

Chapter 19

Angular momentum

In this chapter, we discuss the theory of angular momentum in quantum mechanics and applications of the theory to many practical problems. The relationship between group theory and the generators of the group are much simpler for the rotation group than the complete Galilean group we studied in Chapter 7 on symmetries. The use of angular momentum technology is particularly important in applications in atomic and nuclear physics. Unfortunately there is a lot of overhead to learn about before one can become reasonably knowledgeable in the field and a proficient calculator. But the effort is well worth it — with a little work, you too can become an “angular momentum technician!”

We start in this chapter with the eigenvalue problem for general angular momentum operators, followed by a discussion of spin one-half and spin one systems. We then derive the coordinate representation of orbital angular momentum wave functions. After defining parity and time-reversal operations on eigenvectors of angular momentum, we then discuss several classical descriptions of coordinate system rotations, followed by a discussion of how eigenvectors of angular momentum are related to each other in rotated systems. We then show how to couple two, three, and four angular momentum systems and introduce $3j$, $6j$, and $9j$ coupling and recoupling coefficients. We then define tensor operators and prove various theorems useful for calculations of angular momentum matrix elements, and end the chapter with several examples of interest from atomic and nuclear physics.

You will find in Appendix G, a presentation of Schwinger’s harmonic oscillator theory of angular momentum. This method, which involves Boson algebra, is very useful for calculation of rotation matrices and Clebsch-Gordan coefficients, but is not necessary for a general understanding of how to use angular momentum technology. We include it as a special topic, and use it to derive some general formulas.

A delightful collection of early papers on the quantum theory of angular momentum, starting with original papers by Pauli and Wigner, can be found in Biedenharn and Van Dam [1]. We adopt here the notation and conventions of the *latest edition* of Edmonds[2], which has become one of the standard reference books in the field.

19.1 Eigenvectors of angular momentum

The Hermitian angular momentum operators J_i , $i = 1, 2, 3$, obey the algebra:

$$[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \quad (19.1)$$

In this section, we prove the following theorem:

Theorem 33. *The eigenvalues and eigenvectors of the angular momentum operator obey the equations:*

$$\begin{aligned} J^2 |j, m\rangle &= \hbar^2 j(j+1) |j, m\rangle, \\ J_z |j, m\rangle &= \hbar m |j, m\rangle, \\ J_{\pm} |j, m\rangle &= \hbar A(j, \mp m) |j, m \pm 1\rangle, \end{aligned} \quad (19.2)$$

where $J_{\pm} = J_x \pm iJ_y$, and

$$A(j, m) = \sqrt{(j+m)(j-m+1)}, \quad A(j, 1 \pm m) = A(j, \mp m), \quad (19.3)$$

with

$$j = 0, 1/2, 1, 3/2, 2, \dots, \quad -j \leq m \leq j.$$

Proof. It is easy to see that $J^2 = J_z^2 + J_y^2 + J_x^2$ commutes with J_z : $[J^2, J_z] = 0$. Of course, J^2 commutes with any other component of \mathbf{J} . Thus, we can simultaneously diagonalize J^2 and any component of \mathbf{J} , which we choose to be J_z . We write these eigenvectors as $|\lambda, m\rangle$. They satisfy:

$$\begin{aligned} J^2 |\lambda, m\rangle &= \hbar^2 \lambda |\lambda, m\rangle, \\ J_z |\lambda, m\rangle &= \hbar m |\lambda, m\rangle. \end{aligned}$$

We now define operators, J_{\pm} by linear combinations of J_x and J_y : $J_{\pm} = J_x \pm iJ_y$, with the properties:

$$J_{\pm}^{\dagger} = J_{\mp}, \quad [J_z, J_{\pm}] = \pm \hbar J_{\pm}, \quad [J_+, J_-] = 2\hbar J_z$$

The total angular momentum can be written in terms of J_{\pm} and J_z in several ways. We have:

$$J^2 = \frac{1}{2}(J_- J_+ + J_+ J_-) + J_z^2 = J_+ J_- + J_z^2 - \hbar J_z = J_- J_+ + J_z^2 + \hbar J_z. \quad (19.4)$$

The ladder equations are found by considering,

$$J_z \{J_{\pm} |\lambda, m\rangle\} = (J_{\pm} J_z + [J_z, J_{\pm}]) |\lambda, m\rangle = \hbar(m \pm 1) \{J_{\pm} |\lambda, m\rangle\}.$$

Therefore $J_{\pm} |\lambda, m\rangle$ is an eigenvector of J_z with eigenvalue $\hbar(m \pm 1)$. So we can write:

$$\begin{aligned} J_+ |\lambda, m\rangle &= \hbar B(\lambda, m) |\lambda, m+1\rangle, \\ J_- |\lambda, m\rangle &= \hbar A(\lambda, m) |\lambda, m-1\rangle. \end{aligned} \quad (19.5)$$

But since $J_- = J_+^{\dagger}$, it is easy to show that $B(\lambda, m) = A^*(\lambda, m+1)$.

Using (19.4), we find that m is bounded from above and below. We have:

$$\langle \lambda, m | \{J^2 - J_z^2\} | \lambda, m \rangle = \hbar^2 (\lambda - m^2) = \frac{1}{2} \langle \lambda, m | (J_+^{\dagger} J_+ + J_-^{\dagger} J_-) | \lambda, m \rangle \geq 0.$$

So $0 \leq m^2 \leq \lambda$. Thus, for fixed $\lambda \geq 0$, m is bounded by: $-\sqrt{\lambda} \leq m \leq +\sqrt{\lambda}$. Thus there must be a maximum and a minimum m , which we call m_{\max} , and m_{\min} . This means that there must exist some ket, $|\lambda, m_{\max}\rangle$, such that:

$$\begin{aligned} J_+ |\lambda, m_{\max}\rangle &= 0, \\ \text{or, } J_- J_+ |\lambda, m_{\max}\rangle &= (J^2 - J_z^2 - \hbar J_z) |\lambda, m_{\max}\rangle \\ &= \hbar^2 (\lambda - m_{\max}^2 - m_{\max}) |\lambda, m_{\max}\rangle = 0, \end{aligned}$$

so $m_{\max}(m_{\max} + 1) = \lambda$. Similarly, there must exist some other ket, $|\lambda, m_{\min}\rangle$ such that:

$$\begin{aligned} J_- |\lambda, m_{\min}\rangle &= 0, \\ \text{or, } J_+ J_- |\lambda, m_{\min}\rangle &= (J^2 - J_z^2 + \hbar J_z) |\lambda, m_{\min}\rangle \\ &= \hbar^2 (\lambda - m_{\min}^2 + m_{\min}) |\lambda, m_{\min}\rangle = 0, \end{aligned}$$

so we find that $m_{\min}(m_{\min} - 1) = \lambda$. Therefore we must have

$$m_{\max}(m_{\max} + 1) = \lambda = m_{\min}(m_{\min} - 1),$$

Which means that either $m_{\min} = -m_{\max}$, which is possible, or $m_{\min} = m_{\max} + 1$, which is impossible! So we set $j = m_{\max} = -m_{\min}$, which defines j . Then $\lambda = m_{\max}(m_{\max} + 1) = m_{\min}(m_{\min} - 1) = j(j + 1)$. Now we must be able to reach $|\lambda, m_{\max}\rangle$ from $|\lambda, m_{\min}\rangle$ by applying J_+ in unit steps. This means that $m_{\max} - m_{\min} = 2j = n$, where $n = 0, 1, 2, \dots$ is an integer. So $j = n/2$ is *half-integral*.

