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Chapter 2

Theory of Group Representation

2.1 Basic Definitions

This chapter is not about the legalities of class action lawsuits. Rather, when we speak of a *group representation*, we mean a map from the space of elements of some abstract group G to a space of operators $\hat{D}(G)$ which act linearly on some vector space \mathcal{V} . The fancy way to say this is that a representation is a map from G to $\text{End}(\mathcal{V})$, the space of *endomorphisms* of \mathcal{V} .¹

2.1.1 Group elements cry out for representation

Check it:

DEFINITION : Let G be a group and let \mathcal{V} be a vector space. A *linear representation*² of G is a homomorphism $\hat{D} : G \mapsto \text{End}(\mathcal{V})$. The *dimension* of the representation is $\dim(\mathcal{V})$. The representation is *faithful* if $\hat{D}(G)$ is an isomorphism. Otherwise it is said to be *degenerate*.

In plain English: each group element $g \in G$ maps to an operator³ $\hat{D}(g)$ which acts on the vector space \mathcal{V} . For us, \mathcal{V} will be a finite-dimensional subspace of the full Hilbert space \mathcal{H} , for some quantum mechanical Hamiltonian, which transforms into itself under symmetry group operations. If \mathcal{V} is n -dimensional, we can choose a basis $\{|e_i\rangle\}$ with $i \in \{1, \dots, n\}$. The action of $\hat{D}(g)$ on each basis state is given by

$$\hat{D}(g)|e_k\rangle = |e_i\rangle D_{ik}^{(n)}(g) \quad , \quad (2.1)$$

where $D^{(n)}(g) \in \text{GL}(n, \mathbb{C})$ is an $n \times n$ matrix. That \hat{D} is a homomorphism means $\hat{D}(g)\hat{D}(g') = \hat{D}(gg')$, which entails $D^{(n)}(g)D^{(n)}(g') = D^{(n)}(gg')$: We shall interchangeably refer to both $\hat{D}(G)$ as well as

¹An endomorphism is a map from a set to itself. An automorphism is an invertible endomorphism.

²We use the term "linear representation" to distinguish it from what is called a "projective representation", which we introduce in §2.1.5. Most of the time we shall abbreviate the former as simply "representation".

³Here and henceforth we shall endeavor to properly attire all our operators with stylish hats.

$D^{(n)}(G)$ as representations, though formally one is in terms of operators acting on \mathcal{V} and the other in terms of matrices, which presumes some choice of basis for \mathcal{V} . If the representation is unitary, we may write it as $\hat{U}(G)$.

2.1.2 Equivalent and reducible representations

Let $D^{(n)}(G)$ and $\tilde{D}^{(n)}(G)$ be two n -dimensional matrix representations of G , and suppose $\exists S \in \text{GL}(n, \mathbb{C})$ such that $\tilde{D}^{(n)}(g) = S^{-1}D^{(n)}(g)S$ for all $g \in G$. Then D and \tilde{D} are said to be *equivalent* representations.

How can we test for equivalence? One diagnostic we can apply is based on the identity $\text{Tr}(S^{-1}AS) = \text{Tr}A$. We call

$$\chi(g) \equiv \text{Tr}D(g) \quad (2.2)$$

the *character* of g in the representation $D(G)$. Note that all group elements in a given equivalence class have the same character, because $\chi(h^{-1}gh) = \chi(g)$. So one thing we can say at this point is that if the characters of the same class differ in D and \tilde{D} , then the representations are not equivalent.

Now let's talk about reducibility. Two definitions:

DEFINITION : Let $\hat{D}(G)$ be a representation of G acting on the vector space \mathcal{V} . A subspace $\mathcal{V}_1 \subset \mathcal{V}$ is *invariant* if $\hat{D}(g)|\psi\rangle \in \mathcal{V}_1 \forall |\psi\rangle \in \mathcal{V}_1$. An invariant subspace is called *minimal* (or *proper*) if it contains no nontrivial invariant subspaces⁴.

DEFINITION : A representation $\hat{D}(G)$ acting on \mathcal{V} is *irreducible* if there is no nontrivial invariant subspace $\mathcal{V}_1 \subset \mathcal{V}$ under the action of $\hat{D}(G)$. Otherwise the representation is *reducible*. If the orthogonal complement⁵ \mathcal{V}_1^\perp is also invariant, the representation is said to be *fully reducible*.

What does reducibility entail for a matrix representation $D^{(n)}(G)$? Let the reducible subspace \mathcal{V}_1 be spanned by vectors $\{|e_1\rangle, \dots, |e_{n_1}\rangle\}$, with its complement \mathcal{V}_1^\perp spanned by $\{|e_{n_1+1}\rangle, \dots, |e_{n_1+n_2}\rangle\}$, where $n_1 + n_2 \equiv n = \dim(\mathcal{V})$. According to Eqn. 2.1, we must have

$$D^{(n)}(g) = \left[\begin{array}{c|c} D^{(n_1)}(g) & C^{(n_1, n_2)}(g) \\ \hline 0 & D^{(n_2)}(g) \end{array} \right] \quad (2.3)$$

where $D^{(n_1)}(G)$ and $D^{(n_2)}(G)$ are each smaller matrix representations of G , and, adopting an obvious and simplifying notation,

$$C(gh) = D_1(g)C(h) + C(g)D_2(h) \quad , \quad (2.4)$$

with $C(E) = 0$. Note that transitivity is then satisfied, *i.e.*

$$\begin{aligned} C(ghk) &= D_1(gh)C(k) + C(gh)D_2(k) \\ &= D_1(g)C(hk) + C(g)D_2(hk) \\ &= D_1(gh)C(k) + D_1(g)C(h)D_2(k) + C(g)D_2(hk) \quad . \end{aligned} \quad (2.5)$$

⁴*I.e.* no invariant subspaces other than \mathcal{V}_1 itself and the null vector $\{0\}$.

⁵An unexpected and out-of-context accolade. For example, "Get the hell out of this lane before we run into that truck!!" followed by "Dude, those are really nice cufflinks."

If \mathcal{V}_1^\perp is invariant, then $C^{(n_1, n_2)}(g) = 0$ for all g and $D^{(n)}(G)$ is block diagonal, meaning that $D^{(n)}(G)$ is fully reducible.

We may now prove the following theorem:

◇ Any unitary representation $\hat{D}(G)$ that is reducible is fully reducible.

The proof is trivial. In Eqn. 2.3, the upper right $n_1 \times n_2$ rectangular block of $D^\dagger D = \mathbb{1}$ is $D_1^\dagger C = 0$. But D_1 is invertible, hence $C = 0$. Full reducibility means that we can express any unitary representation as a *direct sum* over irreducible representations, viz.

$$\begin{aligned} D(g) &= \overbrace{D^{\Gamma_1}(g) \oplus \cdots \oplus D^{\Gamma_1}(g)}^{n_{\Gamma_1} \text{ times}} \oplus \overbrace{D^{\Gamma_2}(g) \oplus \cdots \oplus D^{\Gamma_2}(g)}^{n_{\Gamma_2} \text{ times}} \oplus \cdots \\ &= \bigoplus_{\Gamma} n_{\Gamma} D^{\Gamma}(g) \quad , \end{aligned} \quad (2.6)$$

where each irreducible representation Γ_j appears $n(\Gamma_j) \equiv n_{\Gamma_j}$ times. If we call $D(g) \equiv D^\Psi(g)$ the matrix of g in the Ψ representation, then the reduction of Ψ is

$$\Psi = n_{\Gamma_1} \Gamma_1 \oplus n_{\Gamma_2} \Gamma_2 \oplus \cdots . \quad (2.7)$$

2.1.3 Conjugate and adjoint representations

If the matrices $D(G)$ form a representation Γ of the group G , then their complex conjugates $D(G)^*$ also form a representation of G , which we call Γ^* , called the *conjugate representation* of Γ . This is because, defining $D^*(g) = [D(g)]^*$,

$$D^*(g) D^*(h) = [D(g) D(h)]^* = D^*(gh) \quad . \quad (2.8)$$

If $D(G)$ is a real representation, then $\Gamma^* \cong \Gamma$.

Similarly, the matrices $[D(G)^\top]^{-1}$, i.e. the inverse transposes of $D(G)$, also form a representation, called the *adjoint representation* of Γ . This is because, with $D^\top(g) \equiv [D(g)]^\top$ and $\overline{D}(g) \equiv [D^\top(g)]^{-1}$,

$$\overline{D}(g) \overline{D}(h) = [D^\top(g)]^{-1} [D^\top(h)]^{-1} = [D^\top(h) D^\top(g)]^{-1} = [[D(g) D(h)]^\top]^{-1} = [D^\top(gh)]^{-1} = \overline{D}(gh) \quad . \quad (2.9)$$

Note that for unitary representations, the complex and adjoint representations are one and the same.

It is left as an exercise to the student to prove that $D(G)$, $D^*(G)$, and $\overline{D}(G)$ are either all reducible or all irreducible.

2.1.4 Unitary representations of finite groups

So it turns out that every representation $D^{(n)}(G)$ of a finite group is equivalent to a unitary representation. To show this, we need to find an invertible matrix S such that $S^{-1} D^{(n)}(g) S \in \text{U}(n)$ for all $g \in G$. It

almost seems too much to ask, but as we're about to see, it is quite easy to construct such an S . We'll suppress the superscript on $D^{(n)}(g)$ and remember throughout that we are talking about an n -dimensional representation.

Start by forming the matrix

$$H = \sum_{g \in G} D^\dagger(g) D(g) \quad . \quad (2.10)$$

Clearly $H = H^\dagger$ is Hermitian, which means it can be diagonalized by a unitary matrix $V \in U(n)$. We write

$$V^\dagger H V = \Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \quad , \quad (2.11)$$

with $\lambda_j > 0$ for all j (you should prove this). Now define $\tilde{D}(g) = V^\dagger D(g) V$, in which case

$$\Lambda = V^\dagger H V = \sum_{g \in G} \tilde{D}^\dagger(g) \tilde{D}(g) \quad , \quad \lambda_k = \sum_{g \in G} \sum_{l=1}^n |\tilde{D}_{lk}(g)|^2 \quad . \quad (2.12)$$

We may now form the matrices $\Lambda^{\pm 1/2}$, and define

$$B(g) = \Lambda^{1/2} \tilde{D}(g) \Lambda^{-1/2} \quad . \quad (2.13)$$

We now show that $B(g)$ is unitary for all g :

$$\begin{aligned} B^\dagger(g) B(g) &= \Lambda^{-1/2} \tilde{D}^\dagger(g) \Lambda \tilde{D}(g) \Lambda^{-1/2} = \Lambda^{-1/2} \sum_{h \in G} \tilde{D}^\dagger(g) \tilde{D}^\dagger(h) \tilde{D}(h) \tilde{D}(g) \Lambda^{-1/2} \\ &= \Lambda^{-1/2} \overbrace{\sum_{h \in G} \tilde{D}^\dagger(hg) \tilde{D}(hg)}^{\Lambda} \Lambda^{-1/2} = \mathbf{1} \quad , \end{aligned} \quad (2.14)$$

where we have invoked the rearrangement theorem to write the sum over all hg for fixed g as a sum over group elements. So we have shown $B(g) = S^{-1} D(g) S$ is unitary for all g , with $S = V \Lambda^{-1/2}$. Note that not all symmetries can be realized unitarily. For example, time-reversal, which we shall discuss in due time, is an anti-unitary symmetry.

The above proof relies on the convergence of the sum for H in Eqn. 2.10. For discrete groups of finite order, or for compact continuous (Lie) groups, this convergence is guaranteed. But for groups of infinite order or noncompact Lie groups, convergence is not guaranteed. The Lorentz group, for example, has nonunitary representations.

2.1.5 Projective representations

I highly recommend you skip this section.

What? You're still here? OK, but strap in as we introduce the concept of a *projective representation*⁶. In a projective representation, the multiplication rule is preserved up to a phase, *i.e.*

$$\hat{D}(g) \hat{D}(h) = \omega(g, h) \hat{D}(gh) \quad , \quad (2.15)$$

⁶I am grateful to my colleague John McGreevy for explaining all sorts of crazy math shit to me.

where $\omega(g, h) \in \mathbb{C}$ for all $g, h \in G$ is called a *cocycle*. Hence $\hat{D}(G)$ is no longer a homomorphism. We still require associativity, meaning

$$\begin{aligned} \hat{D}(g)\hat{D}(h)\hat{D}(k) &= [\hat{D}(g)\hat{D}(h)]\hat{D}(k) = \omega(g, h)\hat{D}(gh)\hat{D}(k) = \omega(g, h)\omega(gh, k)\hat{D}(ghk) \\ &= \hat{D}(g)[\hat{D}(h)\hat{D}(k)] = \omega(h, k)\hat{D}(g)\hat{D}(hk) = \omega(g, hk)\omega(h, k)\hat{D}(ghk) \quad , \end{aligned} \quad (2.16)$$

which therefore requires

$$\frac{\omega(g, h)}{\omega(h, k)} = \frac{\omega(g, hk)}{\omega(gh, k)} \quad . \quad (2.17)$$

Perhaps the simplest discrete example is that of the abelian group $\mathbb{Z}_2 \times \mathbb{Z}_2$, which consists of the elements $\{E, \sigma, \tau, \sigma\tau\}$, with $\sigma^2 = \tau^2 = E$ and $\sigma\tau = \tau\sigma$. Consider now the projective representation where

$$D(\sigma) = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad D(\tau) = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad D(\sigma\tau) = iY \equiv \Lambda = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad , \quad (2.18)$$

where X, Y, Z are the familiar Pauli matrices, and $D(E)$ is of course the 2×2 identity matrix. Then $\omega(\sigma, \tau) = \omega(\sigma, \sigma\tau) = \omega(\sigma\tau, \tau) = 1$ but $\omega(\tau, \sigma) = \omega(\sigma\tau, \sigma) = \omega(\tau, \sigma\tau) = -1$. Below we shall find that representation of abelian groups are always one-dimensional. Not so for projective representations! Here we have an example of an abelian group with a two-dimensional irreducible projective representation. Incidentally, we can *lift* the projective representation to a conventional linear representation, of a different group \tilde{G} , acting on the same two-dimensional vector space. \tilde{G} is called a *central extension* of G .⁷ In our case, $\tilde{G} \subset \text{SU}(2)$ consists of the eight elements $\{\pm E, \pm Z, \pm X \pm \Lambda\}$, with the multiplication table given by

$$(\pm E)^2 = (\pm Z)^2 = (\pm X)^2 = E \quad , \quad (\pm \Lambda)^2 = -E \quad (2.19)$$

and

$$ZX = -XZ = \Lambda \quad , \quad Z\Lambda = -\Lambda Z = X \quad , \quad \Lambda X = -X\Lambda = Z \quad . \quad (2.20)$$

Clearly \tilde{G} is nonabelian, and as we remarked in chapter 1, there are only two distinct nonabelian groups of order eight. So \tilde{G} must either be the dihedral group D_4 or the quaternion group Q . You should figure out which one it is for yourself before proceeding to the next paragraph.

