

Chapter 3

Representations

3.1 Basic definitions

The main ingredients that are necessary to develop *representation theory* are introduced in this section. Some basic theorems about representations of groups are presented in the following section. Most of the results will be quoted without a proof. The interested reader can refer to [Tun85].

3.1.1 Representations

Definition 3.1.1 A *representation* D of a group G is a homomorphism from G into the set of linear operators acting on a vector space V :

$$\begin{aligned} D : G &\longrightarrow \text{GL}(V) \\ g &\longrightarrow \hat{g}, \end{aligned}$$

where $g \in G$ is an abstract element of the group G , while $\hat{g}$ is an operator acting linearly on the elements (vectors) of V .

Since D is a homomorphism, the linear operators verify:

$$D(g)D(g') = D(gg'); \quad (3.1)$$

as usual, note that the product on the LHS is a product between linear operators acting on the vectors in V , while the product inside the parenthesis on the RHS is the product of group elements in G . The representation $D(g)$ corresponds to an explicit realization of the group structure of G . If V is a d -dimensional vector space, the representation is called d -dimensional. Having chosen a basis in the vector space V , $\hat{g}$ can be written as $d \times d$ matrix.

Faithful representation The representation is called *faithful* if the mapping $G \rightarrow \text{GL}(V)$ is an isomorphism.

Matrix representation Let $\{|e_i\rangle\}_{i=1,\dots,d}$ be a basis of V , complete and orthonormal, $\langle e_i | e_j \rangle = \delta_{ij}$. Acting with $\hat{g}$ on one of the vectors $|e_i\rangle$ yields some other vector in V . Since the basis is complete, we can write this new vector as a linear combination of the basis vectors. If we call $D(g)_i^j$ its coordinates in the $\{|e_i\rangle\}$ basis, we obtain:

$$\hat{g}|e_i\rangle = \sum_{j=1}^d |e_j\rangle D(g)_i^j. \quad (3.2)$$

The set of all the $D(g)_i^j$ as i varies from 1 to d defines a matrix representing the element g .

Exercise 3.1.1 Prove that the mapping $D(g)_i^j$ defined above is a homomorphism from G into the group of $d \times d$ matrices.

Unfaithful representation We can write down for every group G at least one trivial representation, known as the *identity representation*:

$$\forall g \in G, D(g) = \mathbb{I}. \quad (3.3)$$

You can readily check that the equation above defines a homomorphism, which is obviously not a one-to-one correspondence.

Equivalent representations

Definition 3.1.2 Two matrix representations $\{D(g)\}, \{D'(g)\}$ of the same dimension are called *equivalent* if and only if there exist a matrix S , $d \times d$, non-singular, such that:

$$\forall g \in G, D'(g) = SD(g)S^{-1}. \quad (3.4)$$

Note that the same matrix S has to connect the matrices $D(g)$ and $D'(g)$ for all the elements of G . The two representations correspond to the same realization of the group structure seen in two different bases. The matrix S is the matrix that implements the transformation from one basis to the other.

Exercise 3.1.2 Let D, D' be two equivalent representations, and let S be the transformation that relates them. Prove that $D'(ab) = SD(ab)S^{-1}$.

Unitary representations

Definition 3.1.3 A *unitary representation* of a group G is a representation such that the matrix $D(g)$ is unitary for all $g \in G$, i.e.

$$\forall g \in G, D(g)D(g)^\dagger = \mathbb{I}. \quad (3.5)$$

Unitary representations are important in quantum mechanics since they preserve transition amplitudes.

Theorem 3.1.1 Any matrix representation of a *finite* group is equivalent to a unitary representation.

3.1.2 Reducible representations

We have seen that symmetry transformations naturally embody a group structure. It is important to identify subsets of the vector space of physical states such that the states in these subsets are transformed into each other by symmetry transformations. These structures are called invariant subspaces.

Definition 3.1.4 Let us consider a representation of a group G , acting on a vector space V . If $L_s \subset V$ is a subspace of V , such that:

$$\forall g \in G, \forall |\phi\rangle \in L_s, \hat{g}|\phi\rangle \in L_s, \quad (3.6)$$

then L_s is called an *invariant subspace*, and the V is *reducible* under G .

The subspace L_s is also called *closed* under G .

The existence of invariant subspaces defines the reducible representations. Let $\{D(g), g \in G\}$ be a representation of G in V , and let $\dim V = d$. If V has an invariant subspace L_s , $\dim L_s = s < d$, then there exists a basis in V such that:

$$\forall g \in G, D(g) = \begin{pmatrix} D^{(1)}(g) & 0 \\ 0 & D^{(2)}(g) \end{pmatrix}, \quad (3.7)$$

where $D^{(1)}$ is a $s \times s$ matrix, and $D^{(2)}$ is a $(d-s) \times (d-s)$ matrix.

Definition 3.1.5 In the case described above, the representation D is called a *reducible representation*. Conversely, if there is no invariant subspace in V , the representation is called *irreducible*.