We can find $A(j, m)$ and $B(j, m)$ by squaring the second of (19.5). We find:

$$\begin{aligned} \hbar^2 |A(j, m)|^2 \langle j, m-1 | j, m-1 \rangle &= \langle j, m | J_+ J_- | j, m \rangle, \\ &= \langle j, m | (J^2 - J_z^2 + \hbar J_z) | j, m \rangle, \\ &= \hbar^2 \{j(j+1) - m^2 + m\}, \\ &= \hbar^2 (j+m)(j-m+1). \end{aligned}$$

Taking $A(j, m)$ to be real (this is conventional), we find:

$$A(j, m) = \sqrt{(j+m)(j-m+1)},$$

which also determines $B(j, m) = A(j, m+1)$. This completes the proof. \square

Remark 28. Note that we used only the commutation properties of the components of angular momentum, and did not have to consider any representation of the angular momentum operators.

Remark 29. The appearance of half-integer quantum numbers for j is due to the fact that there exists a two-dimensional representation of the rotation group. We will discuss this connection in Section 19.2.4 below.

Remark 30. The eigenvectors of angular momentum $|j, m\rangle$ refer to a particular coordinate frame Σ , where we chose to find common eigenvectors of J^2 and J_z in that frame. We can also find common angular momentum eigenvectors of J^2 and $J_{z'}$, referred to some other frame Σ' , which is rotated with respect to Σ . We write these eigenvectors as $|j, m'\rangle$. They have the same values for j and m , and are an equivalent description of the system, and so are related to the eigenvectors $|j, m\rangle$ by a unitary transformation. We find these unitary transformations in Section 19.3 below.

19.1.1 Spin

The spin operator \mathbf{S} is a special case of the angular momentum operator. It may *not* have a coordinate representation. The possible eigenvalues for the magnitude of intrinsic spin are $s = 0, 1/2, 1, 3/2, \dots$

Spin one-half

The case when $s = 1/2$ is quite important in angular momentum theory, and we have discussed it in great detail in Chapter 13. We only point out here that the Pauli spin-1/2 matrices are a special case of the general angular momentum problem we discussed in the last section. Using the results of Theorem 33 for the case of $j = 1/2$, the matrix elements of the spin one-half angular momentum operator is given by:

$$\begin{aligned} \langle 1/2, m | (J_x + iJ_y) | 1/2, m' \rangle &= \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, & \langle 1/2, m | (J_x - iJ_y) | 1/2, m' \rangle &= \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \\ \langle 1/2, m | J_z | 1/2, m' \rangle &= \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \end{aligned}$$

So the matrices for spin-1/2 can be written in terms of the Pauli matrices by writing: $\mathbf{S} = (\hbar/2)\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = \sigma_x \hat{\mathbf{x}} + \sigma_y \hat{\mathbf{y}} + \sigma_z \hat{\mathbf{z}}$ is a matrix of unit vectors, and where the Pauli matrices are given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (19.6)$$

The Pauli matrices are Hermitian, traceless matrices which obey the algebra:

$$\begin{aligned} \sigma_i \sigma_j + \sigma_j \sigma_i &= 2\delta_{ij}, & \sigma_i \sigma_j - \sigma_j \sigma_i &= 2i\epsilon_{ijk}\sigma_k, \\ \text{or: } \sigma_i \sigma_j &= \delta_{ij} + i\epsilon_{ijk}\sigma_k, \end{aligned} \quad (19.7)$$

A spin one-half particle is fully described by a spinor $\chi(\theta, \phi)$ with two parameters of the form:

$$\chi(\theta, \phi) = \begin{pmatrix} e^{-i\phi/2} \cos(\theta/2) \\ e^{+i\phi/2} \sin(\theta/2) \end{pmatrix}, \quad (19.8)$$

where (θ, ϕ) is the direction of a unit vector $\hat{\mathbf{p}}$. $\chi(\theta, \phi)$ is an eigenvector of $\hat{\mathbf{p}} \cdot \boldsymbol{\sigma}$ with eigenvalue $+1$, i.e. spin-up in the $\hat{\mathbf{p}}$ direction. Here $\hat{\mathbf{p}}$ is called the **polarization** vector. The density matrix for spin one-half can be written in terms of just one unit vector ($\hat{\mathbf{p}}$) described by two polar angles (θ, ϕ) :

$$\rho(\hat{\mathbf{p}}) = \chi(\theta, \phi) \chi^\dagger(\theta, \phi) = \frac{1}{2} (1 + \hat{\mathbf{p}} \cdot \boldsymbol{\sigma}). \quad (19.9)$$

This result will be useful for describing a beam of spin one-half particles.

Spin one

The Deuteron has spin one. The spinor χ describing a spin one particle is a 3×1 matrix with three complex components. Since one of these is an overall phase, it takes eight real parameters to fully specify a spin-one spinor. In contrast, it takes only two real parameters to fully describe a spin one-half particle, as we found in the last section. The density matrix $\rho = \chi \chi^\dagger$ is a 3×3 Hermitian matrix and so requires nine basis matrices to describe it, one of which can be the unit matrix. That leaves eight more independent matrices which are needed. It is traditional to choose these to be combinations of the spin-one angular momentum matrices. From the results of Theorem 33, the matrix elements for the $j = 1$ angular momentum operator is given by:

$$\begin{aligned} \langle 1, m | (J_x + iJ_y) | 1, m' \rangle &= \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, & \langle 1, m | (J_x - iJ_y) | 1, m' \rangle &= \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \\ \langle 1, m | J_z | 1, m' \rangle &= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \end{aligned}$$

So let us put $\mathbf{J} = \hbar \mathbf{S}$, where

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (19.10)$$

The spin one angular momentum matrices obey the commutation relations: $[S_i, S_j] = i\epsilon_{ijk}S_k$. Also they are Hermitian, $S_i^\dagger = S_i$, and traceless: $\text{Tr}[S_i] = 0$. They also obey $\text{Tr}[S_i^2] = 2$ and $\text{Tr}[S_i S_j] = 0$. An additional five independent matrices can be constructed by the traceless symmetric matrix of Hermitian matrices S_{ij} , defined by:

$$S_{ij} = \frac{1}{2} (S_i S_j + S_j S_i) - \frac{1}{3} \mathbf{S} \cdot \mathbf{S}, \quad S_{ij}^\dagger = S_{ij}. \quad (19.11)$$

We also note here that $\text{Tr}[S_{ij}] = 0$ for all values of i and j . So then the density matrix for spin one particles can be written as:

$$\rho = \frac{1}{3} (1 + \mathbf{P} \cdot \mathbf{S} + \sum_{ij} T_{ij} S_{ij}), \quad (19.12)$$

and where \mathbf{P} is a real vector with three components and T_{ij} a real symmetric traceless 3×3 matrix with five components. So P_i and T_{ij} provide *eight* independent quantities that are needed to fully describe a beam of spin one particles.