To be more clear, an *extension* \tilde{G} of a group G by an abelian group A is given by an *exact sequence* of homomorphisms,

$$1 \longrightarrow A \xrightarrow{\psi} \tilde{G} \xrightarrow{\pi} G \longrightarrow 1 \quad . \quad (2.21)$$

Exactness means that the kernel of every map in the sequence is the image of the map which precedes it, and that ψ is injective while π is surjective. Furthermore $\text{im}(\psi) \triangleleft \tilde{G}$, i.e. the image of ψ in \tilde{G} is a normal subgroup. The extension is said to be *central* if $\text{im}(\psi) \subseteq Z(\tilde{G})$, i.e. if the image $\psi(A)$ lies within the center of \tilde{G} . The first map in the sequence, $1 \longrightarrow A$, is a trivial injection of the one element group $\mathbb{Z}_1 = \{1\}$ to the identity in A (it is so trivial we don't bother distinguishing it with a name). Similarly the last map $G \longrightarrow 1$ is the trivial surjection onto \mathbb{Z}_1 .

In our previous example, the group $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ is lifted to $\tilde{G} = D_4$ by means of the abelian group $A = \mathbb{Z}_2$. Thus, let $\mathbb{Z}_2 = \{1, m\}$, $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, \tau, \sigma, \sigma\tau\}$, and $D_4 = \{E, -E, \Lambda, -\Lambda, X, -X, Z, -Z\}$. We

⁷For example, the central extension for UCSD is 858-534-2230.

Clearly $R \in \text{SO}(3)$, and each $R(\xi, \hat{\mathbf{n}})$ labels a unique such group element, aside from the identification $R(\pi, \hat{\mathbf{n}}) = R(\pi, -\hat{\mathbf{n}})$. Yet both $\pm U$ map to R , hence the double cover. Another way to say this is $\text{SU}(2)/\mathbb{Z}_2 \cong \text{SO}(3)$.

A more familiar example to condensed matter physicists is that of the *magnetic translation group*, which is the group of space translations in the presence of a uniform magnetic field. Let's first consider ordinary translations in $d = 3$ dimensions. The translation operator is $\hat{t}(\mathbf{d}) = \exp(i\mathbf{p} \cdot \mathbf{d}/\hbar) = \exp(\mathbf{d} \cdot \nabla)$. Note that $\hat{t}(\mathbf{d})\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{d})$. Since the different components of \mathbf{p} commute, we have $\hat{t}(\mathbf{d})\hat{t}(\mathbf{d}') = \hat{t}(\mathbf{d} + \mathbf{d}')$, hence $\hat{t}(\mathbb{R}^3, +)$ is a representation of the group \mathbb{R}^3 , where the group operation is vector addition.

In the presence of a uniform magnetic field \mathbf{B} , the kinetic energy becomes $\hat{T} = \pi^2/2m$, where the *cyclotron momentum* π is given by $\pi = \mathbf{p} + \frac{e}{c}\mathbf{A}$ and $\nabla \times \mathbf{A} = \mathbf{B}$. Its different components in general do not commute. Rather, $[\pi^\alpha, \pi^\beta] = -i(\hbar e/c)\varepsilon_{\alpha\beta\gamma}B^\gamma$. One then defines the *guiding center momentum* operator $\kappa \equiv \pi - \frac{e}{c}\mathbf{B} \times \mathbf{r}$, and finds $[\kappa^\alpha, \kappa^\beta] = +i(\hbar e/c)\varepsilon_{\alpha\beta\gamma}B^\gamma$ as well as $[\kappa^\alpha, \pi^\beta] = 0$. The *magnetic translation operator* is then defined as $\hat{t}_{\mathbf{B}}(\mathbf{d}) \equiv \exp(i\kappa \cdot \mathbf{d}/\hbar)$. This commutes with the kinetic energy, but one finds

$$\hat{t}_{\mathbf{B}}(\mathbf{d})\hat{t}_{\mathbf{B}}(\mathbf{d}') = \exp(-i\pi\mathbf{B} \cdot \mathbf{d} \times \mathbf{d}'/\phi_0)\hat{t}_{\mathbf{B}}(\mathbf{d} + \mathbf{d}') \quad , \quad (2.26)$$

where $\phi_0 = hc/e$ is the Dirac flux quantum. In this case, then, we have a projective representation of the abelian group of translations in \mathbb{R}^3 . Note that $[\hat{t}_{\mathbf{B}}(\mathbf{d}), \hat{t}_{\mathbf{B}}(\mathbf{d}')] = 0$ if and only if $\mathbf{B} \cdot \mathbf{d} \times \mathbf{d}' = q\phi_0$, where $q \in \mathbb{Z}$, which says that the parallelogram with sides \mathbf{d} and \mathbf{d}' encloses an area containing an integer number of Dirac quanta.

2.2 The Great Orthogonality Theorem

We now return to the warm, comforting safe-space of discrete groups with finite dimension, and their proper representations, and embark on a path toward a marvelous result known as the "Great Orthogonality Theorem". To reach this sublime state of enlightenment, we first need two lemmas⁸ due to I. Schur⁹.

2.2.1 Schur's first lemma

LEMMA : Let $\hat{D}(G)$ be an irreducible representation of G on a vector space \mathcal{V} , and \hat{C} an arbitrary linear operator on \mathcal{V} . If $[\hat{D}(g), \hat{C}] = 0$ for all $g \in G$, then $\hat{C} = \lambda\hat{1}$ is a multiple of the identity.

We've already seen how any irreducible representation of a finite group is equivalent to a unitary representation, hence without loss of generality we may assume $\hat{D}(G)$ is unitary. We will also assume \hat{C} is Hermitian. This imposes no restriction, because from an arbitrary \hat{C} we may form $\hat{C}_+ = \frac{1}{2}(\hat{C} + \hat{C}^\dagger)$ and $\hat{C}_- = \frac{1}{2i}(\hat{C} - \hat{C}^\dagger)$, both of which are Hermitian, and prove the theorem for \hat{C}_\pm separately.

⁸"[A lemma] is a stepping stone on the path to proving a theorem" - some math blog.

⁹Awful pun: We can trust in these lemmas because their author was Schur.

With $\hat{C} = \hat{C}^\dagger$, we may find a unitary operator \hat{W} such that $\hat{W}^\dagger \hat{C} \hat{W} = \hat{\Lambda}$, where $\hat{\Lambda}$ is diagonal in our basis. In other words, we may use \hat{W} to transform to a new basis $|\tilde{e}_{a\mu}\rangle$ where $\hat{C}|\tilde{e}_{a\mu}\rangle = \lambda_a|\tilde{e}_{a\mu}\rangle$. Here a labels the distinct eigenvalues of \hat{C} , and μ is an auxiliary index parameterizing the subspace $\mathcal{V}_a \subset \mathcal{V}$ with eigenvalue λ_a . Since $\hat{D}(g)$ commutes with \hat{C} for all $g \in G$, each \mathcal{V}_a is an invariant subspace. But by assumption $\hat{D}(G)$ is an irreducible representation, in which case the only invariant subspace is \mathcal{V} itself. In that case, \hat{C} can only have one eigenvalue, hence $\hat{C} = \lambda\hat{1}$ for some $\lambda \in \mathbb{R}$. QED

COROLLARY : If G is abelian, its irreducible representations are all of dimension one.

To prove the corollary, note that if G is abelian, then for any $h \in G$, we have $[\hat{D}(g), \hat{D}(h)] = 0$ for all $g \in G$. By the lemma, $\hat{D}(h) = \lambda_h \hat{1}$ for all $h \in G$. As an example, consider the cyclic group C_n , consisting of elements $\{E, R, R^2, \dots, R^{n-1}\}$. The operator \hat{R} must then correspond to a unimodular complex number $e^{i\theta}$, and $\hat{R}^n = 1$ requires $\theta = 2\pi j/n$ with $j \in \{0, 1, \dots, n-1\}$ labeling the representation. Thus, C_n has n one-dimensional representations, each of which is of course irreducible.

2.2.2 Schur's second lemma

LEMMA : Let $\hat{D}_1(G)$ and $\hat{D}_2(G)$ be two irreducible representations of a finite group G , acting on vector spaces \mathcal{V}_1 and \mathcal{V}_2 , respectively. Let $\hat{L} : \mathcal{V}_2 \mapsto \mathcal{V}_1$ be a linear operator such that $\hat{L}\hat{D}_2(g) = \hat{D}_1(g)\hat{L}$ for all $g \in G$. Then either (i) $\hat{L} = 0$ or (ii) $\mathcal{V}_1 \cong \mathcal{V}_2$ and $\hat{D}_1(G)$ is equivalent to $\hat{D}_2(G)$.

Note that this means that the matrices $D_1^{(n_1)}(g)$ and $D_2^{(n_2)}(g)$ satisfy $LD_1^{(n_1)}(g) = D_2^{(n_2)}(g)L$, where L is a $n_2 \times n_1$ rectangular matrix corresponding to \hat{L} .

To prove this lemma, we start by considering the space $\text{im}(\hat{L}) = \{\hat{L}|\psi_2\rangle \mid |\psi_2\rangle \in \mathcal{V}_2\}$, which is the image of the operator \hat{L} . This is an invariant subspace for $\hat{D}_1(G)$ because

$$\hat{D}_1(g)\hat{L}|\psi_2\rangle = \hat{L}\hat{D}_2(g)|\psi_2\rangle = \hat{L}|\tilde{\psi}_2\rangle \in \text{im}(\hat{L}) \quad \forall g \in G \quad . \quad (2.27)$$

But if $\hat{D}_1(G)$ is an irreducible representation, either $\text{im}(\hat{L}) = 0$ or $\text{im}(\hat{L}) = \mathcal{V}_1$.

Next, consider the kernel $\ker(\hat{L}) = \{|\psi_2\rangle \in \mathcal{V}_2 \mid \hat{L}|\psi_2\rangle = 0\}$. This is invariant under $\hat{D}_2(G)$ because

$$\hat{L}\hat{D}_2(g)|\psi_2\rangle = \hat{D}_1(g)\hat{L}|\psi_2\rangle = 0 \quad . \quad (2.28)$$

So either $\ker(\hat{L}) = 0$ or $\ker(\hat{L}) = \mathcal{V}_2$.

So we conclude that either

$$(i) \text{im}(\hat{L}) = 0 \text{ and } \ker(\hat{L}) = \mathcal{V}_2 \quad \text{or} \quad (ii) \text{im}(\hat{L}) = \mathcal{V}_1 \text{ and } \ker(\hat{L}) = 0 \quad .$$

Case (i) says $\hat{L} = 0$, i.e. every vector \mathcal{V}_2 maps to zero. Case (ii) says $\mathcal{V}_1 \cong \mathcal{V}_2$ and \hat{L} is an isomorphism. Hence \hat{L} is invertible and we may write $\hat{D}_2(g) = \hat{L}^{-1}\hat{D}_1(g)\hat{L}$ for all $g \in G$, which is to say the two representations are equivalent¹⁰.

¹⁰Mathematicians call a lemma like this where there are two possible cases a *dilemma*.

2.2.3 Great Orthogonality Theorem

Someone wise once said, "when life gives you lemmas, make a proof".

THEOREM : Let G be a finite group, Γ an irreducible representation of G , and $D^\Gamma(g)$ the matrix of g in the representation Γ . Then

$$\sum_{g \in G} D_{ki}^\Gamma(g^{-1}) D_{i'k'}^{\Gamma'}(g) = \frac{N_G}{d_\Gamma} \delta_{\Gamma\Gamma'} \delta_{ii'} \delta_{kk'} \quad (2.29)$$

where $N_G = |G|$ is the order of G and $d_\Gamma = \dim(\Gamma)$ is the dimension of the representation Γ .

It is important to stress that equivalent representations are not distinguished; they are considered to be the same representation. Also, note that if the representations are all unitary, we may write

$$\sum_{g \in G} D_{ik}^{\Gamma*}(g) D_{i'k'}^{\Gamma'}(g) = \frac{N_G}{d_\Gamma} \delta_{\Gamma\Gamma'} \delta_{ii'} \delta_{kk'} \quad , \quad (2.30)$$

where $D^{\Gamma*}(g) = [D^\Gamma(g)]^*$, i.e. the matrix of g in the conjugate representation Γ^* is the complex conjugate of the matrix of g in the representation Γ . Note that the matrices $D^{\Gamma*}(g)$ and $D_{ik}^\Gamma(g)$ are not necessarily of the same dimension. I.e. i and k in Eqns. 2.29, 2.30 run from 1 to d_Γ while i' and k' run from 1 to $d_{\Gamma'}$. We say that two general (not necessarily irreducible) representations Ψ and Ψ' are *orthogonal* if

$$\sum_{g \in G} D_{ik}^{\Psi*}(g) D_{i'k'}^{\Psi'}(g) = 0 \quad . \quad (2.31)$$

We will see that this means that Ψ and Ψ' , when fully reduced into IRREPS, contain no IRREPS in common.

