7. Products and matrix elements

Based on the properties of group representations, a number of useful results can be derived. Consider a vector space $\mathcal{V}$ with an inner product $\langle\psi|\phi\rangle$ of vectors $\psi, \phi \in \mathcal{V}$ and suppose a group action $\mathsf{D}(\mathcal{G})$ of the group $\mathcal{G}$ has been defined on $\mathcal{V}$. Any vector $\psi \in \mathcal{V}$ can be used to generate a subspace, spanned by $\{\mathsf{D}_R\psi$ for all $R \in \mathcal{G}\}$, which is invariant under $\mathcal{G}$ and hence carries a representation, generally reducible, of $\mathcal{G}$. This representation can be reduced to a direct sum of irreps, generating a basis for the invariant subspace in which each basis vector is a basis vector of some irrep of $\mathcal{G}$. These basis vectors can be denoted $\psi_i^{(\mu)}$, where μ identifies the relevant irrep and i, which can range from 1 to d_μ, the dimension of the irrep, is said to label the *row* of the irrep.

This procedure can be repeated, starting with a vector in $\mathcal{V}$ which is not in the invariant subspace already analysed. In this way, a basis of $\mathcal{V}$ can be generated in which every basis vector is labeled with an irrep index μ and a row index i. Linear combinations of basis vectors, all having the same irrep and row indices, will then have well defined irrep and row indices. Such vectors are of considerable interest.

Consider, for instance, the inner product of two vectors belonging to specified rows of irreps of the group $\mathcal{G}$ of order g. A typical inner product is $\langle\psi_i^{(\mu)}|\phi_j^{(\nu)}\rangle$. If the elements of $\mathcal{G}$ operate as unitary operators in $\mathcal{V}$, then $\langle\psi_i^{(\mu)}|\phi_j^{(\nu)}\rangle = \langle\mathsf{D}_R\psi_i^{(\mu)}|\mathsf{D}_R\phi_j^{(\nu)}\rangle$ for each $R \in \mathcal{G}$. It follows that

$$\begin{aligned}
\langle\psi_i^{(\mu)}|\phi_j^{(\nu)}\rangle &= \sum_{R\in\mathcal{G}} \langle\mathsf{D}_R\psi_i^{(\mu)}|\mathsf{D}_R\phi_j^{(\nu)}\rangle/g \\
&= \sum_{R\in\mathcal{G}}\sum_{kl} \langle(\mathcal{D}_R^{(\mu)})_{ki}\psi_k^{(\mu)}|(\mathcal{D}_R^{(\nu)})_{lj}\phi_l^{(\nu)}\rangle/g \\
&= \sum_{R\in\mathcal{G}}\sum_{kl} (\mathcal{D}_R^{(\mu)})^*_{ki}(\mathcal{D}_R^{(\nu)})_{lj}\langle\psi_k^{(\mu)}|\phi_l^{(\nu)}\rangle/g \\
&= \sum_{kl} \langle\psi_k^{(\mu)}|\phi_l^{(\nu)}\rangle\delta_{\mu\nu}\delta_{kl}\delta_{ij}/d_\mu \\
&= \delta_{\mu\nu}\delta_{ij}\sum_k \langle\psi_k^{(\mu)}|\phi_k^{(\nu)}\rangle/d_\mu. \qquad (1)
\end{aligned}$$

This inner product is diagonal in the irrep (vanishes unless $\mu = \nu$), diagonal in the row (vanishes unless $i = j$) and its value is independent of the row (because of the average over the row index k). Vectors belonging to different irreps or to different rows of the same irrep are orthogonal and the overlap between vectors belonging to the same row of an irrep is independent of the row.

