Group Theory for Solid State Physics Xingyu Ren 250120 https://github.com/Phy-Ren

This note is mostly based on Wiki and the (unpublished) lecture note of Jianjun Xu(徐建军) at Fudan University. We recommend the interest readers to look at some textbooks on "group theory for physicists" for further studies.

1. Basics

Definition 1 A group, denoted as (G, \cdot) , is a non-empty set G together with a binary operation on G, here denoted " \cdot ", that combines any two elements a and b of G to form an element of G, denoted $a \cdot b$, such that the following three requirements, known as group axioms, are satisfied:

- 1. Associativity: $(a \cdot b) \cdot c = a \cdot (b \cdot c), \ \forall a, b, c \in G$.
- 2. Identity element: $\exists e \in G \text{ s.t. } a \cdot e = e \cdot a = a, \ \forall a \in G.$
- 3. Inverse element: $\forall a \in G, \exists a^{-1} \in G \text{ s.t. } a \cdot a^{-1} = a^{-1} \cdot a = e$.

We will usually omit the multiplication ' \cdot ' and just denote the group as G and write $ab := a \cdot b$. Note that in this definition the multiplication is not required to be commutative, i.e., $a \cdot b \neq b \cdot a$ is possible.

Definition 2 A group A is Abelian if the multiplication is commutative $a \cdot b = b \cdot a$, $\forall a, b \in A$.

Definition 3 A homomorphism from a group (G, \cdot) to a group (H, *) is a function $f: G \to H$ s.t. $f(a \cdot b) = f(a) * f(b), \forall a, b \in G$.

Group homomorphisms are functions that respect group structure. If the map is one-to-one correspondence, then this homomorphism is called an isomorphism.

Definition 4 A subgroup (H, \cdot) of group (G, \cdot) is a subset of G s.t. H is also a group under the same multiplication.

The inclusion map $H \hookrightarrow G$ is a group homomorphism with the same multiplication operation. This means that the identity element e of G must be contained in H.

Theorem 1 Rearrangement Theorem: Each row and each column in the group multiplication table lists each of the group elements once and only once. From this, it follows that no two elements may be in the identical location in two rows or two columns. Thus, each row and each column is a rearranged list of the group elements.

This theorem can be also formulated as gG = Gg = G, $\forall g \in G$, where $gG := \{g \cdot h \mid h \in G\}$.

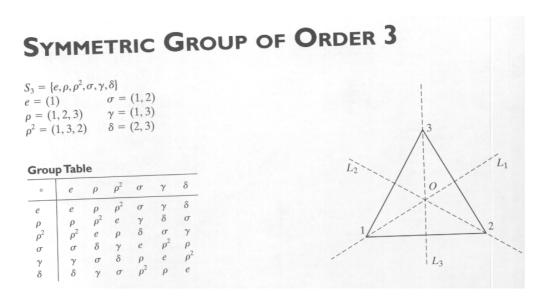


Figure 1: Multiplication table of the permutation group S_3 .

Definition 5 Two elements g_i, g_j in group G is conjugate to each other if $\exists g \in G$ s.t. $g_i = g \cdot g_j \cdot g^{-1}$.

The conjugate relation is an equivalence relation (also called binary relation) \sim , which is reflective, symmetric and transitive. That is, $\forall a, b, c \in G$:

- 1. Reflexivity: $a \sim a$.
- 2. Symmetry: $a \sim b$ iff $b \sim a$.
- 3. Transitivity: If $a \sim b$ and $b \sim c$ then $a \sim c$.

Once we have an equivalence relation, we can quotient out this equivalence relation to get the equivalence class.

Definition 6 The equivalence class of conjugate relation in group G is called conjugate class.

We usually use [g] to denote the conjugate class of the element $g \in G$, which is a set containing all the elements conjugate to g. For Abelian group, every element is a conjugate class.

Definition 7 Given a subgroup H of group G, the left and right cosets of H, containing an element g, are $gH := \{g \cdot h \mid h \in H\}$ and $Hg := \{h \cdot g \mid h \in H\}$, respectively. In many situations it is desirable to consider two group elements the same if they differ by an element of a given subgroup. Cosets are used to formalize this insight: a subgroup H determines left and right cosets, which can be thought of as translations of H by an arbitrary group element g. Note that in general a coset is not a group because there may be no identity element. The left coset may not be the same with the right coset, i.e., $gH \neq Hg$ is possible.

