The rhombohedral and hexagonal lattice systems are not fully compatible with point group symmetries. Knowing the point group doesn’t uniquely determine the lattice systems. Sometimes we can resolve this incompatibility using one of the following two methods: (1) merge rhombohedral + hexagonal lattice systems into one and (2) regroup crystals in these two lattice systems into two classes, which are compatible with point groups.

- **6 crystal families**: Similar to lattice systems, but rhombohedral and hexagonal lattice systems are merged into 1 crystal family, known as the hexagonal crystal family.

- **7 crystal systems**: similar to lattice systems, but regroup rhombohedral and hexagonal lattice systems into trigonal and hexagonal crystal systems.

  trigonal crystal systems:\[
  C_3 + S_6 + D_3 + C_{3v} + D_{3d}
  \]

  hexagonal crystal systems:\[
  C_h + C_{3h} + C_{6h} + D_6 + C_{6v} + D_{3h} + D_{6h}
  \]

  The trigonal crystal system is slightly larger than the rhombohedral lattice system. The hexagonal crystal system is slightly smaller than the hexagonal lattice systems.

### 5.5. Representations

#### 5.5.1. Definition

To describe non-commutative products \((A \neq B \neq A)\), a very convenient tool is matrices.

A representation of a group is a map from the group to a set of \(N \times N\) matrices,

\[
g \rightarrow \rho(g)
\]

where \(g\) is an element of the group and \(\rho(g)\) is a \(N \times N\) matrix, such that

\[
\rho(g_1) \rho(g_2) = \rho(g_1 g_2)
\]

for any two elements \(g_1\) and \(g_2\) in this group.

**Example: rotations**

Rotations along \(z\)

\[
\begin{pmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
\begin{pmatrix}
x' \\
y' \\
z'
\end{pmatrix}
= \begin{pmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
\]

We can define similar matrices for rotations along \(x\) and \(y\), or any directions. This is a representation for the \(SO(3)\) rotational group.

#### 5.5.2. N is called the dimensions of the representations

If \(\rho(g)\) are \(N \times N\) matrices, we say that such a mapping is a \(N\)-dimensional representation.

#### 5.5.3. The trivial presentation

There is an obvious representation for any groups: Mapping all group elements to the number 1 (it is a \(1 \times 1\) matrix)

\[
g_1 \rightarrow 1
\]

\[
g_2 \rightarrow 1
\]

\[
g_1 g_2 \rightarrow 1
\]

Obviously,

\[
\rho(g_1) \rho(g_2) = \rho(g_1 g_2)
\]
5.5.4. Faithful representations
A faithful representation: if the map \( g \rightarrow \rho(g) \) is a one-to-one correspondence [i.e. if \( g_1 \neq g_2 \), then \( \rho(g_1) \neq \rho(g_2) \)], the representation is called faithful.
- Not all representations are faithful (e.g. the trivial representation is not faithful, as long as the group has more than one element).
- A faithful representation carvers all the information about the group.
- If a representation is NOT faithful, it lost some information about the group (e.g. the trivial representation lost almost all information about the group).

5.5.5. Abelian representations and non-abelian representations
As mentioned above, in general, we don’t require a group to be abelian,

\[
g_1 \neq g_2 \Rightarrow \rho(g_1) \neq \rho(g_2)
\]

However, even for a nonabelian group, with \( g_1 \neq g_2 \), the presentation may be abelian.

\[
\rho(g_1) \rho(g_2) = \rho(g_2) \rho(g_1)
\]

One example is the trivial presentation above. It is obviously commutable (abelian).
- Any presentation of a abelian group is abelian
- Any group has at least one abelian representation
- A 1D representation for any group is an abelian representation

5.5.6. Equivalent representations
If we have on representation, \( \rho(g) \), then

\[
g \rightarrow M \rho(g) M^{-1}
\]

is also a representation, where \( M \) is an arbitrary invertible matrix.

If

\[
\rho(g_1) \rho(g_2) = \rho(g_1 g_2)
\]

then obviously

\[
M \rho(g_1) M^{-1} M \rho(g_2) M^{-1} = M \rho(g_1) \rho(g_2) M^{-1} = M \rho(g_1 g_2) M^{-1}
\]

We call these two representations “equivalent”.

In the language of quantum mechanics, two equivalent representations are identical, except that they are written in two different basis.

When we consider representations of a group, we only need one representation from each equivalent family, because each presentation in this family carry the same information (just in a different basis).

