Symmetry: Appendices and examples

A Résumé of matrix terminology and formulae

An $n \times m$ matrix is an array of numbers (possibly complex) with n rows and m columns. We shall need only square matrices $(n \times n)$ and row and column vectors ($1 \times n$ and $n \times 1$):

$$A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}; \quad \boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}.$$

Addition of matrices: $(A+B)_{ij} = A_{ij} + B_{ij}$.

Multiplication of matrices: $(AB)_{ij} = \sum_k A_{ik} B_{kj}$.

Transposition: The transpose A^T has elements $A^T{}_{ij} = A_{ji}$.

Complex conjugate: $(A^*)_{ij} = A_{ij}{}^*$.

Hermitian conjugate: $A^\dagger = (A^T)^*$.

The *inverse* of a matrix A is a matrix A^{-1} such that $AA^{-1} = A^{-1}A = I$, where I is the *unit matrix* with ones along the diagonal and zeros elsewhere. A has an inverse if and only if $\det(A) \neq 0$.

Note that $(AB)^T = B^T A^T$; $(AB)^\dagger = B^\dagger A^\dagger$; $(AB)^{-1} = B^{-1} A^{-1}$.

A matrix is *diagonal*	if all its off-diagonal elements are zero;
real	if $A = A^*$;
symmetric	if $A = A^T$;
Hermitian	if $A = A^\dagger$;
orthogonal	if $A^T = A^{-1}$, so that $AA^T = I$;
unitary	if $A^\dagger = A^{-1}$, so that $AA^\dagger = I$;
singular	if $\det(A) = 0$.

The *scalar product* of two vectors is $\boldsymbol{u}^\dagger \boldsymbol{v} = u_1^* v_1 + u_2^* v_2 + \ldots + u_n^* v_n$. Two vectors are *orthogonal* if their scalar product vanishes; $\boldsymbol{u}$ is *normalized* if $\boldsymbol{u}^\dagger \boldsymbol{u} = 1$.

Any non-singular matrix T can be used to transform vectors: $\boldsymbol{v}' = T\boldsymbol{v}$, or matrices: $A' = TAT^{-1}$. This is a *similarity* or *equivalence* transformation. If T is orthogonal (or unitary) we get an orthogonal (or unitary) transformation.

The *trace* of a matrix is the sum of its diagonal elements. It is invariant under any similarity transformation:

$$\mathrm{trace}(A') = \sum_i A'_{ii} = \sum_{ijk} T_{ij} A_{jk} (T^{-1})_{ki} = \sum_{ijk} (T^{-1})_{ki} T_{ij} A_{jk} = \sum_k A_{kk} = \mathrm{trace}(A).$$

The eigenvectors $\boldsymbol{u}^{(i)}$ of a matrix A satisfy $A\boldsymbol{u}^{(i)} = \lambda^{(i)} \boldsymbol{u}^{(i)}$. If A is Hermitian then the eigenvalues are real; moreover the eigenvectors are orthogonal to each other, so if they are also normalized they satisfy $\boldsymbol{u}^{(i)\dagger} \boldsymbol{u}^{(j)} = \delta_{ij}$. The matrix U whose columns are the eigenvectors (i.e. $U_{ki} = u_k^{(i)}$) is therefore unitary, and A is transformed to diagonal form by the matrix U^{-1}: $U^{-1}AU = \Lambda$. The diagonal elements of the matrix Λ are the eigenvalues $\lambda^{(i)}$.

