6 Applications of finite groups

6.5 Perturbation and degeneracy splitting

Now suppose that the Hamiltonian of the system is perturbed by a term V. How does the spectrum change? In particular, we want to know if the degeneracy structure of the system changes. This will depend on the symmetry property of V. The short answer is: if V has the same symmetry as H, then the degeneracy required by symmetry is preserved while the accidental degeneracies may be lifted (removed); on the other hand, if V breaks some of the symmetries of H, then it is possible to lift non-accidental degeneracies as well. (Recall that non-accidental degeneracies exist among different basis states of the same irrep while accidental degeneracies exist among different irreps (which may or may not be equivalent).)

This can be shown by considering the symmetry of the perturbed Hamiltonian $H' = H + V$. If V has the same symmetry as H, then so does H'. Our previous argument regarding the eigen spectrum of H still applies. Therefore, inequivalent irreps of $D(g)$ remain separate under H'. It is possible that V mix equivalent irreps which originally belong to different eigen sectors of H. This has two consequences. First, it can change the linear combination of the irreps that form eigen sectors of the Hamiltonian; Secondly, it can change the eigenvalues of the sectors and thereby remove or introduce accidental degeneracy. However, the degeneracy required by symmetry with higher dimensional irreps remains intact.

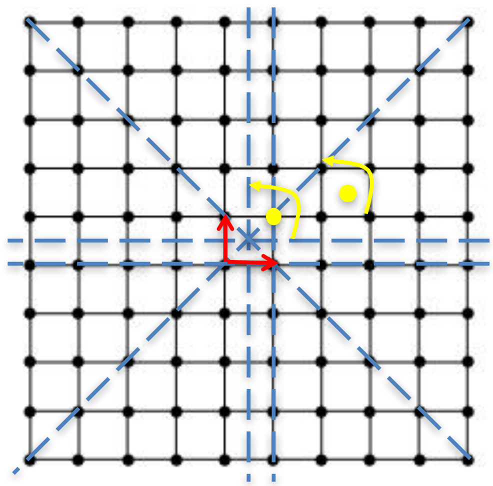
On the other hand, if V has a smaller symmetry than H, then the symmetry of H' will generally be a subgroup of that of H ($G' \subset G$). In this case, some higher dimensional irreps of G can break down to the direct sum of multiple irreps of G', therefore the degeneracy is not protected by symmetry any more and can be lifted.

Suppose that we start with an H with D_3 symmetry and add a perturbation V with only the subgroup Z_3 symmetry. H' has only Z_3 symmetry. The symmetry representation of D_3 naturally restricts to a representation of Z_3 by only keeping the representation matrices in the Z_3 subgroup. Under this restriction, each irreducible block in the representation becomes a representation of Z_3, but not necessarily an irreducible one. The trivial irrep of D_3 restricts to the trivial irrep of Z_3. The 1D nontrivial irrep of D_3 also restricts to the trivial irrep of Z_3. The 2D irrep of D_3 on the other hand is reducible when restricted to Z_3. When the character of the 2D irrep is restricted to the Z_3 subgroup, it becomes $\chi = \{2, -1, -1\}$, which can be decomposed into two 1D irreps of Z_3 with character $\{1, \omega, \omega^2\}$ and $\{1, \omega^2, \omega\}$. Therefore, the 2D irrep of D_3 splits into two inequivalent irreps of Z_3. On the spectrum side, all the trivial irreps of Z_3 can remix and form a set of (generically nondegenerate) eigenstates. The degeneracy associated with the 2D irreps are now completely lifted, and each eigenstate corresponds to a nontrivial irrep of Z_3.

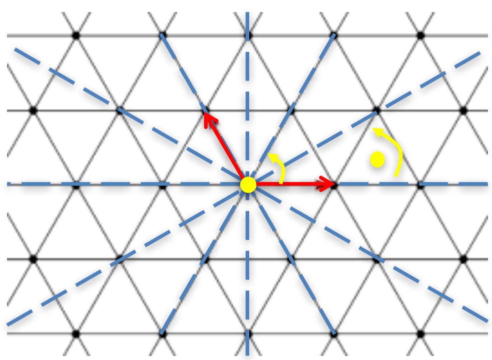
6.6 Crystal tensor properties

6.6.1 Point Group Symmetries

A crystal can have more symmetries than just translation symmetry. Let's consider some popular lattices and find out their symmetry.