Q: How do we know whether two representations are equivalent or not?
A: Look at the trace of the matrices (known as the character). If two representations have the same characters, then they are equivalent. Otherwise, they are not.

Note: for a 1D representation, characters = representations.

5.5.7. Reducible and irreducible representations
If \( \rho(g) \) is a representation and \( \rho'(g) \) is another representation of the same group, then obviously,

\[
\begin{pmatrix}
\rho(g) & 0 \\
0 & \rho'(g)
\end{pmatrix}
\]

is also a representation.

This representation, as well as all representations that are equivalent to this representation, is called a reducible representation, because it can be reduced to two separate representations.

If a representation cannot be made block diagonal (by any similar transformations), then it is called irreducible.
When we consider representations of a group, we will only focus on irreducible representations. Because reducible ones doesn’t carry addition information. They are composed by irreducible ones.

5.5.8. All possible representations

From the previous two sections, we can see immediately, if we want to know all possible representation of a group, we only need to consider irreducible and inequivalent representations (to avoid repeating the same information).

Q: How many irreducible and inequivalent representations does a group have?

A: For a finite group (a group with finite number of elements), there is only a finite number of representations

If we list all possible representations for a finite group, \( (\rho_i(g)) \ i=1,2,\ldots,m \) marks different representations, one can prove that

\[
N = d_1^2 + d_2^2 + \ldots d_m^2
\]  

(5.27)

where \( N \) is the number of elements in the group (name as the order of the group). \( d_i \) is the dimensions of the \( i \)th representation.

Because \( d_i \) are all positive integers, for any finite \( N, m \) must be finite

5.5.9. Example:

- \( C_1 \): only one operator: the identity \( \{E\} \). Examples: some crystals with triclinic Bravais lattices. (NOT all crystals with triclinic lattices have \( C_1 \) symmetry. Some of them have \( C_i \) )

The order of the group \( N=1 \). So there can be only one presentation with \( d_1 = 1 \). That is the trivial representation: \( E \to 1 \)

- \( C_2 \): two operators:\( \{E, I\} \). The symmetry of a triclinic Bravais lattice (ignoring any structure inside each unit cell)

The order of the group \( N=1 \). There is only one possible way to split \( N \) as sum of \( d_i^2 \)

\[
2 = 1^2 + 1^2
\]

(5.28)

Only two representations. One of them is obvious (trivial), where \( E \to 1 \) and \( I \to 1 \). The other is \( E \to 1 \) and \( I \to -1 \). The second representation is faithful.

- \( C_2 \): two operations: \( \{E, C_2\} \), where \( C_2 \) is 180-degree rotation along \( z \). Examples: some of the crystals with a monoclinic Bravais lattice.

Same as \( C_i \)

- \( D_2 \): if we add 180-degree rotation along \( x \) to \( C_2 \), then we must also add 180-degree rotation along \( y \), because a \( C_2 \) rotation along \( x \) followed by a \( C_2 \) rotation along \( y \) is equivalent to a \( C_2 \) rotation along \( y \). The closure condition requires us to add the fourth element to the group. This group is known as \( D_2 \).

Four elements \( (N = 4) \). There are two ways to split 4

\[
4 = 1^2 + 1^2 + 1^2 + 1^2
\]

(5.29)

and

\[
4 = 2^2
\]

(5.30)

which one should we use here?

A: must be \( 4 = 1^2 + 1^2 + 1^2 + 1^2 \). Because we know that any group has a (trivial 1d representation). So there must be at least one \( d_i = 1 \).

The four representations:

Character table:

\[
\begin{array}{cccc}
D_2 & E & C_2(x) & C_2(y) \\
\Gamma_1 & 1 & 1 & 1 \\
\Gamma_2 & 1 & -1 & 1 \\
\Gamma_3 & 1 & 1 & -1 \\
\Gamma_4 & 1 & -1 & -1 \\
\end{array}
\]

(5.31)

None of the irreducible representations are faithful.

Note: because \( 4 = 1^2 + 1^2 + 1^2 + 1^2 \), all representations of \( D_2 \) are 1-dimensional. Because 1D representations are abelian, we can see immediately, all representations of \( D_2 \) are abelian. Because all representations of \( D_2 \) are abelian, \( D_2 \) must be an abelian group.

A nonabelian group must have at least 5 elements \( N > 4 \).