Exercise 42. Find all independent matrix components of S_{ij} . Find all values of $\text{Tr}[S_i S_{jk}]$ and $\text{Tr}[S_{ij} S_{kl}]$. Use these results to find $\text{Tr}[\rho S_i]$ and $\text{Tr}[\rho S_{ij}]$ in terms of P_i and T_{ij} .

Exercise 43. Show that for spin one, the density matrix is idempotent: $\rho^2 = \rho$. Find any restrictions this places on the values of P_i and T_{ij} .

19.1.2 Orbital angular momentum

The orbital angular momentum for a single particle is defined as:

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}, \quad (19.13)$$

where \mathbf{R} and \mathbf{P} are operators for the position and momentum of the particle, and obey the commutation rules: $[X_i, P_i] = i\hbar \delta_{ij}$. Then it is easy to show that:

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k, \quad (19.14)$$

as required for an angular momentum operator. Defining as before $L_{\pm} = L_x \pm i L_y$, we write the eigenvalues and eigenvectors for orbital angular momentum as:

$$\begin{aligned} L^2 |\ell, m\rangle &= \hbar^2 \ell(\ell+1) |\ell, m\rangle, \\ L_z |\ell, m\rangle &= \hbar m |\ell, m\rangle, \\ L_{\pm} |\ell, m\rangle &= \hbar A(\ell, \mp m) |\ell, m \pm 1\rangle, \end{aligned} \quad (19.15)$$

for $-\ell \leq m \leq +\ell$, and $\ell = 0, 1, 2, \dots$. We will show below that ℓ has only integer values. We label eigenvectors of spherical coordinates by $|\hat{\mathbf{r}}\rangle \mapsto |\theta, \phi\rangle$, and define:

$$Y_{\ell, m}(\hat{\mathbf{r}}) = \langle \hat{\mathbf{r}} | \ell, m \rangle = \langle \theta, \phi | \ell, m \rangle = Y_{\ell, m}(\theta, \phi). \quad (19.16)$$

In the coordinate representation, $\tilde{\mathbf{L}}$ is a differential operator acting on functions:

$$\tilde{\mathbf{L}} Y_{\ell, m}(\theta, \phi) = \langle \hat{\mathbf{r}} | \mathbf{L} | \ell, m \rangle = \frac{\hbar}{i} \hat{\mathbf{r}} \times \nabla Y_{\ell, m}(\theta, \phi), \quad (19.17)$$

We can easily work out the orbital angular momentum in spherical coordinates. Using

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta,$$

with spherical unit vectors defined by:

$$\begin{aligned} \hat{\mathbf{r}} &= \sin \theta \cos \phi \hat{\mathbf{x}} + \sin \theta \sin \phi \hat{\mathbf{y}} + \cos \theta \hat{\mathbf{z}} \\ \hat{\phi} &= -\sin \phi \hat{\mathbf{x}} + \cos \phi \hat{\mathbf{y}} \\ \hat{\theta} &= \cos \theta \cos \phi \hat{\mathbf{x}} + \cos \theta \sin \phi \hat{\mathbf{y}} - \sin \theta \hat{\mathbf{z}}, \end{aligned}$$

we find that the gradient operator is given by:

$$\nabla = \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta}.$$

So the angular momentum vector is given by:

$$\tilde{\mathbf{L}} = \frac{\hbar}{i} \mathbf{r} \times \nabla = \frac{\hbar}{i} \left\{ \hat{\mathbf{r}} \times \hat{\phi} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + \hat{\mathbf{r}} \times \hat{\theta} \frac{\partial}{\partial \theta} \right\} = \frac{\hbar}{i} \left\{ -\hat{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} + \hat{\phi} \frac{\partial}{\partial \theta} \right\},$$

which is independent of the radial coordinate r . So from (19.17), we find:

$$\begin{aligned}\tilde{L}_x Y_{\ell,m}(\theta, \phi) &= \frac{\hbar}{i} \left\{ -\sin \phi \frac{\partial}{\partial \theta} - \frac{\cos \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi), \\ \tilde{L}_y Y_{\ell,m}(\theta, \phi) &= \frac{\hbar}{i} \left\{ +\cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\tan \theta} \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi), \\ \tilde{L}_z Y_{\ell,m}(\theta, \phi) &= \frac{\hbar}{i} \left\{ \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi),\end{aligned}$$

where $Y_{\ell,m}(\theta, \phi) = \langle \theta, \phi | \ell, m \rangle$. So we find

$$\tilde{L}_{\pm} Y_{\ell,m}(\theta, \phi) = \frac{\hbar}{i} e^{\pm i\phi} \left\{ \pm i \frac{\partial}{\partial \theta} - \frac{1}{\tan \theta} \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi),$$

and so

$$\begin{aligned}\tilde{L}^2 Y_{\ell,m}(\theta, \phi) &= \left\{ \frac{1}{2}(L_+ L_- + L_- L_+) + L_z^2 \right\} Y_{\ell,m}(\theta, \phi), \\ &= -\hbar^2 \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} Y_{\ell,m}(\theta, \phi),\end{aligned}$$

Single valued eigenfunctions of L^2 and L_z are the spherical harmonics, $Y_{\ell m}(\theta, \phi)$, given by the solution of the equations,

$$\begin{aligned}- \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right\} Y_{\ell,m}(\theta, \phi) &= \ell(\ell+1) Y_{\ell,m}(\theta, \phi), \\ \frac{1}{i} \left\{ \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi) &= m Y_{\ell,m}(\theta, \phi), \\ \frac{1}{i} e^{\pm i\phi} \left\{ \pm i \frac{\partial}{\partial \theta} - \frac{1}{\tan \theta} \frac{\partial}{\partial \phi} \right\} Y_{\ell,m}(\theta, \phi) &= A(\ell, \mp m) Y_{\ell, m \pm 1}(\theta, \phi),\end{aligned}\tag{19.18}$$

where $\ell = 0, 1, 2, \dots$, with $-\ell \leq m \leq \ell$, and $A(\ell, m) = \sqrt{(\ell+m)(\ell-m+1)}$. Note that the eigenvalues of the orbital angular momentum operator are integers. The half-integers eigenvalues of general angular momentum operators are missing from the eigenvalue spectra. This is because wave functions in coordinate space must be single valued.

Definition 33 (spherical harmonics). We define spherical harmonics by:

$$Y_{\ell,m}(\theta, \phi) = \begin{cases} \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} (-)^m e^{im\phi} P_{\ell}^m(\cos \theta), & \text{for } m \geq 0, \\ (-)^m Y_{\ell,-m}^*(\theta, \phi), & \text{for } m < 0. \end{cases}\tag{19.19}$$

where $P_{\ell}^m(\cos \theta)$ are the associated Legendre polynomials which are *real* and depend only on $|m|$. This is Condon and Shortly's definition [3], which is the same as Edmonds [2][pages 19–25] and is now standard.