Note that $D^{(1)}$ and $D^{(2)}$ are also representations of G , of dimension d and $d-s$ respectively. Moreover, the invariant subspace L_s may contain further subspaces that are left invariant by the matrices $D^{(1)}(g)$. In this case the representation $D^{(1)}$ can be further reduced, *i.e.* each matrix $D^{(1)}(g)$ can be written into two diagonal sub-blocks. When all the invariant subspaces have been mapped out, the representation D is said to have been fully decomposed, each matrix $D(g)$ can be written in a block diagonal form, which we shall write as:

$$\forall g \in G, D(g) = \begin{pmatrix} \Gamma^{(1)}(g) & 0 & \dots \\ 0 & \Gamma^{(2)}(g) & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}, \quad (3.8)$$

where $\Gamma^{(i)}$ represent irreducible representation of G . Note that the same $\Gamma^{(i)}$ can appear more than once in the decomposition of a given reducible representation D . In general we denote the decomposition of D by:

$$D = m_1 \Gamma^{(1)} \oplus m_2 \Gamma^{(2)} \oplus \dots \oplus m_n \Gamma^{(n)}, \quad (3.9)$$

where m_i are positive integers.

A representation D is called *simply reducible* if the coefficients are all $m_i = 0, 1$.

3.2 Schur's lemma

Schur's lemma plays a fundamental role in the classification of group representations. In the first part of this section, we state the theorem and prove it. The rest of the section is devoted to the discussion of some of the major consequences of Schur's lemma.

Theorem 3.2.1 Let G be a group, Γ an *irrep* (irreducible representation) on V , and let T be a complex vector space. If there exist a matrix $T \in \text{GL}(V)$ such that

$$T\Gamma(g) = \Gamma(g)T, \quad \forall g \in G, \quad (3.10)$$

then necessarily

$$T = \lambda \mathbb{I}. \quad (3.11)$$

(Schur's lemma)

A matrix that commutes with all the elements of an irrep must be a multiple of the identity matrix. Given the importance of Schur's lemma, we shall present here its proof for the interested reader.

Proof of Schur's lemma First we need to prove that, under the assumptions above, the kernel of T ,

$$\ker T = \{|v_0\rangle \in V : T|v_0\rangle = |0\rangle\} \quad (3.12)$$

is closed under G . Let us consider $|v_0\rangle \in \ker T$, and $g \in G$, then:

$$T\Gamma(g)|v_0\rangle = \Gamma(g)T|v_0\rangle = |0\rangle, \quad (3.13)$$

and therefore $\Gamma(g)|v_0\rangle \in \ker T$.

Now we can use the fact that Γ is an irrep, and therefore there can not be non-trivial invariant subspaces. The only two options are either $\ker T = V$, or $\ker T = \{|0\rangle\}$. In the first case we have proved Schur's lemma, since $T = \lambda \mathbb{I}$, with $\lambda = 0$.

If $\ker T = \{|0\rangle\}$, then $\lambda = 0$ is not an eigenvalue of T . Let $\lambda \neq 0$ be an eigenvalue of T , with eigenvector $|v_1\rangle$, and let us define the operator $T_\lambda = T - \lambda \mathbb{I}$. From the definition of T_λ you can easily check that:

$$T_\lambda \Gamma(g) = \Gamma(g)T_\lambda, \quad \forall g \in G, \quad (3.14)$$

but now we know that $\ker T_\lambda \neq \{|0\rangle\}$, because by definition $|v_1\rangle \in \ker T_\lambda$. Since Γ is an irrep, the only other possibility is:

$$\ker T_\lambda = V \iff T = \lambda \mathbb{I}. \quad (3.15)$$

Exercise 3.2.1 Prove the following corollary of Schur's lemma. All the irreps of an Abelian group G are 1-dimensional.

Using Schur's lemma, we can prove the following

Theorem 3.2.2 Let $\Gamma^{(i)}, \Gamma^{(j)}$ be inequivalent irreps of dimension d_i, d_j respectively, if there exists a $(d_i \times d_j)$ matrix M such that:

$$\Gamma^{(i)}(g)M = M\Gamma^{(j)}(g), \quad \forall g \in G, \quad (3.16)$$

then $M = 0$.

(Schur's second lemma)

We shall not prove explicitly this theorem. However it plays a central role in establishing the so-called *orthogonality theorem*.

Theorem 3.2.3 Let $\Gamma^{(i)}, \Gamma^{(j)}$ be irreps of a finite group G , $|G| = g$, and let us assume that the two representations are inequivalent for $i \neq j$, and identical for $i = j$, then

$$\sum_{a \in G} \Gamma^{(i)}(a)_{pq} \Gamma^{(j)}(a)_{rs}^* = \frac{g}{d_i} \delta_{ij} \delta_{pr} \delta_{qs}, \quad (3.17)$$

where $d_i = \dim \Gamma^{(i)}$.

3.3 Characters of a representation

Let us now introduce some more mathematical tools that are useful to study the representations of a group.

Definition 3.3.1 The *characters* of a matrix representation $\{D(g)\}$ of a group G are defined as:

$$\chi(g) = \text{Tr} D(g) = \sum_k D(g)_k^k, \quad \forall g \in G. \quad (3.18)$$

The set of all characters is called the *character system*. For a finite group, $|G| = n$, $\chi(g)$ is a vector with n components.

Properties Characters satisfy the following properties:

1. for a 1-dim representation, the character system is the representation itself:

$$D(g) = \lambda(g) \in \mathbb{C}, \quad \text{Tr} D(g) = \lambda(g). \quad (3.19)$$

2. characters of conjugate elements are the same;
if $\exists g \in G, b = gag^{-1}$, then

$$\chi(a) = \text{Tr}[D(g)D(b)D(g^{-1})] = \chi(b);$$

i.e. all elements of a class have the same character. The character χ is called a *class function*, and will sometimes be denoted as χ_k , where the subscript k identifies the class C_k .