- \( D_3 \): symmetry of a equilateral triangle
It has 6 elements: \( E \) (doing nothing), \( C_3 \) 120 degree rotation along \( z \). \( C_3^2 = C_3^{-1} \)-120 degree rotation, and 3 \( C_2 \) rotations in the \( xy \) plane.

\[
4 = 1^2 + 1^2 + 2^2
\]

(5.32)

\textbf{Character table:}

\[
\begin{array}{cccc}
D_3 & E & C_3(z) & C_3^{-1}(z) \\
\Gamma_1 & 1 & 1 & 1 \\
\Gamma_2 & 1 & 1 & 1 \\
\Gamma_3 & 2 & -1 & 0 \\
\end{array}
\]

(5.33)

For \( \Gamma_3 \), which is the only faithful irreducible representation for \( D_3 \), we have

\[
E = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}
\]

(5.34)

\[
C_3 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}
\]

(5.35)

\[
C_3^{-1} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}
\]

(5.36)

\[
C_2^a = \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}
\]

(5.37)

\[
C_2^b = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}
\]

(5.38)

\[
C_2^c = \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}
\]

(5.39)

\section*{5.6. Applications of group theory in physics}

- Classify physics systems based on their symmetries

Create a list of all possible groups. Then each physics systems should belong to one of the classes. (Example: 32 point groups. So we can classify crystals in these 32 families)

Systems in each class show different physical properties (e.g. if we apply an \( E \) field along \( x \), whether there is a current flow along \( y \)?)

- Symmetries provide strong constraints on physical observables (utilizing representations).

Sometimes, solving a problem is hard (or even impossible). But without bothering to solve the problem, we can get qualitative properties by thinking physics observables as a representation of the corresponding symmetry group.

Sometimes, we don’t know the details of a system. But as long as we know its symmetry, we can make strong predictions, which is right for sure, even if we don’t fully know the details of the system.

\section*{5.7. Representations and degeneracy}

In QM, we learned that in general a QM system sometimes shows degeneracy (i.e. more than one eigenstates share the same eigenenergy). There are two types of degeneracy (a) accidental and (b) protected.

\subsection*{5.7.1. Accidental degeneracy:}

Accidental degeneracy: different states have the same energy level for no reason other than pure luck. Eigenenergies are functions of control parameters: \( \epsilon(a, b, c, ...) \) and \( \epsilon_2(a, b, c, ...) \). For two different functions, they are not expected to take the same value. However, if our control parameters happen to take some very special values, these two functions may have the same value (only for this set of control parameters). If we are slightly away from the this special points, the degeneracy will be gone.
In physics, accidental degeneracy is not a “real” degeneracy, for two reasons:

(1) Because in physics, there is always some error. There is no way to put all control parameters to exactly these values with no error. The small errors will imply that these two energies are not really the same. The best we can do is to make them close. With high enough experimental resolution, we will always find that the two levels have a (small) energy difference.

(2) A model is different from a real system. A model is simplified reality. The Hamiltonian in our theory calculation always differs from the reality

\[ H_{\text{real}} = H_{\text{model}} + \delta H \]  

(5.40)

If the difference is small, we can treat \( \delta H \) as perturbation. If we find accidental degeneracy theoretically (in \( H_{\text{model}} \)), it doesn’t mean that the real system will have the degeneracy. Degenerate perturbation told us, a small perturbation \( \delta H \), will usually lift the degeneracy (unless there is a reason tell it not to).

### 5.7.2. Protected degeneracy:

Protected degeneracy: different states with the same energy for a reason. If some “reason” says that regardless of details (such as the values of control parameters), these states must have the same energy, we say that this degeneracy is protected by this “reason”. As long as the reason remains, the degeneracy cannot be lifted. Equivalently, if we want to lift the degeneracy, we have to get ride of the reason. The “reason” is often certain symmetry.

### 5.7.3. Energy levels and representations of the symmetry group

Consider eigenstates of \( H \), \( |a\rangle \), \( |b\rangle \), \( |c\rangle \), ... Under a symmetry operation (e.g. rotation or translation) \( X \), these quantum states will be transformed to a other set of states, and the transformation is described by a unitary matrix

\[
\begin{pmatrix}
|a\rangle \\
|b\rangle \\
|c\rangle \\
...
\end{pmatrix}
= U(X)
\begin{pmatrix}
|a\rangle \\
|b\rangle \\
|c\rangle \\
...
\end{pmatrix}
\]  

(5.41)

In quantum mechanics, if \( X \) is a symmetry operation, it means that \( U(X)H U(X)^{-1} = H \), which means that

\[ UH = HU \]  

(5.42)

Thus

\[ [U , H] = 0 \]  

(5.43)

All symmetry operators form a group. \( U(X) \) is a representation of the group. In general, \( U(X) \) is reducible. In the bases shown above, \( U(x) \) is block diagonal, and quantum states in each energy level form a block. Each block form a representation of the group.