The spherical harmonics defined here have the properties:

- The spherical harmonics are orthonormal and complete:

$$\int Y_{\ell m}^*(\Omega) Y_{\ell' m'}(\Omega) d\Omega = \delta_{\ell, \ell'} \delta_{m, m'}, \quad \sum_{\ell m} Y_{\ell m}^*(\Omega) Y_{\ell m}(\Omega') = \delta(\Omega - \Omega'),$$

where $d\Omega = d(\cos \theta) d\phi$.

- Under complex conjugation,

$$Y_{\ell,m}^*(\theta, \phi) = (-)^m Y_{\ell,-m}(\theta, \phi). \quad (19.20)$$

- Under space inversion:

$$Y_{\ell,m}(\pi - \theta, \phi + \pi) = (-)^{\ell} Y_{\ell,m}(\theta, \phi). \quad (19.21)$$

- We also note that since $P_{\ell}^m(\cos \theta)$ is real,

$$Y_{\ell,m}(\theta, -\phi) = Y_{\ell,m}(\theta, 2\pi - \phi) = Y_{\ell,m}^*(\theta, \phi). \quad (19.22)$$

- At $\theta = 0$, $\cos \theta = 1$, $P_{\ell}^m(1) = \delta_{m,0}$ so that:

$$Y_{\ell,m}(0, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m,0}, \quad (19.23)$$

independent of ϕ .

Other properties of the spherical harmonics can be found in Edmonds [2] and other reference books. It is useful to know the first few spherical harmonics. These are:

$$\begin{aligned} Y_{0,0}(\theta, \phi) &= \sqrt{\frac{1}{4\pi}}, & Y_{1,0}(\theta, \phi) &= \sqrt{\frac{3}{4\pi}} \cos \theta, & Y_{1,\pm 1}(\theta, \phi) &= \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}, \\ Y_{2,0}(\theta, \phi) &= \sqrt{\frac{5}{16\pi}} (2 \cos^2 \theta - \sin^2 \theta), & Y_{2,\pm 1}(\theta, \phi) &= \mp \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta e^{\pm i\phi}, \\ Y_{2,\pm 2}(\theta, \phi) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}. \end{aligned} \quad (19.24)$$

Definition 34 (Reduced spherical harmonics). Sometimes it is useful to get rid of factors and define reduced spherical harmonics (Racah [4]) $C_{\ell,m}(\theta, \phi)$ by:

$$C_{\ell,m}(\theta, \phi) = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell,m}(\theta, \phi). \quad (19.25)$$

Remark 31. The orbital angular momentum states for $\ell = 0, 1, 2, 3, 4, \dots$ are often referred to as s, p, d, f, g, \dots states.

19.1.3 Parity and Time reversal

We discussed the effects of parity and time reversal transformations on the generators of Galilean transformations, including the angular momentum generator, in Chapter 7. We study the effect of these transformations on angular momentum states in this section.

Parity

For parity, we found in Section 7.7.1 that \mathcal{P} is linear and unitary, with eigenvalues of unit magnitude, and has the following effects on the angular momentum, position, and linear momentum operators:

$$\begin{aligned} \mathcal{P}^{-1} \mathbf{X} \mathcal{P} &= -\mathbf{X}, \\ \mathcal{P}^{-1} \mathbf{P} \mathcal{P} &= -\mathbf{P}, \\ \mathcal{P}^{-1} \mathbf{J} \mathcal{P} &= \mathbf{J}. \end{aligned} \quad (19.26)$$

We also found that $\mathcal{P}^{-1} = \mathcal{P}^{\dagger} = \mathcal{P}$. So under parity, we can take:

$$\mathcal{P} |\mathbf{x}\rangle = |-\mathbf{x}\rangle, \quad \mathcal{P} |\mathbf{p}\rangle = |-\mathbf{p}\rangle. \quad (19.27)$$

The angular momentum operator does not change under parity, so \mathcal{P} operating on a state of angular momentum $|jm\rangle$ can only result in a phase. If there is a coordinate representation of the angular momentum eigenstate, we can write:

$$\begin{aligned}\langle \hat{\mathbf{r}} | \mathcal{P} | \ell, m \rangle &= \langle \mathcal{P}^\dagger \hat{\mathbf{r}} | \ell, m \rangle = \langle \mathcal{P} \hat{\mathbf{r}} | \ell, m \rangle = \langle -\hat{\mathbf{r}} | \ell, m \rangle \\ &= Y_{\ell, m}(\pi - \theta, \phi + \pi) = (-)^\ell Y_{\ell, m}(\theta, \phi) = (-)^\ell \langle \mathbf{x} | \ell, m \rangle,\end{aligned}$$

where we have used (19.21). Therefore:

$$\mathcal{P} | \ell, m \rangle = (-)^\ell | \ell, m \rangle. \quad (19.28)$$

For spin 1/2 states, the parity operator must be the unit matrix. The phase is generally taken to be unity, so that:

$$\mathcal{P} | 1/2, m \rangle = | 1/2, m \rangle. \quad (19.29)$$

So parity has different results on orbital and spin eigenvectors.

Time reversal

For time reversal, we found in Section 7.7.2 that \mathcal{T} is anti-linear and anti-unitary, $\mathcal{T}^{-1}i\mathcal{T} = -i$ with eigenvalues of unit magnitude, and has the following effects on the angular momentum, position, and linear momentum operators:

$$\begin{aligned}\mathcal{T}^{-1} \mathbf{X} \mathcal{T} &= \mathbf{X}, \\ \mathcal{T}^{-1} \mathbf{P} \mathcal{T} &= -\mathbf{P}, \\ \mathcal{T}^{-1} \mathbf{J} \mathcal{T} &= -\mathbf{J}.\end{aligned} \quad (19.30)$$

Under time-reversal,

$$\mathcal{T} | \mathbf{x} \rangle = | \mathbf{x} \rangle, \quad \mathcal{T} | \mathbf{p} \rangle = | -\mathbf{p} \rangle. \quad (19.31)$$

The angular momentum operator reverses sign under time reversal, so \mathcal{T} operating on a state of angular momentum can only result in a phase. Because of the anti-unitary property, the commutation relations for angular momentum are invariant under time reversal. However since $\mathcal{T} J^2 \mathcal{T}^{-1} = J^2$, $\mathcal{T} J_z \mathcal{T}^{-1} = -J_z$, and $\mathcal{T} J_\pm \mathcal{T}^{-1} = -J_\mp$, operating on the eigenvalue equations (19.2) by \mathcal{T} gives:

$$\begin{aligned}J^2 \{ \mathcal{T} | j, m \rangle \} &= \hbar^2 j(j+1) \{ \mathcal{T} | j, m \rangle \}, \\ J_z \{ \mathcal{T} | j, m \rangle \} &= -\hbar m \{ \mathcal{T} | j, m \rangle \}, \\ J_\mp \{ \mathcal{T} | j, m \rangle \} &= -A(j, \mp m) \{ \mathcal{T} | j, m \rangle \}.\end{aligned} \quad (19.32)$$

These equations have the solution:

$$\mathcal{T} | j, m \rangle = (-)^{j+m} | j, -m \rangle. \quad (19.33)$$

Here we have introduced an arbitrary phase $(-)^j$ so that for half-integer values of j , the operation of parity will produce a sign, not a complex number. Let us investigate time reversal on both spin-1/2 and integer values of j .

