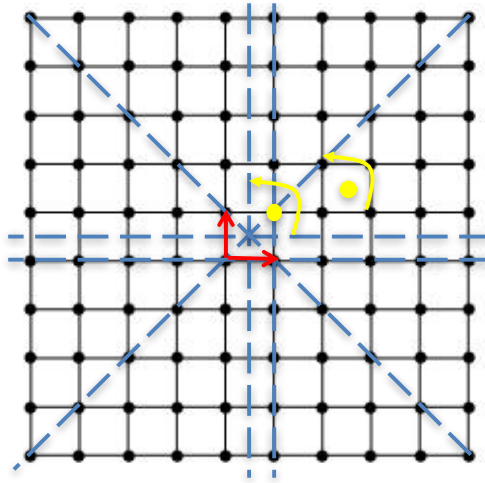


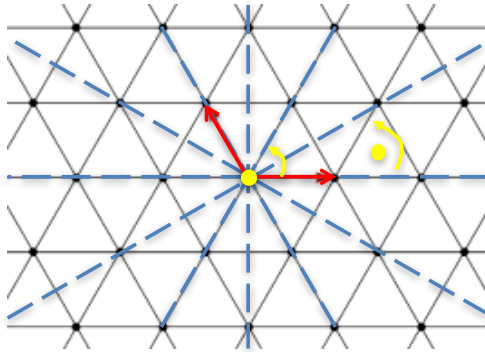
## 6 Applications of finite groups

### 6.6 Crystal tensor properties

Let's consider some popular lattices and find out their symmetry.



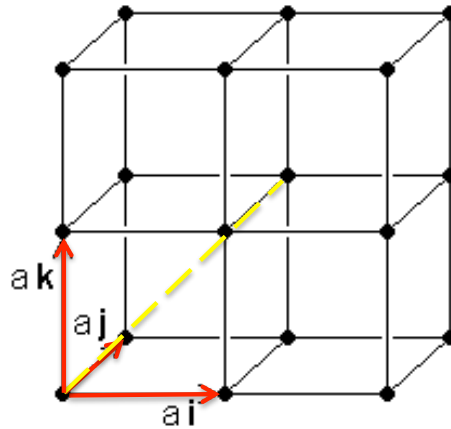
The square lattice is invariant under the following transformations: a. rotation by  $\pi/2$  (yellow arrow around the yellow dot rotation center); b. reflection (with respect to the blue axes); c. translation by unit distance in  $x$  or  $y$  directions (red arrows).



The triangular lattice is invariant under the following transformations: a. rotation by  $\pi/3$  around lattice points and rotation by  $2\pi/3$  around plaquette center; b. reflection (with respect to the blue axes); c. translation by unit distance in the two directions specified by red arrows.

The cubic lattice in  $3D$  is invariant under: a. translation by unit distance in  $i, j, k$  directions (red arrows); b. reflection with respect to the  $ij, jk, ki$  planes; c. rotation around  $i, j, k$  axis by  $\pi/2$ ; d. rotation around the diagonal axis of the cube by  $2\pi/3$ ; e. inversion ( $i \rightarrow -i, j \rightarrow -j, k \rightarrow -k$ ) centered at any lattice site.

The symmetry transformation of an infinite lattice falls into two types: **point group symmetry**, transformations which keep at least one point fixed; **translation symmetry**, transformation which



moves every point in the same direction by the same amount. Put together, they form the full **space group symmetry** of the lattice.

According to their symmetries,  $2D$  lattices are classified into five **Bravais lattices**, including oblique, rectangular, centered rectangular, hexagonal, and square lattices.  $3D$  lattices are classified into 14 Bravais lattices, including for example primitive cubic, body-centered cubic, face-centered cubic, hexagonal lattice, etc.

Moreover, each point in the lattice can have a structure of its own instead of just being a rotationally invariant ball. For example, each point in the lattice can host a molecule with internal structures. This will in general reduce the symmetry of the system and further distinguish among the lattices. Taking this into consideration, there are 230 different lattices in  $3D$ .

