Rotation Matrices

If a rotation \( R \) is specified by \( \theta \) and \( \phi \), we can define the matrix elements by

\[
D^{(j)}_{m', m} (R) = \langle j, m' | \exp \left( -i \hat{O} \cdot \mathbf{\hat{R}} \right) | j, m \rangle
\]

These matrix elements are sometimes called Wigner functions after E.P. Wigner.

Note that

\[
J^2 D(R) | j, m \rangle = J(\hat{J} J) D(R) | j, m \rangle
\]

since \( J^2 \) commutes with \( \hat{J} \).

Often the \((2j+1)(2j+1)\) matrix formed by \( D^{(j)}_{m', m} (R) \) is referred to as the \((2j+1)\)-dimensional irreducible representation of \( D(R) \).

Properties

\[
\sum_{m'} (j) D^{(j)}_{m', m} (R) D^{(j)}_{m', m} (R') = D^{(j)}_{m', m} (R R')
\]

\[
D_{m', m} (R^{-1}) = D_{m', m} (R) \quad \text{unitary}
\]

If we make a rotation of a state \( | j, m \rangle \)

\[
| j, m \rangle \rightarrow D(R) | j, m \rangle \quad \text{the state can contain } m' \text{ values different to } m. \text{ To obtain that}
\]
\[ D(\mathbf{R})_{i,m} = \sum_{m'} D^{(3)}_{i,m'} \mathbf{R}_{m',m} \]

We can also write \( D(\mathbf{R}) \) in terms of the Euler angles:

\[ D_{m,m} (\theta, \phi, \chi) = \langle m, m' \mid \exp(-i\phi \mathbf{J}_2) \exp(-i\chi \mathbf{J}_3) \exp(-i\theta \mathbf{J}_1) \rangle_{m'} \]

\[ = \varepsilon^{(m, m + \chi)} \langle m, m' \mid \exp(-i\phi \mathbf{J}_2) \rangle_{m'} \]

**Vector Operator:**

Classical Physics: vector means \( \mathbf{V}_i \rightarrow \frac{\partial}{\partial \mathbf{R}_i} \mathbf{V}_i \)

under rotation \( \mathbf{R} \):

Quantum Physics:

\[ \langle \mathbf{d} \mid \mathbf{V}_i \rangle_{\mathbf{d}} = \frac{\partial}{\partial \mathbf{R}_i} \mathbf{V}_i \]

Covariant Tensors vs Irreducible Tensors

Classical Physics

Task: \( \varepsilon_{ij} \frac{\partial}{\partial \mathbf{R}_i} \mathbf{R}_j \rightarrow \varepsilon_{ij} \frac{\partial}{\partial \mathbf{R}_i} \mathbf{R}_j \mathbf{R}_k \)

Cartesian Tensor

The number of indices is called the rank of the tensor.
The simplest example of a Cartesian tensor of rank 2 is a dyadic formed out of \( \mathbf{u} \) and \( \mathbf{v} \):

\[
T_{ij} = U_i V_j
\]

- Have 9 components
- Each transforms under rotation

The issue with Cartesian tensors is that they are reducible: They can be decomposed into objects that transform differently under rotation.

Specifically for the dyadic,

\[
U_i U_j = \frac{\mathbf{u} \cdot \mathbf{v}}{3} \delta_{ij} + \left( \frac{U_i U_j - U_i V_j}{U_i + U_j - 2 \mathbf{u} \cdot \mathbf{v}} \right)
\]

- The first term \( \mathbf{u} \cdot \mathbf{v} \) is a scalar: invariant under rotation
- The second is an antisymmetric tensor which can be written as a vector \( E_i (\mathbf{u} \times \mathbf{v}) \). It has 3 independent components
- The third one is a 3x3 symmetric traceless vector with 5 independent components

\[3 \times 3 = 1 + 3 + 5\]

The number of independent components checks as

Note the r.h.s are explicitly multiplicities
\( \ell = 0 \quad \ell = 1 \quad \ell = 2 \)
Thus suggest that the dyadic can be "reduced" into "irreducible" spherical tensors. One can identify a spherical tensor as

\[ T_{\ell q} = Y_{\ell=-q}^{m} (\mathbf{v}) \]

To see the transformation of spherical tensors under rotation

\[ (\mathbf{n}) \rightarrow \mathbf{D}(\mathbf{R}) \mathbf{n} = \mathbf{n}' \]

We note that

\[ y_{\ell}^{m} (\mathbf{n}') = \langle \mathbf{n}' | \ell m \rangle \]

thus the tensors of \( T_{\ell m} (\mathbf{n}) \)

\[ \mathbf{D}(\mathbf{R})^{(\ell m)} = \sum_{m'} y_{\ell}^{m'} (\mathbf{n}) \mathbf{D}_{m m'} (\mathbf{R})^{(\ell m')} \]

Then one expects that for an operator that acts linearly

\[ \mathbf{D}^{+ (\ell m)} T_{\ell m} (\mathbf{R}) = \sum_{m'} y_{\ell}^{m'} (\mathbf{n}) \mathbf{D}_{m m'} (\mathbf{R})^{(\ell m')} \]

Motivated by this we define a spherical tensor of rank \( k \) as
\[ D^+(R) T_{q}^{(2)} D(R) = \sum_{q=1}^{n} D_{q}^{(2) \leftarrow (k)} T_{q}^{(2)} \]

or

\[ D(R) T_{q}^{(2)} D^+(R) D^+(R) = \sum_{q=1}^{n} D_{q}^{(2) \leftarrow (k)} T_{q}^{(2)} \]

Explicit Spherical Tensors

\[ T_{00}^{(2)} = -\frac{U_{0} V_{0}}{3} \left( U_{0} V_{0} + U_{1} V_{0} - U_{0} V_{0} \right) \]

\[ T_{11}^{(2)} = \frac{(U x V)_{y}}{\sqrt{2}} \]

\[ T_{12}^{(2)} = U_{0} V_{0} \]

\[ T_{-11}^{(2)} = U_{0} V_{0} + U_{0} V_{0} \]

\[ T_{0}^{(2)} = \frac{U_{0} V_{0} + 2 U_{0} V_{0} + U_{1} V_{0}}{\sqrt{2}} \]
The Wigner–Eckart Theorem

m-selecion rule

\[ \langle d', i', m' | T_q^{(\omega)} | d, i, m \rangle = 0 \text{ unless } m' = g \pm m \]

Wigner–Eckart Theorem

\[ \langle d', i', m' | T_q^{(\omega)} | d, i, m \rangle = C(q, g | q, m, m') \frac{(-1)^{i'-g} / (2g+1)} \]

\[ \text{Dynamical element (e.g. rotoval #) independent of } m, m' \]

In other words, such a matrix element factors into a dynamical part: the reduced matrix element and a geometrical part: the Clebsch–Gordan coefficient that contains the rotational properties.

To evaluate \[ \langle d', i', m' | T_q^{(\omega)} | d, i, m \rangle \] it is sufficient to know only one of them, and we can know the value for all combinations of \( m', m \) and \( g \).