For spin-1/2 states, in a 2×2 matrix representation, we require:

$$\mathcal{T}^{-1} \sigma_i \mathcal{T} = -\sigma_i, \quad (19.34)$$

for $i = 1, 2, 3$. Now we know that σ_2 changes the sign of any σ_i , but it also takes the complex conjugate, which we do not want in this case. So for spin 1/2, we take the following matrix representation of the time reversal operator:

$$\mathcal{T} = i \sigma_2 \mathcal{K} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathcal{K}, \quad (19.35)$$

where \mathcal{K} is a complex conjugate operator acting on functions. This makes \mathcal{T} anti-linear and anti-unitary. Now since $(i\sigma_y)\sigma_x(i\sigma_y) = \sigma_x$, $(i\sigma_y)\sigma_y(i\sigma_y) = -\sigma_y$, and $(i\sigma_y)\sigma_z(i\sigma_y) = \sigma_z$, and recalling that σ_x and σ_z are real, whereas $\sigma_y^* = -\sigma_y$, so that:

$$\mathcal{T}^{-1} \sigma_i \mathcal{T} = -\sigma_i, \quad (19.36)$$

as required. Now the matrix representation of \mathcal{T} on spinor states have the effect:

$$\begin{aligned} \mathcal{T} |1/2, 1/2\rangle &= i\sigma_2 \mathcal{K} |1/2, 1/2\rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathcal{K} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = -\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -|1/2, -1/2\rangle. \\ \mathcal{T} |1/2, -1/2\rangle &= i\sigma_2 \mathcal{K} |1/2, -1/2\rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathcal{K} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = +\begin{pmatrix} 1 \\ 0 \end{pmatrix} = +|1/2, +1/2\rangle, \end{aligned}$$

so that

$$\mathcal{T} |1/2, m\rangle = (-)^{1/2+m} |1/2, -m\rangle, \quad (19.37)$$

in agreement with (19.33).

Exercise 44. For the spin \mathcal{T} operator defined in Eq. (19.35), show that:

$$\mathcal{T}^{-1} = \mathcal{T}^\dagger = \mathcal{T}. \quad (19.38)$$

For integer values of the angular momentum, there is a coordinate representation of the angular momentum vector. If we choose

$$\langle \hat{\mathbf{r}} | \ell, m \rangle = Y_{\ell, m}(\theta, \phi), \quad (19.39)$$

then we can write:

$$\begin{aligned} \langle \hat{\mathbf{r}} | \mathcal{T} | \ell, m \rangle &= \langle \mathcal{T}^\dagger \hat{\mathbf{r}} | \ell, m \rangle^* = \langle \mathcal{T} \hat{\mathbf{r}} | \ell, m \rangle^* = \langle \hat{\mathbf{r}} | \ell, m \rangle^* \\ &= Y_{\ell, m}^*(\theta, \phi) = (-)^m Y_{\ell, -m}(\theta, \phi) = (-)^m \langle \hat{\mathbf{r}} | \ell, -m \rangle. \end{aligned}$$

So we conclude that:

$$\mathcal{T} | \ell, m \rangle = (-)^m | \ell, -m \rangle, \quad (19.40)$$

which does *not* agree with (19.33). However if we choose:

$$\langle \hat{\mathbf{r}} | \ell, m \rangle = i^\ell Y_{\ell, m}(\theta, \phi), \quad (19.41)$$

then

$$\begin{aligned} \langle \hat{\mathbf{r}} | \mathcal{T} | \ell, m \rangle &= \langle \mathcal{T}^\dagger \hat{\mathbf{r}} | \ell, m \rangle^* = \langle \mathcal{T} \hat{\mathbf{r}} | \ell, m \rangle^* = \langle \hat{\mathbf{r}} | \ell, m \rangle^* \\ &= [i^\ell Y_{\ell, m}(\theta, \phi)]^* = (-)^{\ell+m} Y_{\ell, -m}(\theta, \phi) = (-)^{\ell+m} \langle \hat{\mathbf{r}} | \ell, -m \rangle. \end{aligned}$$

which gives:

$$\mathcal{T} | \ell, m \rangle = (-)^{\ell+m} | \ell, -m \rangle, \quad (19.42)$$

which *does* agree with (19.33). We will see in Section 19.4 that when orbital and spin eigenvectors are coupled together by a Clebsch-Gordan coefficient, the operation of time reversal on the coupled state is preserved if we choose the spherical functions defined in Eq. (19.41). However, Eq. (19.39) is generally used in the literature.

19.2 Rotation of coordinate frames

A fixed point P in space, described by Euclidean coordinates (x, y, z) and (x', y', z') in two frames Σ and Σ' , are related to each other by a rotation if lengths and angles are preserved. We have described this portion of the more general Galilean transformation in Chapter 7 by a linear orthogonal transformation between the coordinates: $x'_i = R_{ij} x_j$, with $R_{ij} R_{ik} = \delta_{jk}$. Proper transformations which preserve orientation are those with $\det[R] = +1$. The set of all orthogonal matrices R describing rotations form a three-parameter group called $SO(3)$. There are several ways to describe the relative orientation of these two coordinate frames. Some of the common ones are: an axis and angle of rotation, denoted by $(\hat{\mathbf{n}}, \theta)$, Euler angles, denoted by three angles (α, β, γ) , and the Cayley-Kline parameters. We will discuss these parameterizations in this section.

There are two alternative ways to describe a rotation: the *active* meaning where each point in space is transformed into a new point, which we can think of as a physical rotation of a vector or object, and the *passive* meaning where the point remains fixed and the coordinate system is rotated. We use passive rotation here, which was our convention for the general Galilean transformations of Chapter 7. Edmonds [2] uses passive rotation, whereas Biedenharn [5], Rose [6], and Merzbacher [7] all use active rotations.¹

19.2.1 Rotation matrices

Let Σ and Σ' be two coordinate systems with a common origin, and let a point P described by a vector \mathbf{r} from the origin to the point and let (x, y, z) be Cartesian coordinates of the point in Σ and (x', y', z') be Cartesian coordinates of the *same* point in Σ' . Let us further assume that both of these coordinate systems are oriented in a *right* handed sense.² Then we can write the vector \mathbf{r} in either coordinate system using unit vectors:³

$$\mathbf{r} = x_i \hat{\mathbf{e}}_i = x'_i \hat{\mathbf{e}}'_i, \quad (19.43)$$

where $\hat{\mathbf{e}}_i$ and $\hat{\mathbf{e}}'_i$ are orthonormal sets of unit vectors describing the two Cartesian coordinate systems: $\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \hat{\mathbf{e}}'_i \cdot \hat{\mathbf{e}}'_j = \delta_{ij}$. So we find that components of the vector \mathbf{r} in the two systems are related by:

$$x'_i = R_{ij} x_j, \quad \text{where} \quad R_{ij} = \hat{\mathbf{e}}'_i \cdot \hat{\mathbf{e}}_j, \quad (19.44)$$

where R must satisfy the orthogonal property:

$$R_{ik}^T R_{kj} = R_{ki} R_{kj} = \delta_{ij}. \quad (19.45)$$

That is $R^{-1} = R^T$. The unit vectors transform in the opposite way:

$$\hat{\mathbf{e}}'_i = \hat{\mathbf{e}}_j R_{ji} = R_{ij}^T \hat{\mathbf{e}}_j, \quad (19.46)$$

so that, using the orthogonality relation, Eq. (19.43) is satisfied. From Eq. (19.45) we see that $\det[R] = \pm 1$, but, in fact, for rotations, we must restrict the determinant to $+1$ since rotations can be generated from the unit matrix, which has a determinant of $+1$.