As an example of the G.O.T. in action, consider the cyclic group C_n , with elements $\{E, R, R^2, \dots, R^{n-1}\}$. We know that there are n irreducible representations (IRREPS), all of which are one-dimensional. Each IRREP Γ is labeled by an integer j_Γ , with $D^\Gamma(R^k) = \exp(2\pi i j_\Gamma k/n)$. Then

$$\sum_{k=0}^{n-1} D^{\Gamma*}(R^k) D^{\Gamma'}(R^k) = \sum_{k=0}^{n-1} e^{2\pi i (j_\Gamma - j_{\Gamma'}) k/n} = n \delta_{\Gamma\Gamma'} \quad . \quad (2.32)$$

To prove the theorem, let M be a $d_\Gamma \times d_{\Gamma'}$ matrix, and

$$L = \sum_{g \in G} D^\Gamma(g^{-1}) M D^{\Gamma'}(g) \quad , \quad (2.33)$$

which is also of dimensions $d_\Gamma \times d_{\Gamma'}$. By the rearrangement theorem, $D^\Gamma(h^{-1}) L D^{\Gamma'}(h) = L$ for all $h \in G$, i.e. $L D^{\Gamma'}(h) = D^\Gamma(h) L$. We now appeal to Schur's lemmas, and conclude that either (i) $\Gamma \neq \Gamma'$ and $L = 0$, or (ii) $\Gamma = \Gamma'$ and $L = \lambda E$. Now choose the matrix $M_{jj'}^{(kk')} = \delta_{jk} \delta_{j'k'}$, where $k \in \{1, \dots, d_\Gamma\}$ and $k' \in \{1, \dots, d_{\Gamma'}\}$ are arbitrary. Here (kk') is a label for a family of $d_\Gamma d_{\Gamma'}$ matrices. We then have

$$L_{ii'}^{(kk')} = \sum_{g \in G} D_{ik}^\Gamma(g^{-1}) D_{k'i'}^{\Gamma'}(g) \quad . \quad (2.34)$$

We've already noted that if $\Gamma \neq \Gamma'$, then $L^{(kk')} = 0$. If $\Gamma = \Gamma'$, we must have $L_{ii'}^{(kk')} = \lambda_{kk'} \delta_{ii'}$, with

$$\lambda_{kk'} = \frac{1}{d_\Gamma} \text{Tr} L^{(kk')} = \frac{1}{d_\Gamma} \sum_{g \in G} D_{ik}^\Gamma(g^{-1}) D_{k'i}^\Gamma(g) = \frac{1}{d_\Gamma} \sum_{g \in G} [D^\Gamma(g) D^\Gamma(g^{-1})]_{k'k} = \frac{N_G}{d_\Gamma} \delta_{kk'} \quad , \quad (2.35)$$

and we are done!

Without loss of generality, we may restrict our attention to unitary representations. Let us define the vector

$$\psi_g^{(\Gamma ik)} \equiv \sqrt{\frac{d_\Gamma}{N_G}} D_{ik}^\Gamma(g) \quad , \quad (2.36)$$

where (Γik) is a label, with $i, k \in \{1, \dots, d_\Gamma\}$, and where the group element g indexes the components of ψ . The GOT can then be restated as an orthonormality condition on these vectors, *i.e.*

$$\langle \psi^{(\Gamma ik)} | \psi^{(\Gamma' i' k')} \rangle = \delta_{\Gamma \Gamma'} \delta_{ii'} \delta_{kk'} \quad , \quad (2.37)$$

which is kind of cool. Since each $\psi^{(\Gamma ik)}$ lives in a vector space of N_G dimensions, we know that the total number of these vectors cannot exceed N_G , *i.e.*

$$\sum_{\Gamma} d_\Gamma^2 \leq N_G \quad . \quad (2.38)$$

Indeed, after we discuss the *regular representation*, we shall prove that the set $\{\psi^{(\Gamma ik)}\}$ is complete as well as orthonormal. Completeness then entails the equality $\sum_{\Gamma} d_\Gamma^2 = N_G$, as well as

$$\sum_{\Gamma} \sum_{i,k=1}^{d_\Gamma} \psi_g^{(\Gamma ik)} (\psi_{g'}^{(\Gamma ik)})^* = \frac{1}{N_G} \sum_{\Gamma} d_\Gamma \sum_{i,k=1}^{d_\Gamma} D_{ik}^\Gamma(g) D_{ik}^{\Gamma*}(g') = \delta_{gg'} \quad , \quad (2.39)$$

which is also quite wonderful¹¹.

2.3 Group Characters

Recall the definition of the *character* of the group element g in the representation Γ , $\chi^\Gamma(g) = \text{Tr} D^\Gamma(g)$, where $D^\Gamma(G)$ are the matrices of the representation Γ , which may be taken to be unitary. We remarked earlier that $\chi^\Gamma(h^{-1}gh) = \chi^\Gamma(g)$, due to cyclic invariance of the trace, means that two elements g and g' in the same conjugacy class have the same character¹². Therefore, it is convenient to focus on the conjugacy classes themselves, labeling them \mathcal{C} . The expression $\chi^\Gamma(\mathcal{C})$ then will refer to the character of each element in the conjugacy class \mathcal{C} . The identity element always forms its own class, and we accordingly have the following important result:

◇ *The dimension of any representation Γ is the character of the identity: $d_\Gamma \equiv \dim(\Gamma) = \chi^\Gamma(E)$.*

Note also that if a class \mathcal{C} contains the inverse of each of its elements, then $\chi^\Gamma(\mathcal{C})$ is real in every unitary representation, since then $\chi^\Gamma(g) = \chi^\Gamma(g^{-1}) = [\chi^\Gamma(g)]^*$.

¹¹We might well call this the "Great Completeness Theorem".

¹²The fact that character is so intimately associated with class may seem politically incorrect and even distressful to some. If this makes you feel unsafe, try to remember that we are talking about group theory.

$\mathcal{C} \rightarrow$	\mathcal{C}_1	$3\mathcal{C}_2$	$2\mathcal{C}_3$
$\Gamma \downarrow$	$\{E\}$	$\{\sigma, \sigma', \sigma''\}$	$\{R, W\}$
A_1	1	1	1
A_2	1	-1	1
E	2	0	-1
\mathcal{Y}	3	1	0

Table 2.1: Character table for $C_{3v} \cong D_3$. The representations A_1, A_2 , and E are irreducible.

2.3.1 Example: D_3

Recall the dihedral group $D_3 \cong C_{3v} \cong S_3$, with elements $(E, R, W, \sigma, \sigma', \sigma'')$. In chapter one, we identified its three conjugacy classes, $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{\sigma, \sigma', \sigma''\}$, and $\mathcal{C}_3 = \{R, W\}$, and we met up with *four* of its representations. The first two are one-dimensional, and we call them A_1 and A_2 . The 1×1 matrices of the A_1 representation are given by

$$D^{A_1}(E) = 1 \quad , \quad D^{A_1}(R) = 1 \quad , \quad D^{A_1}(W) = 1 \quad , \quad D^{A_1}(\sigma) = 1 \quad , \quad D^{A_1}(\sigma') = 1 \quad , \quad D^{A_1}(\sigma'') = 1 \quad . \quad (2.40)$$

In the A_2 representation, the 1×1 matrices are

$$D^{A_2}(E) = 1 \quad , \quad D^{A_2}(R) = 1 \quad , \quad D^{A_2}(W) = 1 \quad , \quad D^{A_2}(\sigma) = -1 \quad , \quad D^{A_2}(\sigma') = -1 \quad , \quad D^{A_2}(\sigma'') = -1 \quad . \quad (2.41)$$

The third representation, called E , is two-dimensional, with

$$\begin{aligned} D^E(E) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & D^E(R) &= \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} & D^E(W) &= \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \\ D^E(\sigma) &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & D^E(\sigma') &= \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} & D^E(\sigma'') &= \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \quad . \end{aligned} \quad (2.42)$$

Finally, recall the defining representation of S_3 , which we call \mathcal{Y} :

$$\begin{aligned} D^{\mathcal{Y}}(E) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} & D^{\mathcal{Y}}(R) &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} & D^{\mathcal{Y}}(W) &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \\ D^{\mathcal{Y}}(\sigma) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} & D^{\mathcal{Y}}(\sigma') &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} & D^{\mathcal{Y}}(\sigma'') &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad . \end{aligned} \quad (2.43)$$

Let's construct the character table for D_3 . Taking the traces, we obtain the results in Tab. 2.1. Note the notation $3\mathcal{C}_2$ and $2\mathcal{C}_3$, which refer to the 3-element class \mathcal{C}_2 and the 2-element class \mathcal{C}_3 , respectively. The

representation \mathcal{Y} is reducible, and it turns out that $\mathcal{Y} = A_1 \oplus E$. Indeed, one sees that

$$\chi^{\mathcal{Y}}(g) = \chi^{A_1}(g) + \chi^E(g) \quad . \quad (2.44)$$

We shall see how reducible representations may be decomposed further below.

Remark about reality of characters

If a class \mathcal{C} contains the inverse of each of its elements, then $\chi^{\Gamma}(\mathcal{C})$ is real in every unitary representation, since then $\chi^{\Gamma}(g) = \chi^{\Gamma}(g^{-1}) = [\chi^{\Gamma}(g)]^*$. This is the case for all classes of $C_{3v} \cong D_3$, for example. It is *not* the case in general, and certainly not for most abelian groups in particular, because in an abelian group, all classes contain a single element, but the only elements which are their own inverses are those elements of order $n = 1$ or $n = 2$. For example, if we eliminate the reflection symmetries, C_{3v} is broken down to $C_3 \cong Z_3$. Without the mirrors, we lose the conjugacy of R and W , since $\sigma R \sigma^{-1} = \sigma R \sigma = W$, which also holds when σ is replaced by either of the other mirrors σ' and σ'' . Thus, the class $2C_3$ in C_{3v} breaks up into two distinct classes C_3 (R) and C_3^{-1} (W) within C_3 . In two of the IRREPS, the $C_3^{\pm 1}$ classes have complex characters, as shown in Tab. 2.2.

2.3.2 Orthogonality theorem for characters

Taking the trace of each of the matrices in Eqn. 2.29, we obtain¹³

$$\sum_{g \in G} \chi^{\Gamma}(g^{-1}) \chi^{\Gamma'}(g) = N_G \delta_{\Gamma\Gamma'} \quad . \quad (2.45)$$

Henceforth we shall assume all representations are unitary, in which case $\chi^{\Gamma}(g^{-1}) = [\chi^{\Gamma}(g)]^* = \chi^{\Gamma*}(g)$. We may replace the above sum over group elements by a sum over conjugacy classes \mathcal{C} , resulting in

$$\sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma*}(\mathcal{C}) \chi^{\Gamma'}(\mathcal{C}) = N_G \delta_{\Gamma\Gamma'} \quad , \quad (2.46)$$

where $N_{\mathcal{C}}$ is the number of elements in class \mathcal{C} . If we set $\Gamma = \Gamma'$, we have

$$\sum_{\mathcal{C}} N_{\mathcal{C}} |\chi^{\Gamma}(\mathcal{C})|^2 = N_G \quad . \quad (2.47)$$

Note that for D_3 , which has six elements, the representations A_1 and A_2 in Tab. 2.1 appropriately yield $1 \cdot 1^2 + 3 \cdot 1^2 + 2 \cdot 1^2 = 6$. Similarly, for E we have $1 \cdot 2^2 + 3 \cdot 0^2 + 2 \cdot (-1)^2 = 6$. But for \mathcal{Y} the LHS of Eqn. 2.47 gives $1 \cdot 3^2 + 3 \cdot 1^2 + 2 \cdot 0^2 = 12$, hence we can immediately tell that \mathcal{Y} must be reducible. For irreducible representations, we have the following:

THEOREM : Two IRREPS Γ and Γ' are equivalent if and only if $\chi^{\Gamma}(g) = \chi^{\Gamma'}(g)$ for all $g \in G$.

This proof is left as an exercise to the reader. Note that an IRREP Γ is equivalent to its complex conjugate Γ^* if and only if Γ is real.

¹³In Eqn. 2.29, recall that $i, k \in \{1, \dots, d_{\Gamma}\}$ and $i', k' \in \{1, \dots, d_{\Gamma'}\}$.

2.3.3 Dirac characters

Recall from chapter 1 the notion of a group algebra \mathfrak{G} , which consists of linear combinations of the form $\mathbf{x} = \sum_{g \in G} x_g g$. Consider now the quantity

$$\Omega_a = \sum_{g \in \mathcal{C}_a} g \quad , \quad (2.48)$$

where the sum is over all group elements in the conjugacy class \mathcal{C}_a , where a ranges from 1 to the total number of classes. Ω_a is known as a *Dirac character*. Unlike the group characters we have discussed thus far, which are complex numbers, Dirac characters are elements of the group algebra. What makes them special is that each Ω_a commutes with every element of G , because taking $g^{-1}\Omega_a g$ simply reorders the terms in the above sum. We shall now prove that any element of \mathfrak{G} which commutes with the entire group G must be a linear combination of the Dirac characters. To see this, write a general element $\mathbf{x} \in \mathfrak{G}$ as $\mathbf{x} = \sum_{g \in G} x_g g$, where each $x_g \in \mathbb{C}$. Then for any $r \in G$,

$$r^{-1} \mathbf{x} r = \sum_{h \in G} x_h r^{-1} h r = \sum_{g \in G} x_{rgr^{-1}} g \quad , \quad (2.49)$$

and therefore if $r^{-1} \mathbf{x} r = \mathbf{x}$, then equating the coefficients of g we have $x_g = x_{rgr^{-1}}$ for all $r \in G$, which says that x_g is a *class function*, i.e. it takes the same value for every element of a given conjugacy class.

Since each Ω_a commutes with all group elements, so does the product $\Omega_a \Omega_b$, and the above result then entails a relation of the form

$$\Omega_a \Omega_b = \sum_c F_{abc} \Omega_c \quad , \quad (2.50)$$

where the F_{abc} are called the *class coefficients*. Recall that the identity element E forms its own class, which we can always call Ω_1 , so that $F_{1bc} = F_{b1c} = \delta_{bc}$.

