For the analysis of a symmetry group or algebra it is helpful to define the ALL-COMMUTING or CENTRAL operators $\{\mathbb{C}, \mathbb{C}', \ldots\}$. These are any operators

$$\mathbb{C} = \sum_g \gamma_g g \tag{3.2.8}$$

in the group algebra which commute with all group operators $[\mathbb{C}h = h\mathbb{C}]$. By averaging over all group operators using commutativity $[\mathbb{C} = h\mathbb{C}h^{-1}]$ we obtain

$$\mathbb{C} = (1/{}^\circ G)\sum_h h\mathbb{C}h^{-1} = (1/{}^\circ G)\sum_g \gamma_g\left(\sum_h hgh^{-1}\right). \tag{3.2.9}$$

By appealing to Lagrange's theorem and Eq. (3.2.7) one derives

$$\mathbb{C} = (1/{}^\circ G)\sum_g \gamma_g {}^\circ N_g c_g = \sum_g (\gamma_g/{}^\circ c_g)c_g. \tag{3.2.10}$$

This proves that any all-commuting operator $\mathbb{C}$ must be a linear combination of class operators. The $\mathbb{C}$'s make up the commutative class algebra for which the c_g's are a basis. Since any product $c_g c_h$ belongs to the algebra it must be a combination,

$$c_g c_h = \sum_j \gamma^j_{gh} c_j, \tag{3.2.11}$$

of c_g's, as well. The coefficients γ^j_{gh} are called algebraic STRUCTURE CONSTANTS.

B. Idempotent Analysis of Class Algebras

It is possible to write all the class operators c_g as a combination of a single set of idempotents P^α, as was done for Abelian groups of operators in Chapter 2. The only difference here is that the minimal equations are more complicated.

For example, using the C_{3v} class algebra table [Eq. (3.2.1b)] we find the minimal equation of c_3. This is the lowest-degree equation that involves just powers of c_3. [It may also involve $c_1 = \mathbf{1}$; however, c_1 may be thought of as the zeroth power $(c_3)^0$.] The degree of the following equation is not yet high enough, since an unwanted $3c_2$ term appears:

$$(c_3)^2 = 3c_1 + 3c_2.$$

Multiplying by c_3 again gives the desired minimal equation

$$(c_3)^3 = 3c_3 + 3c_2c_3 = 9c_3. \tag{3.2.12}$$

Note that the degree of a minimal equation for class operators cannot exceed the number of classes, since that is the dimension of the algebra. The cubic minimal equation for c_3 factors into the following form:

$$(c_3 - 3\mathbf{1})(c_3 + 3\mathbf{1})(c_3 - 0\mathbf{1}) = 0. \tag{3.2.13}$$

The three roots $c_3^{(1)} = 3$, $c_3^{(2)} = -3$, and $c_3^{(3)} = 0$ yield three idempotents $\mathbb{P}^1$, $\mathbb{P}^2$, and $\mathbb{P}^3$, respectively, when substituted into the general formula (1.2.15)

$$\mathbb{P}^\alpha = \prod_{\gamma\neq\alpha}(c_3 - c_3^{(\gamma)}\mathbf{1}) / \prod_{\gamma\neq\alpha}(c_3^{(\alpha)} - c_3^{(\gamma)}). \tag{3.2.14}$$

The desired idempotents are given as follows.

$$\begin{aligned}
\mathbb{P}^1 &= [(c_3 + 3\mathbf{1})(c_3 - 0)]/[(3+3)(3-0)] = \left[(c_3)^2 + 3c_3\right]/18,\\
\mathbb{P}^1 &= (c_1 + c_2 + c_3)/6 = (\mathbf{1} + r + r^2 + \sigma_1 + \sigma_2 + \sigma_3)/6,\\
\mathbb{P}^2 &= (c_1 + c_2 - c_3)/6 = (\mathbf{1} + r + r^2 - \sigma_1 - \sigma_2 - \sigma_3)/6,\\
\mathbb{P}^3 &= (2c_1 - c_2)/3 = (2\mathbf{1} - r - r^2)/3.
\end{aligned} \tag{3.2.15}$$

The $\mathbb{P}^\alpha$ are called ALL-COMMUTING, CENTRAL, or CLASS idempotents of C_{3v}. The original class operators can be expanded in terms of all-commuting idempotents according to spectral decomposition, where

$$\begin{aligned}
c_j &= \sum_\alpha c_j^{(\alpha)}\mathbb{P}^\alpha,\\
c_j\mathbb{P}^\alpha &= c_j^{(\alpha)}\mathbb{P}^\alpha.
\end{aligned} \tag{3.2.16}$$