3. if two representations $D^{(1)}$ and $D^{(2)}$ are equivalent, they have the same character system:

$$\begin{aligned} D^{(1)}(g) &= S D^{(2)}(g) S^{-1}, \quad \forall g \in G, \\ \Rightarrow \text{Tr} D^{(1)}(g) &= \text{Tr}[S D^{(2)}(g) S^{-1}] = \text{Tr} D^{(2)}(g); \end{aligned}$$

even though we are not going to prove it explicitly, the implication in the opposite direction is also true. Two representations are equivalent if and only if they have the same character system.

First orthogonality relation Starting from the orthogonality theorem, setting $p = q, r = s$, and summing over p and r yields:

$$\sum_{a \in G} \sum_p \Gamma^{(i)}(a)_p^p \sum_r \left(\Gamma^{(j)}(a)_r^r \right)^* = \frac{g}{d_i} \delta_{ij} d_i, \quad (3.20)$$

i.e.

$$\sum_{a \in G} \chi^{(i)}(a) \chi^{(j)}(a)^* = g \delta_{ij}, \quad (3.21)$$

where g is the order of the group G . Using the fact that the character is a class function, and collecting the elements $a \in G$ in classes C_k , with c_k elements in each class C_k , we can rewrite the above relation as:

$$\sum_{k=1}^{N_c} c_k \chi_k^{(i)} \left(\chi_k^{(j)} \right)^* = g \delta_{ij}, \quad (3.22)$$

where N_c indicates the number of classes.

Exercise 3.3.1 Prove the following, useful result. For the trivial representation:

$$\sum_{a \in G} \chi^{(0)}(a) = g; \quad (3.23)$$

while for any other irreducible representation:

$$\sum_{a \in G} \chi^{(i)}(a) = 0. \quad (3.24)$$

3.4 Reduction of reducible representations

We have seen that a reducible representation can be decomposed as:

$$D(a) = \bigoplus_i m_i \Gamma^{(i)}(a), \quad a \in G, \quad (3.25)$$

where $\Gamma^{(i)}$ are irreps and m_i are integers, that indicate how many times the representation $\Gamma^{(i)}$ appears in the decomposition of D .

The matrix D is a block diagonal matrix, with the matrices $\Gamma^{(i)}$ appearing in the diagonal blocks. Taking the trace of D , we find:

$$\chi(a) = \sum_i m_i \chi^{(i)}(a). \quad (3.26)$$

We can use the first orthogonality relation to determine the coefficients m_i ; if we multiply Eq. (3.26) by $\chi^{(j)}(a)^*$, and sum over $a \in G$, we obtain:

$$\sum_{a \in G} \chi(a) \chi^{(j)}(a)^* = \sum_i \sum_{a \in G} \chi^{(i)}(a) \chi^{(j)}(a)^* = g m_i \quad (3.27)$$

i.e.

$$m_j = \frac{1}{g} \sum_{a \in G} \chi(a) \chi^{(j)}(a)^*, \quad (3.28)$$

where g is the order of the finite group G .

Reducibility criterion The previous result can be used to establish a useful criterion to identify an irreducible representation. Let D be a generic representation of a group G , with character system $\chi(a)$, and of order g , then:

$$\frac{1}{g} \sum_{a \in G} \chi(a) \chi(a)^* = \sum_i m_i^2 > 0. \quad (3.29)$$

The only way this sum can be equal to one, is if all the m_i are equal to zero, except for one which we denote m_k . Then the representation D corresponds to $\Gamma^{(k)}$ and is irreducible. Therefore:

$$D \text{ is irreducible} \iff \sum_{a \in G} \chi(a) \chi(a)^* = g. \quad (3.30)$$

The following relation is useful to identify the irreps of finite group.

Theorem 3.4.1 Let G be a finite group of order g , and let N_i be the number of irreps of G , then:

$$\sum_{i=1}^{N_i} d_i^2 = g, \quad (3.31)$$

i.e. the sum of the squares of the dimensions of all the irreps of G is equal to the order of the group.

Second orthogonality relation The second orthogonality relation is a completeness relation for the characters:

$$\sum_{i=1}^{N_i} \chi_k^{(i)} \chi_l^{(i)*} = \frac{g}{c_k} \delta_{kl}, \quad (3.32)$$

where k, l are indices that identify classes of G , while $\Gamma^{(i)}$ are the irreps as usual.

Finally we state one more theorem, which you can use without worrying about its proof.

Theorem 3.4.2 For a finite group G the number of inequivalent irreps is *equal* to the number of classes.

Character tables The character system of a group is conveniently summarized in the *character table*.

Definition 3.4.1 A *character table* is a square matrix of characters $\chi_k^{(i)}$, where the rows of the matrix are labelled by the distinct irreps of G , $i = 1, \dots, N_i$, and the columns are labelled by the distinct classes of G , $k = 1, \dots, N_c$.

We shall always label C_1 the class of the identity, $[e] = \{e\}$.

Exercise 3.4.1 Prove that $\chi_1^{(i)} = d_i$, where d_i is the dimension of the irreducible representation $\Gamma^{(i)}$. In solving the exercise, check that you remember the definition of a class, of an irreducible representation, and of the dimension of a representation. Remember that the character is a class function. Deduce that the first column of the character tables is made of the dimensions of the irreps.

Exercise 3.4.2 Consider the trivial representation (1-dimensional), $\Gamma^{(1)}(g) = 1, \forall g \in G$, prove that $\chi_k^{(1)} = 1, \forall k = 1, \dots, N_c$. Deduce that the first row of the character table is made of 1's.

