2. Representation theory and basic theorems

2.1 Matrix representatives

The point group symmetry operations introduced in the previous chapter are transformations defined in $\mathbb{R}^3$. As such, their representation takes the move from the vectorial space structure of $\mathbb{R}^3$.

Def: VECTORIAL SPACE on $\mathbb{R}$ or $\mathbb{C}$ is a set V on which we have consistently defined 2 operations

- sum: $v_1, v_2 \in V \Rightarrow v_1 + v_2 = v_3$,
- product with a scalar $a \in \mathbb{R}$ (or $\mathbb{C}$) $a v_1$.

The sum and product with scalar operations satisfy the following properties:

$$\forall\, u\ v\ w \in V \quad (u+v)+w = u+(v+w)$$
$$\exists\, 0 \in V \cdot \forall v \in V \quad 0+v = v$$
$$\forall\, v \in V \quad \exists -v \in V : -v+v = 0$$
$$\forall\, v, w \in V \quad v+w = w+v$$

$\{V,+\}$ is an Abelian group

$$\forall \lambda \in \mathbb{R}\ (\text{or } \mathbb{C})\ \forall v, w \in V \quad \lambda(v+w) = \lambda v + \lambda w$$
$$\forall \lambda, \mu \in \mathbb{R}\ (\text{or } \mathbb{C})\ \forall v \in V \quad (\lambda+\mu)v = \lambda v + \mu v$$
$$\forall \lambda, \mu \in \mathbb{R}\ (\text{or } \mathbb{C})\ \forall v \in V \quad (\lambda\mu)v = \lambda(\mu v)$$
$$\forall v \in V \quad 1v = v \quad \text{and} \quad 0v = 0$$

Notice that $\mathbb{R}$ or $\mathbb{C}$ can be substituted by whatever other field $\mathbb{K}$.

All point symmetry operations are linear applications on $\mathbb{R}^3$.

Def: LINEAR APPLICATION $f : V \to V$ is linear if

$$f(\alpha v + \beta w) = \alpha f(v) + \beta f(w) \quad \forall v, w \in V \text{ and } \alpha, \beta \in \mathbb{K}.$$

Theorem: The space of linear applications $V \to V$ is isomorphous to the space of matrices $n \times n$ taken from $\mathbb{K}$. n is the size of V.

$$\mathrm{Hom}_{\mathbb{K}}(V, V) \simeq \mathrm{Mat}(n, n; \mathbb{K})$$

Turning to our specific problem $V = \mathbb{R}^3$ on $\mathbb{R}$ with dimension 3. In order to determine the 3×3 real matrix associated to the point symmetry operations.

i) Apply the symmetry operation on the element of a basis and expand on the basis itself. (for simplicity we take an orthonormal basis).

$\mathbb{R}^3 \to \hat{e}_x \; \hat{e}_y \; \hat{e}_z$

$$f(\hat{e}_x) = a\hat{e}_x + b\hat{e}_y + c\hat{e}_z$$
$$f(\hat{e}_y) = d\,\hat{e}_x + e\,\hat{e}_y + f\,\hat{e}_z$$
$$f(\hat{e}_z) = g\hat{e}_x + h\,\hat{e}_y + i\,\hat{e}_z$$

ii) Using linearity of f apply on a linear combination

$$f(\alpha\hat{e}_x + \beta\hat{e}_y + \gamma\hat{e}_z) = \alpha'\hat{e}_x + \beta'\hat{e}_y + \gamma'\hat{e}_z$$
$$\begin{aligned} &\| \\ &(\alpha a + \beta d + \gamma g)\,\hat{e}_x \\ &(\alpha b + \beta e + \gamma h)\,\hat{e}_y \\ &(\alpha c + \beta f + \gamma i)\,\hat{e}_z\,. \end{aligned}$$

iii) Collect the components

$$\begin{pmatrix} \alpha' \\ \beta' \\ \gamma' \end{pmatrix} = \underbrace{\begin{pmatrix} a & d & g \\ b & e & h \\ c & f & i \end{pmatrix}}_{\Gamma(f)} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

The matrix transformation for the coefficients is the transpose of the one for the basis.

All point symmetry operations conserve the norm. It follows that all associated matrices $\Gamma(f)$ are orthogonal.