Given an $n \times n$ matrix $\mathcal{A}$ and an $m \times m$ matrix $\mathcal{B}$, their *outer product* or *Kronecker product* is an $nm \times nm$ matrix $\mathcal{A} \times \mathcal{B}$, where $(\mathcal{A} \times \mathcal{B})_{ij,kl} = (\mathcal{A})_{ik}(\mathcal{B})_{jl}$. The Kronecker product of two representations, $\mathsf{D}_R^{(\mu)} \times \mathsf{D}_R^{(\nu)}$, sometimes denoted $\mathsf{D}_R^{(\mu\times\nu)}$, is itself a representation, in which the representation matrices are Kronecker products of the matrices of the component representations.

$[(\mathcal{D}_R^{(\mu\times\nu)}\mathcal{D}_S^{(\mu\times\nu)})_{ij,kl} = \sum_{mn}(\mathcal{D}_R^{(\mu\times\nu)})_{ij,mn}(\mathcal{D}_S^{(\mu\times\nu)})_{mn,kl}$
$= \sum_{mn}(\mathcal{D}_R^{(\mu)})_{im}(\mathcal{D}_R^{(\nu)})_{jn}(\mathcal{D}_S^{(\mu)})_{mk}(\mathcal{D}_S^{(\nu)})_{nl} = (\mathcal{D}_{RS}^{(\mu)})_{ik}(\mathcal{D}_{RS}^{(\nu)})_{jl}$
$= (\mathcal{D}_{RS}^{(\mu\times\nu)})_{ij,kl}.]$

In general, the $d_\mu d_\nu$-dimensional representation $\mathsf{D}^{(\mu\times\nu)}$ is reducible, even when $\mathsf{D}^{(\mu)}, \mathsf{D}^{(\nu)}$ are both irreps. In particular, when $\mu = \nu$, the product representation can always be reduced to symmetric and antisymmetric parts.

[If $\{\psi_i^{(\mu)}\}, \{\phi_j^{(\nu)}\}$ are bases for the irreps $\mathsf{D}^{(\mu)}, \mathsf{D}^{(\nu)}$, then $\{\psi_i^{(\mu)}\phi_j^{(\nu)}\}$ is a basis for $\mathsf{D}^{(\mu\times\nu)}$. When $\mu = \nu$, $\{\psi_i^{(\mu)}\phi_j^{(\mu)} + \psi_j^{(\mu)}\phi_i^{(\mu)}\}$ is a basis for the $d_\mu(d_\mu+1)/2$-dimensional symmetric representation $\mathsf{D}^{[\mu\times\mu]}$ and $\{\psi_i^{(\mu)}\phi_j^{(\mu)} - \psi_j^{(\mu)}\phi_i^{(\mu)}\}$ is a basis for the $d_\mu(d_\mu-1)/2$-dimensional antisymmetric representation $\mathsf{D}^{\{\mu\times\mu\}}$. For the special case $\psi = \phi$, only the symmetric representation exists. (See further details in the appendix.)]

From the definition of the Kronecker product, the character $\sum_{ij}(\mathcal{D}_R^{(\mu\times\nu)})_{ij,ij}$ is $\chi_R^{(\mu\times\nu)} = \chi_R^{(\mu)}\chi_R^{(\nu)}$, for all $R \in \mathcal{G}$. [For $\mu = \nu$, $\chi_R^{[\mu\times\mu]} = (\chi_R^{(\mu)})^2/2 + \chi_{R^2}^{(\mu)}/2$ and $\chi_R^{\{\mu\times\mu\}} = (\chi_R^{(\mu)})^2/2 - \chi_{R^2}^{(\mu)}/2$.]

If one of the irreps (say ν) in the product is one-dimensional, then its characters all satisfy $|\chi_R^{(\nu)}| = 1$ and the sum $\sum_{R\in\mathcal{G}}|\chi_R^{(\mu\times\nu)}|^2 = \sum_{R\in\mathcal{G}}|\chi_R^{(\mu)}|^2|\chi_R^{(\nu)}|^2 = \sum_{R\in\mathcal{G}}|\chi_R^{(\mu)}|^2 = g$ (since μ is an irrep), which means the product representation $\mu \times \nu$ is irreducible. The product of an irrep with a one-dimensional irrep is an irrep.