For the group C_{3v} , with classes $\mathcal{C}_1 = \{E\}$, $\mathcal{C}_2 = \{R, W\}$, and $\mathcal{C}_3 = \{\sigma, \sigma', \sigma''\}$,

$$\begin{aligned} \Omega_2 \Omega_2 &= (R + W)(R + W) = 2E + R + W = 2\Omega_1 + \Omega_2 \\ \Omega_2 \Omega_3 &= (R + W)(\sigma + \sigma' + \sigma'') = \sigma'' + \sigma + \sigma' + \sigma' + \sigma'' + \sigma = 2\Omega_3 \\ \Omega_3 \Omega_3 &= (\sigma + \sigma' + \sigma'')(\sigma + \sigma' + \sigma'') = 3E + 3R + 3W = 3\Omega_1 + 3\Omega_2 \quad . \end{aligned} \quad (2.51)$$

Thus,

$$\begin{aligned} F_{111} &= F_{122} = F_{212} = F_{133} = F_{313} = 1 \\ F_{221} &= 2 \quad , \quad F_{222} = 1 \quad , \quad F_{233} = F_{323} = 2 \quad , \quad F_{331} = 3 \quad , \quad F_{332} = 3 \quad , \end{aligned} \quad (2.52)$$

with all other $F_{abc} = 0$. Because the Dirac characters all commute, any equation solved by the Ω_a will be solved by their eigenvalues ω_a ¹⁴. We always have $\omega_1 = 1$. We then must solve the three equations

$$\omega_2^2 = 2 + \omega_2 \quad , \quad \omega_2 \omega_3 = 2\omega_3 \quad , \quad \omega_3^2 = 3 + 3\omega_2 \quad . \quad (2.53)$$

¹⁴*Eigenvalues?!* How are we suddenly talking about *eigenvalues*? Well, you see, as we noted toward the end of §1.3.1, the group algebra \mathfrak{G} is in fact a vector space \mathcal{A} with basis vectors $g \in G$, endowed with a linear multiplication law $\mathcal{A} \times \mathcal{A} \rightarrow \mathcal{A}$. Thus, any element of the algebra is also a linear operator, and linear operators have eigenvalues. So there.

If $\omega_3 = 0$, the third of these gives $\omega_2 = -1$, which is consistent with the first, and therefore $\omega = (1, -1, 0)$. If $\omega_3 \neq 0$, the second equation gives $\omega_2 = 2$, again consistent with the first, and thus $\omega_3^2 = 9$, and so there are two possible solutions $\omega = (1, 2, 3)$ and $\omega = (1, 2, -3)$.

Relation to group characters

Suppose $D^\Gamma(G)$ is an irreducible matrix representation of G , and define the matrix

$$\Lambda_a = \sum_{g \in \mathcal{C}_a} D^\Gamma(g) \quad . \quad (2.54)$$

Then for all $h \in G$, we have $D^\Gamma(h^{-1}) \Lambda_a D^\Gamma(h) = \Lambda_a$, and by Schur's first lemma it must be that each $\Lambda_a = \lambda_a \mathbf{1}$ is a multiple of the identity matrix. But then

$$\text{Tr } \Lambda_a = d_\Gamma \lambda_a = \sum_{g \in \mathcal{C}_a} \chi^\Gamma(g) = N_{\mathcal{C}_a} \chi^\Gamma(\mathcal{C}_a) \quad , \quad (2.55)$$

and therefore

$$\Lambda_a = \frac{N_{\mathcal{C}_a}}{d_\Gamma} \chi^\Gamma(\mathcal{C}_a) \mathbf{1} \quad . \quad (2.56)$$

But clearly the Λ_a satisfy the same algebra as the Ω_a , *i.e.*

$$\Lambda_a \Lambda_b = \sum_c F_{abc} \Lambda_c \quad , \quad (2.57)$$

which yields the following relation for group characters:

$$\chi^\Gamma(\mathcal{C}_a) \chi^\Gamma(\mathcal{C}_b) = d_\Gamma \sum_l f_{abc} \chi^\Gamma(\mathcal{C}_c) \quad , \quad (2.58)$$

where $f_{abc} \equiv (N_{\mathcal{C}_c} / N_{\mathcal{C}_a} N_{\mathcal{C}_b}) F_{abc}$.

2.4 Decomposition of Representations

2.4.1 Reducible representations

We claim that the reduction of a reducible representation Ψ into IRREPS is unique. To see this, suppose

$$\Psi = \bigoplus_{\Gamma} n_{\Gamma}(\Psi) \Gamma \quad \Rightarrow \quad \chi^\Psi(\mathcal{C}) = \sum_{\Gamma} n_{\Gamma}(\Psi) \chi^\Gamma(\mathcal{C}) \quad . \quad (2.59)$$

We now derive an explicit formula for the decomposition $\{n_{\Gamma}(\Psi)\}$. Using the character orthogonality equation, we have

$$\sum_c N_c \chi^{\Gamma^*}(\mathcal{C}) \chi^\Psi(\mathcal{C}) = \sum_{\Gamma'} n_{\Gamma'}(\Psi) \overbrace{\sum_c N_c \chi^{\Gamma^*}(\mathcal{C}) \chi^{\Gamma'}(\mathcal{C})}^{N_G \delta_{\Gamma\Gamma'}} = N_G n_{\Gamma}(\Psi) \quad . \quad (2.60)$$

Thus, the number of times the IRREP Γ appears in the decomposition of Ψ is

$$n_{\Gamma}(\Psi) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma*}(\mathcal{C}) \chi^{\Psi}(\mathcal{C}) \quad . \quad (2.61)$$

Note that if $\Psi = \Gamma'$ is itself an IRREP, the above formula correctly gives $n_{\Gamma}(\Gamma') = \delta_{\Gamma\Gamma'}$.

Note further that we can define the vectors

$$V_{\mathcal{C}}^{\Gamma} = \sqrt{\frac{N_{\mathcal{C}}}{N_G}} \chi^{\Gamma}(\mathcal{C}) \quad , \quad (2.62)$$

which are labeled by IRREPS Γ , and whose indices run over the equivalence classes \mathcal{C} . Character orthogonality then entails

$$\langle \mathbf{V}^{\Gamma} | \mathbf{V}^{\Gamma'} \rangle = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma*}(\mathcal{C}) \chi^{\Gamma'}(\mathcal{C}) = \delta_{\Gamma\Gamma'} \quad . \quad (2.63)$$

Note that the vector space $\{\mathbf{V}^{\Gamma}\}$ is spanned by the vectors corresponding to all IRREPS, and that these vectors must be complete if every representation can be decomposed into IRREPS. Thus, we conclude the following:

◇ *The number of IRREPS is the number of classes: $\sum_{\Gamma} 1 = \sum_{\mathcal{C}} 1$.*

Completeness then entails $\sum_{\Gamma} |\mathbf{V}^{\Gamma}\rangle\langle \mathbf{V}^{\Gamma}| = \mathbf{1}$, i.e.

$$\sum_{\Gamma} \chi^{\Gamma*}(\mathcal{C}) \chi^{\Gamma}(\mathcal{C}') = \frac{N_G}{N_{\mathcal{C}}} \delta_{\mathcal{C}\mathcal{C}'} \quad , \quad (2.64)$$

from which it follows that

$$\chi^{\Psi}(\mathcal{C}) = \sum_{\Gamma} n_{\Gamma}(\Psi) \chi^{\Gamma}(\mathcal{C}) \quad , \quad (2.65)$$

i.e. the characters of a reducible representation are given by the sums of the characters of their constituents. This is quite obvious when one considers that any reducible representation may be brought to block diagonal form, where the individual blocks are the constituent IRREPS.

2.4.2 Projection onto a particular representation

Suppose, on your birthday, you are given a unitary matrix representation $\Delta(G)$ of a popular finite discrete group. You have reason to believe $\Delta(G)$ is reducible¹⁵, and you are a very impatient person, so you don't want to spend your time sifting through $\Delta(G)$ for your favorite IRREPS – especially not on your birthday. You would like to access them directly! How to do it?

The first thing to do is to go borrow a set of matrices $D_{\mu\nu}^{\Gamma}$ for all the IRREPS of G . Then construct the following expressions:

$$\Pi_{\mu\nu}^{\Gamma} = \frac{d_{\Gamma}}{N_G} \sum_{g \in G} D_{\mu\nu}^{\Gamma*}(g) \Delta(g) \quad , \quad (2.66)$$

¹⁵It may have come in a very large box, for example.

which for each set of labels (Γ, μ, ν) is a matrix of the same rank as $\Delta(G)$. The $\Pi_{\mu\nu}^\Gamma$ are *projection matrices* onto the μ^{th} row of the IRREP Γ . The following three marvelous things are true:

(i) The product of projectors is

$$\Pi_{\mu\nu}^\Gamma \Pi_{\mu'\nu'}^{\Gamma'} = \delta_{\Gamma\Gamma'} \delta_{\nu\mu'} \Pi_{\mu\nu}^\Gamma \quad . \quad (2.67)$$

(ii) Hermitian conjugate: $(\Pi_{\mu\nu}^\Gamma)^\dagger = \Pi_{\nu\mu}^\Gamma$, *i.e.*

$$(\Pi_{\mu\nu}^\Gamma)^*_{ji} = (\Pi_{\nu\mu}^\Gamma)_{ij} \quad . \quad (2.68)$$

(iii) Resolution of identity (where there is an implied sum on μ):

$$\sum_{\Gamma} \Pi_{\mu\mu}^\Gamma = \mathbf{1} \quad , \quad (2.69)$$

You will have fun proving these results for yourself! Note that $P_\mu^\Gamma \equiv \Pi_{\mu\mu}^\Gamma$ with no sum on μ satisfies

$$P_\mu^\Gamma P_{\mu'}^{\Gamma'} = \delta_{\Gamma\Gamma'} \delta_{\mu\mu'} P_\mu^\Gamma \quad , \quad (2.70)$$

i.e. each P_μ^Γ is a rank one projector onto the μ row of the Γ IRREP. Summing over all rows of all IRREPs yields $\sum_{\Gamma, \mu} P_\mu^\Gamma = \mathbf{1}$. However, note that it is the projectors of *fixed column index* which transform according to a particular IRREP, because¹⁶

$$\Delta(g) \Pi_{\mu\nu}^\Gamma = \sum_{\rho} \Pi_{\rho\nu}^\Gamma D_{\rho\mu}^\Gamma(g) \quad . \quad (2.71)$$

Finally let's take the trace on μ and ν in Eqn. 2.66 and form $\Pi^\Gamma = \sum_{\mu} \Pi_{\mu\mu}^\Gamma = \sum_{\mu} P_\mu^\Gamma$, *i.e.*

$$\Pi^\Gamma \equiv \frac{d_\Gamma}{N_G} \sum_{g \in G} \chi^{\Gamma*}(g) \Delta(g) \quad . \quad (2.72)$$

This also acts as a projection matrix onto Γ , since $\Pi^\Gamma \Pi^{\Gamma'} = \delta_{\Gamma\Gamma'} \Pi^\Gamma$.

Consider now an arbitrary vector ψ , and form the vector $\psi^{(\Gamma\mu)} = \Pi_{\mu\nu}^\Gamma \psi$. The index ν is fixed and suppressed in $\psi^{(\Gamma\mu)}$. That is, we form the vector whose i^{th} component is

$$\psi_i^{(\Gamma\mu)} = \frac{d_\Gamma}{N_G} \sum_{g \in G} D_{\mu\nu}^{\Gamma*}(g) \Delta_{ij}(g) \psi_j \quad . \quad (2.73)$$

Then, appealing to Eqn. 2.71,

$$\Delta_{ij}(g) \psi_j^{(\Gamma\mu)} = \psi_i^{(\Gamma\rho)} D_{\rho\mu}^\Gamma(g) \quad , \quad (2.74)$$

with implied sums on j and ρ . We've just projected an arbitrary vector ψ onto one which transforms according to the μ^{th} row of the IRREP Γ , *i.e.* $\psi^{(\Gamma\mu)}$.

¹⁶Prove it!

2.4.3 The regular representation

The regular representation of any finite discrete group is defined as follows. Define the group multiplication table so that the entry for row g_a and column g_b is $g_a^{-1}g_b$ rather than the usual $g_a g_b$. By this convention, all diagonal entries will be the identity element, E . The matrices of the regular representation are all of rank N_G , which is of course the rank of the multiplication table, and $D_{g,g'}^{\text{reg}}(h)$ is defined to be one everywhere h occurs in the above reorganized table, and zero otherwise. In other words,

$$D_{g,g'}^{\text{reg}}(h) = \delta_{g',gh} = \begin{cases} 1 & \text{if } g' = gh \\ 0 & \text{if } g' \neq gh \end{cases} . \quad (2.75)$$

Note that

$$\sum_{g' \in G} D_{g,g'}^{\text{reg}}(h) D_{g',g''}^{\text{reg}}(k) = \sum_{g' \in G} \delta_{g',gh} \delta_{g'',g'k} = \delta_{g'',ghk} = D^{\text{reg}}(hk) , \quad (2.76)$$

and so $D^{\text{reg}}(G)$ is a valid representation. We may now prove the following:

$$\text{THEOREM : } \Gamma_{\text{reg}} = \bigoplus_{\Gamma} d_{\Gamma} \Gamma .$$

In other words, each IRREP appears in Γ_{reg} as many times as its dimension. To show this, first note that

$$\chi^{\Gamma_{\text{reg}}}(h) = \sum_{g \in G} \delta_{g,gh} = N_G \delta_{h,E} \quad (2.77)$$

since $g = gh$ entails $h = E$. Next, we invoke Eqn. 2.61 with $\Psi = \Gamma_{\text{reg}}$. From the above result, only the identity class contributes to the sum over equivalence classes \mathcal{C} , in which case

$$n_{\Gamma}(\Gamma_{\text{reg}}) = \chi^{\Gamma}(E) = d_{\Gamma} . \quad (2.78)$$

As a bonus, we can now establish the equality in Eqn. 2.38, since

$$N_G = \chi^{\Gamma_{\text{reg}}}(E) = \sum_{\Gamma} n_{\Gamma}(\Gamma_{\text{reg}}) \chi^{\Gamma}(E) = \sum_{\Gamma} d_{\Gamma}^2 . \quad (2.79)$$

Therefore the order of any finite group is the sum of the squares of the dimensions of its irreducible representations. QED