<u>proof</u>: We use the scalar product $(\hat{e}_i, \hat{e}_j) = \delta_{ij}$ extended bilinearly over the entire vector space $\mathbb{R}^3$.

$$(f(v), f(w)) = \Big(f\big(\sum_i \alpha_i \hat{e}_i\big), f\big(\sum_j \beta_j \hat{e}_j\big)\Big) =$$

$$= \sum_{ij} \alpha_i \beta_j \big(f(\hat{e}_i), f(\hat{e}_j)\big) =$$

$$= \sum_{ij} \alpha_i \beta_j \Big(\sum_\ell \Gamma(f)_{\ell i} \hat{e}_\ell , \sum_k \Gamma(f)_{kj} \hat{e}_k \Big)$$

$$= \sum_{ij} \alpha_i \beta_j \sum_{\ell k} \Gamma(f)_{\ell i} \Gamma(f)_{kj} \delta_{\ell k} = \sum_{ijk} \alpha_i \beta_j \Gamma^T(f)_{ik} \Gamma(f)_{kj}$$

$$(v, w) = \sum_{ij} (\alpha_i \hat{e}_i , \beta_j \hat{e}_j) = \sum_i \alpha_i \beta_i$$

$$\Rightarrow \boxed{\sum_k \Gamma^T(f)_{ik} \Gamma(f)_{kj} = \delta_{ij}}$$

■

<u>Theorem</u> Let $\mathcal{G} = \{A, B, \dots\}$ be a point symmetry group $\Rightarrow$ the set of matrix representatives $\{\Gamma(A), \Gamma(B), \dots\}$ on the vectorial space $\mathbb{R}^3$ is a group isomorphous to $\mathcal{G}$.

<u>proof</u>: Being the mapping bijective (no 2 distinct point symmetry operations transform $\hat{e}_x, \hat{e}_y$ and $\hat{e}_z$ in the same way) it is enough to prove the homomorphism

$$\Gamma(A)_{ij}: \quad v = \sum_i \alpha_i \hat{e}_i \qquad A(v) = \sum_i \hat{e}_i \sum_j \Gamma(A)_{ij} \alpha_j$$

$$\Gamma(AB) = ? \quad A(B(v)) = A\Big(\sum_k \hat{e}_k \sum_j \Gamma(B)_{kj} \alpha_j \Big) = \sum_{kj} \Gamma(B)_{kj} \alpha_j A(\hat{e}_k)$$

$$= \sum_{kj} \Gamma(B)_{kj} \alpha_j \sum_{i\ell} \hat{e}_i \Gamma(A)_{i\ell} \delta_{\ell k} = \sum_i \hat{e}_i \sum_{jk} \Gamma(A)_{ik} \Gamma(B)_{kj} \alpha_j$$

$$= \sum_i \hat{e}_i \sum_j \big[\Gamma(A) \cdot \Gamma(B)\big]_{ij} \alpha_j \Rightarrow \Gamma(AB) = \Gamma(A) \cdot \Gamma(B).$$

■

<u>exemple 1</u> C_{2v} the group of the water molecule

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \Gamma(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(\sigma_{xz}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(\sigma_{yz}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

<u>example 2</u> C_4

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(C_4^+) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(C_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \Gamma(C_4^-) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} C_4(\hat{e}_x) &= \hat{e}_y \\ C_4(\hat{e}_y) &= -\hat{e}_x \\ C_4(\hat{e}_z) &= \hat{e}_z \end{aligned} \quad = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{e}_x \\ \hat{e}_y \\ \hat{e}_z \end{pmatrix}$$

2.2 Function transformation

Each point symmetry operation R maps every point P in $\mathbb{R}^3$ into the transformed one R(P). We can now consider the set of functions $f: \mathbb{R}^3 \to \mathbb{C}$ and associate to the point symmetry operation the function transformation (functional) defined as:

$$\hat{R} f(R(P)) = f(P)$$

alternatively

$$\hat{R} f(P) = f(R^{-1}(P))$$

which is equivalent since $R \ \mathbb{R}^3 \to \mathbb{R}^3$ is bijective.
The first definition given above ensures that the transformed function calculated in the transformed point coincide with the original function calculated in the original point.