**Proof:**

If \( |a\rangle \) is an eigenstate with energy \( E \), after a symmetry transformation, \( U(X) |a\rangle \) must also be an eigen state with the same eigenenergy.

\[ H (U |a\rangle) = U H |a\rangle = U E |a\rangle = E (U |a\rangle) \]  

(5.44)

In other words, a symmetry transformation can only transfer a eigenstate to some eigenstates with the same eigenenergy, i.e. \( U(X) \) is block diagonal. Each block remains inside a group of degenerate states.

### 5.7.4. Reducible and irreducible representations

Now, lets zoom into one specific energy level with \( n \)-fold degeneracy. Assuming that we have \( n \) degenerate states at this energy level:

\[
\begin{pmatrix}
|1\rangle \\
|2\rangle \\
...
|n\rangle
\end{pmatrix}
= U_n(X)
\begin{pmatrix}
|1\rangle \\
|2\rangle \\
...
|n\rangle
\end{pmatrix}
\]  

(5.45)

Here, \( U_n(X) \) is the corresponding \((n \times n)\) transfer matrix. It is easy to check that this matrix form a representation of the group. This representation could be reducible or irreducible. If it is a reducible one, then the degeneracy here is accidental. If it is a irreducible one, then it is protected.

**Proof:**

We introduce some small perturbation to the system

\[ H + \delta H \]  

(5.46)
and we make sure that the perturbation preserves the same symmetry. If the perturbation lifts the degeneracy, than using the eigenstates of \( H + \delta H \), \( U_{\delta}(X) \) becomes block-diagonal. This means that \( U_{\delta}(X) \) must be a reducible representation.

Irreducible representation are impossible to break into smaller pieces, and thus degeneracy cannot be lifted. Reducible representation can break, and in general the degeneracy will be lifted.

5.7.5. Implications:

- If the symmetry group of a quantum system has a n-dimensional representation, then this system could have n-fold protected degeneracy.
- Similarly, if the symmetry group doesn’t have a n-dimensional representation, then it is impossible for the system to have a n-fold degeneracy (i.e. if you see one, it must be either due to an accident, or the system has some symmetry that we haven’t figured out yet).
- If the representation with highest dimension is \( n_{\text{max}} \) dimensional, the system can at most have \( n_{\text{max}} \)-fold presentation (unless there is another reason to require a higher degeneracy).
- If the symmetry group is abelian, then there should be no degeneracy.

5.7.6. Example: a particle in a square well.

Consider a 2D potential well. Here, we only require the potential well to have the symmetry of a square (\( D_4 \)), but we don’t care about the detailed functional form.

\[
V(x, y) = V(\pm y, \pm x) = V(\pm x, \pm y)
\]

The symmetry group for a square is \( D_4 \), which has four 1D representations and one 2D representation. Thus the eigenstates for this system should have some 1 or 2 fold degeneracy.

Example: an infinite square potential \( V = 0 \) for \( 0 < x < a \) and \( 0 < y < a \) and \( V = +\infty \) otherwise.

It is easy to show that eigenstates are

\[
\psi_{mn}(x, y) = \sin \left( \frac{2 m + 1}{a} \pi x \right) \sin \left( \frac{2 n + 1}{a} \pi y \right)
\]

Eigenenergies are

\[
E_{mn}(x, y) = \frac{\hbar^2}{2 \mu} \left( \frac{2 m + 1}{a} \pi \right)^2 + \left( \frac{2 n + 1}{a} \pi \right)^2 = \frac{\hbar^2 \pi^2}{2 \mu a^2} \left( 4 m^2 + 4 n^2 + 4 m + 4 n + 1 \right)
\]

For \( m = n \), it is one-fold degeneracy (or say non-degenerate). For \( m \neq n \), there is a two fold degeneracy \( E_{mn} = E_{nm} \). In agreement with the symmetry prediction.

5.7.7. Example: a particle in a rectangular well.

Consider a rectangular potential well:

\[
V(x, y) = V(\pm x, \pm y)
\]

The symmetry group is \( D_2 \), which is an abelian group, and thus all representations are 1D. Thus there should be no degeneracy in this system.