Theorem 2 The left cosets of any subgroup H form a partition of G; that is, the union of all left cosets is equal to G and two left cosets are either equal or have an empty

intersection.

This means the representative element of a coset can be chosen to be any element in this coset.

Definition 8 The order of a group G is the number of elements in this group, denoted as |G|.

If the order of a group is finite, we call this group a finite group, otherwise it is called infinite group.

Theorem 3 Lagrange Theorem: The order |G| of a finite group G is dividable by the order |H| of its subgroup H, i.e., $|G|/|H| = l_H$ is an integer called the index of subgroup H.

This theorem tells us the structure of group G can be organized by its subgroup H as

$$G = H \oplus g_1 H \oplus g_2 H \oplus \cdots \oplus g_{l-1} H \tag{1}$$

for a collection of elements g_i . Obviously, if the order n is a prime number, then the group G can not have an proper subgroup.

Theorem 4 Given an element a of group G, the set of all elements that commute with a, denoted as $Z(a) := \{g \in G \mid g \cdot a \cdot g^{-1} = a\}$, is also a group, called the centralizer of a in G.

By the Orbit-Stabilizer Theorem, the orbit of a is the conjugate class [a], while the stabilizer of a is just the centralizer Z(a), so the theorem states |[a]| = |Z(a)|. Since Z(a) is a subgroup of G, |Z(a)| should be a factor of |G| by the Lagrange Theorem. Above theorems immediately implies that the number of elements |[a]| in any conjugate class [a] of group G is a factor of the order |G|.

Theorem 5 The center of a group G is the set of all elements in G that commute with every element of G, denoted as $Z(G) := \{z \in G | z \cdot g = g \cdot z, \forall g \in G\}$, which is also a group.

Definition 9 For a subgroup H of group G, if gH = Hg, $\forall g \in G$, then H is called a normal (or invariant) subgroup.

If H is a subgroup of group G, then gHg^{-1} should also be a subgroup of G for any $g \in G$ with the same order as H. This structure motivates the following theorem.

Theorem 6 H is a normal subgroup of group G iff H contains some full conjugate classes of G.

If G is an Abelian group, then every subgroup is normal. Similarly, if the index of a subgroup is 2, then it is normal. For a normal subgroup H, we can define the multiplication * of its cosets as

$$(g_i H) * (g_j H) := g_i \cdot H \cdot g_j \cdot H = g_i \cdot g_j \cdot H \cdot H = (g_i g_j) H.$$

Definition 10 For a subgroup H of group G, the quotient set $G/H = \{H, g_1H, \dots, g_{l-1}H\}$ forms a group of order $l_H = |G|/|H|$ if H is normal, called quotient group.

If a group G does not contain any nontrivial normal subgroup, then it is called single group. The classification of finite single groups is a great milestone in the history of mathematics. The proof consists of tens of thousands of pages in several hundred journal articles written by about 100 authors, published mostly between 1955 and 2004.

Theorem 7 Homomorphism Theorem: For a group homomorphism $f: G \to G'$, the kernel $H := \{h \in G \mid f(h) = e'\}$ of f is a normal subgroup of G, and the quotient group G / H is isomorphic to the image $\{f(g) \mid g \in G\}$ in G'.

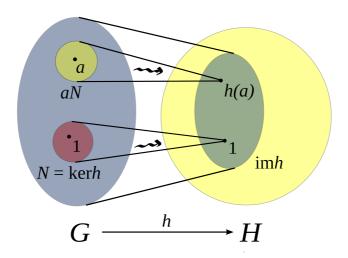


Figure 2: Structure of group homomorphism.

Theorem 8 Cayley Theorem: Every group of order n is isomorphic to a subgroup of the permutation group S_n .

This theorem comes directly from the Rearrangement Theorem. This theorem is important because we have many tools to study permutation groups.

