CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 23: Combining Rotation and Translation Symmetries

In the last lecture, we looked at the combination of a reflection operation and a translation operation.

In this lecture, we examine what happens when we combine a rotation with a translation in two dimensions. Suppose we have a rotation about a point A through an angle α, followed by a translation vector $T = (T_x, T_y)$. We want to determine the resulting symmetry operation.

Using matrices, the translation matrix in homogeneous coordinates is:

$$T = \begin{pmatrix} 1 & 0 & T_x \\ 0 & 1 & T_y \\ 0 & 0 & 1 \end{pmatrix}$$

The rotation matrix about the origin is:

$$R_\alpha = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying the translation and rotation matrices gives:

$$TR_\alpha = \begin{pmatrix} \cos\alpha & -\sin\alpha & T_x \\ \sin\alpha & \cos\alpha & T_y \\ 0 & 0 & 1 \end{pmatrix}$$

We now compare this with the general rotation matrix about a point (a, b), which we derived earlier:

$$R_\alpha(a,b) = \begin{pmatrix} \cos\alpha & -\sin\alpha & a(1-\cos\alpha)+b\sin\alpha \\ \sin\alpha & \cos\alpha & -a\sin\alpha + b(1-\cos\alpha) \\ 0 & 0 & 1 \end{pmatrix}$$

By comparing element by element, we equate the relevant components to find the coordinates (a, b) of the rotation point corresponding to the combination of rotation and translation:

1. First row, third column:

$$a(1 - cos\alpha) + bsin\alpha = T$$

2. Second row, third column:

$$-\ asin\alpha + b(1 - cos\alpha) = 0$$

From the second equation, solving for b in terms of a:

$$b = \frac{asin\alpha}{1-cos\alpha}$$

Substitute this into the first equation:

$$a(1 - cos\alpha) + \frac{asin^2\alpha}{1-cos\alpha} = T$$

Simplifying:

$$a\frac{(1-cos\alpha)^2+sin^2\alpha}{1-cos\alpha} = T$$

Expanding $(1 - cos\alpha)^2 + sin^2\alpha = 2(1 - cos\alpha)$, so:

$$a\frac{2(1-cos\alpha)}{1-cos\alpha} = 2a = T \quad \Rightarrow \quad a = \frac{T}{2}$$

Now substituting $a = T/2$ into the equation for b:

$$bsin\alpha = T - a(1 - cos\alpha) = T - \frac{T}{2}(1 - cos\alpha) = \frac{T}{2}(1 + cos\alpha)$$

Thus:

$$b = \frac{T}{2}\frac{1+cos\alpha}{sin\alpha}$$

Using the half-angle formulas:

$$b = \frac{T}{2} cot \frac{\alpha}{2}$$

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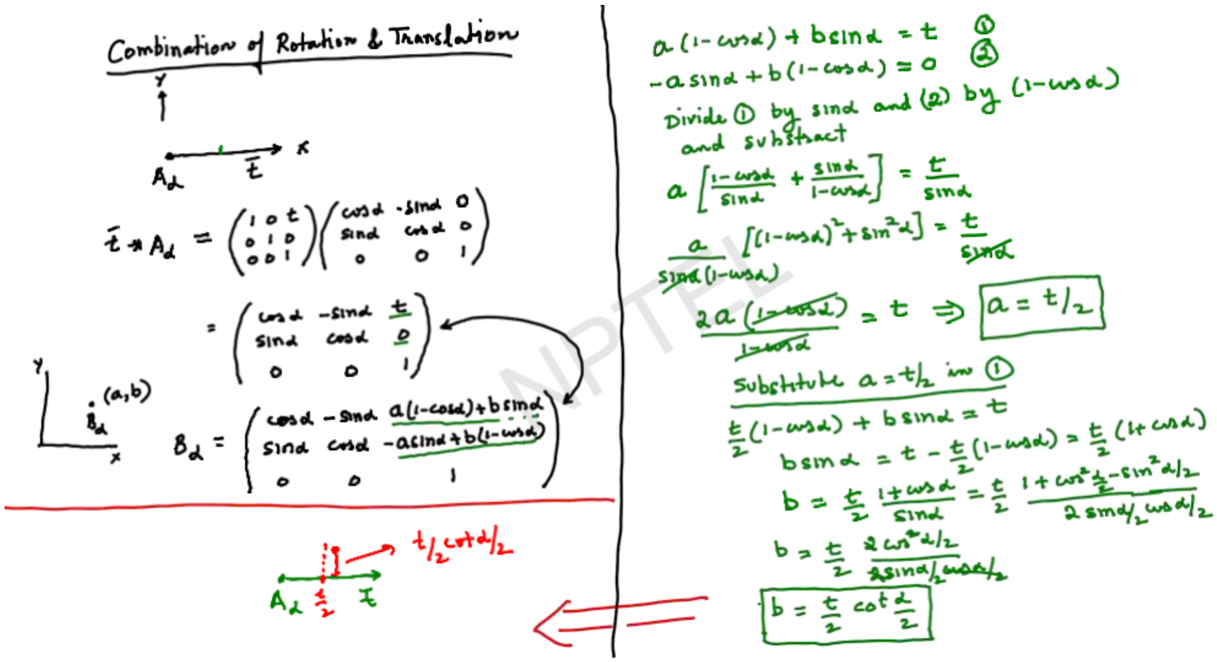