2.4.4 Induced and subduced representations

The regular representation is a special case of something called an *induced representation*. Suppose $H \subset G$ is a subgroup. As we saw in chapter 1, this entails that N_G/N_H is an integer, and there is a unique *coset construction* where we can write

$$G = \sum_{j=1}^{N_G/N_H} r_j H . \quad (2.80)$$

Uniqueness means that the set $\{r_j\}$ is fixed by H . Now suppose we have a representation $D_{ab}(H)$. We now define

$$\tilde{D}_{ia,jb}(g) = \sum_{h \in H} D_{ab}(h) \delta_{r_i h, gr_j} \quad , \quad (2.81)$$

where

$$\delta_{r_i h, gr_j} = \begin{cases} 1 & \text{if } r_i h = gr_j \\ 0 & \text{otherwise} \end{cases} \quad . \quad (2.82)$$

Then one finds

$$\begin{aligned} \tilde{D}_{ia,jb}(g) \tilde{D}_{jb,kc}(g') &= \sum_{h, h' \in H} D_{ab}(h) D_{bc}(h') \delta_{r_i h, gr_j} \delta_{r_j h', g'r_k} \\ &= \sum_{\tilde{h} \in H} D_{ac}(\tilde{h}) \delta_{r_i \tilde{h}, gg'r_k} = \tilde{D}_{ia,kc}(gg') \quad , \end{aligned} \quad (2.83)$$

and so $\tilde{D}(G)$ is a representation of the larger group G . Note that if $D_{ab}(h) = 1$, then $\tilde{D}_{ij}(g) = \sum_{h \in H} \delta_{r_i h, gr_j}$ and that if $H = \{E\}$ then $\tilde{D}(G)$ is just the regular representation. The character of g in the induced representation is then

$$\tilde{\chi}(g) = \text{Tr } \tilde{D}(g) = \sum_{h \in H} \chi(h) \sum_i \delta_{g, r_i h r_i^{-1}} \quad . \quad (2.84)$$

Let G be a group and $H \subset G$ a proper subgroup of G . Then any representation $D^\Psi(G)$ is also a representation of H , called the *subduced representation* $\Psi^\downarrow(H)$, with

$$D^{\Psi^\downarrow}(h) = D^\Psi(h) \quad . \quad (2.85)$$

Even if $D^\Psi(G)$ is reducible, the subduced representation $D^{\Psi^\downarrow}(H)$ need not necessarily be irreducible. For example, the subduced representation on to the identity is the unit matrix of rank $d_{\Psi'}$, which is clearly reducible since it is a direct sum of $d_{\Psi'}$ one-dimensional trivial representations. If $D^\Psi(G)$ is reducible, then so is $D^{\Psi^\downarrow}(H)$. Thus, if $D^{\Psi^\downarrow}(H)$ is irreducible, then necessarily $D^\Psi(G)$ be reducible. Furthermore, if Ψ and Ψ' are two IRREPS of G , if there exists a subgroup $H \subset G$ such that Ψ^\downarrow and Ψ'^\downarrow are orthogonal, meaning they contain no common IRREPS of H , then Ψ and Ψ' are orthogonal. This is easily proven using the coset decomposition, writing $G = \sum_a r_a H$, so that

$$D_{ik}^\Psi(g) = D_{ik}^\Psi(rh) = \sum_m D_{im}^\Psi(r) D_{mk}^\Psi(h) \quad (2.86)$$

for some $h \in H$ and $r \notin H$. Multiplying the complex conjugate of this expression by the corresponding expression for $D_{i'k'}^{\Psi'}(g)$, and then summing over $g \in G$, we have

$$\sum_{g \in G} D_{ik}^{\Psi^*}(g) D_{i'k'}^{\Psi'}(g) = \sum_{m, m'} \sum_r D_{im}^{\Psi^*}(r) D_{i'm'}^{\Psi'}(r) \sum_{h \in H} D_{mk}^{\Psi^*}(h) D_{m'k'}^{\Psi'}(h) \quad , \quad (2.87)$$

which vanishes if Ψ^\downarrow and Ψ'^\downarrow are orthogonal representations on H .

2.4.5 Summary of key results

Here we summarize the key results. For unitary representations of a finite group G :

- **Great Orthogonality Theorem**: $\sum_{g \in G} D_{ik}^{\Gamma^*}(g) D_{i'k'}^{\Gamma'}(g) = (N_G/d_{\Gamma}) \delta_{\Gamma\Gamma'} \delta_{ii'} \delta_{kk'}$.
- **Great Completeness Theorem**: $\sum_{\Gamma, i, k} d_{\Gamma} D_{ik}^{\Gamma^*}(g) D_{ik}^{\Gamma}(g') = N_G \delta_{gg'}$.
- **Group characters**: $\chi^{\Gamma}(\mathcal{C}) \equiv \text{Tr } D^{\Gamma}(g)$, where g is any element in the conjugacy class \mathcal{C} .
- **Character tables**: Rows indexed by IRREPS Γ , columns indexed by classes \mathcal{C} . Identity IRREP row entries are all 1's. Identity class column entries are $d_{\Gamma} = \text{Tr } D^{\Gamma}(E)$.
- **Row orthogonality**: $\sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma^*}(\mathcal{C}) \chi^{\Gamma'}(\mathcal{C}) = N_G \delta_{\Gamma\Gamma'}$.
- **Column orthogonality**: $\sum_{\Gamma} \chi^{\Gamma^*}(\mathcal{C}) \chi^{\Gamma}(\mathcal{C}') = (N_G/N_{\mathcal{C}}) \delta_{\mathcal{C}\mathcal{C}'}$.
- **Decomposition**: The IRREP Γ appears $n_{\Gamma}(\Psi) = N_G^{-1} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma^*}(\mathcal{C}) \chi^{\Psi}(\mathcal{C})$ times in Ψ .
- **Projection matrices**: If $\Delta(G)$ is a reducible representation, $\Pi_{\mu\nu}^{\Gamma} = (d_{\Gamma}/N_G) \sum_{g \in G} D_{\mu\nu}^{\Gamma^*}(g) \Delta(g)$ projects onto the μ^{th} row of the Γ IRREP.

Here $N_G = |G|$ is the number of elements in G , $d_{\Gamma} = \text{dim}(\Gamma)$ is the dimension of the representation Γ , and $N_{\mathcal{C}}$ is the number of group elements in the conjugacy class \mathcal{C} .

2.4.6 Example character tables

Thus far we have not encountered any complex values of $\chi^{\Gamma}(g)$, but such cases are quite common. Consider, for example, the cyclic group C_3 consisting of $\{E, R, W\}$. C_n is abelian for all n , hence each element is its own class. We've seen how the 1×1 matrix $D^{\Gamma}(R^k)$ is given by $\omega^{kj_{\Gamma}}$ with $\omega = \exp(2\pi i/n)$, where $j_{\Gamma} \in \{0, \dots, n-1\}$ labels the IRREP, and $k \in \{0, \dots, n-1\}$. Tab. 2.2 shows the character table for C_3 . Note that $\Gamma_3 = \Gamma_2^*$ is the complex conjugate of the Γ_2 representation.

C_3	E	R	W
Γ_1	1	1	1
Γ_2	1	ω	ω^2
Γ_3	1	ω^2	ω

Table 2.2: Character table for C_3 .

We saw in chapter one that the eight element quaternion group, $Q = \{\pm E, \pm i, \pm j, \pm k\}$ has five conjugacy classes. Aside from the trivial one-dimensional identity representation Γ_1 , it has three other inequivalent one-dimensional IRREPs, called *sign representations*. The first of these we call Γ_2 , the 1×1 matrices for which are $D^{\Gamma_2}(\pm E, \pm i) = +1$ while $D^{\Gamma_2}(\pm j, \pm k) = -1$. One can check this is a valid group

Q	$\{E\}$	$\{-E\}$	$\{i, -i\}$	$\{j, -j\}$	$\{k, -k\}$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	1	-1	1	-1
Γ_4	1	1	-1	-1	1
Ψ	2	-2	0	0	0

Table 2.3: Character table for the quaternion group Q .

homomorphism. Permuting $\pm i$, $\pm j$, and $\pm k$ gives the other two one-dimensional IRREPS. One can then easily infer that there is one remaining IRREP of dimension 2. The character table for the quaternion group Q is shown in Tab. 2.3.

While the character table for a group G contains a wealth of important information, it does not always distinguish G up to isomorphism. That is, it is possible for two different groups to have the same character table. Such is the case with Q and D_4 , for example. The dihedral group D_4 also has five classes, which we can call E (the identity), C_2 (rotation by π), C_4 (rotations by $\pm\frac{1}{2}\pi$), C'_2 (reflections in $y = 0$ and in $x = 0$), and C''_2 (reflections in $y = x$ and in $y = -x$). Tab. 2.4 shows its character table¹⁷, which you should compare with Tab. 2.3.

D_4	E	C_2	$2C_4$	$2C'_2$	$2C''_2$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

Table 2.4: Character table for the dihedral group D_4 .

Recall that the eight matrices $\{\pm E, \pm Z, \pm X, \pm A\}$ from §2.1.5 form a real two-dimensional representation of either D_4 or Q (you were supposed to figure out which). Applying the GOT with $N_G = 8$ and $d_\Gamma = 2$, we have

$$2 E_{ik} E_{i'k'} + 2 Z_{ik} Z_{i'k'} + 2 X_{ik} X_{i'k'} + 2 A_{ik} A_{i'k'} = 4 \delta_{ii'} \delta_{kk'} \quad . \quad (2.88)$$

Recall $A = iY = -A^\top$, hence we may write the above relation as

$$X_{ik} X_{k'i'} + Y_{ik} Y_{k'i'} + Z_{ik} Z_{k'i'} = 2 \delta_{ii'} \delta_{kk'} - \delta_{ik} \delta_{i'k'} \quad , \quad (2.89)$$

which is recognized as the familiar Pauli matrix identity $\sigma_{\alpha\beta}^a \sigma_{\mu\nu}^a = 2 \delta_{\alpha\nu} \delta_{\beta\mu} - \delta_{\alpha\beta} \delta_{\mu\nu}$.

¹⁷Note that there is a representation labeled E , which you should take care not to confuse with the identity element.

2.4.7 Character table for $\mathbb{Z}_2 \times G$

Consider any group G with classes \mathcal{C}_j and representations Γ_a and take its direct product with \mathbb{Z}_2 , whose elements are written $\{E, \varepsilon\}$ with $\varepsilon^2 = 1$. Then $\varepsilon g = g\varepsilon$ for all $g \in G$, i.e. the operation ε commutes with all elements of G , hence ε forms its own class. Clearly $\mathbb{Z}_2 \times G$ has $2N_G$ elements, $\{E, g_2, \dots, g_{N_G}, \varepsilon, \varepsilon g_2, \dots, \varepsilon g_{N_G}\}$. The representation matrices in any representation satisfy $D(\varepsilon g) = D(\varepsilon)D(g)$, with $D(\varepsilon) = \pm \mathbb{1}$. Thus, each IRREP Γ_a of G spawns two IRREPS in $\mathbb{Z}_2 \times G$, labeled $\Gamma_{a\pm}$, whose representation matrices are

$$D^{\Gamma_{a\pm}}(g) = D^{\Gamma_a}(g) \quad , \quad D^{\Gamma_{a\pm}}(\varepsilon g) = \pm D^{\Gamma_a}(g) \quad . \quad (2.90)$$

Note that $\dim(\Gamma_{a\pm}) = \dim(\Gamma_a)$. The character table for $\mathbb{Z}_2 \times G$ is given in Tab. 2.5 in terms of the characters of G .

$\mathbb{Z}_2 \times G$	\mathcal{C}_j	$\varepsilon \mathcal{C}_j$
Γ_{a+}	$\chi^{\Gamma_a}(\mathcal{C}_j)$	$\chi^{\Gamma_a}(\mathcal{C}_j)$
Γ_{a-}	$\chi^{\Gamma_a}(\mathcal{C}_j)$	$-\chi^{\Gamma_a}(\mathcal{C}_j)$

Table 2.5: Character table for $\mathbb{Z}_2 \times G$.

In solid state physics, there are many structures which possess an *inversion symmetry* under $\mathbf{r} \rightarrow -\mathbf{r}$. Clearly this commutes with all rotations. Thus, the cubic group $O \cong S_4$ has 24 elements, but upon adding inversion, it becomes O_h with 48 elements. The dihedral group D_n is the symmetry group of the n -gon. Adding inversion or a horizontal reflection plane doubles its size from $2n$ to $4n$ elements, yielding the group D_{nh} .

2.4.8 Direct product representations

Given two representations (not necessarily IRREPS) Ψ_a and Ψ_b of a group G , we can form a new representation of G , written $\Psi_a \times \Psi_b$, and called the direct product representation. Given basis vectors $|e_i\rangle \in \mathcal{V}$ and $|\tilde{e}_p\rangle \in \mathcal{V}'$, with $1 \leq i \leq d_{\Psi_a}$ and $1 \leq p \leq d_{\Psi_b}$, the action of $\hat{D}(g)$ on the vector space $\mathcal{V} \otimes \mathcal{V}'$ in the product representation is given by

$$\hat{D}(g) |e_k\rangle \otimes |\tilde{e}_q\rangle = |e_i\rangle \otimes |\tilde{e}_p\rangle D_{ik}^{\Psi_a}(g) D_{pq}^{\Psi_b}(g) \quad . \quad (2.91)$$

Thus, the matrix form of $\hat{D}(g)$ in the product representation is

$$D_{ip, kq}^{\Psi_a \times \Psi_b}(g) = D_{ik}^{\Psi_a}(g) D_{pq}^{\Psi_b}(g) \quad . \quad (2.92)$$

The characters are then given by taking the trace, i.e. contracting with $\delta_{ik} \delta_{pq}$, yielding

$$\chi^{\Psi_a \times \Psi_b}(g) = \chi^{\Psi_a}(g) \chi^{\Psi_b}(g) \quad . \quad (2.93)$$

So the character of $g \in G$ in the product representation is the product of the characters of g in the initial representations.