Definition 11 Given two groups G_1, G_2 , the direct product of them is defined as $G_1 \otimes G_2 := \{(g_1, g_2) \mid g_1 \in G_1, g_2 \in G_2\}$, while the multiplication * is defined as $(g_1, g_2) * (g'_1, g'_2) := (g_1 \cdot g'_1, g_2 \cdot g'_2)$. The direct product of two groups is still a group.

2. Group Representation

A group may be abstract to manipulate, while vector spaces are something physicists familiar with. To represent a group by matrices, we need to introduce group representation theory. The essence of representation theory is that we study the action of

the group on vector spaces to study the group itself.

Definition 12 If V is a vector space over the field K, the general linear group of V, written GL(V) or Aut(V), is the group of all automorphisms of V, i.e. the set of all bijective linear transformations $V \to V$, together with functional composition as group operation.

If V has finite dimension n, then $\operatorname{GL}(V)$ and $\operatorname{GL}(n,K)$ (the group of $n\times n$ invertible matrices on field K) are isomorphic. The isomorphism is not canonical; it depends on a choice of basis in V. Given a basis (e_1, \dots, e_n) of V and an automorphism Γ in $\operatorname{GL}(V)$, we have then for every basis vector e_i that $\Gamma(e_i) = D_{ii}e_i$ (we will use Einstein sum rule).

Definition 13 A representation of a group G on a vector space V over a field K is a group homomorphism from G to GL(V), the general linear group on V. That is, a representation is a map $\rho: G \to GL(V)$ s.t. $\rho(g_1g_2) = \rho(g_1)\rho(g_2), \ \forall g_1, g_2 \in G$.

Here V is called the representation space and the dimension of V is called the dimension or degree of the representation. It is common practice to refer to V itself as the representation when the homomorphism is clear from the context. The field K is usually chosen to be real number \mathbb{R} or complex number \mathbb{C} for real representation and complex representation, respectively. If a basis of V is chosen, we will have $\Gamma_g(e_i) = D_{ji}(g)e_j$, i.e., represent the group element $g \in G$ by a matrix D(g) in GL(V) or GL(n, K). The group multiplication is given by matrix multiplication in GL(V): $D(g_1g_2) = D(g_1)D(g_2)$. Obviously, $D(e) = \mathbb{I}$ and $D(g^{-1}) = [D(g)]^{-1}$. We will usually just denote a representation by D(G).

Definition 14 If D(G) is a d-dimensional representation of group G, then the $SD(G)S^{-1}$ is also a d-dimensional representation for any $d \times d$ non-singular matrix S, called the equivalent or isomorphic representation of D(G).

Definition 15 If the representation D(G) of group G can be block diagonalized, i.e., can be written as

$$D(g) = \begin{pmatrix} D_1(g) & \\ & D_2(g) \end{pmatrix}, \ \forall g \in G \tag{2}$$

by some basis transformation S, then $D(G) = D_1(G) \oplus D_2(G)$ is a reducible representation. Here $D_1(G)$ and $D_2(G)$ are all representations of G.

If $D_1(G)$ and $D_2(G)$ are still reducible representations, we can further decompose them until that D(G) is a direct sum of irreducible representations

$$D(G) = \sum_{p=1}^{\oplus} a_p D^{(p)}(G),$$
 (3)

where a_p counts the number of the p-th irreducible representation $D^{(p)}(G)$.

Definition 16 Given a representation D(G) of group G, the character of D(g) for any

group element g is defined as $\chi(g) := \operatorname{Tr} D(g)$.

Note that the trace of matrix has the cyclic permutation property

$$\operatorname{Tr}(ABC) = \operatorname{Tr}(BCA) = \operatorname{Tr}(CAB).$$
 (4)

Obviously, elements in the same conjugate class have the same character. Similarly, equivalent representations have the same character. The character $\chi(e) = \text{Tr}(\mathbb{I}_d) = d$ of identity element e is always the dimension d of this representation. These properties make it a good quantity to study.

Theorem 9 If group G has a nontrivial normal subgroup H, then any representation D(K) of the quotient group K = G / H is also a (unfaithful) representation of G. On the other hand, if there is an unfaithful representation D'(G) of G, then there should be at least one normal subgroup H' of G s.t. D'(K') is faithful representation of the quotient group K' = G / H'.

