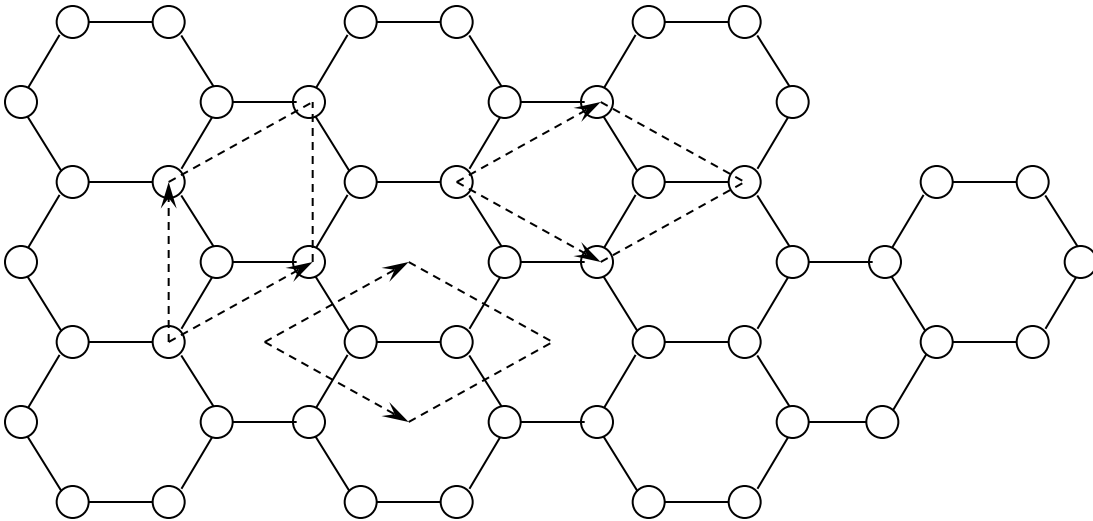


# Problem 1

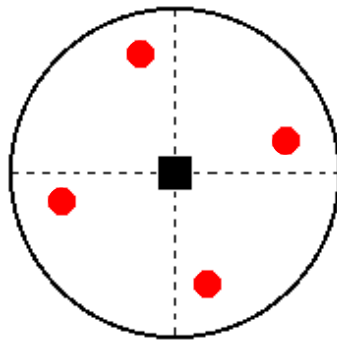


A **primitive basis** is a crystallographic basis of the vector lattice  $\mathbf{L}$  such that every lattice vector  $\mathbf{t}$  of  $\mathbf{L}$  may be obtained as an integral linear combination of the basis vectors,  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ .

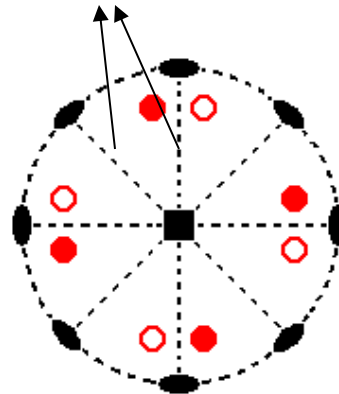
A **primitive cell** is a unit cell built on the basis vectors of a primitive basis of the direct lattice

# Problem 2

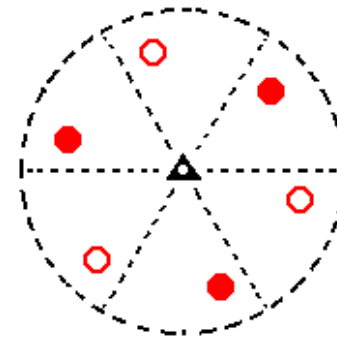
The two axis here are different from each other.



$C_4$



$D_4$

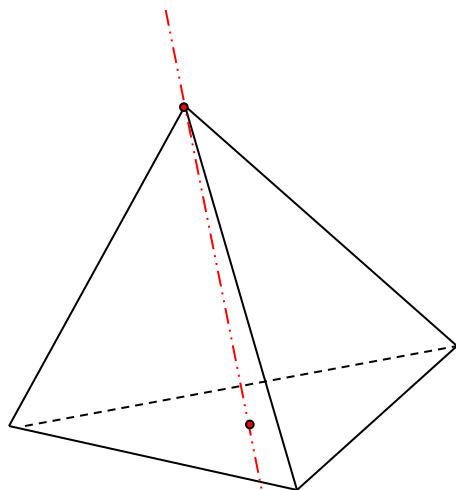


$C_{3i} (S_6)$

$D_4$  is also called 422 because it is composed of 4-fold rotation and 2 different 2-fold rotation