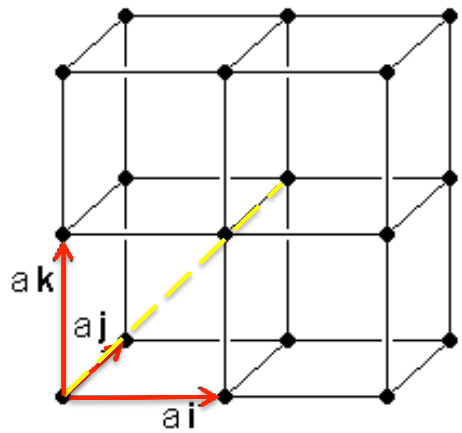
The square lattice is invariant under the following transformations: a. rotation by $\pi/2$ (yellow arrow around the yellow dot rotation center); b. reflection (with respect to the blue axises); c. translation by unit distance in x or y directions (red arrows).



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 axises); 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 ($i \to -i$, $j \to -j$, $k \to -k$) centered at any lattice site. (Note that inversion in $3D$ is not equivalent to a rotation transformation.)

The symmetry transformations 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 $3D$.

6.6.2 Operators forming a representation of symmetry

Before we talk about tensor properties of crystals, we need to talk about in quantum mechanics how operators transform under symmetry and how operators can form a representation of the symmetry group.

In a Hilbert space, the state of the system is given by a wave function $|\psi\rangle$. Suppose that symmetries of group G act on the Hilbert space as $D(g)$. The wave function transforms under symmetry as $|\psi\rangle \to D(g)|\psi\rangle$. Suppose that O is an operator acting on the Hilbert space. For example, O can be a Hermitian operator corresponding to some measurable quantity. As a linear operator on the Hilbert space, O takes the form $O = \sum_{ij} O_{ij}|\psi_i\rangle\langle\psi_j|$. Therefore, under symmetry transformation, O transforms as $O \to D(g)OD^\dagger(g)$.

For example, translation by a in the x direction is implemented by $e^{ip_x a}$, where p_x is the momentum operator in the x direction. This can be seen from the following relation

$$e^{ip_x a} x e^{-ip_x a} = x + a \tag{1}$$

This relation can be proven as follows: define $f(a) \equiv e^{ip_x a} x e^{-ip_x a}$.

$$\frac{d}{da} f(a) = e^{ip_x a} i p_x x e^{-ip_x a} + e^{ip_x a}(-ixp_x)e^{-ip_x a} = e^{ip_x a} i[p_x, x] e^{-ip_x a} = 1 \tag{2}$$

Therefore,

$$f(a) = f(0) + a \tag{3}$$

Similarly, rotation around the z direction is implemented by $e^{iL_z\theta}$ where L_z is the angular momentum operator in the z direction, $L_z = xp_y - yp_x$. How do the operators x and y transform under such rotations? Intuitively, x and y should rotate into some linear combinations of the two inside the two dimensional space spanned by themselves. We can check that this is indeed true. In particular, if we define

$$s_x(\theta) \equiv e^{iL_z\theta} x e^{-iL_z\theta}, s_y(\theta) \equiv e^{iL_z\theta} y e^{-iL_z\theta} \tag{4}$$

then

$$\frac{d}{d\theta} s_x(\theta) = e^{iL_z\theta} i[L_z, x] e^{-iL_z\theta} = -s_y(\theta), \frac{d}{d\theta} s_y(\theta) = e^{iL_z\theta} i[L_z, y] e^{-iL_z\theta} = s_x(\theta) \tag{5}$$

from which we see

$$s(x) = \cos\theta x - \sin\theta y, \;\; s(y) = \cos\theta y + \sin\theta x \tag{6}$$

In general, if a set of operators $\{O_1, ..., O_M\}$ transform under symmetry $D(g)$, $g \in G$, as

$$D(g) O_m D^\dagger(g) = \sum_{m'} E(g)_{mm'} O_{m'} \tag{7}$$

then we say that the operators form a representation of the symmetry given by $E(g)$. Therefore, x and y form a 2-dimensional representation of the circle group given by $E(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$.