Definition 17 A representation D(G) of group G is unitary if $D(g)^{\dagger} = D(g)^{-1}, \ \forall g \in G, \ where \dagger \ means \ Hermit \ conjugate \ D_{ij}^{\dagger} = D_{ji}^*.$

Note that here is a nice property for the Hermit matrix: every Hermite matrix can be diagonalized by some unitary similar transformations.

Theorem 10 For finite group G, every representation D(G) has an equivalent unitary representation.

This theorem can be generalized to compact Lie group. Based on this theorem, from now on we will only talk about unitary representation.

Lemma 1 Schur's Lemma: Given a d-dimensional irreducible representation D(G) of group G, if an arbitrary $d \times d$ matrix M satisfies MD(g) = D(g)M, $\forall g \in G$, then $M = \lambda \mathbb{I}_d$, where λ is a constant.

The proof depends on the unitarity of the representation. The Schur's Lemma can be generalized to the following theorem.

Theorem 11 Given two irreducible representations $D^{(p)}(G)$, $D^{(q)}(G)$ with dimensions d_p, d_q , if there is an non-zero $d_q \times d_p$ matrix M satisfying $MD^{(p)}(g) = D^{(q)}(g)M$, $\forall g \in G$, then $D^{(p)}(G)$, $D^{(q)}(G)$ are equivalent representations with M being the similar transformation.

Theorem 12 Generalized Orthogonality Theorem: Given two inequivalent irreducible unitary representations $D^{(p)}(G)$, $D^{(q)}(G)$ with dimensions d_p , d_q , we have

$$\sum_{q \in G} D_{\mu\nu}^{(p)*}(g) D_{\mu'\nu'}^{(q)}(g) = \frac{|G|}{d_p} \delta_{pq} \delta_{\mu\mu'} \delta_{\nu\nu'}.$$
 (5)

This theorem is proved by Theorem 11, and the hint is that we can construct

 $M = \sum_{g \in G} D^{(q)}(g) S D^{(p)} \left(g^{-1}\right)$ for an arbitrary non-singular matrix S.

Theorem 13 Burnside Theorem: If group G has r inequivalent irreducible representations in total, we have

$$d_1^2 + d_2^2 + \dots + d_r^2 = |G|, (6)$$

where d_i is the dimension of i-th irreducible representation.

In fact, Theorem 12 immediately implies $d_1^2 + d_2^2 + \cdots + d_r^2 \leq |G|$. To prove the equality, we need to introduce the canonical representation in Definition 18, and the theorem is proved by Eq. (12).

Theorem 14 (First) Character Orthogonality Theorem: Given two nonequivalent irreducible unitary representations $D^{(p)}(G)$, $D^{(q)}(G)$, we have

$$\sum_{q \in G} \chi^{(p)*}(g)\chi^{(q)}(g) = |G|\delta_{pq}. \tag{7}$$

This theorem is obvious when starting from Theorem 12 and taking trace. We mentioned before that the group elements in the same conjugate class will have the same character, so Eq. (7) can be rewritten as

$$\sum_{[g]\in G} |[g]| \chi^{(p)*}([g]) \chi^{(q)}([g]) = |G| \delta_{pq}, \tag{8}$$

where the summation is over the conjugate class [g], and |[g]| is the number of elements in this class.

Theorem 15 For a group G, the number r of the inequivalent irreducible representations equals to the number k of the conjugate classes, i.e., r = k.

Similarly as Theorem 13, Eq. (8) immediately implies $r \leq k$. We emphasize that Theorem 13 plus Theorem 15 can uniquely determine the number and dimensions of all inequivalent irreducible representations of a group G.

Theorem 16 Two representations of the same group are equivalent iff they have the same characters.

Starting from Eq. (3), we can take the trace

$$\chi(G) = \sum_{p=1}^{\oplus} a_p \chi^{(p)}(G), \tag{9}$$

then the multiplicity a_p can be obtained by the orthogonality relation of characters

$$a_p = \frac{1}{|G|} \sum_{g \in G} \chi^{(p)*}(g) \chi(g). \tag{10}$$

Using Theorem 14, we can further calculate

$$\sum_{g \in G} |\chi(g)|^2 = \sum_{g \in G} \sum_{p,q}^{\oplus} a_p a_q \chi^{(p)*}(g) \chi^{(q)}(g) = |G| \sum_p a_p^2 \geqslant |G|, \tag{11}$$

which tells us $\sum_{g \in G} |\chi(g)|^2 > n$ for a reducible representation, while

 $\sum_{g \in G} |\chi(g)|^2 = |G|$ for an irreducible representation.