Character table for D_3 Let us consider the symmetry group of the equilateral triangle, D_3 , and let us construct the character table step by step.

D_3 is a finite group of order $g = 6$, and we will denote the 6 elements $G = \{e, a, b, c, d, f\}$, where e is the identity, a, b are rotations by $2\pi/3$, and $4\pi/3$, and c, d, f are reflexions.

Exercise 3.4.3 Show by explicit calculations that there are three classes in D_3 . They are: $C_1 = [e] = \{e\}$, $C_2 = [a] = \{a, b\}$, $C_3 = [c] = \{c, d, f\}$.

Since the number of classes equals the number of irreps, we know that there are three irreps of D_3 , which we denote by $\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}$.

The relation between the dimension of the irreps and the order of the group yields:

$$\sum_{i=1}^{N_i} d_i^2 = 6; \quad (3.33)$$

remember that the coefficients d_i are integers – they are the dimension of the irreps – and therefore Eq. (3.33) has a unique solution: $d_1 = 1, d_2 = 1, d_3 = 2$.

We shall identify $\Gamma^{(1)}$ with the trivial representation, which associates 1 to every element of D_3 .

A second inequivalent (and one-dimensional) irrep of D_3 of dimension 1 is provided by

$$\Gamma^{(2)}(e) = 1, \Gamma^{(2)}(a) = 1, \Gamma^{(2)}(b) = 1, \Gamma^{(2)}(c) = -1, \Gamma^{(2)}(d) = -1, \Gamma^{(2)}(f) = -1. \quad (3.34)$$

Exercise 3.4.4 Check that the above is a genuine representation of D_3 .

Finally the 2-dimensional irreducible representation $\Gamma^{(3)}$ is given by the matrices that implement the geometrical transformations in two-dimensional Euclidean space:

$$\Gamma^{(3)}(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \Gamma^{(3)}(a) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \quad (3.35)$$

$$\Gamma^{(3)}(b) = \begin{pmatrix} x & x \\ x & x \end{pmatrix} \quad \Gamma^{(3)}(c) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad (3.36)$$

$$\Gamma^{(3)}(d) = \begin{pmatrix} x & x \\ x & x \end{pmatrix} \quad \Gamma^{(3)}(f) = \begin{pmatrix} x & x \\ x & x \end{pmatrix} \quad (3.37)$$

We now have all the ingredients for the following exercise.

Exercise 3.4.5 Write the character table for D_3 . First write the first column, then complete the first two lines. Finally complete the remaining entries by using the orthogonality relation. You can check the entries in the last line against the traces of the matrices $\Gamma^{(3)}$.

3.5 Direct product of representations

Let G be a group, $\{D^{(p)}\}, \{D^{(q)}\}$ two representations of dimensions p, q . For a generic $a \in G$, $D^{(p)}(a)$ is a $p \times p$ matrix, and $D^{(q)}(a)$ is a $q \times q$ matrix. We can define a $(pq) \times (pq)$ matrix as follows:

$$D(a) = \begin{pmatrix} D^{(p)}(a)_{11}D^{(q)}(a) & D^{(p)}(a)_{12}D^{(q)}(a) & \dots \\ D^{(p)}(a)_{21}D^{(q)}(a) & & \ddots \\ \vdots & & \end{pmatrix} \quad (3.38)$$

where each block represents a $q \times q$ matrix.

The set of matrices constructed in this way define the *direct product* of the representations $D^{(p)}$ and $D^{(q)}$:

$$D = D^{(p)} \otimes D^{(q)}. \quad (3.39)$$

Clearly the representation D has dimension pq .

In dealing with direct products of representations, it is useful to introduce collective indices, denoted by capital latin letters $A, B, \dots$, that represent the pair of indices (i, r) , where $i = 1, \dots, p$, $r = 1, \dots, q$. The action of $D(a)$ on a vector can be written as:

$$\sum_B D(a)_B^A v^B = \sum_{j,s} D(a)_{js}^{ir} v^{js} \quad (3.40)$$

$$= D^{(p)}(a)_j^i D^{(q)}(a)_s^r v^{js}. \quad (3.41)$$

Clebsch–Gordan series The product of two irreps yields a larger representation, which in general will not be irreducible. Such larger representation can be decomposed in a series of irreps according to:

$$\Gamma^{(i)} \otimes \Gamma^{(j)} = \bigoplus_k c_k^{ij} \Gamma^{(k)}, \quad (3.42)$$

where the c_k^{ij} are non-negative integers that count how many times the irrep $\Gamma^{(k)}$ appears in the direct product. They can be computed as discussed in the previous section using characters.

Note that the character of the direct product representation is given by:

$$\chi(D(a)) = \text{Tr}(\Gamma^{(i)}(a) \otimes \Gamma^{(j)}(a)) = \sum_A D(a)_A^A \quad (3.43)$$

$$= \sum_{k,r} \Gamma^{(i)}(a)_k^k \Gamma^{(j)}(a)_r^r \quad (3.44)$$

$$= \chi^{(i)}(a) \chi^{(j)}(a). \quad (3.45)$$

From Eq. (3.42) we obtain:

$$\chi^{(i)}(a) \chi^{(j)}(a) = \sum_k c_k^{ij} \chi^{(k)}(a). \quad (3.46)$$

Finally using the orthogonality relation:

$$c_k^{ij} = \frac{1}{g} \sum_{a \in G} \chi^{(k)}(a)^* \chi^{(i)}(a) \chi^{(j)}(a), \quad (3.47)$$

or, equivalently:

$$c_k^{ij} = \frac{1}{g} \sum_{l=1}^{N_c} c_l (\chi_l^{(k)})^* \chi_l^{(i)} \chi_l^{(j)}, \quad (3.48)$$

where l runs over the classes of the group G , and c_l is the number of elements in the l -th class. The coefficients c_k^{ij} are called *Clebsch–Gordan* coefficients.