## 6.7 Constrains on macroscopic measurements

The macroscopic properties of a crystal is constrained by the underlying lattice symmetry. To understand how such a constraint works, we need to distinguish between scalar properties, vector properties and tensor properties.

Some properties of a crystal is just described by a number. For example, the mass, temperature, specific heat or free energy of the system.

Some properties of a crystal is a three dimensional vector. For example, the electric polarization  $P$  with three components  $(P_x, P_y, P_z)$ , and the current density  $(J_x, J_y, J_z)$ . The vectors have a single index, labeling the three dimensions of space. We say that a vector is a tensor of rank 1.

Some properties are described by tensors, i.e. quantities with more than one index. For example, the conductivity of a material is in general a two-index tensor. Usually, we think of conductivity as a scalar which measures the proportionality constant between current density  $J$  and applied electric field  $E$ . Both  $J$  and  $E$  are three dimensional vectors. Conductivity defined as the ratio between two vectors is a scalar only when  $J$  and  $E$  points in the same direction and their ratio is independent of the direction. But this is not necessarily true in a material. There are materials whose induced current can lie in a different direction from the applied electric field. Then to describe conductivity, we need to specify the proportionality constant between current density in every direction  $(x, y,$

$z$ ) and applied electric field in every direction ( $x, y, z$ ). Therefore, the conductivity becomes a two index tensor

$$\sigma_{ij} = J_i/E_j, \quad i, j = x, y, z \quad (1)$$

In the most general case, all nine entries in the tensor can be nonzero. Tensors with two indices are of rank 2.

Some other useful example of two index tensor properties are the stress and strain. The strain tensor describes the deformation (change in shape) of a body with respect to its original configuration. Suppose that the original position of each particle is given by  $(r_x, r_y, r_z)$  and after deformation each particle moves by  $(\delta_x, \delta_y, \delta_z)$ . The displacement of each particle can be different, therefore,  $(\delta_x, \delta_y, \delta_z)$  is in general a function of  $(r_x, r_y, r_z)$ . If  $(\delta_x, \delta_y, \delta_z)$  is independent of  $(r_x, r_y, r_z)$ , then the deformation amounts to a global translation of the body and we are not interested in that. We are interested in the case where every point has different displacement and hence the whole body deforms. Therefore, the strain tensor is defined as

$$\epsilon_{ij} = \frac{\partial \delta_i}{\partial r_j}, \quad i, j = x, y, z \quad (2)$$

The stress tensor on the other hand, is defined as the force acting in  $i$  direction on a unit surface in the  $j$  direction

$$\sigma_{ij} = \frac{\partial F_i}{\partial S_j}, \quad i, j = x, y, z \quad (3)$$

Combining these tensors, we can get tensors of even higher rank. For example, stress can induce electric polarization in piezoelectric materials. When the stress is small, the induced polarization has a linear relation to the stress. Their proportionality constant, called the piezoelectric modulus, is a rank three tensor and is defined as

$$d_{ijk} = \frac{\partial P_i}{\partial \sigma_{jk}}, \quad i, j, k = x, y, z \quad (4)$$

Similarly, in an elastic material under small stress, strain and stress have a linear relation and their proportionality constant, called the Young's modulus, is a rank four tensor and is defined as

$$\lambda_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \epsilon_{kl}}, \quad i, j, k, l = x, y, z. \quad (5)$$

As these properties depends on the coordinate system  $x, y, z$ , if we rotate the coordinate system, they should transform accordingly. In particular, in a quantum mechanical system at a thermal equilibrium state of temperature  $T$ , the measured quantity is given by

$$\langle O \rangle = \text{Tr}(e^{-H/k_B T} O) \quad (6)$$

If the Hamiltonian of the system is invariant under certain symmetry,  $D(g)H = HD(g)$ , then the measured quantity should transform according to how  $O$  transforms.