The product representation can be decomposed as $\mathsf{D}^{(\mu\times\nu)} = \sum_\rho a_\rho \mathsf{D}^{(\rho)}$, which is known as the *Clebsch-Gordan series*, where the non-negative integer $a_\rho = \sum_k g_k \chi_k^{(\mu)}\chi_k^{(\nu)}\chi_k^{(\rho)*}/g$ and $\sum_\rho a_\rho d_\rho = d_\mu d_\nu$. Irreps ρ for which $a_\rho = 0$ do not appear in the Clebsch-Gordan series.The basis functions of the irreps are $\Psi_l^{\rho,\alpha_\rho} = \sum_{ij}(\mu i \nu j|\rho\alpha_\rho l)\psi_i^{(\mu)}\phi_j^{(\nu)}$, which defines the *Clebsch-Gordan* *coefficients* $(\mu i\nu j|\rho\alpha_\rho l)$. The additional index α_ρ is a multiplicity index, since the same irrep $\mathsf{D}^{(\rho)}$ may occur a number of times in the decomposition. If a particular irrep ρ does not appear in the Clebsch-Gordan series, the corresponding Clebsch-Gordan coefficient can be taken to vanish. If attention is restricted to unitary representations, the Clebsch-Gordan transformation is itself unitary and can be inverted, $\psi_i^{(\mu)}\phi_j^{(\nu)} = \sum_{\rho,\alpha_\rho,l}(\mu i\nu j|\rho\alpha_\rho l)^*\Psi_l^{\rho,\alpha_\rho}$.

[Now $\mathsf{D}_R(\psi_i^{(\mu)}\phi_j^{(\nu)}) = \sum_{mn}(\mathcal{D}_R^{(\mu)})_{mi}(\mathcal{D}_R^{(\nu)})_{nj}\psi_m^{(\mu)}\phi_n^{(\nu)}$ and $\mathsf{D}_R\Psi_l^{\rho,\alpha_\rho} = \sum_r(\mathcal{D}_R^{(\rho)})_{rl}\Psi_r^{\rho,\alpha_\rho} = \sum_{rmn}(\mathcal{D}_R^{(\rho)})_{rl}(\mu m\nu n|\rho\alpha_\rho r)\psi_m^{(\mu)}\phi_n^{(\nu)}$. The basis vectors are linearly independent, so
$(\mathcal{D}_R^{(\mu)})_{mi}(\mathcal{D}_R^{(\nu)})_{nj} = \sum_{\rho,\alpha_\rho,lr}(\mu m\nu n|\rho\alpha_\rho r)(\mu i\nu j|\rho\alpha_\rho l)^*(\mathcal{D}_R^{(\rho)})_{rl}$,
where it is assumed that the same representation matrices $\mathcal{D}^{(\rho)}(R)$ are used for each occurrence of the irrep $\mathsf{D}^{(\rho)}$.]

Suppose some physical operator acts in the carrier space $\mathcal{V}$. The matrix elements $\langle\psi|\mathcal{O}|\phi\rangle$ are of interest. For a unitary group action, $\langle\psi|\mathcal{O}|\phi\rangle = \langle\mathsf{D}_R\psi|\mathsf{D}_R\mathcal{O}|\phi\rangle = \langle\mathsf{D}_R\psi|\mathsf{D}_R\mathcal{O}\mathsf{D}_{R^{-1}}|\mathsf{D}_R\phi\rangle$. It is evident that operators will transform under the action of the group as $\mathsf{D}_R\mathcal{O}(D_R)^{-1}$. The set of transformed operators $\{\mathsf{D}_R\mathcal{O}(D_R)^{-1}\}$, for all $R\in\mathcal{G}$, is closed under the action of the group and generates an invariant space of operators which carries a (generally reducible) representation of $\mathcal{G}$. This representation can be decomposed into a sum of irreps, the bases of which are *tensor operators* $\mathcal{O}_i^{(\mu)}$ transforming as $\mathsf{D}_R\mathcal{O}_i^{(\mu)}\mathsf{D}_{R^{-1}} = \sum_{j=1}^{d_\mu}(\mathcal{D}_R^{(\mu)})_{ji}\mathcal{O}_j^{(\mu)}$.