Matrices describing coordinate systems that are related by *positive* rotations about the x -, y -, and z -axis by an amount α , β , and γ respectively are given by:

$$R_x(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \alpha & \sin \alpha \\ 0 & -\sin \alpha & \cos \alpha \end{pmatrix}, \quad R_y(\beta) = \begin{pmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{pmatrix}, \quad R_z(\gamma) = \begin{pmatrix} \cos \gamma & \sin \gamma & 0 \\ -\sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (19.47)$$

Notice the location of negative *signs!* One can easily check that these matrices are orthogonal and have determinants of $+1$.

¹Biedenharn [5] states that the Latin terms for these distinctions are “alibi” for active and “alias” for passive descriptions.

²We do not consider space inversions or reflections in this chapter.

³In this section, we use a summation convention over repeated indices.

Eq. (19.44) describes a general rotation in terms of nine direction cosines between the coordinate axes,

$$R_{ij} = \hat{\mathbf{e}}'_i \cdot \hat{\mathbf{e}}_j = \cos(\theta_{ij}).$$

These direction cosines, however, are not all independent. The orthogonality requirement, and the fact that the determinant of the matrix must be +1, provides six constraint equations, which then leave *three* independent quantities that are needed to describe a rotation.

Exercise 45. Show that if Σ and Σ' are related by a rotation matrix R and Σ' and Σ'' are related by a rotation matrix R' , the coordinate systems Σ and Σ'' are related by another orthogonal rotation matrix R'' . Find R'' in terms of R and R' , and show that it has determinant +1.

Definition 35 (The $O^+(3)$ group). The last exercise shows that all three-dimensional rotational matrices R form a three parameter group, called $O^+(3)$, for orthogonal group with positive determinant in three-dimensions.

The direction cosines are not a good way to parameterize the rotation matrices R since there are many relations between the components that are required by orthogonality and unit determinant. In the next sections, we discuss ways to parameterize this matrix.

19.2.2 Axis and angle parameterization

Euler's theorem in classical mechanics states that "the general displacement of a rigid body with one point fixed is a rotation about some axis." [8, p. 156] We show in this section how to parameterize the rotation matrix R by an axis and angle of rotation. We start by writing down the form of the rotation matrix for infinitesimal transformations:

$$R_{ij}(\hat{\mathbf{n}}, \Delta\theta) = \delta_{ij} + \epsilon_{ijk} \hat{n}_k \Delta\theta + \dots \equiv \delta_{ij} + i (L_k)_{ij} \hat{n}_k \Delta\theta + \dots, \quad (19.48)$$

where $\hat{\mathbf{n}}$ is the axis of rotation, $\Delta\theta$ the magnitude of the rotation. Here we have introduced three imaginary Hermitian and antisymmetric 3×3 matrices $(L_k)_{ij}$, called the classical generators of the rotation. They are defined by:

$$(L_k)_{ij} = \frac{1}{i} \epsilon_{ijk}. \quad (19.49)$$

Explicitly, we have:

$$L_x = \frac{1}{i} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad L_y = \frac{1}{i} \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad L_z = \frac{1}{i} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (19.50)$$

Note that these angular momentum matrices are *not* the same as the spin one angular momentum matrices S_i found in Eqs. (19.10), even though they are both 3×3 matrices! The matrices L_k are called the **adjoint** representation of the angular momentum generators. The matrix of unit vectors \mathbf{L} is defined by:

$$\mathbf{L} = L_i \hat{\mathbf{e}}_i = \frac{1}{i} \begin{pmatrix} 0 & \hat{\mathbf{e}}_3 & -\hat{\mathbf{e}}_2 \\ -\hat{\mathbf{e}}_3 & 0 & \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 & -\hat{\mathbf{e}}_1 & 0 \end{pmatrix}. \quad (19.51)$$

so that we can write, in matrix notation:

$$R(\hat{\mathbf{n}}, \Delta\theta) = 1 + i \mathbf{L} \cdot \hat{\mathbf{n}} \Delta\theta + \dots. \quad (19.52)$$

So $\mathbf{L}^\dagger = -\mathbf{L}^T = \mathbf{L}$. So $R^T(\hat{\mathbf{n}}, \Delta\theta) = 1 - i \mathbf{L} \cdot \hat{\mathbf{n}} \Delta\theta + \dots$. The \mathbf{L} matrix is imaginary, but the $R(\hat{\mathbf{n}}, \Delta\theta)$ matrix is still real. The classical angular momentum generators have *no units* and satisfy the commutation relations:

$$[L_i, L_j] = i \epsilon_{ijk} L_k, \quad (19.53)$$

which is identical to the ones for the quantum angular momentum operator, except for the fact that in quantum mechanics, the angular momentum operator has units and the commutation relations a factor of \hbar . There is no quantum mechanics or \hbar here!

Exercise 46. Carefully explain the differences between the adjoint representation of the angular momentum matrices L_i defined here, and the angular momentum matrices S_i discussed in Section 19.1.1. Can you find a unitary transformation matrix U which relates the S_i set to the L_i set?

We can now construct a finite classical transformation matrix $R(\hat{\mathbf{n}}, \theta)$ by compounding N infinitesimal transformation of an amount $\Delta\theta = \theta/N$ about a fixed axis $\hat{\mathbf{n}}$. This gives:

$$R(\hat{\mathbf{n}}, \theta) = \lim_{N \rightarrow \infty} \left[1 + i \frac{\hat{\mathbf{n}} \cdot \mathbf{L} \theta}{N} \right]^N = e^{i \hat{\mathbf{n}} \cdot \mathbf{L} \theta} . \quad (19.54)$$

The difficulty here is that the matrix of vectors \mathbf{L} appears in the exponent. We understand how to interpret this by expanding the exponent in a power series. In order to do this, we will need to know the value of powers of the L_i matrices. So we compute:

$$\begin{aligned} (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} &= \frac{1}{i} n_k \epsilon_{ijk} , \\ (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^2 &= -n_k n_{k'} \epsilon_{ilk} \epsilon_{ljk'} = n_k n_{k'} \epsilon_{ikl} \epsilon_{ljk'} = n_k n_{k'} (\delta_{ij} \delta_{kk'} - \delta_{ik'} \delta_{kj}) \\ &= \delta_{ij} - n_i n_j \equiv P_{ij} \\ (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^3 &= (\hat{\mathbf{n}} \cdot \mathbf{L})_{il}^2 (\hat{\mathbf{n}} \cdot \mathbf{L})_{lj} = \frac{1}{i} (\delta_{il} - n_i n_l) n_k \epsilon_{ljk} = \frac{1}{i} (n_k \epsilon_{ijk} - n_i n_l n_k \epsilon_{ljk}) \\ &= \frac{1}{i} n_k \epsilon_{ijk} = (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} , \\ (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^4 &= (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^2 = P_{ij} , \quad \text{etc} \dots \end{aligned} \quad (19.55)$$