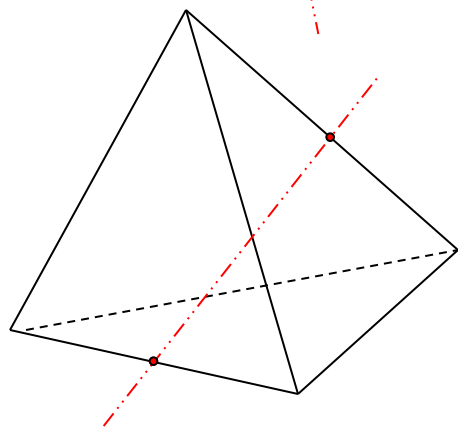
- Central symbol: rotational symmetry around vertical axis
- Symbols on edge: rotational symmetry around horizontal axes
- Lines through centre point: mirror planes
- Inner symbols (red in these diagrams): faces on the crystal
  - filled circle: lower face
  - open circle: upper face

# Problem 3a



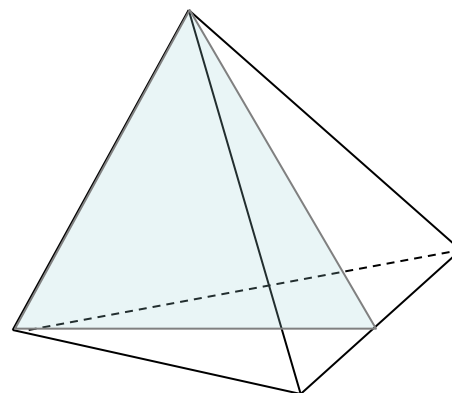
4 x  $C_3$  rotations

Axis from one apex to the centre of the opposite face through the centre of the tetrahedron



3 x  $C_2$  rotations

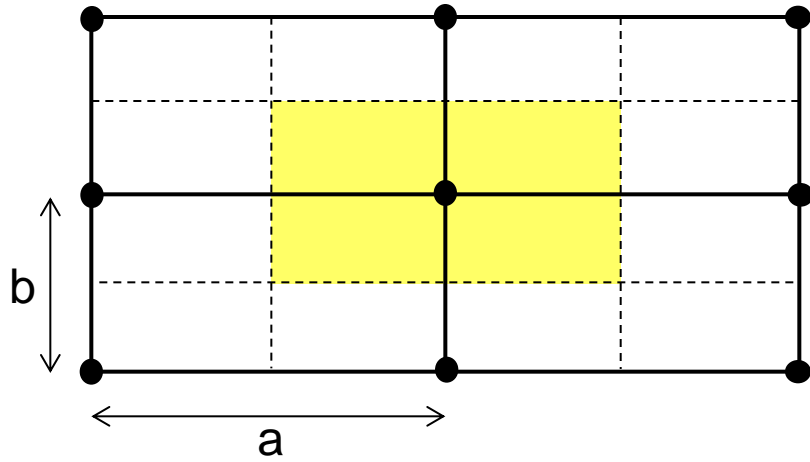
Axis from midpoint on one side to the midpoint of the opposite side