Example of function transformation

$$f(P) = x\, e^{-r} \qquad P = x\hat{e}_x + y\hat{e}_y + z\hat{e}_z$$
$$r = (x^2 + y^2 + z^2)^{1/2}$$

We take the point symmetry operation C_4^+. The question is the construction of $\hat{C}_4^+ f$. According to the definition:

$$\hat{C}_4^+ f(P) = f(C_4^-(P))$$

The matrix representative of C_4^- is $\Gamma(C_4^-) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$$= \hat{C}_4^+ f\begin{pmatrix} x \\ y \\ z \end{pmatrix} = f\left(\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}\right) = f\begin{pmatrix} y \\ -x \\ z \end{pmatrix} = y\, e^{-(y^2+x^2+z^2)^{1/2}} = y\, e^{-r}.$$

<u>Theorem</u>: Let's consider the point symmetry group $G = \{R, T, S, \dots\}$. The set of functionals $\{\hat{R}, \hat{T}, \hat{S}, \dots\}$ defined on the set of analytical functions $f: \mathbb{R}^3 \to \mathbb{C}$

$$\hat{R} f(P) = f(R^{-1}(P)) \qquad \forall P \in \mathbb{R}^3$$

is a group (with respect to functional composition) isomorphous to G.

<u>Proof</u>: the mapping $R \to \hat{R}$ preserves the product: let's define $S = RT$

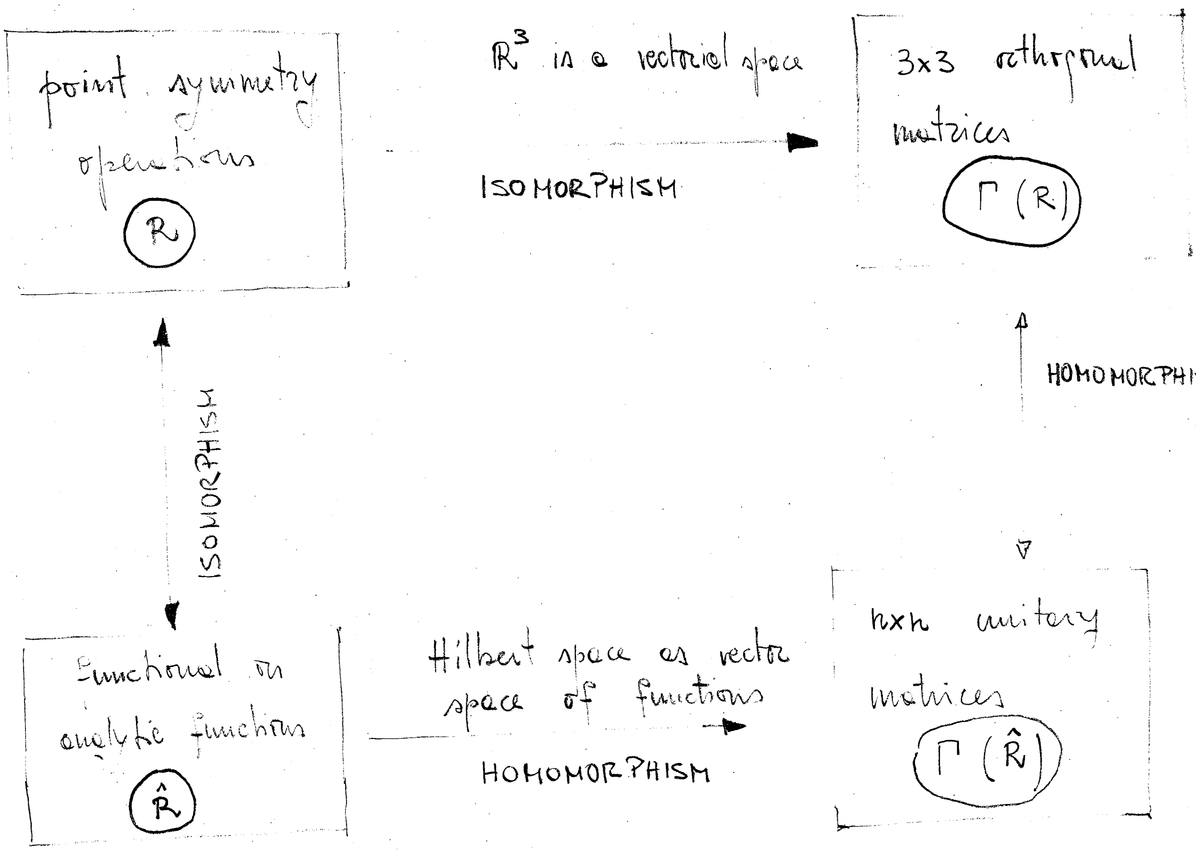
- $$\hat{R}[\hat{T} f(P)] = \hat{R} f(T^{-1}(P)) = f(T^{-1}(R^{-1}(P))) =$$
$$= f\left(\Gamma(T)^{-1}\,\Gamma(R)^{-1}\begin{pmatrix} x \\ y \\ z \end{pmatrix}\right) = f\left((\Gamma(R)\,\Gamma(T))^{-1}\begin{pmatrix} x \\ y \\ z \end{pmatrix}\right) =$$
$$= f((RT)^{-1}(P)) = f(S^{-1}(P)) = \hat{S} f(P).$$

all other relations follow immediately. The isomorphism is ensured by the enormous freedom in the choice of f which can be taken as e.g. a gaussian centered around an arbitrary point P in $\mathbb{R}^3$.