There are two basic representations to consider: canonical representation and coset representation.

Definition 18 Using group elements of a group G as a basis $\{e_i = g_i, g_i \in G\}$, the action of group element g on this linear space is constructed as the linear operator $\{\Gamma_g = g, g \in G\}$, i.e., $\Gamma_g e_i := gg_i = g_j = e_j$. This representation is called canonical representation $D^{(c)}(g)$.

The representation matrix $D^{(c)}(g)$ can be directly read out from the $g_i \sim g_j^{-1}$ multiplication table: if g appears in the i-th row and j-th column, then $D^{(c)}_{ij}(g) = 1$, otherwise the matrix entry is zero. Then the character is $\chi^{(c)}(e) = |G|$, otherwise it is zero. The canonical representation is |G|-dimensional and it is obviously reducible because $\sum_{g \in G} |\chi^{(c)}(g)|^2 = |G|^2 > |G|$. Using Eq. (10), we can decompose the character as

$$\chi^{(c)}(g) = \sum_{p} a_p \chi^{(p)}(g) = \sum_{p} d_p \chi^{(p)}(g), \tag{12}$$

where $a_p = d_p$ (the dimension of representation) is a nontrivial result.

Definition 19 Follow Eq. (1), using cosets of a subgroup H of group G as a basis $\{e_i = g_i H\}$, the action of group element g on this linear space is constructed as the linear operator $\{\Gamma_g = g, g \in G\}$, i.e., $\Gamma_g e_i := gg_i H = g_j H = e_j$. This representation is called coset representation $D^{(d)}(g)$.

Similarly, the representation matrix $D^{(d)}(g)$ can be directly read out from the coset $g_i H \sim H g_j^{-1}$ multiplication table: if g appears in the i-th row and j-th column, then $D_{ij}^{(d)}(g) = 1$, otherwise the matrix entry is zero. The coset representation is useful because it can be used to construct the induced representation.

Definition 20 Chosen a subgroup H of group G, if we have a representation $D^{(H)}(H)$ of H and a coset representation $D^{(d)}(G)$ of group G on H, then we can use their direct product to construct an induced representation $D^{(I)}(G)$ as

$$D^{(I)}(g)_{\beta\alpha} = D^{(d)}_{\beta\alpha}(g)D^{(H)}(g_{\beta}^{-1}gg_{\alpha}), \tag{13}$$

where every entry of this super matrix $D^{(I)}(g)_{etalpha}$ is the matrix $D^{(H)}ig(g_{eta}^{-1}gg_{lpha}ig)$ (

 $g_{\beta}^{-1}gg_{\alpha} \in H$ if $D_{\beta\alpha}^{(d)}(g) = 1$). Here α, β labels the conjugate class, and g_{α}, g_{β} are representatives of corresponding conjugate classes, respectively.

In general, this induced representation is reducible. Given a subgroup H of group G, its induced representation $D^{(I)}(g) = \sum_G a_G D^{(G)}(g)$ can be decomposed into irreducible representations of G, while irreducible representations of G are in general reducible for H, which can be further decomposed into the irreducible representations of H:

$$D^{(G)}(h) = \sum_{H} b_{H} D^{(H)}(h).$$

Theorem 17 Frobenius Reciprocity Theorem: $a_G = b_H$.