We may now use Eqn. 2.61 to decompose the product representation into IRREPs, viz.

$$n_{\Gamma}(\Psi_a \times \Psi_b) = \frac{1}{N_G} \sum_{\mathcal{C}} N_{\mathcal{C}} \chi^{\Gamma^*}(\mathcal{C}) \chi^{\Psi_a}(\mathcal{C}) \chi^{\Psi_b}(\mathcal{C}) \quad . \quad (2.94)$$

We then have

$$\Psi_a \times \Psi_b = \bigoplus_{\Gamma} n_{\Gamma}(\Psi_a \times \Psi_b) \Gamma \quad . \quad (2.95)$$

Eqns. 2.94 and 2.95 are extremely useful! Note that

$$d_a d_b = \sum_{\Gamma} n_{\Gamma}(\Psi_a \times \Psi_b) d_{\Gamma} \quad , \quad (2.96)$$

where $d_{a,b} = \dim(\Psi_{a,b})$. This is because the original matrices on the LHS of Eqn. 2.92 are of rank $d_a d_b$. If they are decomposed into blocks of rank d_{Γ} with each such block appearing n_{Γ}^{ab} times, the matrices must be the same size.

For practice, consider the product representation $E \times E$ of the group D_4 . Consulting the character table Tab. 2.4, we see that $[\chi^E(\mathcal{C})]^2 = 4$ for $\mathcal{C} = E$ and $\mathcal{C} = C_2$, and is otherwise zero. Performing the decomposition, we find $n_{\Gamma}(E \times E) = 1$ for $\Gamma \in \{A_1, A_2, B_1, B_2\}$ but $n_E(E \times E) = 0$. Thus,

$$E \times E = A_1 \oplus A_2 \oplus B_1 \oplus B_2 \quad . \quad (2.97)$$

One also finds $A_2 \times B_1 = B_2$, $B_1 \times B_2 = A_1$, $B_2 \times E = B_2$, etc. For the group C_3 , we have $\Gamma_2 \times \Gamma_2 = \Gamma_3$. All these results are consistent with the following fun fact:

◇ The product of two IRREPs $\Gamma_a \times \Gamma_b$ contains the identity representation if and only if $\Psi_b = \Psi_a^*$.

Direct products of different groups

Recall that the direct product $F = G \times H$ of groups G and H consists of elements (g, h) obeying the multiplication rule $(g, h)(g', h') = (gg', hh')$. Consider now a direct product of representations $\Psi_a^G \times \Psi_b^H$. The matrix representation of the product group element (g, h) is then

$$D_{ip, kq}^{\Psi_a^G \times \Psi_b^H}(g, h) = D_{ik}^{\Psi_a^G}(g) D_{pq}^{\Psi_b^H}(h) \quad , \quad (2.98)$$

with $1 \leq i, k \leq d_{\Psi_a^G}$ and $1 \leq p, q \leq d_{\Psi_b^H}$. The operators $\hat{D}(G \times H)$ act on basis vectors $|e_i\rangle \otimes |\tilde{e}_p\rangle \in \mathcal{V} \otimes \tilde{\mathcal{V}}$, according to

$$\hat{D}(g, h) |e_i\rangle \otimes |\tilde{e}_p\rangle = |e_i\rangle \otimes |\tilde{e}_p\rangle D_{ik}^{\Psi_a^G}(g) D_{pq}^{\Psi_b^H}(h) \quad . \quad (2.99)$$

In other words, $D^{\Psi_a^G \times \Psi_b^H}(g, h) = D^{\Psi_a^G}(g) \otimes D^{\Psi_b^H}(h)$. Thus, the character of (g, h) in this representation is

$$\chi^{\Psi_a^G \times \Psi_b^H}(g, h) = \chi^{\Psi_a^G}(g) \chi^{\Psi_b^H}(h) \quad , \quad (2.100)$$

and once again the character of the direct product is the product of the characters. Note that our earlier discussion fits in here if we apply the group homomorphism $G \mapsto G \times G$ where $\phi(g) = (g, g)$.

2.5 Real Representations

Here we follow the very clear discussion in §5-5 of Hammermesh. Consider an irreducible matrix representation $D(G)$ of a finite group G . We may, without loss of generality, assume $D(G)$ is a unitary, hence $D^*(G) = \overline{D}(G)$, i.e. the complex and adjoint representations coincide. If $D(G) = D^*(G)$, i.e. if $D(G)$ is real, then $\chi(g) \in \mathbb{R}$ for all $g \in G$. Conversely, if all the characters are real, then $\chi^*(g) = \chi(g) \forall g \in G$, which means that $D(G) \cong D^*(G)$ ¹⁸. The only case where $D(G)$ and $D^*(G)$ are *not* equivalent is when there are complex characters, i.e. $\text{Im } \chi(g) \neq 0$ for some $g \in G$.

There are then three possibilities for the IRREPS of any finite group G :

- (1) $D(G)$ is real or can be brought to real form. All characters are real: $\chi(g) \in \mathbb{R} \forall g \in G$.
- (2) $D(G) \cong D^*(G)$, but cannot be brought to real form. Again, $\chi(g) \in \mathbb{R} \forall g \in G$.
- (3) $D(G) \not\cong D^*(G)$. Not all characters are real: $\exists g \in G$ s.t. $\text{Im } \chi(g) \neq 0$.

Suppose $\chi(G) \in \mathbb{R}$, i.e. all the characters are real. Then we are dealing with cases (1) and (2), in which case there exists $S \in \text{GL}(n, \mathbb{C})$ such that $SD(g)S^{-1} = \overline{D}(g) = D^*(g)$ for all $g \in G$.¹⁹ Furthermore, this relation can be manipulated to give $S = D^\top(g)SD(g)$, which entails²⁰

$$S^{-1}S^\top = D^{-1}(g)S^{-1}S^\top D(g) \quad (2.101)$$

for all $g \in G$. By Schur's first lemma, we must have $S^{-1}S^\top = \varepsilon \mathbf{1}$, i.e. $S^\top = \varepsilon S$. But taking the transpose of this equation gives $S = \varepsilon S^\top = \varepsilon^2 S$, which means $\varepsilon = \pm 1$. If $\varepsilon = -1$, we must have that $D(G)$ is even-dimensional, because $\det S = \det S^\top = \det(-S) = (-1)^n \det S$, where $n = \dim(G)$.

$\varepsilon = +1$ corresponds to case (1). In this case, S is both unitary and symmetric, and by Takagi's factorization²¹, there exists a unitary matrix U such that $S = UU^\top$. Then $S^{-1} = U^*U^{-1}$, in which case $U^\top U D(g) U^\dagger U^* = D^*(g)$, which gives $UD(g)U^\dagger = U^*D^*(g)U^\top = [UD(g)U^\dagger]^*$ for all $g \in G$. Thus, $D(G)$ is unitarily equivalent to a real representation.

Note that any matrix of the form

$$S = \sum_{g \in G} D^\top(g) X D(g) \quad (2.102)$$

with X arbitrary satisfies $D^\top(h) S D(h) = S$ for all $h \in G$, by rearrangement. This would guarantee that $D(G) \cong D^*(G)$, so if case (3) pertains, we must have that *the RHS in Eqn. 2.102 vanishes for any X* . Thus, we must have $\sum_{g \in G} D_{ik}(g) D_{jl}(g) = 0$ for all $i, j, k, l \in \{1, \dots, n\}$. The other two possibilities are that

¹⁸If $\chi^\Gamma(g) = \chi^{\Gamma^*}(g)$ for all $g \in G$, then applying the decomposition formula eqn. 2.61 gives $n_\Gamma(\Gamma^*) = 1$, which says that Γ and Γ^* are the same IRREP.

¹⁹This also tells us $\chi(g^{-1}) = \chi(g)$, since $\overline{D}(g) = D^\top(g^{-1})$.

²⁰Taking the transpose, one has $D^\top(g)S^\top D(g) = S^\top$. Taking the inverse, $D^{-1}(g)S^{-1}\overline{D}(g) = S^{-1}$. Multiply to get Eqn. 2.101.

²¹Takagi [1927] proved that any complex symmetric matrix $A = A^\top \in \mathbb{C}^{n \times n}$ may be written in the form $A = VB V^\top$, where $V \in \text{U}(n)$ and B is real and diagonal with all nonnegative entries. Thus $A = WBW^\top$ with $W \equiv V^{-1}$, in which case $B^\dagger B = W^* A^\dagger W^\dagger W A W^\top = W^* A^\dagger A W^\top$. It follows that if A is also unitary, then $B^\dagger B = \mathbf{1}$, hence $B = \mathbf{1}$ and so $A = VV^\top$. We pause to sadly recall how Mr. Takagi was ruthlessly murdered by Hans Gruber in the Bruce Willis action film *Die Hard*.

$S^T = \varepsilon S$ with $\varepsilon = \pm 1$, corresponding to cases (1) and (2), respectively²². We can combine all three cases in the following equation:

$$\sum_{g \in G} D_{ik}(g) D_{jl}(g) = \varepsilon \sum_{g \in G} D_{jk}(g) D_{il}(g) \quad , \quad (2.103)$$

where $\varepsilon = 0, \pm 1$. Contracting the indices k with j and i with l then yields

$$\sum_{g \in G} \chi(g^2) = \varepsilon \sum_{g \in G} \chi^2(g) \quad . \quad (2.104)$$

For cases (1) and (2), we may invoke the GOT, taking the traces of both matrices on the LHS of Eqn. 2.30, which says $\sum_{g \in G} \chi^2(g) = N_G$. We then arrive at the following result, which is valid for any IRREP Γ :

$$\varepsilon_\Gamma = \frac{1}{N_G} \sum_{g \in G} \chi^\Gamma(g^2) \quad , \quad (2.105)$$

where $\varepsilon_\Gamma = +1, -1$, and 0 for cases (1), (2), and (3), respectively, is known as the *Frobenius-Schur indicator*.

We may immediately apply this result to C_3 , whose character table is provided in Tab. 2.2 above. Note $R^2 = W$ and $W^2 = R$, so for the Γ_2 and Γ_3 representations, we have $\chi(E^2) + \chi(R^2) + \chi(W^2) = 0$, which says that neither Γ_2 nor Γ_3 is equivalent to a real representation. As a second example, consider the two-dimensional Ψ representation of the quaternion group Q , whose character table appears in Tab. 2.3. We have $(\pm E)^2 = E$ but $(\pm i)^2 = (\pm j)^2 = (\pm k)^2 = -E$, and since $\chi(\pm E) = \pm 2$, we have $\sum_{g \in Q} \chi(g^2) = 2 \cdot 2 + 6 \cdot (-2) = -8 = -N_G$, corresponding to $\varepsilon_\Psi = -1$. Thus $\Psi \cong \Psi^*$, but cannot be brought to real form. Indeed, we know that the elements i, j , and k in this representation may be represented by the 2×2 matrices $-iX, -iY$, and $-iZ$, respectively, where $\{X, Y, Z\}$ are the Pauli matrices. Thus, $D^\Psi(\pm i)$ and $D^\Psi(\pm k)$ contain complex matrix elements. Note that all the characters are still real.

There is one last bonus from this analysis. Consider an element $g \in G$ and let us ask how many elements h are there for which $g = h^2$. In other words, how many "square roots" does g have within the group? (Equivalently, how many times does g appear along the diagonal of the group multiplication table?) Call this number $\zeta(g)$. Then from Eqn. 2.105, we have

$$\sum_{g \in G} \zeta(g) \chi^\Gamma(g) = \varepsilon_\Gamma N_G \quad . \quad (2.106)$$

Note that $\zeta(g)$ does not depend on the representation Γ . Now we can use character orthogonality and the fact that $\zeta(g^{-1}) = \zeta(g)$ to derive

$$\zeta(g) = \sum_{\Gamma} \varepsilon_\Gamma \chi^\Gamma(g) \quad , \quad (2.107)$$

where the sum is now over IRREPS. For example, the number of square roots of the identity E is

$$\zeta(E) = \sum_{\Gamma} \varepsilon_\Gamma d_\Gamma \quad . \quad (2.108)$$

²²Since $\varepsilon = 1$ is proven to correspond to case (1) and case (3) requires $\varepsilon = 0$, it must be that $\varepsilon = -1$ corresponds to case (2).

2.6 Representations of the Symmetric Group

Recall that the symmetric group S_n consists of all permutations σ on the set of n distinct elements, which we conventionally take to be the set $\{1, \dots, n\}$. Thus i gets mapped to $\sigma(i)$. Under group multiplication, $\mu\sigma$ is the permutation mapping i to $\mu(\sigma(i))$.

In §1.3.2, we learned how any element of the symmetric group S_n could be expressed as a product of cycles $(i_1 i_2 \cdots i_k)$, which means $\sigma(i_1) = i_2, \sigma(i_2) = i_3, \text{etc.}$, until finally $\sigma(i_k) = i_1$. For example,

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 7 & 2 & 6 & 8 & 1 & 3 & 5 & 4 \end{pmatrix} = (175)(2)(36)(48) \quad . \quad (2.109)$$

We require that in the cyclic decomposition of any $\sigma \in S_n$, each integer $i \in \{1, \dots, n\}$ occur exactly once. Cyclic decompositions remain invariant under cyclic permutation within the individual cycles, and under changing the order of the cycles. Thus, $(175)(2)(36)(48)$ is the same permutation as $(48)(2)(36)(175)$ or $(63)(571)(84)(2)$.

2.6.1 Partitions, Young diagrams and Young tableaux

A *partition* of a positive integer $n \in \mathbb{N}$ is a (necessarily finite) non-decreasing sequence of positive integers $\lambda = \{\lambda_1, \dots, \lambda_k\}$ such that $\sum_{j=1}^k \lambda_j = n$. There is no known closed formula for the total number of partitions $p(n)$, although Hardy and Ramanujan proved the asymptotic formula²³

$$p(n) \sim \frac{\exp\left(\pi\sqrt{2n/3}\right)}{4\sqrt{3}n} \quad . \quad (2.110)$$

Any cyclic decomposition of a permutation $\sigma \in S_n$ may be associated with a partition of n , where the $\{\lambda_i\}$ are the lengths of the individual cycles. Thus, in our earlier example, $\sigma = (175)(2)(36)(48)$ and $\lambda = \{3, 2, 2, 1\}$. We can express this partition using a *Young diagram*, which is a set of empty boxes arranged in rows such that there are λ_1 boxes in row 1, *etc.*, and where the first boxes from each row are aligned in a single leftmost column. Thus,

$$\{3, 2, 2, 1\} = \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \square & & \\ \hline \end{array} \quad . \quad (2.111)$$

For obvious reasons, we call λ the *shape* of the permutation. Note that for a shape $\lambda = \{\lambda_1, \dots, \lambda_k\}$, there are λ_1 columns and k rows in the associated Young diagram. If we want to specify a *particular* permutation, we need to label the boxes, yielding a *Young tableau*. Thus,

$$\sigma = (175)(2)(36)(48) = \begin{array}{|c|c|c|} \hline 1 & 7 & 5 \\ \hline 3 & 6 & \\ \hline 4 & 8 & \\ \hline 2 & & \\ \hline \end{array} \quad . \quad (2.112)$$

²³Ramanujan managed to prove several other remarkable results, such as $p(5k + 4) \equiv 0 \pmod{5}$, $p(7k + 5) \equiv 0 \pmod{7}$, and $p(11k + 6) \equiv 0 \pmod{11}$. Given these results, one might suspect that $p(13k + 7) \equiv 0 \pmod{13}$, but in fact there are no additional congruences of the form $p(ak + b) \equiv 0 \pmod{k}$ for any prime a other than 5, 7, or 11. Number theory is often weird.