Exercise 3.5.1 Write the character table for D_3 . Deduce the character for the product representation $\Gamma^{(3)} \otimes \Gamma^{(3)}$, where $\Gamma^{(3)}$ is the two-dimensional irrep of D_3 .

3.6 Restriction to a subgroup

Let $H \subset G$ be a subgroup, and $\Gamma^{(i)}$ an irrep of G , then

$$\left\{ \Gamma^{(i)}(a), a \in H \right\} \quad (3.49)$$

defines a representation of H . However this representation is not necessarily irreducible; since there are *less* elements in H than there are in G , there could be subspaces of V that are not invariant under the full group G , but are invariant under the smaller set of transformations H .

When this happens, the induced representation can be reduced:

$$\Gamma^{(i)} = \oplus_j m_j^i \gamma^{(j)}, \quad (3.50)$$

where $\gamma^{(j)}$ are irreps of H .

Exercise 3.6.1 Let us consider $Z_3 \subset D_3$. Write down the character table for the irreps of Z_3 . Write down the restriction of the irreps of D_3 to Z_3 (in doing so note that elements that are conjugate to each other in D_3 , and therefore belong to the same class in the character table of D_3 , are no longer conjugate in Z_3 . They define distinct classes, which appear as additional columns in the character table.

Decompose the induced representation of Z_3 in terms of irreps of Z_3 .

3.7 Representations of the product group

Consider the product group $G = H \otimes K$, whose elements can be written as $g = hk$, where the elements of H and K are assumed to commute with each other.

The irreps of the product group are fully classified by the following theorem.

Theorem 3.7.1 If Γ_H, Γ_K are representations of H and K respectively, then $\Gamma_H \otimes \Gamma_K$ is a representation of G .

Moreover if $\Gamma_H^{(i)}, \Gamma_K^{(j)}$ are irreps, then $\Gamma_H^{(i)} \otimes \Gamma_K^{(j)}$ is also an irrep of G . Such irreps exhaust *all* the irreps of G .

Exercise 3.7.1 Using the reducibility criterion, prove that the representations $\Gamma_H^{(i)} \otimes \Gamma_K^{(j)}$ are indeed irreps.

By computing the sum of their dimensions squared, prove that they do exhaust all possible irreps of G .

3.8 Representations in Quantum Mechanics

We shall now discuss how representations appear in the study of physical systems. Let us consider a quantum system, whose states are described by vectors (*kets*) in a complex vector space with a scalar product (*Hilbert space*).

Any state $|\psi\rangle$ can be expanded on an orthonormal complete basis $\{|\psi_n\rangle\}$:

$$\langle\psi_n|\psi_m\rangle = \delta_{nm}, \quad (3.51)$$

$$\sum_n |\psi_n\rangle\langle\psi_n| = 1, \quad (3.52)$$

$$|\psi\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n c_n |\psi_n\rangle, \quad (3.53)$$

where the coefficients c_n represent the probability amplitude for $|\psi\rangle$ to be in a state $|\psi_n\rangle$.

Physical observables are described by hermitean operators:

$$O^\dagger = O \quad (\text{real eigenvalues}). \quad (3.54)$$

The energy eigenstates are defined as:

$$H|u_n\rangle = E_n|u_n\rangle, \quad (3.55)$$

and can be expanded in the $\{|\psi_n\rangle\}$ basis:

$$|u_m\rangle = \sum_n |\psi_n\rangle \langle \psi_n | u_m \rangle. \quad (3.56)$$

Let us now consider a group G , acting on the states of the Hilbert space:

$$a \in G, \quad |\psi\rangle \mapsto \hat{a}|\psi\rangle, \quad (3.57)$$

$$\hat{a}|\psi_n\rangle = \sum_m |\psi_m\rangle \Gamma(a)_n^m. \quad (3.58)$$

Let us see how H transforms under G . Remember that H is the generator of time translations:

$$i\partial_t|\psi\rangle = H|\psi\rangle, \quad (3.59)$$

and that under the action of G :

$$|\psi\rangle \mapsto |\psi'\rangle = \hat{a}|\psi\rangle. \quad (3.60)$$

By looking at the time evolution of the transformed state:

$$i\partial_t|\psi'\rangle = i\partial_t\hat{a}|\psi\rangle = \hat{a}H|\psi\rangle \quad (3.61)$$

$$= (\hat{a}H\hat{a}^\dagger)\hat{a}|\psi\rangle = (\hat{a}H\hat{a}^\dagger)|\psi'\rangle, \quad (3.62)$$

we deduce the transformed Hamiltonian:

$$H' = \hat{a}H\hat{a}^\dagger. \quad (3.63)$$

If the group describes a symmetry of the system, then $H' = H$, *i.e.*

$$[H, \hat{a}] = 0, \quad \forall a \in G, \quad (3.64)$$

and therefore:

$$H\hat{a}|u^\alpha\rangle = \hat{a}H|u^\alpha\rangle = E_\alpha(\hat{a}|u^\alpha\rangle), \quad (3.65)$$

i.e. the transformation $\hat{a}$ connects states with the same energy.

