CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES
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Lecture 11: Restrictions on Rotational Symmetries

In this lecture, the discussion focuses on certain restrictions on rotational symmetries in a lattice or crystal. These restrictions arise due to the presence of translation symmetry. To understand this clearly, it is useful to begin with a specific example before generalizing the idea.

Consider a five-fold rotational symmetry. The minimum angle of rotation required in this case is given by $2\pi/5$, which is equal to 72°. Now imagine a row of equally spaced lattice points, and assume that each lattice point carries a five-fold rotational axis. Let points A and B be two such lattice points, and let the spacing between them be t, which represents the translation magnitude from A to B. Since every lattice point is assumed to possess five-fold rotational symmetry, a rotation of 72° must be valid about each point.

A counterclockwise rotation of 72° about point A acts on the entire space and hence on point B as well, carrying B to a new position C. Because rotational symmetry must map lattice points onto lattice points, C must also be a lattice point. Similarly, a clockwise rotation of 72° about point B must also be allowed. This operation carries point A to another point D, which again must be a lattice point. Thus A, B, C, and D are all lattice points.

By construction, segment AB is the shortest distance between lattice points, since it connects adjacent lattice points along that direction. Because the rotational operations map AB to CD, the direction AB must be parallel to the direction CD. If translation symmetry is to be preserved, the minimum spacing of lattice points in the direction of CD must be identical to the minimum spacing in the direction of AB.

However, from the geometry of the construction, it is evident that the distance CD is strictly smaller than AB, which contradicts the requirement that lattice points maintain a constant minimum spacing. Therefore, it becomes impossible to place lattice points at C and D while simultaneously preserving translation symmetry, and the conclusion follows that five-fold rotational symmetry cannot exist in a lattice.

To generalize this argument, consider two lattice points separated by a distance t, and assume that each point possesses a rotational symmetry characterized by a minimum rotation angle α. Let these points be denoted A_α and B_α.

A rotation of α about A carries B to a new lattice point C, and a rotation of α about B in the opposite (clockwise) direction carries A to another lattice point D. The line segments AB and CD must therefore be parallel. To analyze the length CD, draw perpendiculars from A and B to the line CD, meeting it at points E and F respectively. The total length CD can then be written as

$$CD = CE + EF + FD.$$

Thus, by examining the geometric contributions of CE, EF, and FD, one can determine whether CD is equal to, greater than, or less than AB. This geometric approach reveals the precise conditions under which rotational symmetry is compatible with translation symmetry, and ultimately shows why only certain rotational symmetries are permitted in a lattice.

In this continuation, we analyze the distances in the lattice under rotational symmetry. The segment EF is equal to t, the spacing between adjacent lattice points. To determine CE, consider triangle ACE. The angle $\angle ACE$ is given by $\pi - \alpha$ because $\angle CAE = \alpha - \pi/2$. Similarly, in triangle FDB, the angle $\angle FDB$ is also $\pi - \alpha$. Given that AB $= t$, a rotation about A maps line AB to AC, so that $AC = t$. Likewise, $BD = t$. Applying the cosine rule in triangle ACE, we find

$$CE = t\cos(\pi - \alpha).$$

Similarly, $FD = tcos(\pi - \alpha)$ and $EF = t$. Therefore, the total length CD is

$$CD = CE + EF + FD = tcos(\pi - \alpha) + t + tcos(\pi - \alpha) = t(1 - 2cos\alpha).$$

Since C and D must be lattice points, the distance CD must be an integer multiple of the translation t, say mt, where m is an integer. Thus, we have

$$mt = t(1 - 2cos\alpha) \quad \Rightarrow \quad cos\alpha = \frac{1-m}{2}$$

To determine the allowed rotational symmetries, we consider integer values of m. For $m =- 2$, $cos\alpha = 3/2$, which is invalid because $cos\alpha$ must lie between -1 and 1. Similarly, $m =- 3$ yields an even larger invalid value. For $m =- 1$, $cos\alpha = 1$ and $\alpha = 0$ or 2π. For $m = 0$, $cos\alpha = 1/2$ and $\alpha = \pi/3$ or $60°$. For $m = 1$, $cos\alpha = 0$ and $\alpha = \pi/2$ or $90°$. For $m = 2$, $cos\alpha =- 1/2$ and $\alpha = 2\pi/3$ or $120°$. For $m = 3$, $cos\alpha =- 1$ and $\alpha = \pi$. For $m = 4$, $cos\alpha =- 3/2$, which is invalid. Larger integers lead to even more invalid values. Therefore, the only allowed values of m are $- 1, 0, 1, 2, 3$.

Rewriting these angles in the standard $2\pi/n$ form, we find: $2\pi/1$ gives a 1-fold rotational axis, $2\pi/6$ gives 6-fold rotational symmetry, $2\pi/4$ gives 4-fold, $2\pi/3$ gives 3-fold, and $2\pi/2$ gives 2-fold. Hence, only 1-, 2-, 3-, 4-, and 6-fold rotational symmetries are possible in a lattice or crystal. Without translation symmetry, any value of n would be possible; in nature, many more rotational symmetries can be observed in flowers or plants, such as 5- or 8-fold symmetry. These are referred to as crystallographic rotational symmetries.

Graphical symbols are used to represent these rotational symmetries: the 2-fold is often depicted as a lens or ellipse, the 3-fold as an equilateral triangle representing $120°$ rotation, the 4-fold as a square, and the 6-fold as a regular hexagon. A 5-fold symbol would correspond to a pentagon, but this is not a crystallographic symmetry and therefore does not occur in lattice structures.

Restrictions on Rotational Symmetry

- due to presence of translation symmetry
- consider 5-fold rotation symmetry:
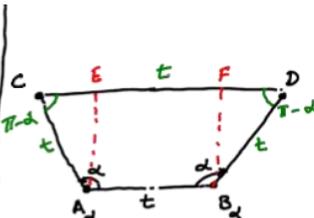
$$\alpha = \frac{2\pi}{5} = 72°$$
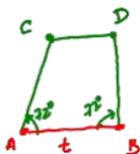
A, B, C, D → Lattice Points

AB = minimum distance

AB || CD → same spacing of lattice points in both cases

CD < AB → Contradiction

⇒ 5-fold symmetry cannot exist in a lattice

AB || CD

$$CD = CE + EF + FD$$
$$= t\cos(\pi - \alpha) + t + t\cos(\pi - \alpha)$$
$$= t - 2t\cos\alpha = t(1 - 2\cos\alpha)$$

$$CD = mt = t(1 - 2\cos\alpha)$$

$$\Rightarrow \boxed{\cos\alpha = \frac{1 - m}{2}}$$

$$m \in \mathbb{Z}$$

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m	cos α	α	
-2	3/2	—	
-1	1	$2\pi = \frac{2\pi}{1}$	1-fold
0	1/2	$\frac{\pi}{3} = \frac{2\pi}{6}$	6-fold
1	0	$\frac{\pi}{2} = \frac{2\pi}{4}$	4-fold
2	-1/2	$2\pi/3$	3-fold
3	-1	$\pi = \frac{2\pi}{2}$	2-fold
4	-3/2	—	

Only 1, 2, 3, 4 and 6-fold rotational symmetries possible in a lattice / crystal

→ Crystallographic Rotational Symmetries

2 → ⬗
3 → △
4 → ▢
6 → ⬡

5 → ⬠   t Not Crystallographic