Due to the nature of cyclic permutations, this tableau is equivalent to any of the following:

$$\begin{array}{|c|c|c|} \hline 1 & 7 & 5 \\ \hline 3 & 6 & \\ \hline 4 & 8 & \\ \hline 2 & & \\ \hline \end{array}, \quad
 \begin{array}{|c|c|c|} \hline 5 & 1 & 7 \\ \hline 8 & 4 & \\ \hline 3 & 6 & \\ \hline 2 & & \\ \hline \end{array}, \quad
 \begin{array}{|c|c|c|} \hline 7 & 5 & 1 \\ \hline 6 & 3 & \\ \hline 8 & 4 & \\ \hline 2 & & \\ \hline \end{array}, \quad \text{etc.} \quad (2.113)$$

One important feature of cyclic permutations is that their length is preserved under conjugation. Thus,

$$\mu(175)(36)(48)(2) \mu^{-1} = (\mu(1) \mu(7) \mu(5)) (\mu(3) \mu(6)) (\mu(4) \mu(8)) (\mu(2)) \quad . \quad (2.114)$$

Thus, each shape λ specifies an equivalence class \mathcal{C}_λ , which we will simply abbreviate as λ . Recall from §1.3.2 that the number of possible decompositions of any $\sigma \in S_n$ into ν_1 1-cycles, ν_2 2-cycles, etc. is

$$N(\nu_1, \nu_2, \dots, \nu_n) = \frac{n!}{1^{\nu_1} \nu_1! 2^{\nu_2} \nu_2! \dots n^{\nu_n} \nu_n!} \quad . \quad (2.115)$$

Thus $|\lambda| = N(\nu_1, \nu_2, \dots, \nu_n)$, where the shape $\lambda = \{\lambda_1, \dots, \lambda_k\}$ uniquely determines the set $\{\nu_1, \dots, \nu_n\}$, according to

$$\nu_l = \sum_{i=1}^k \delta_{\lambda_i, l} \quad . \quad (2.116)$$

I.e. ν_l is the number of cycles of length l . We showed in §1.3.2 that

$$\sum_{\nu_1=0}^{\infty} \dots \sum_{\nu_n=1}^{\infty} N(\nu_1, \nu_2, \dots, \nu_n) \delta_{\nu_1+2\nu_2+\dots+n\nu_n, n} = n! = |S_n| \quad , \quad (2.117)$$

so we have indeed accounted for all the equivalence classes.

2.6.2 S_3 and S_4

For the case $n = 3$, there are three classes, corresponding to the Young diagrams $\begin{array}{|c|} \hline \square \\ \hline \end{array}$, $\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}$, and $\begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \end{array}$, of orders 1, 3, and 2, respectively. What about the IRREPS? We immediately know two one-dimensional IRREPS, namely the trivial IRREP Γ_{triv} and the sign IRREP Γ_{sgn} . In the case of $D_3 \simeq S_3$, we called these IRREPS A_1 and A_2 , respectively (see Tab. 2.1). The remaining representation of D_3 , which we called E , is called the *standard representation* Γ_{std} of the S_3 . Indeed, there is a standard representation for each S_n , and here is how to identify it. Start with the defining representation, which as you should recall from §1.3.2 is the n -dimensional representation in which $D_{ij}(\sigma) = \delta_{i, \sigma(j)}$. Acting on the vector space \mathbb{R}^n , this is clearly reducible because the one-dimensional subspace spanned by the vector ψ where $\psi_i = 1$ for all i is an invariant subspace. Since $D(\sigma) \psi = \psi$ for all $\sigma \in S_n$, we have that $\Gamma_{\text{def}} = \Gamma_{\text{std}} \oplus \Gamma_{\text{triv}}$, i.e. the defining representation is a direct sum of the trivial representation and an $(n - 1)$ -dimensional representation Γ_{std} which turns out to be irreducible. Furthermore, since the characters of representations in direct sums are additive (see eqn. 2.65), we have $\chi^{\Gamma_{\text{std}}}(\lambda) = \chi^{\Gamma_{\text{def}}}(\lambda) - \chi^{\Gamma_{\text{triv}}}(\lambda) = \chi^{\Gamma_{\text{def}}}(\lambda) - 1$. Now in Γ_{def} , the character of any element σ is simply the number of entries in the sequence $\{1 \ 2 \ \dots \ n\}$ which remain fixed by the action of σ . This is the number ν_1 of one-cycles in the corresponding partition λ . Thus

S_3			
N_λ	1	3	2
Γ_{triv}	1	1	1
Γ_{sgn}	1	-1	1
Γ_{std}	2	0	-1

Table 2.6: Character table for the symmetric group S_3 .

$\chi^{\Gamma_{\text{def}}}(\text{[1^3]}) = 3$, $\chi^{\Gamma_{\text{def}}}(\text{[2,1]}) = 1$, and $\chi^{\Gamma_{\text{def}}}(\text{[3]}) = 0$. We thus arrive at the character table in Tab. 2.6, which is of course identical to that of Tab. 2.1 for D_3 . Note that

$$\sum_{\lambda} N_{\lambda} = \sum_{\Gamma} d_{\Gamma}^2 = 6 = |S_3| \quad . \quad (2.118)$$

Now let's consider the case of S_4 . There are now five classes: , , , , and . Regarding the sign representation, we know that $\chi^{\Gamma_{\text{sgn}}}(\lambda)$ is given by $(-1)^{\#}$ of cycles of even length. Regarding the standard representation, of dimension $n - 1 = 3$, we can compute the its characters from the formula $\chi^{\Gamma_{\text{std}}}(\lambda) = \nu_1(\lambda) - 1$ as described above. Thus far we have found three IRREPs, but there are five classes so two IRREPs are missing. One is formed by taking the product $\Gamma_{\text{std}} \times \Gamma_{\text{sgn}}$. This is also of dimension three. Since $1^2 + 1^2 + 3^2 + 3^2 = 20$, we know that the last IRREP, which we call Γ' , is two-dimensional. We arrive at the partial table of Tab. 2.7.

S_4					
N_λ	1	6	3	8	6
Γ_{triv}	1	1	1	1	1
Γ_{sgn}	1	-1	1	1	-1
Γ_{std}	3	1	-1	0	-1
$\Gamma_{\text{std}} \times \Gamma_{\text{sgn}}$	3	-1	-1	0	1
Γ'	2	a	b	c	d

Table 2.7: Partial character table for the symmetric group S_4 .

To determine the missing characters, we invoke row orthogonality, which yields the four equations

$$\begin{aligned}
 0 &= 2 + 6a + 3b + 8c + 6d \\
 0 &= 2 - 6a + 3b + 8c - 6d \\
 0 &= 6 + 6a - 3b - 6d \\
 0 &= 6 - 6a - 3b + 6d \quad .
 \end{aligned}
 \tag{2.119}$$

Solving them is a simple matter and we readily find $a = 0, b = 2, c = -1,$ and $d = 0.$

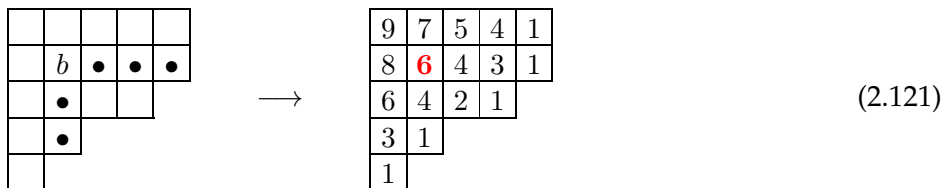
When we get to $S_5,$ we will find that there are seven conjugacy classes, and therefore seven IRREPs. Is there a general way to count the dimensions of the IRREPs of $S_n?$ Funny you should ask.

2.6.3 IRREPs of S_n

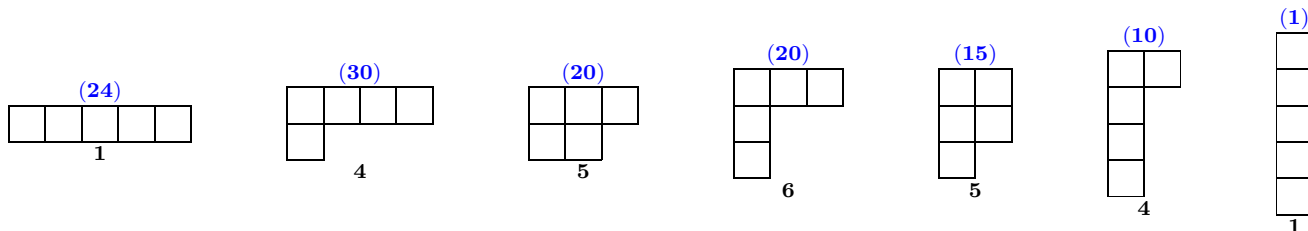
Recall that the number of equivalence classes is the number of IRREPs. For the symmetric group, each shape λ corresponds to an IRREP Γ^λ of S_n ²⁴. What is its dimension $f^\lambda = \dim(\Gamma^\lambda)?$ It may be computed from the *hook length formula*,

$$f^\lambda = \dim(\Gamma^\lambda) = \frac{n!}{\prod_{b \in \lambda} h_\lambda(b)} \quad ,
 \tag{2.120}$$

where the product in the denominator is over all boxes b of the Young diagram for $\lambda,$ and $h_\lambda(b)$ is the *hook length* for the box $b,$ which is the total number of boxes in a 'hook' whose vertex is $b,$ with legs extending rightward and downward. For example,



The proof is technical and interested students may consult the book of B. Sagan for details. For our immediate purposes here, let's just see how all this works in practice. Consider the case $n = 5,$ for which $|S_n| = 5! = 120.$ Behold the seven IRREPs of $S_5:$



These correspond, respectively, to the shapes $\lambda = (5), (4, 1), (3, 2), (3, 1, 1), (2, 2, 1), (2, 1, 1, 1),$ and $(1, 1, 1, 1, 1).$ Each Young diagram is labeled by a subscript which is the dimension $f^\lambda = |\Gamma^\lambda|$

²⁴This is perhaps not obvious, but it turns out that the Young tableaux corresponding to a given partition λ may be arranged into a vector space S^λ on which the elements of S_n act, called a *Specht module*. For details, see the books by B. Sagan and W. Fulton listed in chapter 0.

of the corresponding IRREP as computed from the hook length formula, and a superscript $(|\lambda|)$ which is the number of elements in the corresponding equivalence class, as computed from Eqn. 2.115. Note that the sums of the squares of the dimensions of the IRREPs is equal to the sum of the number of elements of each equivalence class is equal to the order of the group S_5 :

$$1^2 + 4^2 + 5^2 + 6^2 + 5^2 + 4^2 + 1^2 = 24 + 30 + 20 + 20 + 15 + 10 + 1 = 120 = |S_5| \quad .$$

2.7 Application of Projection onto IRREPs : Triatomic Molecule

Fig. 2.1 shows a planar configuration of three equal masses m connected by identical springs k . Each mass may move in the x and y directions, hence the molecule has six degrees of freedom. As a small oscillations problem in classical mechanics, one solves the equation $\omega^2 \mathbf{T} \psi = \mathbf{V} \psi$, where \mathbf{T} and \mathbf{V} are the kinetic energy and potential energy matrices, given by the expressions $T_{nn'} = [\partial^2 T(\mathbf{q}, \dot{\mathbf{q}}) / \partial \dot{q}_n \partial \dot{q}_{n'}]_{\mathbf{q}^0}$ and $V_{nn'} = [\partial^2 V(\mathbf{q}) / \partial q_n \partial q_{n'}]_{\mathbf{q}^0}$, evaluated at equilibrium, with \mathbf{q} the set of generalized coordinates. Here we will find the eigenvectors ψ_a using group theory, without diagonalizing any matrices.