Of particular interest are matrix elements of tensor operators between vectors belonging to specified irreps. Parallel to the earlier treatment of overlaps between vectors, these matrix elements may be seen to satisfy

$$\begin{aligned}
\langle\psi_i^{(\mu)}|\mathcal{O}_k^{(\rho)}|\phi_j^{(\nu)}\rangle &= \sum_{R\in\mathcal{G}}\langle\mathsf{D}_R\psi_i^{(\mu)}|\mathsf{D}_R\mathcal{O}_k^{(\rho)}\mathsf{D}_{R^{-1}}|\mathcal{D}_R\phi_j^{(\nu)}\rangle/g \\
&= \sum_{R\in\mathcal{G}}\sum_{lmn}(\mathcal{D}_R^{(\mu)})_{li}^*(\mathcal{D}_R^{(\rho)})_{nk}(\mathcal{D}_R^{(\nu)})_{mj}\langle\psi_l^{(\mu)}|\mathcal{O}_n^{(\rho)}|\phi_m^{(\nu)}\rangle/g \\
&= \sum_{R\in\mathcal{G}}\sum_{lmn}(\mathcal{D}_R^{(\mu)})_{li}^*\sum_{\sigma\alpha_\sigma rs}(\rho n\nu m|\sigma\alpha_\sigma r)(\rho k\nu j|\sigma\alpha_\sigma s)^*(\mathcal{D}_R^{(\sigma)})_{rs}\langle\psi_l^{(\mu)}|\mathcal{O}_n^{(\rho)}|\phi_m^{(\nu)}\rangle/g \\
&= \sum_{lmn}\sum_{\sigma\alpha_\sigma rs}\delta_{\mu\sigma}\delta_{lr}\delta_{is}(\rho n\nu m|\sigma\alpha_\sigma r)(\rho k\nu j|\sigma\alpha_\sigma s)^*\langle\psi_l^{(\mu)}|\mathcal{O}_n^{(\rho)}|\phi_m^{(\nu)}\rangle/d_\mu \\
&= \sum_{\alpha_\mu}(\rho k\nu j|\mu\alpha_\mu i)^*\left[\sum_{lmn}(\rho n\nu m|\mu\alpha_\mu l)\langle\psi_l^{(\mu)}|\mathcal{O}_n^{(\rho)}|\phi_m^{(\nu)}\rangle\right]/d_\mu. \qquad (2)
\end{aligned}$$

The dependence of the matrix element on the row indices i, j, k is expressed entirely through the Clebsch-Gordan coefficient $(\rho k\nu j|\mu\alpha_\mu i)^*$. This coefficient also contains implicitly selection rules arising from the Clebsch-Gordan series. This very powerful result is the *Wigner-Eckart theorem.* It is often written $\langle\psi_i^{(\mu)}|\mathcal{O}_k^{(\rho)}|\phi_j^{(\nu)}\rangle = \sum_{\alpha_\mu}(\rho k\nu j|\mu\alpha_\mu i)^*\langle\psi^{(\mu)}||\mathcal{O}^\rho||\phi^\nu\rangle$, where the "double-barred" matrix element is called a *reduced matrix element* and depends only on irrep labels, not on row labels.

Given the prominent role played by row labels in the above development, it would clearly be useful to have a more systematic way of labeling the rows of irreps than the simple enumeration $1, 2, \ldots, d_\mu$. A step in this direction is provided by the judicious use of subgroups.

