6 Applications of finite groups

6.6 Crystal tensor properties

6.6.3 Constrains on macroscopic measurements

Now we can talk about how 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 than 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

$$\sigma_{ij} = J_i/E_j, \; i,j = x,y,z \tag{1}$$

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

$$\epsilon_{ij} = \frac{\partial \delta_i}{\partial r_j}, \; i,j = x,y,z \tag{2}$$

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

$$\sigma_{ij} = \frac{\partial F_i}{\partial S_j}, \; i, j = x, y, z \tag{3}$$

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

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

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

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

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

$$< O >= \mathrm{Tr}(e^{-H/k_B T} O) \tag{6}$$

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

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

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

The rank two tensor properties transform as

$$\sigma'_{ij} = \sum_{i'j'} Q^{-1}_{ii'} Q^{-1}_{jj'} \sigma_{i'j'} \tag{8}$$

The rank three tensor properties transform as

$$d'_{ijk} = \sum_{i'j'k'} Q^{-1}_{ii'} Q^{-1}_{jj'} Q^{-1}_{kk'} d_{i'j'k'} \tag{9}$$

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 $Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$, $P \to -P$. 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,

$$\sigma_{ij} = \sigma_{ji} \tag{10}$$

This is due to physics considerations, not symmetry, and it reduces the number of DOF to six. We are left with σ_{11}, σ_{12},σ_{13}, σ_{22}, σ_{23},σ_{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

$$Q = Q^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{11}$$

Under this transformation

$$\sigma_{13} \to -\sigma_{13}, \ \ \sigma_{23} \to -\sigma_{23} \tag{12}$$

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,

$$\sigma_{11} \to \sigma_{22} \to \sigma_{33} \tag{13}$$

and have to be equal. That is, we can conclude that any rank two tensor property in a cubic lattice reduces to a scalar quantity.

7 Continuous Group

Now we are going to move on to continuous groups. We have seen the simplest example of a continuous group, the circle group. Let's first review how that works and see how the idea can be generalized to more complicated groups.

7.1 $SO(2)$

Instead of saying "the circle group", we are going to call it by a more popular name: the $SO(2)$ group. It is a matrix group of two dimensional orthogonal matrices with $+1$ determinant. It represents rotation of a two dimensional vector space and is represented on this two dimensional space as

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{14}$$

$\theta \in [0, 2\pi)$ and the group elements compose as

$$R(\theta_1)R(\theta_2) = R(\theta_1 + \theta_2 \mod 2\pi) \tag{15}$$

Notice that here we are using a particular representation to define the group, but the group is a more general abstract notion. In particular the group can have other kinds of representations. This $2D$ representation is special though in that it is faithful. Other representations may not be faithful. When we say $SO(2)$, in most cases it should be clear from the context whether we are talking about the abstract group or this particular two dimensional representation.

The continuity of the group elements comes from the continuity of the parameter θ. Moreover, the group has a nice property called compact, which roughly means that the parameter takes value in the bounded region of $[0, 2\pi)$.

This is an abelian group and the 2D representation actually decomposes into two 1D irreps through unitary transformation $S = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}$

$$SR(\theta)S^{-1} = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix} \tag{16}$$

Of course there are an infinite number of irreps given by $\{e^{in\theta}\}, n \in \mathbb{Z}$.

Because all irreps are $1D$, the character of the representation is just given by the irrep itself.

$$\chi^{(n)} = e^{in\theta}, \theta \in [0, 2\pi) \tag{17}$$

These characters satisfy an orthogonality condition similar to the finite group case. However, instead of summing over individual group elements, we need to perform an integration over them.

$$\langle \chi^{(n)}, \chi^{(n')} \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in\theta} e^{in'\theta} = \delta_{nn'} \tag{18}$$

Notice that I have chosen a normalization for the inner product of characters so that each character have length 1.

We can use this orthogonality condition of characters in the same way as we have used it for finite groups. For example, we can check that the $2D$ rep given above decomposes into two $1D$ irreps. The character of the $2D$ irrep

$$\chi = 2\cos\theta = e^{i\theta} + e^{-i\theta} \tag{19}$$

Therefore

$$R(\theta) = D^{(1)}(\theta) \oplus D^{(-1)}(\theta) \tag{20}$$

as we have seen above.

The direct product of irreps goes as

$$D^{(n)} \otimes D^{(n')} = D^{(n+n')} \tag{21}$$

Therefore, under direct product, the irreps form a group which is isomorphic to the group of integers.

For finite groups, a useful notion is the generator of the group. Once we have identified the generators of a group and the relations between them, we knows which group it is. For continuous group, can we similarly find such generators? For the $SO(2)$ group, intuition says that the generator of the group is an infinitesimal rotation by a very small angle θ. But of course, no θ is small enough, we can always find a smaller one. What we define instead, is an infinitesimal generator

$$X \equiv i \frac{dR(\theta)}{d\theta}\Big|_{\theta=0} \tag{22}$$

for any representation R. Any group elements in the continuous group can then be obtained by taking the exponential of this infinitesimal generator.

$$R(\theta) = e^{-i\theta X} \tag{23}$$

The exponential of an operator is defined as $e^{-i\theta X} = \sum_{k=0}^{\infty} \frac{(-i\theta X)^k}{k!}$. If we can diagonalize X into $VXV^{-1} = D$, where $D = diag(d_1, d_2, ...)$, then $e^{-i\theta X} = V^{-1} diag(e^{-i\theta d_1}, e^{-i\theta d_2}, ...)V$.

For the irrep labeled by n, $D^{(n)}(\theta) = e^{in\theta}$, $X^{(n)} = -n$. For the $2D$ orthogonal representation, $R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, $X = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Note that X is Hermitian because R is unitary.

In physics, the Hermitian generator X is sometimes identified as the orbital angular momentum J_z around the rotation axis z (e.g. for electron orbits around a nucleus). Suppose that a wave function forms an irrep of the $SO(2)$ group. That is,

$$R(\theta)|\psi\rangle = e^{-in\theta}|\psi\rangle \tag{24}$$

The state is said to have orbital angular momentum $J_z = n$. In other situations, X maybe identified with the number of particles N in the system (e.g. for electrons in metals or insulators) and in this particular state $N = n$.