We choose as generalized coordinates the Cartesian x and y positions of each mass relative to the center of the triangle. The equilibrium coordinates of mass #1 are $(0, 1) \frac{a}{\sqrt{3}}$, of mass #2 $(-\frac{\sqrt{3}}{2}, -\frac{1}{2}) \frac{a}{\sqrt{3}}$, and of mass #3 $(\frac{\sqrt{3}}{2}, -\frac{1}{2}) \frac{a}{\sqrt{3}}$. The symmetry group is D_3 , whose character table is provided in Tab. 2.1. Group elements are represented by matrices $D(g)$ acting on the column vector given by the transpose of $\psi^T = (\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3)$, the vector of displacements relative to equilibrium. This is a six dimensional representation given by $\Gamma = \mathcal{Y} \times E$, where the \mathcal{Y} and E representations are given in §2.3.1. The reason for this is that the group element R , for example, not only rotates the Cartesian coordinates; it also exchanges the positions of the masses, *i.e.* it switches their labels. This is a six-dimensional representation, and using the decomposition formula we find $\mathcal{Y} = A_1 \oplus E$ and $\mathcal{Y} \times E = A_1 \oplus A_2 \oplus E \oplus E$. The matrices are

$$\begin{aligned} D(I) &= \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix} & D(R) &= \begin{pmatrix} 0 & 0 & R \\ R & 0 & 0 \\ 0 & R & 0 \end{pmatrix} & D(W) &= \begin{pmatrix} 0 & W & 0 \\ 0 & 0 & W \\ W & 0 & 0 \end{pmatrix} \\ D(\sigma) &= \begin{pmatrix} \sigma & 0 & 0 \\ 0 & 0 & \sigma \\ 0 & \sigma & 0 \end{pmatrix} & D(\sigma') &= \begin{pmatrix} 0 & 0 & \sigma' \\ 0 & \sigma' & 0 \\ \sigma' & 0 & 0 \end{pmatrix} & D(\sigma'') &= \begin{pmatrix} 0 & \sigma'' & 0 \\ \sigma'' & 0 & 0 \\ 0 & 0 & \sigma'' \end{pmatrix} . \end{aligned} \quad (2.122)$$

where

$$\begin{aligned} I &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & R &= \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} & W &= \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \\ \sigma &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & \sigma' &= \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} & \sigma'' &= \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} . \end{aligned} \quad (2.123)$$

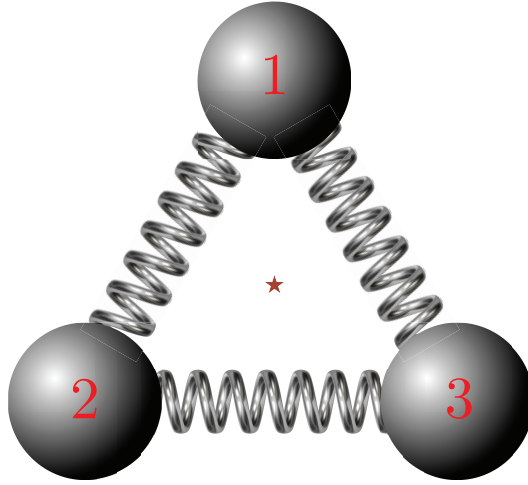


Figure 2.1: A planar molecule modeled as three masses m connected by springs, in the shape of an equilateral triangle. The symmetry is C_{3v} .

We simplify our notation and use g to denote the 2×2 matrix $D^E(g)$ in the E IRREP, and we call the identity I instead of E to obviate any potential confusion with the IRREP E .

Starting with a general rank six vector $\psi^\top = (a \ b \ c \ d \ e \ f)$, we find

$$D(I)\psi = \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ f \end{pmatrix}, \quad D(R)\psi = \frac{1}{2} \begin{pmatrix} -e - \sqrt{3}f \\ \sqrt{3}e - f \\ -a - \sqrt{3}b \\ \sqrt{3}a - b \\ -c - \sqrt{3}d \\ \sqrt{3}c - d \end{pmatrix}, \quad D(W)\psi = \frac{1}{2} \begin{pmatrix} -c + \sqrt{3}d \\ -\sqrt{3}c - d \\ -e + \sqrt{3}f \\ -\sqrt{3}e - f \\ -a + \sqrt{3}b \\ -\sqrt{3}a - b \end{pmatrix} \quad (2.124)$$

and

$$D(\sigma)\psi = \begin{pmatrix} -a \\ b \\ -e \\ f \\ -c \\ d \end{pmatrix}, \quad D(\sigma')\psi = \frac{1}{2} \begin{pmatrix} e + \sqrt{3}f \\ \sqrt{3}e - f \\ c + \sqrt{3}d \\ \sqrt{3}c - d \\ a + \sqrt{3}b \\ \sqrt{3}a - b \end{pmatrix}, \quad D(\sigma'')\psi = \frac{1}{2} \begin{pmatrix} c - \sqrt{3}d \\ -\sqrt{3}c - d \\ a - \sqrt{3}b \\ -\sqrt{3}a - b \\ e - \sqrt{3}f \\ -\sqrt{3}e - f \end{pmatrix}. \quad (2.125)$$

Now let's project! We first project onto A_1 , where, from Eqn. 2.66,

$$\Pi^{A_1} = \frac{1}{6} \left\{ D(I) + D(R) + D(W) + D(\sigma) + D(\sigma') + D(\sigma'') \right\}. \quad (2.126)$$

Adding up the various contributions, we find $\Pi^{A_1}\psi = \frac{1}{2\sqrt{3}}(2b - \sqrt{3}c - d + \sqrt{3}e - f)\hat{e}^{A_1}$, where the components of \hat{e}^{A_1} , expressed as a row vector, are

$$\hat{e}^{A_1} = \frac{1}{\sqrt{3}} \left(0 \quad 1 \quad -\frac{\sqrt{3}}{2} \quad -\frac{1}{2} \quad \frac{\sqrt{3}}{2} \quad -\frac{1}{2} \right). \quad (2.127)$$

Next, we project onto A_2 , with

$$\Pi^{A_2} = \frac{1}{6} \left\{ D(I) + D(R) + D(W) - D(\sigma) - D(\sigma') - D(\sigma'') \right\} . \quad (2.128)$$

Adding up the various contributions, we find $\Pi^{A_2} \psi = \frac{1}{2\sqrt{3}} (2a - c + \sqrt{3}d - e - \sqrt{3}f) \hat{e}^{A_2}$, where the components of \hat{e}^{A_2} are

$$\hat{e}^{A_2} = \frac{1}{\sqrt{3}} \left(1 \quad 0 \quad -\frac{1}{2} \quad \frac{\sqrt{3}}{2} \quad -\frac{1}{2} \quad -\frac{\sqrt{3}}{2} \right) . \quad (2.129)$$

Note that $\hat{e}^{A_1} \cdot \hat{e}^{A_2} = 0$ because the A_1 and A_2 IRREPS correspond to orthogonal subspaces.

Note also that \hat{e}^{A_1} is orthogonal to the following mutually orthogonal vectors:

$$\begin{aligned} \hat{e}^x &= \frac{1}{\sqrt{3}} (1 \quad 0 \quad 1 \quad 0 \quad 1 \quad 0) \\ \hat{e}^y &= \frac{1}{\sqrt{3}} (0 \quad 1 \quad 0 \quad 1 \quad 0 \quad 1) \\ \hat{e}^\phi &= \frac{1}{\sqrt{3}} \left(1 \quad 0 \quad -\frac{1}{2} \quad \frac{\sqrt{3}}{2} \quad -\frac{1}{2} \quad -\frac{\sqrt{3}}{2} \right) . \end{aligned} \quad (2.130)$$

These vectors, as you may have guessed, correspond to the three zero modes for our problem: translations along \hat{x} and \hat{y} , and rotations about the \hat{z} axis through the center of the triangle. These vectors are obtained by the action of the Lie algebra generators for the continuous translation groups \mathbb{R} and rotation group $SO(2)$. Infinitesimal translations result in $x_i \rightarrow x_i + \varepsilon_x$ and $y_i \rightarrow y_i + \varepsilon_y$. To obtain \hat{e}^ϕ , perform an infinitesimal rotation $\exp(\varepsilon_\phi M)$, where $M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma^y$ upon each of the (x_i^0, y_i^0) pairs of equilibrium coordinates:

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -\sqrt{3}/2 \\ -1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix} , \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{3}/2 \\ -1/2 \end{pmatrix} = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix} . \quad (2.131)$$

As for \hat{e}^{A_2} , it too is orthogonal to $\hat{e}^{x,y}$, but we find that $\hat{e}^{A_2} = \hat{e}^\phi$, which tells us that that the infinitesimal rotation transforms according to the A_2 IRREP of D_3 . According to what IRREP do you suppose the two infinitesimal translations transform?

Finally, we come to the E representation, which is two-dimensional. We construct the projectors $\Pi_{\mu\nu}^E$ for $(\mu, \nu) = (1, 1)$ and $(\mu, \nu) = (2, 1)$:

$$\begin{aligned} \Pi_{1,1}^E &= \frac{1}{3} \left\{ D(I) - \frac{1}{2} D(R) - \frac{1}{2} D(W) - D(\sigma) + \frac{1}{2} D(\sigma') + \frac{1}{2} D(\sigma'') \right\} \\ \Pi_{2,1}^E &= \frac{1}{3} \left\{ \frac{\sqrt{3}}{2} D(R) - \frac{\sqrt{3}}{2} D(W) + \frac{\sqrt{3}}{2} D(\sigma') - \frac{\sqrt{3}}{2} D(\sigma'') \right\} . \end{aligned} \quad (2.132)$$

We find

$$\begin{aligned} \Pi_{1,1}^E \psi &= \frac{1}{\sqrt{3}} (a + c + e) \hat{e}^x + \frac{1}{\sqrt{3}} \left(a - \frac{1}{2}c - \frac{\sqrt{3}}{2}d - \frac{1}{2}e + \frac{\sqrt{3}}{2}f \right) \hat{e}^{E,1} \\ \Pi_{2,1}^E \psi &= \frac{1}{\sqrt{3}} (a + c + e) \hat{e}^y + \frac{1}{\sqrt{3}} \left(a - \frac{1}{2}c - \frac{\sqrt{3}}{2}d - \frac{1}{2}e + \frac{\sqrt{3}}{2}f \right) \hat{e}^{E,2} , \end{aligned} \quad (2.133)$$

where

$$\begin{aligned}\hat{\mathbf{e}}^{E,1} &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \\ \hat{\mathbf{e}}^{E,2} &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & -1 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} .\end{aligned}\quad (2.134)$$

Note that the projection onto the rows of E does not annihilate the components parallel to $\hat{\mathbf{e}}^{x,y}$. The student should pause for contemplation to understand why this is so. We now have derived six mutually orthogonal vectors: $\{\hat{\mathbf{e}}^{A_1}, \hat{\mathbf{e}}^{A_2}, \hat{\mathbf{e}}^{E,1}, \hat{\mathbf{e}}^{E,2}, \hat{\mathbf{e}}^x, \hat{\mathbf{e}}^y\}$, with $\hat{\mathbf{e}}^\phi = \hat{\mathbf{e}}^{A_2}$.

Getting back to our small oscillations problem, the potential energy is given by

$$V(\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3) = \frac{1}{2}k (|\mathbf{r}_1 - \mathbf{r}_2| - a)^2 + \frac{1}{2}k (|\mathbf{r}_2 - \mathbf{r}_3| - a)^2 + \frac{1}{2}k (|\mathbf{r}_3 - \mathbf{r}_1| - a)^2 . \quad (2.135)$$

To quadratic order in the displacements from equilibrium, we find

$$\begin{aligned}|\mathbf{r}_1 - \mathbf{r}_2| - a &= \frac{1}{2} \delta x_1 - \frac{1}{2} \delta x_2 + \frac{\sqrt{3}}{2} \delta y_1 - \frac{\sqrt{3}}{2} \delta y_2 + \dots \\ |\mathbf{r}_2 - \mathbf{r}_3| - a &= \delta x_3 - \delta x_2 + \dots \\ |\mathbf{r}_3 - \mathbf{r}_1| - a &= \frac{1}{2} \delta x_3 - \frac{1}{2} \delta x_1 - \frac{\sqrt{3}}{2} \delta y_3 + \frac{\sqrt{3}}{2} \delta y_1 + \dots .\end{aligned}\quad (2.136)$$

The potential energy is then

$$\begin{aligned}V(\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3) &= \frac{1}{2}k \left[\frac{1}{2}(\delta x_1 - \delta x_2) + \frac{\sqrt{3}}{2}(\delta y_1 - \delta y_2) \right]^2 + \frac{1}{2}k (\delta x_2 - \delta x_3)^2 + \\ &\quad \frac{1}{2}k \left[\frac{1}{2}(\delta x_3 - \delta x_1) - \frac{\sqrt{3}}{2}(\delta y_3 - \delta y_1) \right]^2 + \dots\end{aligned}\quad (2.137)$$

and from this one can take the second derivatives by inspection and form the V-matrix. Since we have computed the IRREP projections correctly, we can obtain the eigenvalues of V by performing only one row \times column multiply for each IRREP. One finds that the eigenvalues are $3k$ for the A_1 IRREP and $\frac{3}{2}k$ for the E IRREP. The T-matrix is m times the unit matrix, where m is the mass of each "ion", and therefore the eigenfrequencies are $\omega_{A_1} = \sqrt{3k/m}$ and $\omega_E = \sqrt{3k/2m}$, and of course $\omega_{A_2} = \omega_{E'} = 0$, where E' is a second E doublet corresponding to the translations.

It is instructive to consider the effect of an additional potential,

$$\begin{aligned}V'(\delta x_1, \delta y_1, \delta x_2, \delta y_2, \delta x_3, \delta y_3) &= \frac{1}{2}k' (|\mathbf{r}_1| - \frac{1}{\sqrt{3}}a)^2 + \frac{1}{2}k' (|\mathbf{r}_2| - \frac{1}{\sqrt{3}}a)^2 + \frac{1}{2}k' (|\mathbf{r}_3| - \frac{1}{\sqrt{3}}a)^2 \\ &= \frac{1}{2}k'y_1^2 + \frac{1}{2}k' \left(\frac{\sqrt{3}}{2}x_2 + \frac{1}{2}y_2 \right)^2 + \left(\frac{\sqrt{3}}{2}x_3 - \frac{1}{2}y_3 \right)^2 + \dots ,\end{aligned}\quad (2.138)$$

where $a/\sqrt{3}$ is the distance from the center of the triangle to any of the equilibrium points. This potential breaks the translational symmetry but preserves the rotational symmetry, so we expect only one zero mode to remain, corresponding to $\hat{\mathbf{e}}^{A_2} = \hat{\mathbf{e}}^\phi$. The energy of the A_1 breathing mode will be shifted due to the new potential. It is a good exercise to work out the effect on the E modes. It turns out that V' leads to a coupling between the two E doublets we have derived. The resulting spectrum will then have two finite frequency doublets each transforming as E . Solve to unlock group theory achievement, level D_3 .

2.8 Jokes for Chapter Two

I feel that this chapter was not as funny as the previous one, so I will end with a couple of jokes:

JOKE #1 : A duck walks into a pharmacy and waddles back to the counter. The pharmacist looks down at him and says, "Hey there, little fella! What can I do for you?" "I'd like a box of condoms please," answers the duck. The pharmacist says, "No problem! Would you like me to put that on your bill?" The duck replies, "I'm not that kind of duck."

JOKE #2 : A theorist brings his car to his experimentalist friend and complains that it has been stalling out lately. The experimenter opens the hood and starts poking around. After a few minutes, the engine is idling smoothly. "So what's the story?" asks the theorist. "Meh. Just crap in the carburetor," replies the experimenter. The theorist says, "How often do I have to do that?"