Group	Generators		order	Direct product form	International notation n even	n odd
Non-axial groups						
$\mathcal{C}_1$	E	no symmetry	1		1	
$\mathcal{C}_i$	$\hat{\imath}$		2		$\bar{1}$	
$\mathcal{C}_s$	σ		2		m	
Axial groups						
$\mathcal{C}_n$	C_n		n		n	
$\mathcal{D}_n$	C_n, C_2	$C_2 \perp C_n$	$2n$		$n22$	$n2$
$\mathcal{C}_{nv}$	C_n, σ_v	$\mathcal{C}_{1v} = \mathcal{C}'_s$	$2n$	$\mathcal{C}_{2v} = \mathcal{C}_2 \otimes \mathcal{C}'_s$	nmm	nm
$\mathcal{C}_{nh}$	C_n, σ_h	$\mathcal{C}_{1h} = \mathcal{C}_s$	$2n$	$\mathcal{C}_n \otimes \mathcal{C}_s$	n/m	$\overline{(2n)}$
$\mathcal{S}_n$ (n even)	S_n	$\mathcal{S}_2 = \mathcal{C}_i$	n		$\mathcal{S}_4 = \bar{4}$; $\mathcal{S}_6 = \bar{3}$	
$\mathcal{S}_n$ (n odd)	S_n	$= \mathcal{C}_{nh}$	$2n$			$\overline{(2n)}$
$\mathcal{D}_{nd}$	C_n, C_2, σ_d	$C_2 \perp C_n$	$4n$		$\overline{(2n)}2m$	$\bar{n}m$
$\mathcal{D}_{nh}$	C_n, C_2, σ_h	$C_2 \perp C_n$	$4n$	$\mathcal{D}_n \otimes \mathcal{C}_s$	n/mmm	$\overline{(2n)}m2$
					$\mathcal{D}_{2h} = mmm$	
Cubic groups						
$\mathcal{T}$	$4C_3$		12		23	
$\mathcal{T}_h$	$4C_3, \hat{\imath}$		24	$\mathcal{T} \otimes \mathcal{C}_i$	$m3$	
$\mathcal{T}_d$	$4C_3, \sigma_d$	Each σ_d plane contains 2 C_3 axes	24		$\bar{4}3m$	
$\mathcal{O}$	$4C_3, C_4$	C_4 axes bisect angle	24		432	
$\mathcal{O}_h$	$4C_3, C_4, \hat{\imath}$	between 2 C_3 axes	48	$\mathcal{O} \otimes \mathcal{C}_i$, $\mathcal{T}_d \otimes \mathcal{C}_i$	$m3m$	
Icosahedral groups						
$\mathcal{I}$	$6C_5$		60			
$\mathcal{I}_h$	$6C_5, \hat{\imath}$		120	$\mathcal{I} \otimes \mathcal{C}_i$		

C Proof of the Great Orthogonality Theorem

The proof is given here only in outline. For a full account, see, e.g., Elliott & Dawber, pp. 54ff. The first step is Schur's lemma. If $D^a(R)$ and $D^b(R)$ are the matrices for the irreducible representations Γ_a and Γ_b, of dimensions n_a and n_b, we look for a matrix A that satisfies

$$D^a(R)A = AD^b(R) \tag{C.1}$$

for all R. Schur's lemma states that if $\Gamma_a = \Gamma_b$, then $A = \lambda I$ — that is, it must be a multiple of the $n_a \times n_a$ unit matrix — while if $\Gamma_a \not\sim \Gamma_b$, then A must be the $n_a \times n_b$ zero matrix. We prove it only for the case $\Gamma_a = \Gamma_b$. Consider an eigenvector $\boldsymbol{x}$ of A: $A\boldsymbol{x} = \lambda\boldsymbol{x}$. The vector $x_R \equiv D(R)\boldsymbol{x}$ is also an eigenvector of A, with the same eigenvalue:

$$Ax_R = AD(R)\boldsymbol{x} = D(R)A\boldsymbol{x} = \lambda D(R)\boldsymbol{x} = \lambda x_R, \tag{C.2}$$

since A and $D(R)$ are required to commute. This is true for any R. Now the set of vectors $\boldsymbol{x}_R$ must span the full representation space, since otherwise they would define an irreducible subspace and the representation would be reducible. Hence any vector $\boldsymbol{X}$ in the representation space must be expressible as a linear combination of the $\boldsymbol{x}_R$; that is, $\boldsymbol{X} = \sum_R a_R \boldsymbol{x}_R$ for some set (probably not unique) of coefficients a_R. Then

$$A\boldsymbol{X} = \sum_R a_R A\boldsymbol{x}_R = \lambda \sum_R a_R \boldsymbol{x}_R = \lambda \boldsymbol{X}.$$

If $A\boldsymbol{X} = \lambda\boldsymbol{X}$ for any $\boldsymbol{X}$, then A must be λ times the unit matrix. The proof that $A = 0$ if $\Gamma_a \not\sim \Gamma_b$ follows similar lines; see Elliott & Dawber, p. 60.

The second step in the argument is to observe that the matrix

$$A = \sum_S D^a(S) Z D^b(S^{-1})$$

satisfies eq. (C.1) for any $n_a \times n_b$ matrix Z. The proof uses the homomorphism of the representation matrices several times:

$$\begin{aligned}
D^a(R)A &= \sum_S D^a(R)D^a(S)ZD^b(S^{-1}) \\
&= \sum_S D^a(RS)ZD^b(S^{-1})D^b(R^{-1})D^b(R) \\
&= \sum_S D^a(RS)ZD^b((RS)^{-1})D^b(R) \\
&= \sum_T D^a(T)ZD^b(T^{-1})D^b(R) \\
&= AD^b(R).
\end{aligned} \tag{C.3}$$

We have also used the rearrangement theorem (see Qn. 1), that when S runs through all elements of the group, the set of products $T = RS$ for fixed R contains every element once and only once, so the sum over S in the third line of (C.3) can be replaced by the sum over T in the fourth line.

Finally we choose Z so that $Z_{pq} = 1$ and all other elements are zero, and the G.O.T. follows.