

Lemma 1 *The following two statements are equivalent:*

(P1) *If $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ are partners in a basis for some representation Γ_n of a group G , then there exists an irreducible representation $\Gamma_n^i \in \{\Gamma^i(G)\}$ for which they form partners in its basis.*

(P2) *$\exists \hat{R} \in G$ such that $\langle \Gamma_n A | \hat{R} | \Gamma_n B \rangle \neq 0$*

Proof. We will first prove (P1) \rightarrow (P2) and then (P2) \rightarrow (P1). 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 (P1) \rightarrow (P2) 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 proves (P1) \rightarrow (P2).

Now we prove (P2) \rightarrow (P1) in almost the same fashion: we consider the representation Γ_n of which $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ are partner basis vectors. From (P2) we see that $\hat{P}_{AB}^{(\Gamma_n)} \neq 0$, since all elements $\hat{R} \in G$ are linearly independent in its group-element space. Now:

either Γ_n is itself an irrep of G or it can be decomposed into irreps of G . In the former case, the proof is finished; in the latter case:

$$D^{(\Gamma_n)}(\hat{R}) = \bigoplus_a c_a D^{(\Gamma_a^i)}(\hat{R})$$

such that $D^{(\Gamma_n)}(\hat{R})_{XY} = 0$ if X, Y don't belong to the same subspace of Γ_n —this is the definition of the block-diagonal form. However, if this were the case for A, B , then $\hat{P}_{AB}^{(\Gamma_n)} = 0$, which contradicts (P2). Hence $|\Gamma_n A\rangle, |\Gamma_n B\rangle$ belong to the same subspace of Γ_n and form partners in the basis of one of its constituent irreducible representations, Γ_m^i . QED.