

Lemma 1 *Let $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ be basis function partners for an irreducible representation Γ_n in group G . Then $\exists \hat{R} \in G$ such that $\langle \Gamma_n A | \hat{R} | \Gamma_n B \rangle \neq 0$.*

Proof. From the definition of the basis, we have

$$\langle \Gamma_n A | \hat{R} | \Gamma_n B \rangle = D^{(\Gamma_n)}(\hat{R})_{AB}$$

We will prove the lemma by contradiction. Assume $\forall \hat{R} \in G$ we have $\langle \Gamma_n A | \hat{R} | \Gamma_n B \rangle = 0$. Then $\forall \hat{R} \in G : D^{(\Gamma_n)}(\hat{R})_{AB} = 0$.

Then, following the approach of Dresselhaus, we define the projection operator $\hat{P}_{AB}^{(\Gamma_n)}$ like so:

$$\begin{aligned} \hat{P}_{AB}^{(\Gamma_n)} |\Gamma_n B\rangle &= |\Gamma_n A\rangle \\ \hat{P}_{AB}^{(\Gamma_n)} |\Psi\rangle &= 0 \quad \text{for} \quad \langle \Gamma_n B | \Psi \rangle = 0 \end{aligned}$$

From the orthogonality of basis functions we see immediately that $[\hat{H}, \hat{P}_{AB}^{(\Gamma_n)}]$, hence it can be expressed as the linear combination of the elements of G :

$$\begin{aligned} \hat{P}_{AB}^{(\Gamma_n)} &= \sum_R A_{AB}(\hat{R}) \hat{R} \\ \langle \Gamma_n A | \hat{P}_{AB}^{(\Gamma_n)} | \Gamma_n B \rangle &= \langle \Gamma_n A | \Gamma_n A \rangle = \sum_R A_{AB}(\hat{R}) \langle \Gamma_n A | \hat{R} | \Gamma_n B \rangle \\ 1 &= \sum_R A_{AB}(\hat{R}) D^{(\Gamma_n)}(\hat{R})_{AB} \end{aligned}$$

We have Schur's Wonderful Orthogonality Theorem:

$$\sum_R D^{(\Gamma_n)}(\hat{R})_{AB}^* D^{(\Gamma_n)}(\hat{R})_{AB} = \frac{|G|}{l_n}$$

where l_n is the dimension of Γ_n . Hence we identify

$$A_{AB}(\hat{R}) = \frac{l_n}{|G|} D^{(\Gamma_n)}(\hat{R})_{AB}^*$$

Then

$$\hat{P}_{AB}^{(\Gamma_n)} = \frac{l_n}{|G|} \sum_R D^{(\Gamma_n)}(\hat{R})_{AB}^* \hat{R} = 0$$

But $0 |\Gamma_n B\rangle = 0 \neq |\Gamma_n A\rangle$, which is a contradiction. This finishes the proof—either $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ aren't basis partners of Γ_n or Γ_n is reducible, with $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ belonging to different its subspaces.