Note on orthogonality of partner functions

Steven G. Johnson, MIT Course 18.369

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One useful fact about partner functions of irreducible representations of a symmetry group G is this: **partner functions of different irreps are orthogonal**, for any inner product invariant under G. (For example, any even function is orthogonal to any odd function under any mirror-symmetric inner product, corresponding to the well-known fact that $\int \text{even} \cdot \text{odd} = 0$ if the integration domain is mirror-symmetric.) More precisely:

- A **symmetrical inner product** $\langle \cdot, \cdot \rangle$ is one for which $\langle u, v \rangle = \langle \hat{g}u, \hat{g}v \rangle$ for any $g \in G$ (rotations and/or translations). i.e. the inner product has symmetry G if the symmetry operations $\hat{g}$ are **unitary** in that inner product.
- Let $\phi_i^{(\alpha)}$ be an i-th partner function of irrep $D^{(\alpha)}$ of G (where $i \in 1 \ldots d_\alpha$, the dimension of $D^{(\alpha)}$), and let $\psi_j^{(\beta)}$ be a j-th partner function of irrep $D^{(\beta)}$.
- It follows that $\langle \phi_i^{(\alpha)}, \psi_j^{(\beta)} \rangle = 0$ unless $\alpha = \beta$ and $i = j$, for any symmetrical inner product.

The proof follows straightforwardly from the definition of partner functions and from the "great orthogonality theorem" (also called the Schur orthogonality relations) of the irreps. In particular:

$$\begin{aligned}
\langle \phi_i^{(\alpha)}, \psi_j^{(\beta)} \rangle &= \frac{1}{|G|} \sum_{g \in G} \langle \hat{g}\phi_i^{(\alpha)}, \hat{g}\psi_j^{(\beta)} \rangle && \text{(by symmetry of } \langle \cdot, \cdot \rangle\text{)} \\
&= \frac{1}{|G|} \sum_{g \in G} \left\langle \sum_{i'=1}^{d_\alpha} \phi_{i'}^{(\alpha)} D_{i'i}^{(\alpha)}(g), \sum_{j'=1}^{d_\beta} \psi_{j'}^{(\beta)} D_{j'j}^{(\beta)}(g) \right\rangle && \text{(definition of partner func.)} \\
&= \frac{1}{|G|} \sum_{i',j'} \left[\langle \phi_{i'}^{(\alpha)}, \psi_{j'}^{(\beta)} \rangle \sum_{g \in G} D_{i'i}^{(\alpha)}(g)^* D_{j'j}^{(\beta)}(g) \right] && \text{(bilinearity of } \langle \cdot, \cdot \rangle\text{)} \\
&= \frac{1}{d_\alpha} \sum_{i',j'} \left[\langle \phi_{i'}^{(\alpha)}, \psi_{j'}^{(\beta)} \rangle \delta_{\alpha\beta} \delta_{i'j'} \delta_{ij} \right] && \text{(great orthogonality theorem)} \\
&= 0 \text{ unless } i = j \text{ and } \alpha = \beta. && \text{Q.E.D.}
\end{aligned}$$