The set of eigenvectors $\{u_n^\alpha\}$ associated to each eigenvalue of the energy E_α defines a basis of an invariant subspace which is invariant under G .

The existence of invariant subspaces means that the representation Γ is reducible:

$$\Gamma = \oplus_\alpha m_\alpha \Gamma^{(\alpha)}. \quad (3.66)$$

Each eigenvalue of H , E_α defines an irrep of G . The degeneracy of the eigenvalue E_α is d_α , the dimension of the irrep.

Distinguishing degenerate states Consider now a second operator O , which commutes with H , *i.e.* H and O can be diagonalized simultaneously. There exist a set of common eigenvectors:

$$O|u_i^\alpha\rangle = \lambda_i^\alpha |u_i^\alpha\rangle. \quad (3.67)$$

If O is invariant under G , then by Schur's lemma, O must be proportional to the identity in each subspace spanned by $\{u_n^\alpha\}$ and associated to a given eigenvalue of the Hamiltonian. The matrix associated to O in the basis of the energy eigenstates is block-diagonal, with blocks of size d_α :

$$O = \begin{pmatrix} \lambda_\alpha \mathbb{1}_\alpha & & \\ & \lambda_\beta \mathbb{1}_\beta & \\ & & \ddots \end{pmatrix}. \quad (3.68)$$

On the other hand, if O is invariant under a subgroup $H \in G$, then Schur's lemma does not apply, and the eigenvalues λ_i^α of O can be used to distinguish degenerate energy eigenstates. The blocks in the matrix representation of O are no longer proportional to the identity:

$$O = \begin{pmatrix} \begin{pmatrix} \lambda_1^\alpha & \\ & \lambda_2^\alpha \end{pmatrix} & & \\ & \begin{pmatrix} \lambda_1^\beta & & \\ & \lambda_2^\beta & \\ & & \lambda_3^\beta \end{pmatrix} & \\ & & \ddots \end{pmatrix}. \quad (3.69)$$

We will see an application of this property when we study angular momentum.

Symmetry breaking Another interesting case is when there is a perturbation in the system which breaks the symmetry of the unperturbed Hamiltonian:

$$H = H_0 + \epsilon V \quad (3.70)$$

where H_0 is invariant under G , but V is only invariant under a subgroup $H \in G$, and ϵ is a small parameter.

In this case the perturbation V splits the degenerate energy levels of H_0 , according to the decomposition of the irreps $\Gamma^{(\alpha)}$ of G into irreps $\gamma^{(\beta)}$ of H :

$$\Gamma^{(\alpha)} = \oplus_\beta m_\beta \gamma^{(\beta)}; \quad (3.71)$$

where $\Gamma^{(\alpha)}$ and $\gamma^{(\beta)}$ are irreps of G and H respectively.

Exercise 3.8.1 To illustrate this property, let us consider the crystalline splitting of atomic energy levels, *i.e.* the splitting of atomic levels that appears when atoms are arranged in a crystal.

Free atoms are symmetric under rotations, *i.e.* under the group $SO(3)$ of orthogonal transformations with unit determinant acting on a three-dimensional real vector space. According to

the discussion in the previous sections, the energy levels of the free atoms appear in multiplets with degeneracies that correspond to the dimensions of the irreps of $\text{SO}(3)$. We shall study these representations in more detail later. For the time being we can assume that the irreps are classified by one integer quantum number, $l \in \mathbb{N}$, related to the angular momentum of the state. By convention the irreps with $l = 0, 1, 2$ are called the s, p, d representations respectively. The characters in the l representation are given by:

$$\chi^{(l)}(\theta) = \frac{\sin(l + 1/2)\theta}{\sin \theta/2}, \quad (3.72)$$

where θ is the angle of the rotation. Note that the character does not depend on the axis of rotation. Rotations by the same angle around different axes are conjugate elements of $\text{SO}(3)$, and therefore have the same character.

When $\theta = 0$, the rotation reduces to the identity, and its character yields the dimension of the representation:

$$\lim_{\theta \rightarrow 0} \chi^{(l)}(\theta) = d_l = 2l + 1. \quad (3.73)$$

According to the previous discussion, the energy levels arrange in multiplets according to the dimension of the irreps of $\text{SO}(3)$. The s -wave corresponds to a 1-fold degenerate state, the p -wave to a 3-fold degenerate level, and finally the d -wave yields a 5-fold degenerate level.

When the atoms are arranged in a crystalline structure the symmetry of the system is reduced to the symmetry of the crystal. We will consider as an example a crystal with tetrahedral symmetry, described by the group T . Using the character table constructed in Problem 3.9.4, show that:

1. the 1-fold degeneracy of the s -wave is not lifted;
2. the 3-fold degeneracy of the p -wave is not lifted;
3. the 5-fold degeneracy of the d -wave is lifted, and we obtain three different eigenvalues, which are 1-fold, 1-fold, and 3-fold degenerate respectively.

Selection rules Transformation properties under a symmetry group also determine transition amplitudes. Consider a physical system, whose states are classified by the representations of a symmetry group G . We shall denote these states as ψ_i^α , where α labels the irrep, and i labels the vectors that form a basis of the invariant subspace on which the representation α is acting.