Theorem 18 Second Character Orthogonality Theorem: The summation of all nonequivalent irreducible unitary representations $D^{(p)}(G)$ for $p=1, \dots, r$, we have

$$\sum_{p=1}^{r} |[g_i]| \chi^{(p)*}([g_i]) \chi^{(p)}([g_j]) = |G| \delta_{ij}.$$
(14)

Note that the summation here is over the irreducible representations, while the summation in Eq. (8) is over the conjugate classes. To prove this theorem, we need to construct a matrix $C_i^{(p)} = \sum_{g \in [g_i]} D^{(p)}(g)$, which satisfies $C_i^{(p)} D^{(p)}(g) = D^{(p)}(g) C_i^{(p)}$ for any $g \in G$. Then by the Schur's Lemma, $C_i^{(p)} = \lambda_i^{(p)} \mathbb{I}$. We further point out that $C_i C_j = \sum_k a_{ij}^k C_k$. The proof of this theorem immediately implies that $r \geqslant k$ thus proved Theorem 15. Using these orthogonality relations Theorem 14 and Theorem 18 plus the constraints Theorem 13 and Theorem 15, we can solve the character table of a specific group.

Definition 21 Given two groups G_1, G_2 with irreducible representations $D_1^{(p)}(G_1), D_2^{(q)}(G_2)$, whose dimensions are d_1, d_2 , their direct product $D^{(p,q)}(g_1 \otimes g_2) = D_1^{(p)}(g_1) \otimes D_2^{(q)}(g_2)$ is an irreducible representation of the direct product group $G = G_1 \otimes G_2$ with dimension $d_1 d_2$.

Not that the direct product of groups defined in Definition 11 is commutative, while the direct product of representations are non-commutative. For a group G, the direct product of two irreducible representations $D^{(p,q)}(g) = D^{(p)}(g) \otimes D^{(q)}(g)$ is still a representation of G, but reducible in general

$$D^{(p,q)}(G) = \sum_{\lambda}^{\oplus} a_{\lambda} D^{(\lambda)}(G). \tag{15}$$

The multiplicity can be calculated by the orthogonal relation

$$a_{\lambda} = \frac{1}{|G|} \sum_{g \in G} \chi^{(p)}(g) \chi^{(q)}(g) \chi^{(\lambda)*}(g). \tag{16}$$

The bases of the left and right-hand side of Eq. (15) are $w_{i,j}^{(p,q)}$, $w_l^{(\lambda)\alpha}$ (α labels the multiplicity) respectively, then the (unitary) basis transformation are done by the Clebsch-Gordan coefficient

$$w_l^{(\lambda)\alpha} = \sum_{i,j} \langle {p \atop i} {q \atop j} \mid {\lambda \atop l} \alpha \rangle w_{i,j}^{(p,q)}, \tag{17}$$

$$w_{i,j}^{(p,q)} = \sum_{\lambda,l,\alpha} \langle \frac{\lambda}{l} \alpha \mid \frac{p}{i} \frac{q}{j} \rangle w_l^{(\lambda)\alpha}, \tag{18}$$

$$\langle {\lambda \atop l} \alpha \mid {p \atop i} {q \atop j} \rangle = \langle {p \atop i} {q \atop j} \mid {\lambda \atop l} \alpha \rangle^*.$$
 (19)

The C-G coefficient has the following orthogonality relations

$$\sum_{\lambda,l,\alpha} \langle {p \atop i} {q \atop j} \mid {\lambda \atop l} \alpha \rangle \langle {\lambda \atop l} \alpha \mid {p \atop i'} {q \atop j'} \rangle = \delta_{ii'} \delta_{jj'}, \tag{20}$$

$$\sum_{i,j} \langle \frac{\lambda}{l} \alpha \mid \stackrel{p}{i} \stackrel{q}{j} \rangle \langle \stackrel{p}{i} \stackrel{q}{j} \mid \stackrel{\lambda'}{l'} \alpha' \rangle = \delta_{\lambda \lambda'} \delta_{ll'} \delta_{\alpha \alpha'}. \tag{21}$$

When $a_{\lambda} = 1$ in Eq. (16), the C-G coefficient can be determined up to a U(1) phase

$$|\langle {p \atop i} {q \atop j} | {\lambda \atop l} \rangle|^2 = \frac{d_{\lambda}}{|G|} \sum_{g \in G} D_{ii}^{(p)}(g) D_{jj}^{(q)}(g) D_{ll}^{(\lambda)}(g). \tag{22}$$

When $a_{\lambda} > 1$ in Eq. (16), the C-G coefficient can not be uniquely determined.