One can see that terms in a power series expansion of $R(\hat{\mathbf{n}}, \theta)$ reproduce themselves, so we can collect terms and find:

$$\begin{aligned} R_{ij}(\hat{\mathbf{n}}, \theta) &= [e^{i \theta \hat{\mathbf{n}} \cdot \mathbf{L}}]_{ij} \\ &= \delta_{ij} + i (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} \theta - \frac{1}{2!} (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^2 \theta^2 - \frac{i}{3!} (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^3 \theta^3 + \frac{1}{4!} (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij}^4 \theta^4 + \dots \\ &= n_i n_j + P_{ij} + i (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} \theta - \frac{1}{2!} P_{ij} \theta^2 - \frac{i}{3!} (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} \theta^3 + \frac{1}{4!} P_{ij} \theta^4 + \dots \\ &= n_i n_j + P_{ij} \cos(\theta) + i (\hat{\mathbf{n}} \cdot \mathbf{L})_{ij} \sin(\theta) \\ &= n_i n_j + (\delta_{ij} - n_i n_j) \cos(\theta) + \epsilon_{ijk} n_k \sin(\theta) . \end{aligned} \quad (19.56)$$

In terms of unit vectors, the last line can be written as:

$$\begin{aligned} R_{ij}(\hat{\mathbf{n}}, \theta) &= (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_i) (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_j) + [(\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j) - (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_i) (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_j)] \cos(\theta) + (\hat{\mathbf{n}} \times \hat{\mathbf{e}}_i) \cdot \hat{\mathbf{e}}_j \sin(\theta) \\ &= (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_i) (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_j) + [(\hat{\mathbf{n}} \times (\hat{\mathbf{e}}_i \times \hat{\mathbf{n}})) \cdot \hat{\mathbf{e}}_j] \cos(\theta) + (\hat{\mathbf{n}} \times \hat{\mathbf{e}}_i) \cdot \hat{\mathbf{e}}_j \sin(\theta) . \end{aligned} \quad (19.57)$$

So since $\mathbf{r} = x_i \hat{\mathbf{e}}_i$, we have:

$$\begin{aligned} x'_i &= R_{ij}(\hat{\mathbf{n}}, \theta) x_j = (\hat{\mathbf{n}} \cdot \hat{\mathbf{e}}_i) (\hat{\mathbf{n}} \cdot \mathbf{r}) + [(\hat{\mathbf{n}} \times (\hat{\mathbf{e}}_i \times \hat{\mathbf{n}})) \cdot \mathbf{r}] \cos(\theta) + (\hat{\mathbf{n}} \times \hat{\mathbf{e}}_i) \cdot \mathbf{r} \sin(\theta) \\ &= [(\hat{\mathbf{n}} \cdot \mathbf{r}) \hat{\mathbf{n}} + (\hat{\mathbf{n}} \times (\mathbf{r} \times \hat{\mathbf{n}})) \cos(\theta) + (\mathbf{r} \times \hat{\mathbf{n}}) \sin(\theta)] \cdot \hat{\mathbf{e}}_i , \end{aligned} \quad (19.58)$$

So if we define \mathbf{r}' as a vector with components in the frame Σ' , but with unit vectors in the frame Σ , we find:

$$\mathbf{r}' = x'_i \hat{\mathbf{e}}_i = (\hat{\mathbf{n}} \cdot \mathbf{r}) \hat{\mathbf{n}} + (\hat{\mathbf{n}} \times (\mathbf{r} \times \hat{\mathbf{n}})) \cos(\theta) + (\mathbf{r} \times \hat{\mathbf{n}}) \sin(\theta) . \quad (19.59)$$

Exercise 47. Consider the case of a rotation about the z -axis by an amount θ , so that $\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$, and set $\mathbf{r} = x \hat{\mathbf{e}}_x + y \hat{\mathbf{e}}_y + z \hat{\mathbf{e}}_z$, show that the components of the vector \mathbf{r}' , given by Eq. (19.59), are given by $x'_i = R_{ij}(\hat{\mathbf{e}}_z, \theta) x_j$, as required.

Exercise 48. Show that the trace of $R(\hat{\mathbf{n}}, \theta)$ gives:

$$\sum_i R_{ii}(\hat{\mathbf{n}}, \theta) = 1 + 2 \cos(\theta) = 2 \cos^2(\theta/2), \quad (19.60)$$

where θ is the rotation angle.

Exercise 49. Find the eigenvalues and eigenvectors of $R_{ij}(\hat{\mathbf{e}}_z, \theta)$. Normalize the eigenvectors to the unit sphere, $x^2 + y^2 + z^2 = 1$, and show that the eigenvector with eigenvalue of $+1$ describes the axis of rotation. Extra credit: show that the eigenvalues of an arbitrary orthogonal rotation matrix R are $+1$, 0 , and -1 . (See Goldstein [8].)

Exercise 50. For the double rotation $R'R = R''$, show that the rotation angle θ'' for the combined rotation is given by:

$$2 \cos^2(\theta''/2) = (\hat{\mathbf{n}}' \cdot \hat{\mathbf{n}})^2 + 2 (\hat{\mathbf{n}}' \cdot \hat{\mathbf{n}}) \cos(\theta' + \theta) + [1 - (\hat{\mathbf{n}}' \cdot \hat{\mathbf{n}})^2] [\cos(\theta') + \cos(\theta') \cos(\theta) + \cos(\theta)]. \quad (19.61)$$

It is more difficult to find the new axis of rotation $\hat{\mathbf{n}}''$. One way is to find the eigenvector with unit eigenvalue of the resulting matrix, which can be done numerically. There appears to be no closed form for it.

19.2.3 Euler angles

The Euler angles are another way to relate two coordinate systems which are rotated with respect to one another. We define these angles by the following sequence of rotations, which, taken in order, are:⁴

1. Rotate from frame Σ to frame Σ' an angle α about the z -axis, $0 \leq \alpha \leq 2\pi$.
2. Rotate from frame Σ' to frame Σ'' an angle β about the y' -axis, $0 \leq \beta \leq \pi$.
3. Rotate from frame Σ'' to frame Σ''' an angle γ about the z'' -axis, $0 \leq \gamma \leq 2\pi$.