Example: infinite rectangular well \( V = 0 \) for \( 0 < x < a \) and \( 0 < y < b \), and \( V = +\infty \) otherwise. We know that

\[
E_{mn}(x, y) = \frac{\hbar^2}{2 \mu} \left( \frac{2 m + 1}{a} \pi \right)^2 + \left( \frac{2 n + 1}{b} \pi \right)^2
\]

Here \( E_{mn} \neq E_{nm} \) and thus there is no degeneracy.

It is possible to have accidental degeneracy here, e.g. when \( b = 3a \). However, such an accidental degeneracy is not stable. If there is any error for the ratio \( a/b \), the degeneracy will be lifted.

Symmetry protected degeneracy is different. No matter how we deform the system, as long as the symmetry is preserved, the degeneracy will be there.

5.7.8. Example: Crystal field splitting

In an atom, the eigenstates of electrons are labeled by four indices (ignore spin-orbit coupling)

\[
| n \ell m_s \rangle
\]

where \( n \) is the principle quantum number (positive integers), \( l \) is the total angular momentum quantum number.
\[ L^2 \left| n \ell m s_z \right\rangle = \hbar (\ell + 1) \hbar^2 \left| n \ell m s_z \right\rangle \]  
(5.53)

\( m \) is the quantum number for \( L_z \)

\[ L_z \left| n \ell m s_z \right\rangle = m \hbar \left| n \ell m s_z \right\rangle \]  
(5.54)

\( s_z = \pm \) means spin up (+) or down (-).

We know that energy levels only depends on \( n \) and \( \ell \)

\[ \epsilon(n, \ell) \]  
(5.55)

We will ignore spin index from now on, since it play not role here. For each energy level \( n \), \( \ell \), there are \( 2\ell + 1 \) degenerate quantum states (times 2 if we include spins) labeled by different values of \( m \). This degeneracy is **protected** by the SO(3) rotational symmetry, i.e. an atom is spherically symmetric. Remember that for a fixed \( \ell \), \( \left| l, m \right\rangle \) forms a \( 2\ell + 1 \)-dimensional irreducible representation of the O(3) rotational group.

If we put an atom in a solid with certain point group symmetry, the spherically symmetry will be broken, and thus the \( 2\ell + 1 \)-fold degeneracy will in general be lifted, which is known as crystal field splitting.

In the language of group theory, \( \left| l, m \right\rangle \) form a \( 2\ell + 1 \)-dimensional irreducible representation of the O(3) rotational group. Because a point group is a subgroup of the O(3) group, i.e., any elements in a point group is an element of O(3), \( \left| l, m \right\rangle \) also form a representation of the point group of the lattice. For a point group, this representation is in general reducible, can be broken into smaller irreducible ones. As a result, the energy level with \( 2\ell + 1 \)-fold degeneracy will split into multiple levels with lower degeneracy.

For example:

- The 5 quantum states with \( \ell = 2 \) breaks into \( \Gamma_3 \) (2D) and \( \Gamma_5 \) (3D) representations in a cubic lattice (point group \( O_h \))
  
  \[ 5 = 2 + 3 \]  
  (5.56)

This means that the energy level with 5-fold degeneracy will now split into 2 energy levels with different energies. One of them has 2 fold degeneracy (\( \Gamma_5 \)) and the other 3-fold (\( \Gamma_3 \)).

The triplet (with 3 degenerate states) is often labeled as \( t_{2g} \) and the doublet (with 2 degenerate states) is often called \( e_g \), i.e. the d-wave states split into \( e_g \) and \( t_{2g} \).

- The same 5 quantum states with \( \ell = 2 \) breaks into \( \Gamma_1 \) (1D), \( \Gamma_3 \) (2D) and \( \Gamma_6 \) (2D) representations in a hexagonal lattice (point group \( D_{6h} \))
  
  \[ 5 = 1 + 2 + 2 \]  
  (5.57)

This means that the energy level with 5-fold degeneracy will now split into 3 energy levels with different energies. One of them is non-degeneracy and the other two are 2-fold degenerate.

- The same 5 quantum states with \( \ell = 2 \) breaks into 5 \( \Gamma_1 \) (1D) representations in a triclinic lattice (point group \( C_1 \))
  
  \[ 5 = 1 + 1 + 1 + 1 + 1 \]  
  (5.58)

This means that the energy level with 5-fold degeneracy will now split into 5 energy levels with different energies.

- The 3 states with \( \ell = 1 \) forms the \( \Gamma_4 \) representation of a cubic lattice (point group \( O_h \)). \( \Gamma_4 \) is a 3-d irreducible representation. Thus the energy level will NOT split.
  
  \[ 3 = 3 \]  
  (5.59)