The eigenvalues $c_1^{(\alpha)}$ and $c_2^{(\alpha)}$ are found by multiplying $\mathbb{P}^\alpha$ and c_1 and c_2, respectively, and $c_3^{(\alpha)}$ was given following Eq. (3.2.13). The C_{3v} class spectral decomposition has the following form:

$$\begin{aligned}
\mathbf{1} \equiv c_1 &= \mathbb{P}^1 + \mathbb{P}^2 + \mathbb{P}^3,\\
c_2 &= 2\mathbb{P}^1 + 2\mathbb{P}^2 - \mathbb{P}^3,\\
c_3 &= 3\mathbb{P}^1 - 3\mathbb{P}^2.
\end{aligned} \tag{3.2.17}$$

C. Does the Class Algebra Reduction Work in General?

We can easily prove that a decomposition such as the one for C_{3v} is possible for all finite groups. Since class operators commute, one can follow the procedure which worked for Abelian groups (recall Section 2.9), provided no minimal equation contains a repeated root. But suppose a root is repeated; that is, suppose that

$$(c - c^1\mathbf{1})(\cdots)(c - c^r\mathbf{1})^m(\cdots) = 0 \tag{3.2.18}$$

was the MEq of c with $m \geq 2$ repeated roots. This would imply that one could construct a nonzero operator n,

$$n = (c - c^1\mathbf{1})(\cdots)(c - c^r 1)^{m-1}(\cdots) \neq 0, \tag{3.2.19}$$

which is NILPOTENT, i.e., an operator whose square is zero:

$$n^2 = 0. \tag{3.2.20}$$

If nilpotent n acts on any combination $G = \Sigma\gamma_g g$ of group operators it yields an operator nG which is also nilpotent (note that $nG = Gn$ since n is in the class algebra):

$$nGnG = Gn^2G = 0. \tag{3.2.21}$$

Now setting $G = n^\dagger$, and following the same arguments which are stated in Appendix C, we conclude that $n^\dagger n$ and finally n must be zero. A Hermitian operator cannot be nilpotent without being zero. Hence, a class operator can never have repeated roots; therefore, the class spectral decomposition is always possible.

Finally, the all-commuting or class idempotents can be seen to be unique for the same reasons that applied to Abelian groups (cf. Section 2.9). Also, they may be shown to be Hermitian (see Problem 1.2.7):

$$\mathbb{P}^{\alpha\dagger} = \mathbb{P}^\alpha. \tag{3.2.22}$$

3.5 CHARACTER FORMULAS

For Abelian symmetry analysis the number of repetitions or FREQUENCY of a given irrep $\mathscr{D}^\alpha$ is the number of states of that type still to be separated by means other than symmetry projection. The same is true for multidimensional irreps of non-Abelian groups because different substrates or partners of any irrep will give rise to identical equations. One has only to solve one set for each irrep (α) regardless of its dimension l^α.

Let us now derive some simple formulas for frequency of an irrep of a finite group in a given representation. These are called CHARACTER formulas. Characters of multidimensional irreps are the traces of the $\mathscr{D}^\alpha$ matrices as defined in the following:

$$\chi^\alpha(g) = \text{TRACE}\, \mathscr{D}^\alpha(g) = \sum_{i=1}^{l^\alpha} \mathscr{D}^\alpha_{ii}(g). \tag{3.5.1}$$

For Abelian groups irreps and characters are the same thing, since then $l^\alpha = 1$ always. Nevertheless, every formula given in this section can be applied to either Abelian or non-Abelian groups.

One property of the characters is that they are equal for any two symmetry operators g and g' that are equivalent or from the same class. If g is in the same class with g', then $g' = h^{-1}gh$ for some other symmetry operators h.

Representing this gives

$$\begin{aligned}\chi^\alpha(g') = \sum_i^{l^\alpha} \mathscr{D}^\alpha_{ii}(g') &= \sum_{i,j,k}^{l^\alpha} \mathscr{D}^\alpha_{ij}(h^{-1})\, \mathscr{D}^\alpha_{jk}(g)\, \mathscr{D}^\alpha_{ki}(h) \\ &= \sum_{j,k}^{l^\alpha} \left(\sum_i^{l^\alpha} \mathscr{D}^\alpha_{ki}(h)\, \mathscr{D}^\alpha_{ij}(h^{-1}) \right) \mathscr{D}^\alpha_{jk}(g) \\ &= \sum_j^{l^\alpha} \mathscr{D}^\alpha_{jj}(g),\end{aligned}$$

and finally

$$\chi^\alpha_{g'} \equiv \chi^\alpha(g') = \chi^\alpha(g), \tag{3.5.2}$$

for all g in the class c_g.