Hence, the second rotation axis lies at coordinates:

$$(a, b) = \left(\frac{T}{2}, \frac{T}{2} cot \frac{\alpha}{2}\right)$$

In the previous lecture, we determined the location of a new rotation axis resulting from the combination of a rotation α and a translation T. From the matrix method, we found the coordinates:

$$(a, b) = \left(\frac{T}{2}, \frac{T}{2} cot \frac{\alpha}{2}\right)$$

This places the new rotation axis at the midpoint of the translation vector along the direction of T, and a vertical distance of $T/2cot(\alpha/2)$.

It is instructive to understand this geometrically, which gives a better intuitive feeling of what happens in the two-dimensional plane.

Consider a rotation axis at point A and a translation vector T. Construct a perpendicular to the translation direction and draw a line at an angle $\alpha/2$, which we call line 1. Rotate this line through the angle α about point A; the line moves to a new position, line 2, preserving the angles $\alpha/2$.

Next, translate line 2 along T to obtain line 3. Consider a point P_1 on line 1. After rotation, it moves to P_2 on line 2, and translation moves it to P_3 on line 3.

Point symmetry implies that there is at least one invariant point under this combined operation. For a rotation axis, this invariant point lies on the axis itself. Let us label this point C. After rotation followed by translation, C remains invariant. Therefore, the new rotation axis passes through C.

Dropping a perpendicular from C onto the translation vector shows that it bisects the translation vector, giving the first coordinate:

$$x = \frac{T}{2}$$

The vertical distance along the perpendicular is determined using angles $\alpha/2$ from the geometric construction, giving:

$$y = \frac{T}{2} cot \frac{\alpha}{2}$$

Thus, the new rotation axis C_α is located at:

$$C_\alpha = \left(\frac{T}{2}, \frac{T}{2} cot \frac{\alpha}{2}\right)$$

Now, consider specific cases:

- **Two-fold rotation ($\alpha = \pi$):**

$$y = \frac{T}{2} cot \frac{\pi}{2} = 0$$

The new two-fold axis lies on the translation vector at the midpoint.

- **Three-fold rotation ($\alpha = 2\pi/3$):**

$$y = \frac{T}{2} cot \frac{\pi}{3} = \frac{T}{2\sqrt{3}}$$

The new axis is located perpendicular to the translation and appears both above and below the vector when considering $-\ \alpha$ rotation.

- **Four-fold rotation ($\alpha = \pi/2$):**

$$y = \frac{T}{2} cot \frac{\pi}{4} = \frac{T}{2}$$

The new axes lie on the perpendicular bisector at a distance $T/2$.

- **Six-fold rotation ($\alpha = \pi/3$):**

$$y = \frac{T}{2} cot \frac{\pi}{6} = \frac{\sqrt{3}}{2} T$$

The new six-fold axes lie on the perpendicular bisector at a distance $\sqrt{3}/2\, T$.

In conclusion, combining rotation with translation allows us to determine the precise location of the new rotation axis using both matrix and geometric methods. This provides a clear understanding of symmetry operations in two-dimensional lattices.

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