Suppose $\mathcal{H}$ is a proper subgroup of $\mathcal{G}$. Any irrep of $\mathcal{G}$ is obviously also a representation of $\mathcal{H}$, since all the elements of $\mathcal{H}$ are also elements of $\mathcal{G}$. However, an invariant subspace with respect to $\mathcal{G}$ which contains no smaller invariant subspace relative to $\mathcal{G}$ may contain invariant subspaces relative to $\mathcal{H}$, since the latter is made up of only some of the elements of $\mathcal{G}$. So, in general, an irrep of $\mathcal{G}$ will be a reducible representation of $\mathcal{H}$. Decomposition of this representation into irreps of $\mathcal{H}$ will split the invariant subspace carrying the irrep of $\mathcal{G}$ into invariant subspaces (relative to $\mathcal{H}$) carrying irreps of $\mathcal{H}$. The basis functions of the irrep of $\mathcal{G}$ can be classified according to the irreps of $\mathcal{H}$ to which they belong. This provides an additional label, a partial row label. Repeating the process with a subgroup of $\mathcal{H}$ could further refine the labeling of the basis of the original irrep of $\mathcal{G}$. A chain of nested subgroups could supply rich labels and, in particularly fortunate cases, could even produce a complete labeling of row vectors.

> [Take the symmetric group on n objects $\mathcal{S}_n$ as an example. It contains subgroups isomorphic to $\mathcal{S}_{n-1}$. (Just think of all permutations keeping one object fixed.) These, in turn, contain subgroups $\mathcal{S}_{n-2}$; these, in their turn, $\mathcal{S}_{n-3}$, etc. The irreps of all the $\mathcal{S}_m$ in the chain serve to label completely the rows of every irrep of $\mathcal{S}_n$. In the specific case of $\mathcal{S}_3$, for instance, there is a two-dimensional irrep of mixed symmetry. The subgroup $\mathcal{S}_2$ leaving the first object unpermuted has only one-dimensional irreps, the unit irrep and the alternating irrep. The two basis functions of the two-dimensional irrep of $\mathcal{S}_3$ can be labeled as symmetric or antisymmetric under exchange of the second and third objects.]

Appendix

A. Symmetrised product representation

$$\begin{aligned}
\mathsf{D}_R\left[\psi_i^{(\mu)}\phi_j^{(\mu)}+\psi_j^{(\mu)}\phi_i^{(\mu)}\right] &= \sum_{kl}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}\psi_k^{(\mu)}\phi_l^{(\mu)}+(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\psi_k^{(\mu)}\phi_l^{(\mu)}\right]\\
&= \sum_{kl}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}+(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\right]\psi_k^{(\mu)}\phi_l^{(\mu)}\\
&= \sum_{kl}\frac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}+(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\right]\cdot\left[\psi_k^{(\mu)}\phi_l^{(\mu)}+\psi_l^{(\mu)}\phi_k^{(\mu)}\right]
\end{aligned}$$

$$\Longrightarrow (\mathcal{D}_R^{[\mu\times\mu]})_{ij,kl}=\tfrac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ik}(\mathcal{D}_R^{(\mu)})_{jl}+(\mathcal{D}_R^{(\mu)})_{jk}(\mathcal{D}_R^{(\mu)})_{il}\right]$$

$$\begin{aligned}
\Longrightarrow \chi_R^{[\mu\times\mu]} &= \sum_{ij}\frac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ii}(\mathcal{D}_R^{(\mu)})_{jj}+(\mathcal{D}_R^{(\mu)})_{ji}(\mathcal{D}_R^{(\mu)})_{ij}\right]\\
&= \frac{1}{2}(\chi_R^{(\mu)})^2+\frac{1}{2}\chi_{R^2}^{(\mu)}
\end{aligned}$$