3. Symmetry in Quantum Mechanics

Consider a group G acting on the 3D Euclidean space, the group element g act on the spatial vector \mathbf{r} as $\mathbf{r}' := g \triangleright \mathbf{r}$. Then for a scalar (wave) function $\psi(\mathbf{r})$, the group action will be an operator Γ_g action (note the inverse here)

$$\psi'(\mathbf{r}) := \Gamma_q \psi(\mathbf{r}) \equiv \psi(g^{-1} \rhd \mathbf{r}). \tag{23}$$

Therefore, the scalar function should satisfy $\psi'(\mathbf{r}') = \psi(\mathbf{r})$. This set of operators $\{\Gamma_g \mid g \in G\}$ is isomorphic to the group G. The inner product of the scalar function is defined as

$$(\phi, \psi) := \int d\mathbf{r} \phi^*(\mathbf{r}) \psi(\mathbf{r}). \tag{24}$$

If the operator Γ_g is unitary, we require

$$(\Gamma_q \phi, \Gamma_q \psi) = (\phi, \Gamma_q^{\dagger} \Gamma_q \psi) = (\phi, \psi). \tag{25}$$

Then consider an irreducible representation $D^{(p)}(G)$ with dimension d_p , then we have a

set of scalar functions $\left\{\phi_{\mu}^{(p)} \mid \mu=1, \cdots, d_p\right\}$ as basis of this representation

$$\Gamma_g \phi_{\mu}^{(p)}(\mathbf{r}) = \sum_{\nu=1}^{d_p} \phi_{\nu}^{(p)}(\mathbf{r}) D_{\nu\mu}^{(p)}(g). \tag{26}$$

We call that the function $\phi_{\mu}^{(p)}$ transforms under the μ -the column of the p-th irreducible representation. These basis satisfy the orthogonality relation

$$\left(\phi_{\mu}^{(p)}, \phi_{\nu}^{(q)}\right) = \delta_{pq}\delta_{\mu\nu}.\tag{27}$$

Theorem 19 Given all irreducible representations $\left\{D^{(p)}(G) \mid p=1, \cdots, r\right\}$ of a finite group G acting on the coordinate space with the corresponding normalized basis $\left\{\phi_{\mu}^{(p)}\right\}$, then any square integrable function $\psi(\mathbf{r})$ can be expanded by this basis

$$\psi(\mathbf{r}) = \sum_{p=1}^{r} \sum_{\mu} a_{\mu}^{(p)} \phi_{\mu}^{(p)}(\mathbf{r}).$$
 (28)

Definition 22 Given a Hamiltonian H, the symmetry of H is a set of operators $\{\Gamma_g \mid g \in G\}$ s.t.

$$[H, \Gamma_a] = 0, \ \forall g \in G. \tag{29}$$

The Schrödinger equation is

$$H\psi_{n\lambda} = \epsilon_n \psi_{n\lambda},\tag{30}$$

where n is the energy level, while $\lambda=1, \cdots, d$ labels the degeneracy. The set of all energy eigenstates is complete in the sense that any function can be expanded in this basis. The commutation relation (29) states that $\Gamma_g \psi_{n\lambda}$ is also an energy eigenstate of the same energy level, which means the energy eigenstates $\psi_{n\lambda}$ form an representation of G

$$\Gamma_g \psi_{n\lambda}(\mathbf{r}) = \sum_{\mu=1}^d \psi_{n\mu}(\mathbf{r}) D_{\mu\lambda}(g). \tag{31}$$

In general, this d-dimensional representation is reducible, which can be decomposed into direct sum of irreducible representations $D(G) = \sum_{p=0}^{\oplus} a_p D^{(p)}(G)$ with the new basis

$$\left\{\phi_{\mu\alpha_{p}}^{(p)} \mid p=1, \ \cdots, s; \mu=1, \ \cdots, d_{p}; \alpha_{p}=1, \ \cdots \ a_{p}\right\}, \tag{32}$$

$$a_1 d_1 + a_2 d_2 + \dots + a_s d_s = d. (33)$$

The degenerate energy eigenstates within the same irreducible representations are called normal degeneracy, while the degenerate energy eigenstates between different irreducible representations are called accidental degeneracy. When adding symmetric perturbations, the accidental degeneracy may be lifted, while the normal degeneracy will always be kept.