In general, though, the space of functions in which the functionals $\hat{R}$ are acting is smaller and the relation between the group of point symmetry operations and the group of their associated functionals is just an HOMOMORPHISM.

The Hilbert space of integrable functions $L^2(\mathbb{R}^3)$ is particularly interesting to us as a vectorial space over which $\hat{R}$ admits again a matrix representation.

Schematically



Notice that $\Gamma(\hat{R})$ are matrices of a size completely independent of the 3 dimensional vector space $\mathbb{R}^3$ associated to $\Gamma(R)$.

2.3 | Representations

Def: REPRESENTATION is the group formed by the matrices $\Gamma(R)$ or $\Gamma(\hat{R})$ associated to the point symmetry group $\mathcal{G}$ with generic element R.

Two representations Γ_1 and Γ_2 of the same group $\mathcal{G}$ are equivalent if

$\forall R \in \mathcal{G} \quad \exists! U: \quad \Gamma_1(R) = U^\dagger \Gamma_2(R) U$

<u>Theorem</u>: Every representation of a point group with matrices having non-vanishing determinants is equivalent to a representation made of unitary matrices.

<u>proof</u>:

Let $\Gamma(\hat{R})$ $R \in \mathcal{G}$ be the representation. We start by forming

$$H = \sum_R \Gamma(\hat{R})\,\Gamma(R)^\dagger$$

H is Hermitian since

$$H^\dagger = \sum_R \left[\Gamma(\hat{R})\,\Gamma(\hat{R})^\dagger\right]^\dagger = \sum_R \Gamma(\hat{R})\,\Gamma(\hat{R})^\dagger .$$

Every Hermitian matrix can be diagonalized by a suitable unitary transformation

$$d = U^{-1} H U = \sum_R U^{-1}\Gamma(\hat{R})\Gamma(\hat{R})^\dagger U$$
$$= \sum_R U^{-1}\Gamma(\hat{R})UU^{-1}\Gamma(\hat{R})^\dagger U =: \sum_R \tilde{\Gamma}(\hat{R})\,\tilde{\Gamma}(\hat{R})^\dagger$$

Moreover, notice that d (and also H) is positive definite:

$$d_{kk} = \sum_{Rj} \tilde{\Gamma}(\hat{R})_{kj}\,\tilde{\Gamma}(\hat{R})^\dagger_{jk} = \sum_{Rj} \left|\tilde{\Gamma}(\hat{R})_{kj}\right|^2 > 0$$

We can thus form the matrices $d^{\pm 1/2}$: $(d^{\pm 1/2})_{kk} = (d_{kk})^{\pm 1/2}$. It follows that

$$d^{1/2}\, d^{1/2} = \sum_R \tilde{\Gamma}(\hat{R})\,\tilde{\Gamma}(\hat{R})^\dagger$$
$$\left(d^{\pm 1/2}\right)^\dagger = d^{\pm 1/2}$$
$$d^{1/2}\, d^{-1/2} = \mathbb{1}.$$

We now construct the matrices

$$\tilde{\tilde{\Gamma}}(\hat{R}) = d^{-1/2}\,\tilde{\Gamma}(\hat{R})\,d^{1/2}$$

from which it follows

$$\tilde{\tilde{\Gamma}}(\hat{R})^\dagger = d^{1/2}\,\tilde{\Gamma}(\hat{R})^\dagger\, d^{-1/2}$$

We now show that the matrices $\tilde{\tilde{\Gamma}}(\hat{R})$ are unitary.