B. Antisymmetrised product representation

$$\begin{aligned}
\mathsf{D}_R\left[\psi_i^{(\mu)}\phi_j^{(\mu)}-\psi_j^{(\mu)}\phi_i^{(\mu)}\right] &= \sum_{kl}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}\psi_k^{(\mu)}\phi_l^{(\mu)}-(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\psi_k^{(\mu)}\phi_l^{(\mu)}\right]\\
&= \sum_{kl}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}-(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\right]\psi_k^{(\mu)}\phi_l^{(\mu)}\\
&= \sum_{kl}\frac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ki}(\mathcal{D}_R^{(\mu)})_{lj}-(\mathcal{D}_R^{(\mu)})_{kj}(\mathcal{D}_R^{(\mu)})_{li}\right]\cdot\left[\psi_k^{(\mu)}\phi_l^{(\mu)}-\psi_l^{(\mu)}\phi_k^{(\mu)}\right]
\end{aligned}$$

$$\Longrightarrow (\mathcal{D}_R^{\{\mu\times\mu\}})_{ij,kl}=\tfrac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ik}(\mathcal{D}_R^{(\mu)})_{jl}-(\mathcal{D}_R^{(\mu)})_{jk}(\mathcal{D}_R^{(\mu)})_{il}\right]$$

$$\begin{aligned}
\Longrightarrow \chi_R^{\{\mu\times\mu\}} &= \sum_{ij}\frac{1}{2}\left[(\mathcal{D}_R^{(\mu)})_{ii}(\mathcal{D}_R^{(\mu)})_{jj}-(\mathcal{D}_R^{(\mu)})_{ji}(\mathcal{D}_R^{(\mu)})_{ij}\right]\\
&= \frac{1}{2}(\chi_R^{(\mu)})^2-\frac{1}{2}\chi_{R^2}^{(\mu)}
\end{aligned}$$

C. Clebsch–Gordan coefficients in Dirac notation

In Dirac notation, Clebsch–Gordan coefficients can be treated very naturally. Denote a basis vector belonging to the i-th row of the irrep μ by $|\mu i\rangle$. The basis vectors for the product representation $\mu\times\nu$ are then $|\mu i\rangle|\nu j\rangle$, denoted $|\mu i\nu j)$. The product representation is generally reducible to block diagonal form, with irreps along the main diagonal. The basis vectors for the irreps are denoted $|\mu\nu\rho\alpha_\rho k)$, where ρ labels the irrep, k labels the row and α_ρ labels different occurrences of the same irrep ρ along the diagonal. (Note that the irrep basis vectors still carry the labels μ and ν of the two irreps being multiplied, but not their row labels.) There are $d_\mu d_\nu$ basis vectors all told, where d_σ is the dimension of the irrep σ.

In Dirac notation, the resolution of the identity reads

$$\mathbf{1} = \sum_{ij} |\mu i \nu j)(\mu i \nu j|,$$

from which follows

$$\begin{aligned} |\mu\nu\rho\alpha_\rho k) &= \mathbf{1}|\mu\nu\rho\alpha_\rho k) \\ &= \sum_{ij} |\mu i \nu j)(\mu i \nu j|\mu\nu\rho\alpha_\rho k) \\ &= \sum_{ij} (\mu i \nu j|\mu\nu\rho\alpha_\rho k)|\mu i \nu j). \end{aligned}$$

In this form, it is easy to identify the Clebsch–Gordan coefficient $(\mu i \nu j|\mu\nu\rho\alpha_\rho k)$. In the interest of economy, the superfluous second pair of labels $\mu\nu$ is generally omitted, so the coefficient is written $(\mu i \nu j|\rho\alpha_\rho k)$.

Alternatively, the resolution of the identity could read

$$\mathbf{1} = \sum_{\rho\alpha_\rho k} |\mu\nu\rho\alpha_\rho k)(\mu\nu\rho\alpha_\rho k|,$$

from which follows, in parallel with the same steps as above,

$$|\mu i \nu j) = \sum_{\rho\alpha_\rho k} (\mu\nu\rho\alpha_\rho k|\mu i \nu j)|\mu\nu\rho\alpha_\rho k).$$

By the usual rules of Dirac notation, the expansion coefficient here is related to the previous one by $(\mu\nu\rho\alpha_\rho k|\mu i \nu j) = (\mu i \nu j|\rho\alpha_\rho k)^*$.