GENERAL PROOF OF THE INTEGRAL EVALUATION THEOREM

To prove: $\int_{\substack{\text{all}\\\text{space}}} f_A f_B d\tau = 0$ unless the direct product representation $\{f_x f_y\}$ includes the totally symmetric irreducible representation as one of the components in its direct sum.

The proof will be in two steps:

(1) Show that the integrand $f_A f_B$ can be written as a linear combination of functions, $\{g_k^i\}$ which form the bases for the irreducible representations (i = 1, 2, etc., k = 1 to ℓ_i) contained in the direct sum for $\{f_x f_y\}$.

(2) Show that $\int_{\substack{\text{all}\\\text{space}}} g_k^i d\tau = 0$ unless i = totally symmetric irreducible representation.

STEP 1: The similarity transform $\underline{\underline{S}}$ which takes the direct product matrices into block diagonal form:

$$\underline{\underline{S}}^{-1}\,\underline{\underline{\Gamma}}^{AB}\,\underline{\underline{S}} = \underline{\underline{\Gamma}}_1 \oplus \underline{\underline{\Gamma}}_2 \ \cdots \ \text{etc.}$$

provides a transformation between the direct product basis $\{f_x f_y\}$ and the sets of functions $\{g_k^1\}$, $\{g_m^2\}$, etc. which form bases for the irreducible representations in the direct sum. Thus

$$f_A f_B = \sum_{k=1}^{\ell_1} (S^{-1})_{AB,k_1} g_k^1 + \sum_{m=1}^{\ell_2} (S^{-1})_{AB,m_2} g_m^2 + \text{etc.}$$

or figuratively

$f_A f_B$ = linear combination of [functions of symmetry 1 + functions of symmetry 2 + etc.]

and

$$\int_{\substack{\text{all}\\\text{space}}} f_A f_B d\tau = \text{linear combination}\left[\int_{\substack{\text{all}\\\text{space}}} g_k^i d\tau\right]$$

for the various basis functions (k's) in the irreducible representations (i's) in the direct product.

STEP 2: To prove $\int g_k^i d\tau = 0$ unless i is the totally symmetric irreducible representation.

LEMMA:

$$\sum_{\mathfrak{R}=1}^{h} (\Gamma_i(\hat{\mathfrak{R}}))_{km} = h\delta_{i,T.S.}$$

i.e. The sum of the h components in one of the "GOT" h-tuple vectors is zero unless the vector corresponds to the totally symmetric irreducible representation.

Proof (easy): Since all these vectors must be orthogonal to T.S. vector $(\Gamma_{T.S.}(\hat{\mathfrak{R}}))_{11} = 1$ for all $(\hat{\mathfrak{R}})$:

$$\sum_{\mathfrak{R}=1}^{h} (\Gamma_i(\hat{\mathfrak{R}}))_{km} = \sum_{\mathfrak{R}=1}^{h} (\Gamma_i(\hat{\mathfrak{R}}))_{km} (\Gamma_{T.S.}(\hat{\mathfrak{R}}))_{11} = h\delta_{i,T.S.}$$

A general point in "all space" will be taken into h equivalent points by the operations $\hat{\mathfrak{R}}$. Summing these points in the integrand of

$$\int_{\substack{\text{all} \\ \text{space}}} g_k^i \, d\tau =$$

$$\int_{\text{"unique space"}} \sum_{\mathfrak{R}=1}^{h} \hat{\mathfrak{R}} g_k^i \, d\tau = \int \sum_{\mathfrak{R}=1}^{h} \sum_{m=1}^{\ell_i} (\Gamma_i(\hat{\mathfrak{R}}))_{km} g_m^i \, d\tau = \int \sum_{m=1}^{\ell_i} g_m^i \sum_{\mathfrak{R}=1}^{h} (\Gamma_i(\hat{\mathfrak{R}}))_{km} \, d\tau = 0$$

if i is not T.S.

Thus the values of the integrand at the h symmetry equivalent points will add up to (integrate to) zero unless g_k^i is basis function for totally symmetric irreducible representation, and we have proven the integral theorem.

The only "sticky" point remaining is for "non-general" points in all space, i.e., points lying on symmetry elements. Here the h operations will not yield unique points in the integrand. For these points $g_k^i = 0$ or a subset of the h $\hat{\mathfrak{R}}$ operations will yield a unique set of points in the integrand which sum to zero.