Singular representations of groups also exists they are all equivalent to

$$\begin{vmatrix} 0 & \\ & \Gamma(\hat{R}) \end{vmatrix}$$

with 0 of generic size $n \times n$ where n is the size of the kernel.
The similarity transformation can make the singular transformation not so easily recognizable. Example of singular representation of C_3

$$\Gamma(E) = \frac{1}{3} \begin{vmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{vmatrix}$$

$$\Gamma(C_3^+) = \frac{1}{3} \begin{vmatrix} -1 & -1 & 2 \\ 2 & -1 & -1 \\ -1 & 2 & -1 \end{vmatrix}$$

$$\Gamma(C_3^-) = \frac{1}{3} \begin{vmatrix} -1 & 2 & -1 \\ -1 & -1 & 2 \\ 2 & -1 & -1 \end{vmatrix}$$

$$\tilde{\tilde{\Gamma}}(\hat{R})\,\tilde{\tilde{\Gamma}}(\hat{R})^{\dagger} = d^{-1/2}\,\tilde{\Gamma}(\hat{R})\,d\,\tilde{\Gamma}(\hat{R})^{\dagger} d^{-1/2} =$$

$$= \sum_{S} d^{-1/2}\,\tilde{\Gamma}(\hat{R})\,\tilde{\Gamma}(\hat{S})\,\tilde{\Gamma}(\hat{S})^{\dagger}\,\tilde{\Gamma}(\hat{R})^{\dagger} d^{-1/2} = \quad \text{representation}$$

$$= \sum_{S} d^{-1/2}\,\tilde{\Gamma}(\hat{R}\hat{S})\,\tilde{\Gamma}(\hat{R}\circ\hat{S})^{\dagger} d^{-1/2} = \quad \text{rearrangement theorem}$$

$$= \sum_{S} d^{-1/2}\,\tilde{\Gamma}(\hat{S})\,\tilde{\Gamma}(\hat{S})^{\dagger} d^{-1/2} =$$

$$= d^{-1/2}\,d\,d^{-1/2} = \mathbb{1}.$$

$\Rightarrow$ $\tilde{\tilde{\Gamma}}(\hat{R})$ is a unitary representation of the point group $\mathcal{G}$ and its relation with $\Gamma(\hat{R})$ is:

$$\tilde{\tilde{\Gamma}}(\hat{R}) = d^{-1/2}\,U^{-1}\,\Gamma(\hat{R})\,U\,d^{1/2}$$

where:

$$d = U^{-1} H U \quad \text{is diagonal}$$

$$H = \sum_{R} \Gamma(\hat{R})\,\Gamma(\hat{R})^{\dagger}$$

■

<u>Def</u>: REDUCIBLE REPRESENTATION a representation $\Gamma(\hat{R})$ in which all matrix representatives are brought to the same block diagonal form by the same equivalence transformation.

If the condition above is not fulfilled $\Rightarrow$ the representation Γ is IRREDUCIBLE.

In other words irreducible representations cannot be expressed in terms of representation of lower dimensions.

For a reducible representation:

$$\Gamma_{red}(\hat{T}) = U^{-1}\Gamma(\hat{T})\,U \qquad \text{with} \qquad \Gamma(\hat{T}) = \begin{pmatrix} \Gamma_1(\hat{T}) & 0 \\ 0 & \Gamma_2(\hat{T}) \end{pmatrix} \quad \forall T \in \mathcal{G}.$$

$$T = RS \longrightarrow \begin{pmatrix} \Gamma_1(\hat{R}) & 0 \\ 0 & \Gamma_2(\hat{R}) \end{pmatrix}\begin{pmatrix} \Gamma_1(\hat{S}) & 0 \\ 0 & \Gamma_2(\hat{S}) \end{pmatrix} = \begin{pmatrix} \Gamma_1(\hat{R})\Gamma_1(\hat{S}) & 0 \\ 0 & \Gamma_2(\hat{R})\Gamma_2(\hat{S}) \end{pmatrix}$$

In other terms $\Gamma = \Gamma_1 \oplus \Gamma_2$

2.4 The group of the Hamiltonian

Let's take a physical system, e.g. the benzene molecule, and consider all the point symmetric operations that bring the physical system into itself. They form a group (D_{6h} for benzene).

$\hat{H}$ is the Hamiltonian of the system

$\hat{R}$ the operator associated to one of the sym. operations.

$|\psi_i\rangle$ an eigenstate of $\hat{H}$.

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

But, since the physical system is invariant under R =>

$$\langle\vec{x}|\hat{R}|\psi_i\rangle := \psi_i(R^{-1}(\vec{x}))$$

is also an eigenstate of $\hat{H}$ with the SAME eigenvalue

$$\hat{H}\hat{R}|\psi_i\rangle = E_i\hat{R}|\psi_i\rangle = \hat{R}E_i|\psi_i\rangle = \hat{R}\hat{H}|\psi_i\rangle$$

The same consideration can be repeated $\forall i$ => one can write an operatorial equation:

$$[\hat{H}, \hat{R}] = 0$$

$\forall R \in \mathcal{G}$. => The Hamilton operator commutes with all the elements of the group of operators homomorphous to the group of symmetry operations on the physical system. Viceversa we can define:

<u>Def</u>: THE GROUP OF THE HAMILTONIAN the set of all operators commuting with the Hamiltonian. (prove by exercise that it fulfills the 4 axioms).