Recall the completeness relations between the all-commuting idempotents $\mathbb{P}^\alpha$ and the irreducible or elementary idempotents P^α_{ii}:

$$\mathbb{P}^\alpha = \sum_i P^\alpha_i = \sum_i P^\alpha_{ii}.$$

This leads to a formula for the all-commuting idempotents $\mathbb{P}^\alpha$ in terms of characters using the formula for P^α_{ii} given in Eq. (3.4.19):

$$\begin{aligned}\mathbb{P}^\alpha = \sum_i P^\alpha_{ii} &= (l^\alpha / {}^\circ G) \sum_g \sum_i \mathscr{D}^{\alpha *}_{ii}(g) g \\ &= (l^\alpha / {}^\circ G) \sum_g \chi^{\alpha *}(g) g.\end{aligned}$$

Since the characters are the same for equivalent operators, the preceding sum can be reduced to a sum over just one element from each class $c_g = (g + g' + \cdots)$,

$$\mathbb{P}^\alpha = (l^\alpha / {}^\circ G)\left[\chi^{\alpha *}_g (g + g' + \cdots) + \chi^{\alpha *}_h (h + h' + \cdots) + \cdots\right],$$

or

$$\mathbb{P}^\alpha = (l^\alpha / {}^\circ G) \sum_{\substack{\text{classes} \\ c_g}} \chi^{\alpha *}_g c_g. \tag{3.5.3}$$

This sum is a key to the derivation and application of characters.

A. Derivation of Irrep Characters

The algebra of classes discussed in Section 3.2 gives the all-commuting idempotents

$$\mathbb{P}^{\alpha} = \sum_{\substack{\text{classes} \\ c_g}} p_g^{\alpha} c_g \tag{3.5.4}$$

as a sum of classes. For the example of C_{3v} we obtained

$$\begin{aligned} \mathbb{P}^1 &= \tfrac{1}{6}c_1 + \tfrac{1}{6}c_2 + \tfrac{1}{6}c_3, \\ \mathbb{P}^2 &= \tfrac{1}{6}c_1 + \tfrac{1}{6}c_2 - \tfrac{1}{6}c_3, \\ \mathbb{P}^3 &= \tfrac{2}{3}c_1 - \tfrac{1}{3}c_2, \end{aligned} \qquad (3.5.4)_x$$

in Eq. (3.2.15). Relating the p_g^{α} coefficients in Eqs. (3.5.4) to characters in Eq. (3.5.3) gives

$$\chi_g^{\alpha *} = p_g^{\alpha}(l^{\alpha}/{}^{\circ}G)^{-1}. \tag{3.5.5}$$

To use this one must first determine the dimension l^{α} which is the trace or character of the irrep of the unit class:

$$\chi_1^{\alpha} = l^{\alpha} = \text{Trace}\, \mathscr{D}^{\alpha}(1). \tag{3.5.6}$$

Solving Eq. (3.5.5) gives

$$l^{\alpha} = ({}^{\circ}G p_1^{\alpha *})^{1/2}. \tag{3.5.7}$$

The first column of Eq. $(3.5.4)_x$ gives

$$\begin{aligned} l^1 &= (6 \cdot \tfrac{1}{6})^{1/2} = 1, \\ l^2 &= (6 \cdot \tfrac{1}{6})^{1/2} = 1, \\ l^3 &= (6 \cdot \tfrac{2}{3})^{1/2} = 2, \end{aligned} \qquad (3.5.7)_x$$

which is the first column of the C_{3v} character table in Eq. (3.5.8). The other characters follow from Eqs. $(3.5.4)_x$ and (3.5.5):

$$\begin{array}{r|ccc|} j = & 1 & 2: (r, r^2) & 3: (\sigma_1\sigma_2\sigma_3) \\ \hline \chi_j^{A'} = \chi_j^{A_1} = \chi_j^1 = & 1 & 1 & 1 \\ \chi_j^{A''} = \chi_j^{A_2} = \chi_j^2 = & 1 & 1 & -1 \\ \chi_j^{E} = \chi_j^3 = & 2 & -1 & 0 \\ \hline \end{array}. \tag{3.5.8}$$

The standard notation (1) ≡ A_1, (2) ≡ A_2, and (3) ≡ E for D_3 and C_{3v} irreps will be used from now on. The notation (1) ≡ A' and (2) ≡ A' is sometimes used instead for C_{3v} irreps.

B. Applications of Characters

The power of character theory is great, since it is independent of your choice of basis. Since a matrix trace is invariant to such choice it does not matter how a Hamiltonian is represented or which equivalent version of irreps you chose. Furthermore, sums over symmetry operators are replaced by sums over classes of operators, which can amount to a considerable saving of labor.