In particular, suppose that we do a transformation  $Q_{ij}$  on the coordinate system. Writing  $Q$

in matrix form, for inversion,  $Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ ; for reflection across the  $y - z$  plane  $Q =$

$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ ; for rotation around  $z$  axis,  $Q = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$ .

Under this transformation, the scalar property remains invariant. The vector properties transform as

$$D(Q)P_i D^{-1}(Q) = \sum_{i'} Q_{ii'}^{-1} P_{i'} \quad (7)$$

Note that  $D(Q)$  acts on the Hilbert space of the physical system while  $Q$  is a three dimensional linear transformation acting on the spatial indices.

The rank two tensor properties transform as

$$\sigma'_{ij} = \sum_{i'j'} Q_{ii'}^{-1} Q_{jj'}^{-1} \sigma_{i'j'} \quad (8)$$

The rank three tensor properties transform as

$$d'_{ijk} = \sum_{i'j'k'} Q_{ii'}^{-1} Q_{jj'}^{-1} Q_{kk'}^{-1} d_{i'j'k'} \quad (9)$$

so on and so forth.

Now if the system has certain symmetry, it remains invariant under certain transformations of the coordinate systems. Therefore, all the tensor properties should remain invariant. This puts a strong constrain on which component of the tensor can be nonzero. Consider the following examples.

### 1. Vector property in systems with inversion symmetry.

Suppose that the system has certain vector property  $P_i$ ,  $i = x, y, z$ . Under inversion  $Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ ,  $P \rightarrow -P$ . Therefore, systems with inversion symmetry, like cubic lattice, must have vanishing vector properties. Similarly, in systems with inversion symmetry, all tensor properties of odd rank must vanish. On the other hand, inversion symmetry does not constrain even rank tensors in any way.

### 2. Vector property in systems with rotation symmetry.

Suppose that the system has certain vector property  $P_i$ ,  $i = x, y, z$ . Under rotation the vector will be rotated to a different direction unless it points along the rotation axis. Therefore, in systems with rotation symmetry around a single axis, like the hexagonal lattice or the tetragonal lattice, it is possible to have nonzero vector property (along the axis), while in systems with rotation symmetry around multiple axes, like the cubic lattice, all the vector properties have to be zero.

### 3. Rank two tensor property in cubic lattice.

Suppose that we have a rank two tensor property. Let's try to figure out how many independent degrees of freedom there are of this property in a cubic lattice. A rank two tensor contains nine entries, so originally there are nine degrees of freedom. A large class of these tensors, including stress and strain, are symmetric (under transpose). That is,

$$\sigma_{ij} = \sigma_{ji} \quad (10)$$

This is due to physics considerations, not symmetry, and it reduces the number of DOF to six. We are left with  $\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{22}, \sigma_{23}, \sigma_{33}$ . Now let's use the symmetry properties of the cubic lattice to further reduce the number of DOF.

Inversion symmetry of the cubic lattice does not affect rank two tensors, but reflection and rotation does. Take reflection across  $x - y$  plane for example. The transformation is

$$Q = Q^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (11)$$

Under this transformation

$$\sigma_{13} \rightarrow -\sigma_{13}, \sigma_{23} \rightarrow -\sigma_{23} \quad (12)$$

while the other components remain invariant. Therefore, due to reflection symmetry across  $x - y$  plane,  $\sigma_{13} = \sigma_{23} = 0$ . Similarly, using reflection symmetry across  $y - z$  plane, we get  $\sigma_{12} = 0$ . Therefore, we are only left with the diagonal elements  $\sigma_{11}, \sigma_{22}, \sigma_{33}$ .

Now we use the rotation symmetry around the diagonal axis of the cube. Under a  $2\pi/3$  rotation in this direction,  $x, y, z$  axes are cyclicly permuted. Therefore,

$$\sigma_{11} \rightarrow \sigma_{22} \rightarrow \sigma_{33} \quad (13)$$

and have to be equal. That is, we can conclude that any rank two tensor property in a cubic lattice has to be diagonal and the diagonal elements have to be equal.