The 2 group of operators do NOT coincide. The first one is more reliable since it is independent of the degree of accuracy of the Hamiltonian in the description of the physical system.

2.5 Basic theorems

The basic theorem of representation theory is the orthogonality theorem, due to Issai Schur. The proof of this fundamental theorem is based on 2 lemmas.

First Schur's lemma (1905)

A matrix which commutes with all matrices of an irreducible representation is a constant matrix, i.e. a constant times the unit matrix.

proof: $M\,\Gamma(\hat{R}) = \Gamma(\hat{R})\,M \qquad R \in G \qquad \Gamma$ irreducible.

$$\Downarrow$$

$\Gamma(\hat{R})^{+}M^{+} = M^{+}\Gamma(\hat{R})^{+}$ and, assuming $\Gamma(\hat{R})$ unitary, without loss of generality

$$M^{+}\Gamma(\hat{R}) = \Gamma(\hat{R})\,M^{+}$$

Summarizing, we have $[\Gamma(\hat{R}), M] = 0 = [\Gamma(\hat{R}), M^{+}]$ it follows by linearity of $[\cdot,\cdot]$:

$$[\Gamma(\hat{R}), M + M^{+}] = 0$$

$$[\Gamma(\hat{R}), i(M - M^{+})] = 0$$

Let's introduce the Hermitian matrices $H_1 = M + M^{+}$ and $H_2 = i(M - M^{+})$.

If $[\Gamma(\hat{R}), H] = 0$ and H hermitian $\Rightarrow$ $H = \lambda \mathbb{1}$.

Since H is hermitian $\exists\, U$ unitary: $d = U^{-1}HU$. $\tilde{\Gamma}(\hat{R}) = U^{-1}\Gamma(\hat{R})U$ d = diag

$$[\tilde{\Gamma}(\hat{R}), d] = 0$$

In components $\tilde{\Gamma}(\hat{R})_{nm}\, d_{mm} = d_{nn}\,\tilde{\Gamma}(\hat{R})_{nm} \Rightarrow \tilde{\Gamma}_{nm}(\hat{R})\,(d_{nn} - d_{mm}) = 0 \;\; \forall n,m$

Since $\tilde{\Gamma}(\hat{R})$ is irreducible $\Rightarrow \forall n,m \;\exists\, \hat{R} : \tilde{\Gamma}_{nm}(\hat{R}) \neq 0 \Rightarrow d_{nn} = d_{mm}$.

$$\Rightarrow \quad H_1 = \lambda_1 \mathbb{1}, \quad H_2 = \lambda_2 \mathbb{1} \quad \Rightarrow \quad M = \frac{H_1 - iH_2}{2} = \frac{1}{2}(\lambda_1 - i\lambda_2)\,\mathbb{1}$$

■

A immediate consequence of the lemma is a criterion of reducibility:
If a commuting non-constant matrix exist $\Rightarrow$ the representation is reducible

Second Schur's lemma

Let us consider 2 irreducible representations $\Gamma_1(\hat{R})$ and $\Gamma_2(\hat{R})$ of a group $\mathcal{G}$ with dimensionality l_1 and l_2 respectively. If we can find a matrix M, $l_2 \times l_1$:

$$\boxed{M\,\Gamma_1(\hat{R}) = \Gamma_2(\hat{R})\,M} \qquad (*)$$

$$\Rightarrow \begin{cases} l_1 \neq l_2 \Rightarrow & M = 0 \\ l_1 = l_2 \Rightarrow & \text{either } M = 0 \text{ or } M \text{ is regular } \Gamma_1(\hat{R}) = M^{-1}\Gamma_2(\hat{R})M \simeq \Gamma_2(\hat{R}) \end{cases}$$

proof without loss of generality $l_1 \leq l_2$

$$(*) \Rightarrow \Gamma_1(\hat{R})^{+}M^{+} = M^{+}\Gamma_2(\hat{R})^{+} \qquad \text{but } \Gamma_1 \text{ and } \Gamma_2 \text{ unitary}$$

$$\Gamma_1(\hat{R}^{-1})M^{+} = M^{+}\Gamma_2(\hat{R}^{-1}) \qquad \forall \hat{R} \in \mathcal{G}$$