The transition amplitude due to some interaction V is given by:

$$P(\psi \rightarrow \phi) = \frac{|\langle \phi | V | \psi \rangle|^2}{\langle \phi | \phi \rangle \langle \psi | \psi \rangle}. \quad (3.74)$$

The symmetry of the system implies: $[V, \hat{a}] = 0, \quad \forall a \in G$; therefore we have:

$$\begin{aligned}
 \langle \psi_i^\alpha | V | \phi_j^\beta \rangle &= \frac{1}{g} \sum_{a \in G} \langle \psi_i^\alpha | \hat{a}^\dagger a V | \phi_j^\beta \rangle \\
 &= \frac{1}{g} \sum_{a \in G} \langle \psi_i^\alpha | \hat{a}^\dagger V a | \phi_j^\beta \rangle \\
 &= \frac{1}{g} \sum_{a \in G} \sum_{k,l} \left(\Gamma^{(\alpha)}(a)_i^k \right)^* \left(\Gamma^{(\beta)}(a)_j^l \right) \langle \psi_k^\alpha | V | \phi_l^\beta \rangle \\
 &= \frac{1}{d_\alpha} \delta_{\alpha\beta} \sum_{k,l} \delta_{ij} \delta_{kl} \langle \psi_k^\alpha | V | \phi_l^\alpha \rangle \\
 &= \frac{1}{d_\alpha} \delta_{\alpha\beta} \delta_{ij} \sum_l \langle \psi_l^\alpha | V | \phi_l^\alpha \rangle \\
 &= \delta_{\alpha\beta} \delta_{ij} \langle \psi^\alpha | V | \psi^\alpha \rangle.
 \end{aligned} \tag{3.75}$$

$\langle \psi^\alpha | V | \psi^\alpha \rangle$ is called a reduce matrix element, and only depends on the energy level α , and *not* on the particular state we consider belonging to that multiplet.

The matrix V can be written as:

$$V = \begin{pmatrix} \begin{pmatrix} v^\alpha & & \\ & \ddots & \\ & & v^\alpha \end{pmatrix} & \begin{matrix} d_\alpha \times d_\alpha \text{ matrix} \\ \\ \end{matrix} \\ \begin{pmatrix} v^\beta & & \\ & \ddots & \\ & & v^\beta \end{pmatrix} & \begin{matrix} d_\beta \times d_\beta \text{ matrix} \\ \\ \end{matrix} \\ \vdots & \vdots \end{pmatrix}. \tag{3.76}$$

This is called a *selection rule*; in particular we have:

$$\langle \psi_i^\alpha | V | \psi_j^\beta \rangle = 0, \quad \text{if } \alpha \neq \beta, i \neq j. \tag{3.77}$$

Tensor operators

Definition 3.8.1 *Tensor operators* are multiplets of operators, which transform amongst themselves according to some representations of a group G :

$$T_i^{(\alpha)} \mapsto \hat{a} T_i^{(\alpha)} \hat{a}^\dagger = \sum_j T_j^{(\alpha)} \Gamma^{(\alpha)}(a)_i^j. \tag{3.78}$$

Note that an invariant operator is a special case of a tensor operator, which transforms under the trivial representation $\Gamma^{(1)}$.

Let us now consider tensor operators $T^{(\alpha)}$ transforming as an irrep $\Gamma^{(\alpha)}$, and focus on the transformation properties of the state $T^{(\alpha)} | \psi_j^\beta \rangle$:

$$\begin{aligned}
 \hat{a} T_i^{(\alpha)} | \psi_j^\beta \rangle &= \hat{a} T_i^{(\alpha)} \hat{a}^\dagger \hat{a} | \psi_j^\beta \rangle \\
 &= \sum_{k,l} \Gamma^{(\alpha)}(a)_i^k \Gamma^{(\beta)}(a)_j^l T_k^{(\alpha)} | \psi_l^\beta \rangle
 \end{aligned} \tag{3.79}$$

i.e. the state $T_i^{(\alpha)}|\psi_j^\beta\rangle$ transforms as the product representation $\Gamma^{(\alpha)} \otimes \Gamma^{(\beta)}$.

The product representation can be decomposed in a Clebsch–Gordan series:

$$\Gamma^{(\alpha)} \otimes \Gamma^{(\beta)} = \oplus_k c_k^{\alpha\beta} \Gamma^{(\gamma)}, \quad (3.80)$$

where $\Gamma^{(\gamma)}$ are irreps, and therefore:

$$\langle \psi_k^\delta | T_i^{(\alpha)} | \psi_j^\beta \rangle = 0, \quad (3.81)$$

unless the irrep $\Gamma^{(\delta)}$ appears in the CG series of $\Gamma^{(\alpha)} \otimes \Gamma^{(\beta)}$, *i.e.* $c_\delta^{\alpha\beta} \neq 0$.

Exercise 3.8.2 Consider the transitions between the enrgy levels of an atom in a crystal with D_3 symmetry. The transitions are induced by the operator $T = e\mathbf{R} \cdot \mathbf{E}$. Here $\mathbf{R}$ is an operator acting on the physical states, while $\mathbf{E}$ is an external electric field, and e is the electriccharge of the electron. The generic matrix element for the dipole transition can be written:

$$\langle \psi | T | \phi \rangle = e\mathbf{E} \cdot \langle \psi | \mathbf{R} | \phi \rangle. \quad (3.82)$$

In order to use the above result, we need to find out the transformation properties of the states: $\mathbf{R}|\psi^{(\alpha)}\rangle$.