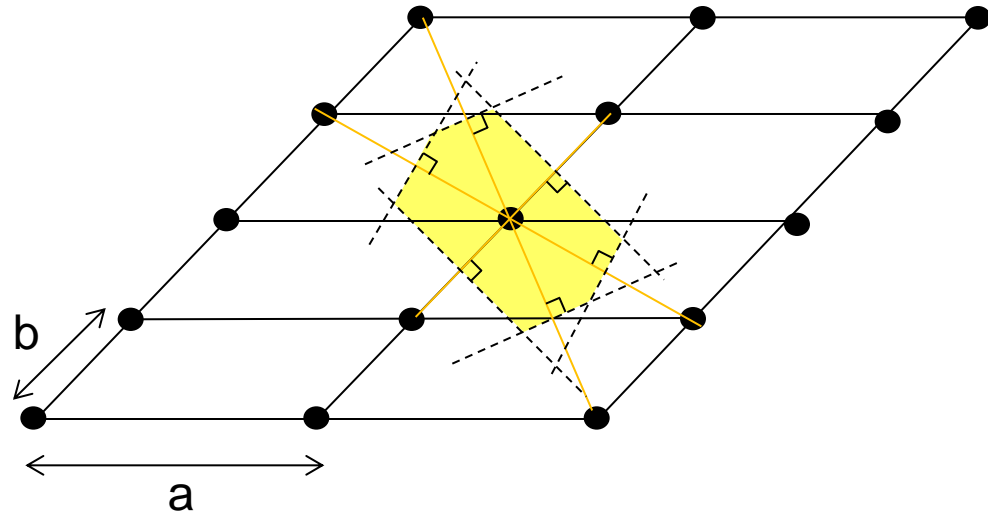
6 x reflections

# Problem 3b

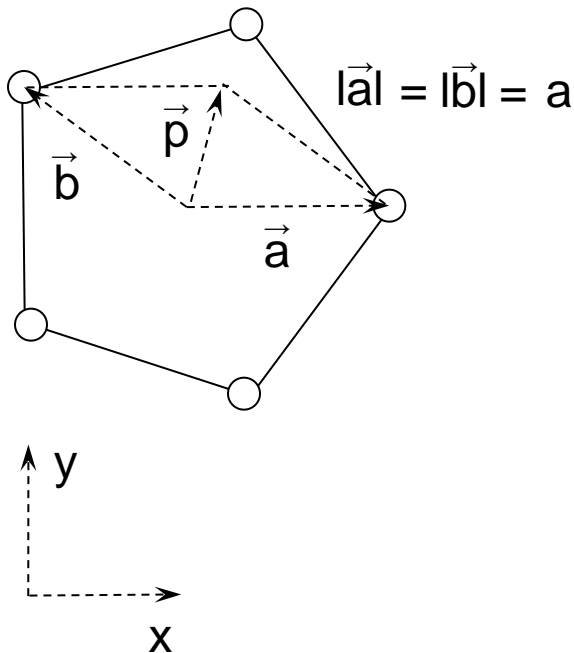
(i)



(ii)



# Problem 4



Obviously,

$$\vec{a} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \vec{b} = a \begin{pmatrix} \cos \theta_b \\ \sin \theta_b \end{pmatrix} \quad \theta_b = \sigma^* 4\pi/5$$

And,

$$\vec{p} = \vec{a} + \vec{b} \quad \text{should still be a part of the lattice under translation operation of a Bravais Lattice}$$

However,

$$|\vec{p}| = a \sqrt{\left(1 + \cos \frac{4\pi}{5}\right)^2 + \sin^2 \frac{4\pi}{5}} = 0.62a < a$$

This means that it is not a part of the lattice, which contradicts with our expectation. So we may come to the conclusion that a 5-fold rotation symmetry is not compatible with the translation properties of a Bravais Lattice.

## Problem 5

Some symmetry transformations of the crystal are also shown here:

$$\text{Rotation by } \theta = 60^\circ, \quad C_6 = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}_{\theta=n \times 60^\circ}$$

$$\text{Mirror symmetry: } \sigma_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The conductivity tensor is invariant under these symmetry transformations of the crystal:

$$\begin{aligned} \sigma &= C^{-1} \sigma C \Rightarrow \sigma_x^{-1} \sigma \sigma_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -\sigma_{11} & \sigma_{12} \\ -\sigma_{21} & \sigma_{22} \end{pmatrix} \\ &= \begin{pmatrix} \sigma_{11} & -\sigma_{12} \\ -\sigma_{21} & \sigma_{22} \end{pmatrix} \equiv \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \end{aligned}$$

no info about  $\sigma_{11}, \sigma_{22}$ ; but from

$$\sigma_{12} = -\sigma_{12} \Rightarrow \sigma_{12} = 0$$

$$\sigma_{21} = -\sigma_{21} \Rightarrow \sigma_{21} = 0$$

$$\therefore \sigma_{12} = \sigma_{21} = 0$$

$$\therefore \sigma = \begin{pmatrix} \sigma_{11} & 0 \\ 0 & \sigma_{22} \end{pmatrix}$$

$$\theta = 60^\circ$$

$$\begin{aligned} \sigma &= C_6^{-1} \sigma C_6 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \sigma_{11} & 0 \\ 0 & \sigma_{22} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{\sigma_{11}}{2} & -\frac{\sqrt{3}\sigma_{11}}{2} \\ \frac{\sqrt{3}\sigma_{22}}{2} & \frac{\sigma_{22}}{2} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\sigma_{11}}{4} + \frac{3\sigma_{22}}{4} & -\frac{\sqrt{3}\sigma_{11}}{4} + \frac{\sqrt{3}\sigma_{22}}{4} \\ -\frac{\sqrt{3}\sigma_{11}}{4} + \frac{\sqrt{3}\sigma_{22}}{4} & \frac{3\sigma_{11}}{4} + \frac{\sigma_{22}}{4} \end{pmatrix} = \begin{pmatrix} \sigma_{11} & 0 \\ 0 & \sigma_{22} \end{pmatrix} \end{aligned}$$

e.g. from first element :

$$\frac{1}{4}(\sigma_{11} + 3\sigma_{22}) = \sigma_{11}$$

$$3\sigma_{22} = 3\sigma_{11}$$

$$\therefore \sigma_{11} = \sigma_{22}$$