$$\boxed{\Gamma_1(\hat{R})M^{+} = M^{+}\Gamma_2(\hat{R})} \qquad (**)$$

$$M\Gamma_1(\hat{R})M^{+} = \begin{cases} \overset{(*)}{} \Gamma_2(\hat{R})MM^{+} \\ \overset{(**)}{} MM^{+}\Gamma_2(\hat{R}) \end{cases} \Rightarrow [\Gamma_2(\hat{R}), MM^{+}] = 0$$

$$M^{+}\Gamma_2(\hat{R})M = \begin{cases} \overset{(*)}{} M^{+}M\Gamma_1(\hat{R}) \\ \overset{(**)}{} \Gamma_1(\hat{R})M^{+}M \end{cases} \Rightarrow [\Gamma_1(\hat{R}), M^{+}M] = 0$$

From the first Schur's lemma $\Rightarrow$ $M^{+}M = \lambda_1 \mathbb{1}_{l_1}$ $\quad MM^{+} = \lambda_2 \mathbb{1}_{l_2}$

Now we consider 2 cases:

(i) $l_1 = l_2$

- $\lambda_1 \neq 0 \qquad \det(M^{+}M) = |\det M|^2 = \lambda_1^{l_1} \neq 0$

  $$M^{-1} = \frac{M^{+}}{\lambda_1} = \frac{M^{+}}{\lambda_2} \Rightarrow \lambda_1 = \lambda_2$$

  from $(*)$ $\quad \Gamma_1(\hat{R}) = M^{-1}\Gamma_2(\hat{R})M \simeq \Gamma_2(\hat{R})$.

- $\lambda_1 = 0 \Rightarrow 0 = \sum_k (M^{+})_{ik} M_{kj}$ if $i=j$ $\quad 0 = \sum_k |M_{ki}|^2 \quad \forall i \Rightarrow \boxed{M=0}$

(ii) $l_1 < l_2$ let us construct

$$N = l_2 \Big\{ \overbrace{M}^{l_1} \quad \overbrace{0}^{l_2 - l_1}$$

$$NN^+ = MM^+ = \lambda_2 \mathbb{1}_{l_2} \quad \text{but } \det N = \det N^+ = 0 \implies \lambda_2 = 0$$

and, using the same argument of the previous case $M = 0$ ∎

With the help of the two Schur's lemmas we can now proceed to the proof of the orthogonality theorem for representations also named by J. van Vleck the wonderful orthogonality theorem (WOT)

Theorem: All pairs of inequivalent irreducible representations $\Gamma^j, \Gamma^{j'}$ of a generic group $\mathcal{G}$ satisfy the orthogonality relation:

$$\sum_{R \in \mathcal{G}} \sqrt{\frac{l_j}{h}} \, \Gamma^j_{\mu\nu}(R) \sqrt{\frac{l_{j'}}{h}} \, \Gamma^{j'}_{\nu'\mu'}(R^{-1}) = \delta_{jj'} \delta_{\mu\mu'} \delta_{\nu\nu'}$$

where the summation runs over the entire set of h elements in the group. Moreover l_j and $l_{j'}$ are, respectively, the dimensionalities of the Γ^j and $\Gamma^{j'}$ representations. If the representation $\Gamma^{j'}$ is unitary, the orthogonality relation becomes

$$\sum_{R \in \mathcal{G}} \sqrt{\frac{l_j}{h}} \, \Gamma^j_{\mu\nu}(R) \sqrt{\frac{l_{j'}}{h}} \, \Gamma^{j'}_{\mu'\nu'}(R)^* = \delta_{jj'} \delta_{\mu\mu'} \delta_{\nu\nu'}$$

proof: Consider an arbitrary matrix X with l_j rows and $l_{j'}$ columns and construct

$$M = \sum_R \Gamma^j(R) \, X \, \Gamma^{j'}(R^{-1}) \qquad M \text{ is } l_j \times l_{j'}$$

$$\Gamma^j(S)M = \Gamma^j(S)\sum_R \Gamma^j(R) \times \Gamma^{j'}(R^{-1}) =$$

$$= \sum_R \Gamma^j(SR) \times \Gamma^{j'}(R^{-1}S^{-1})\,\Gamma^{j'}(S)$$

$$= \sum_R \Gamma^j(SR) \times \Gamma^{j'}((SR)^{-1})\,\Gamma^{j'}(S)$$

$$\stackrel{\text{rear}}{=} \sum_R \Gamma^j(R) \times \Gamma^{j'}(R^{-1})\,\Gamma^{j'}(S) = M\,\Gamma^{j'}(S) \qquad \forall S \in \mathcal{G}$$