The operators $\mathbf{R}$ are a set of tensor operators, which transform as a vector under $SO(3)$, *i.e.* they transform according to the irrep with $l = 1$. Using the formula above we can write the character for a rotation by an angle θ as:

$$\chi_T(\theta) = 1 + 2 \cos \theta. \quad (3.83)$$

We can use the formula above to deduce the character of the transformation in D_3 .

On the other hand, the eigenstates of H for a system with a D_3 symmetry are organized in multiplets that correspond to the irreps of the symmetry group. Remember that there are three irreps for D_3 , with dimensions 1,1, and 2. Therefore we must have two non-degenerate states, corresponding to $\alpha = 1, 2$, and a two-fold degenerate state for $\alpha = 3$.

We obtain the following character table:

D_3	e	2 C_3	3 C_2
$\Gamma^{(1)}$	1	1	1
$\Gamma^{(2)}$	1	1	-1
$\Gamma^{(3)}$	2	-1	0
Γ_T	3	0	-1
$\Gamma_T \otimes \Gamma^{(1)}$	3	0	-1
$\Gamma_T \otimes \Gamma^{(2)}$	3	0	1
$\Gamma_T \otimes \Gamma^{(3)}$	6	0	0

From the character table we can deduce the CG series:

$$\Gamma_T \otimes \Gamma^{(1)} = \Gamma^{(3)} \oplus \Gamma^{(2)} \quad (3.84)$$

$$\Gamma_T \otimes \Gamma^{(2)} = \Gamma^{(3)} \oplus \Gamma^{(1)} \quad (3.85)$$

$$\Gamma_T \otimes \Gamma^{(3)} = \Gamma^{(1)} \oplus \Gamma^{(2)} \oplus 2\Gamma^{(3)} \quad (3.86)$$

Therefore the allowed transitions can be summarized in the following table:

T	$ \psi^{(1)}\rangle$	$ \psi^{(2)}\rangle$	$ \psi^{(3)}\rangle$
$ \psi^{(1)}\rangle$	✗	✓	✓
$ \psi^{(2)}\rangle$	✓	✗	✓
$ \psi^{(3)}\rangle$	✓	✓	✓

3.9 Problems

3.9.1 General properties

- (a) Show that, in any irreducible representation of a finite group, all the elements of the centre of the group are represented by multiples of the unit matrix.
- (b) If Γ is a representation of a finite group, G , show that either Γ and Γ^* are both reducible or they are both irreducible.

3.9.2 Three-dimensional representation of D_3

The elements of D_3 can be seen as geometrical transformations in a three-dimensional Euclidean space, where the third axis is chosen to come out of the plane of the equilateral triangle. Write down the 3×3 matrices that correspond to the elements of D_3 in this representation. Show that such a representation is reducible, and identify explicitly the invariant subspaces.

3.9.3 Character tables

Obtain the character tables and the irreducible representations of

1. the cyclic group of order 3, Z_3 ;
2. the cyclic group of order 4, Z_4 ;
3. the non-cyclic group of order 4, V_4 ;
4. the cyclic group of order n , Z_n .

3.9.4 The tetrahedral group T

The tetrahedral group, T , consists of the set of proper symmetry operations on a regular tetrahedron and is of order 12. Its elements fall into four classes: $\{e\}$, $\{3C_2\}$, $\{4C_{3+}\}$, $\{4C_{3-}\}$, where C_p denotes rotations of magnitude $2\pi/p$ and opposite senses of rotation are indicated by $\pm$.

Find the dimensions of the irreps of T , and complete the character table:

T	$\{e\}$	$\{3C_2\}$	$\{4C_{3+}\}$	$\{4C_{3-}\}$
$\Gamma^{(1)}$	1	1	1	1
$\Gamma^{(2)}$	x	1	ω	ω^*
$\Gamma^{(3)}$	x	1	ω^*	ω
$\Gamma^{(4)}$	x	x	x	x

where $\omega = \exp[i2\pi/3]$.

Using the character table for the tetrahedral group T derived above,

- (a) reduce all the direct products $\Gamma^{(i)} \times \Gamma^{(j)}$, $i, j = 1, \dots, 4$ to direct sums of irreducible representations.
- (b) restrict each $\Gamma^{(i)}$ to the subgroup V_4 , reducing it to a direct sum of irreducible representations $\gamma^{(i)}$ of V_4 . Do the same thing for the subgroup Z_3 .

3.9.5 Direct products

Obtain the direct products of all the irreducible representations of D_3 with each other and reduce them into direct sums of irreducible representations of D_3 .

Using the character table for the tetrahedral group T derived in Q3.6

- (a) reduce all the direct products $\Gamma^{(i)} \times \Gamma^{(j)}$, $i, j = 1, \dots, 4$ to direct sums of irreducible representations.
- (b) restrict each $\Gamma^{(i)}$ to the subgroup V_4 , reducing it to a direct sum of irreducible representations $\gamma^{(i)}$ of V_4 . Do the same thing for the subgroup Z_3 .

3.9.6 More direct products

Let $\Gamma^{(i)}$ and $\Gamma^{(j)}$ be two inequivalent irreducible representations of a finite group, G . Show that the direct product representation $\Gamma^{(i)} \otimes \Gamma^{(j)*}$ does not contain the identity representation.

Show also that the direct product of an irreducible representation with its own complex conjugate representation contains the identity representation once and only once.

Illustrate these results by applying them to the irreducible representations of Z_4 .

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