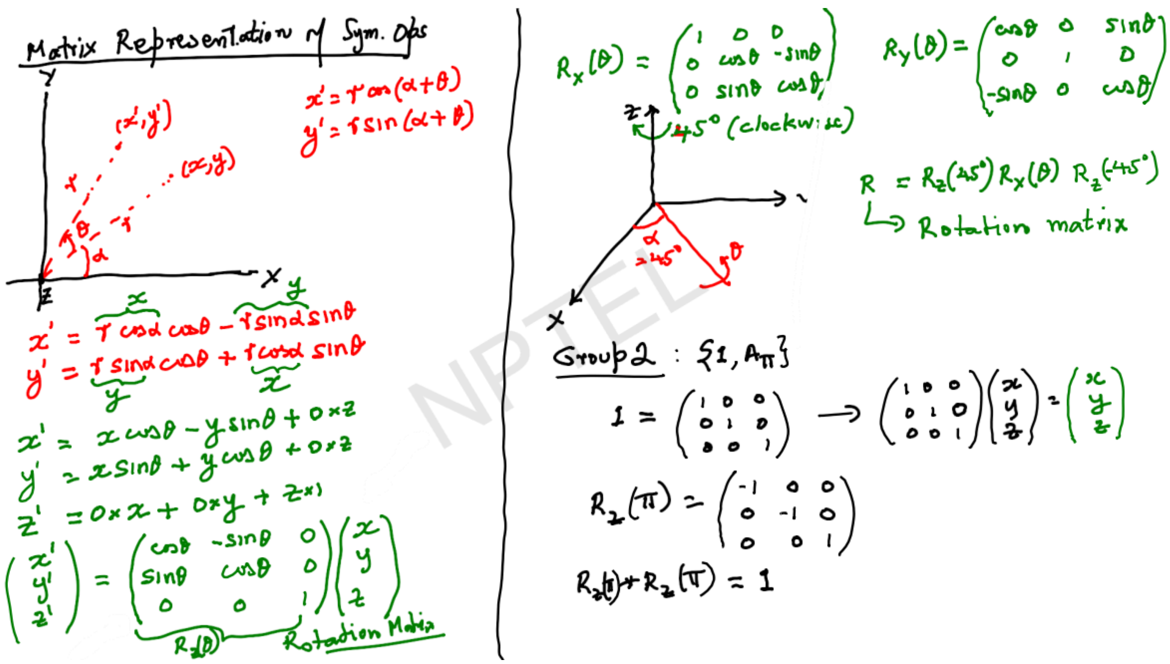

Consider next the group 3, consisting of the identity, a rotation of 120° $(2\pi/3)$, and a rotation of 240°, which we write as -120° $(-2\pi/3)$. These three elements are I, $R_z(2\pi/3)$, and $R_z(-2\pi/3)$. Inserting 120° into the rotation formulas gives $\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Similarly, inserting -120° yields $\begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Thus, all three elements are now expressed as matrices, and the group table can be filled in directly.

In the multiplication table, the element in the first row and first column is the identity. The element in the first row and second column is $R_z(2\pi/3)$, and the element in the first row and third column is $R_z(-2\pi/3)$. Rotating by $+120^\circ$ followed by -120° gives the identity, so the corresponding cells contain I. Likewise, multiplying $R_z(2\pi/3)$ by itself gives $R_z(-2\pi/3)$. This is because adding 120° and 120° yields 240°, which is -120° in standard form. Similarly, multiplying $R_z(-2\pi/3)$ by itself gives $R_z(2\pi/3)$.

As an explicit example, consider multiplying $R_z(2\pi/3)$ by itself. Writing both matrices as $\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$, we multiply the first row of the left matrix with the first column of the right matrix. The product $(-\frac{1}{2})(-\frac{1}{2})$ gives $\frac{1}{4}$, while $(-\frac{\sqrt{3}}{2})(\frac{\sqrt{3}}{2})$ gives $-\frac{3}{4}$, resulting in a sum of $-\frac{1}{2}$.

The third term contributes zero. Repeating the same procedure with the first row and the second column gives $\frac{\sqrt{3}}{2}$, and the first row with the third column gives zero. Performing similar calculations for the second-row yields $-\frac{\sqrt{3}}{2}$ and $-\frac{1}{2}$, and the third row produces 1 in the bottom-right position. The resulting matrix matches the expression for $R_z(-2\pi/3)$ exactly, confirming that the product corresponds to a rotation of -120°.

The remaining entries of the multiplication table can be filled similarly by multiplying the respective matrices. Reflection operations and their corresponding matrices will be discussed separately, as they require additional considerations.

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Group 3 : $\{1, A_{\frac{2\pi}{3}}, A_{-\frac{2\pi}{3}}\}$

$A_{\frac{2\pi}{3}} \to R_z\left(\frac{2\pi}{3}\right)$, $A_{-\frac{2\pi}{3}} \to R_z\left(-\frac{2\pi}{3}\right)$

$$R_z\left(\frac{2\pi}{3}\right) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R_z\left(-\frac{2\pi}{3}\right) = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(product of the two) $= 1$

	1	$R_z\left(\frac{2\pi}{3}\right)$	$R_z\left(-\frac{2\pi}{3}\right)$
1	1	$R_z\left(\frac{2\pi}{3}\right)$	$R_z\left(-\frac{2\pi}{3}\right)$
$R_z\left(\frac{2\pi}{3}\right)$	$R_z\left(\frac{2\pi}{3}\right)$	$R_z\left(-\frac{2\pi}{3}\right)$	1
$R_z\left(-\frac{2\pi}{3}\right)$	$R_z\left(-\frac{2\pi}{3}\right)$	1	$R_z\left(\frac{2\pi}{3}\right)$

$$R_z\left(\frac{2\pi}{3}\right) \times R_z\left(\frac{2\pi}{3}\right) = R_z\left(-\frac{2\pi}{3}\right)$$

$$R_z\left(\frac{2\pi}{3}\right) R_z\left(\frac{2\pi}{3}\right) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = R_z\left(-\frac{2\pi}{3}\right)$$