Case 1 $l_j \neq l_{j'}$ or $l_j = l_{j'}$ but Γ^j not equivalent to $\Gamma^{j'}$. It follows from the second Schur's lemma $M = 0$. We can choose $l_j l_{j'}$ different $X^{\nu\nu'}$ matrices whose elements are $(X^{\nu\nu'})_{\gamma\lambda} = \delta_{\gamma\nu}\delta_{\lambda\nu'}$

$$0 = M_{\mu\mu'} = \sum_R \sum_{\gamma\lambda} \Gamma^j_{\mu\gamma}(R)\,\delta_{\gamma\nu}\delta_{\lambda\nu'}\,\Gamma^{j'}_{\lambda\mu'}(R^{-1}) = \sum_R \Gamma^j_{\mu\nu}(R)\,\Gamma^{j'}_{\nu'\mu'}(R^{-1})$$

Case 2 $l_j = l_{j'}$ and Γ^j is identical to $\Gamma^{j'}$ $\Rightarrow$ from the first Schur's lemma we conclude $M = c\,\mathbb{1}$

$$M_{\mu\mu'} = c^j\,\delta_{\mu\mu'} = \sum_R \sum_{\lambda\gamma} \Gamma^j_{\mu\gamma}(R)\,X_{\gamma\lambda}\,\Gamma^j_{\lambda\mu'}(R^{-1})$$

If we now chose $(X^{\nu\nu'})_{\gamma\lambda} = \delta_{\nu\gamma}\delta_{\nu'\lambda}$

$$M_{\mu\mu'} = c^j_{\nu\nu'}\,\delta_{\mu\mu'} = \sum_R \Gamma^j_{\mu\nu}(R)\,\Gamma^j_{\nu'\mu'}(R^{-1})$$

where we have inserted explicitly the $\nu\nu'$ dependence of the constant c. In order to determine $c_{\nu\nu'}$ we can set $\mu = \mu'$ and $\sum_\mu$

$$c^j_{\nu\nu'}\,l_j = \sum_{R\mu} \Gamma^j_{\nu'\mu}(R^{-1})\,\Gamma^j_{\mu\nu}(R) = \sum_R \Gamma^j_{\nu'\nu}(R^{-1}R) = \sum_R \Gamma^j_{\nu'\nu}(E) = h\,\delta_{\nu'\nu} = h\,\delta_{\nu\nu'}$$

$$\Rightarrow \; c^j_{\nu\nu'} = \frac{h}{l_j}\,\delta_{\nu\nu'} \qquad \Rightarrow \qquad \sum_R \Gamma^j_{\mu\nu}(R)\,\Gamma^j_{\nu'\mu'}(R^{-1}) = \frac{h}{l_j}\,\delta_{\nu\nu'}\,\delta_{\mu\mu'}$$

Summarizing, for every pair of representations Γ^j and $\Gamma^{j'}$ which are identical, not-equivalent or with different dimensionality (i.e. all together inequivalent) one can write the orthogonality relation

$$\sum_{R\in\mathcal{G}} \sqrt{\frac{l_j}{h}}\,\Gamma^{j}_{\mu\nu}(R)\,\sqrt{\frac{l_{j'}}{h}}\,\Gamma^{j'}_{\nu'\mu'}(R^{-1}) = \delta_{jj'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

The case of equivalent representation is easily deduced:

$$\Rightarrow \quad \exists U: \quad \Gamma^{j'}_{\nu'\mu'}(R^{-1}) = \sum_{\lambda\gamma} U^{-1}_{\nu'\lambda}\,\Gamma^{j}_{\lambda\gamma}\,U_{\gamma\mu'}$$

$$\Rightarrow \quad \sum_{R} \sqrt{\frac{l_j}{h}}\,\Gamma^{j}_{\mu\nu}(R)\sqrt{\frac{l_j}{h}}\sum_{\lambda\gamma} U^{-1}_{\nu'\lambda}\,\Gamma^{j}_{\lambda\gamma}(R^{-1})\,U_{\gamma\mu'} = \sum_{\lambda\gamma} U^{-1}_{\nu'\lambda}\,\delta_{\mu\gamma}\,\delta_{\nu\lambda}\,U_{\gamma\mu'} = U^{-1}_{\nu'\nu}\,U_{\mu\mu'}$$