The Euler angles are shown in the Fig 19.1. For this definition of the Euler angles, the y' -axis is called the “line of nodes.” The coordinates of a *fixed* point P in space, a *passive* rotation, is defined by: (x, y, z) in Σ , (x', y', z') in Σ' , (x'', y'', z'') in Σ'' , and $(X, Y, Z) \equiv (x''', y''', z''')$ in Σ''' . Then, in a matrix notation,

$$x''' = R_z(\gamma) x'' = R_z(\gamma) R_y(\beta) x' = R_z(\gamma) R_y(\beta) R_z(\alpha) x \equiv R(\gamma, \beta, \alpha) x, \quad (19.62)$$

where

$$\begin{aligned} R(\gamma, \beta, \alpha) &= R_z(\gamma) R_y(\beta) R_z(\alpha) \\ &= \begin{pmatrix} \cos \gamma & \sin \gamma & 0 \\ -\sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{pmatrix} \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} \cos \gamma \cos \beta \cos \alpha - \sin \gamma \sin \alpha, & \cos \gamma \cos \beta \sin \alpha + \sin \gamma \sin \alpha, & -\cos \gamma \sin \beta \\ -\sin \gamma \cos \beta \cos \alpha - \cos \gamma \sin \alpha, & -\sin \gamma \cos \beta \sin \alpha + \cos \gamma \cos \alpha, & \sin \gamma \sin \beta \\ \sin \beta \cos \alpha, & \sin \beta \sin \alpha, & \cos \beta \end{pmatrix}. \end{aligned} \quad (19.63)$$

Here we have used the result in Eqs. (19.47). The rotation matrix $R(\gamma, \beta, \alpha)$ is real, orthogonal, and the determinant is $+1$.

⁴This is the definition of Euler angles used by Edmonds [2][p. 7] and seems to be the most common one for quantum mechanics. In classical mechanics, the second rotation is often about the x' -axis (see Goldstein [8]). Mathematica uses rotations about the x' -axis. Other definitions are often used for the quantum mechanics of a symmetrical top (see Bohr).

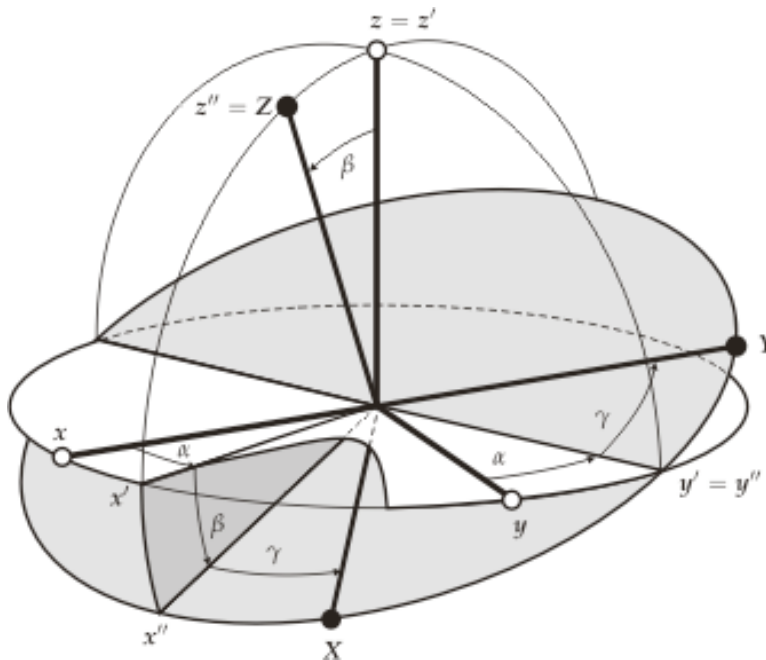


Figure 19.1: Euler angles for the rotations $\Sigma \rightarrow \Sigma' \rightarrow \Sigma'' \rightarrow \Sigma'''$. The final axis is labeled (X, Y, Z) .

We will also have occasion to use the inverse of this transformation:

$$\begin{aligned}
 R^{-1}(\gamma, \beta, \alpha) &= R^T(\gamma, \beta, \alpha) = R_z(-\alpha) R_y(-\beta) R_z(-\gamma) \\
 &= \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{pmatrix} \begin{pmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
 &= \begin{pmatrix} \cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma, & -\cos \alpha \cos \beta \sin \gamma + \sin \alpha \sin \gamma, & \cos \alpha \sin \beta \\ \sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma, & -\sin \alpha \cos \beta \sin \gamma + \cos \alpha \cos \gamma, & \sin \alpha \sin \beta \\ -\sin \beta \cos \gamma, & \sin \beta \sin \gamma, & \cos \beta \end{pmatrix}.
 \end{aligned} \tag{19.64}$$

We note that the coordinates (x, y, z) in the fixed frame Σ of a point P on the unit circle on z''' -axis in the Σ''' frame, $(x''', y''', z''') = (0, 0, 1)$ is given by:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = R_{ij}^{-1}(\alpha, \beta, \gamma) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \sin \beta \cos \alpha \\ \sin \beta \sin \alpha \\ \cos \beta \end{pmatrix}, \tag{19.65}$$

so the polar angles (θ, ϕ) of this point in the Σ frame is $\theta = \beta$ and $\phi = \alpha$. We will use this result later.

19.2.4 Cayley-Klein parameters

A completely different way to look at rotations is to describe them as directed great circle arcs on the unit sphere in three dimensions. Points on the sphere are described by the set of real variables (x_1, x_2, x_3) , with $x_1^2 + x_2^2 + x_3^2 = 1$. These arcs are called **turns** by Biedenharn [5][Ch. 4], and are based on Hamilton's theory of quaternions [9]. Points at the beginning and end of the arc form two reflection planes with the center of the sphere. The line joining these planes is the axis of the rotation and the angle between the planes *half* the angle of rotation. Turns can be added much like vectors, the geometric rules for which are given by Biedenharn [5][p. 184]. Now a stereographic projection from the North pole of a point on the unit sphere

and the equatorial plane maps a unique point on the sphere (except the North pole) to a unique point on the plane, which is described by a *complex* number $z = x + iy$. The geometric mapping can easily be found by similar triangles to be:

$$z = x + iy = \frac{x_1 + ix_2}{1 - x_3} = \frac{1 + x_3}{x_1 - ix_2}. \quad (19.66)$$

Klein [10, 11] and Cayley [12] discovered that a turn, or rotation, described on the unit circle could be described on the plane by a linear fractional transformation of the form:

$$z'^* = \frac{az^* + b}{cz^* + d}, \quad (19.67)$$

where (a, b, c, d) are complex numbers satisfying:

$$|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1, \quad ca^* + db^* = 0. \quad (19.68)$$

The set of numbers (a, b, c, d) are called the *Cayley-Klein* parameters. In order to prove this, we need a way to describe turns on the unit sphere. Let $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ be unit vectors describing the start and end point of the turn. Then we can form a scalar $\xi_0 = \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \equiv \cos(\theta/2)$ and a vector $\boldsymbol{\xi} = \hat{\mathbf{r}} \times \hat{\mathbf{p}} \equiv \hat{\mathbf{n}} \sin(\theta/2)$, which satisfy the property:

$$\xi_0^2 + \boldsymbol{\xi}^2 = 1. \quad (19.69)$$

Thus a turn can be put in one-to-one correspondence with the set of four quantities $(\xi_0, \boldsymbol{\xi})$ lying on a *four*-dimensional sphere. The rule for addition of a sequence of turns can be found from these definitions. Let $\hat{\mathbf{r}}, \hat{\mathbf{p}}$ be unit vectors for the start and end of the first turn described by the parameters $(\xi_0, \boldsymbol{\xi})$, and $\hat{\mathbf{p}}, \hat{\mathbf{s}}$ be the start and end of the second turn described by the parameters $(\xi'_0, \boldsymbol{\xi}')$. This means that:

$$\hat{\mathbf{p}} = \xi_0 \hat{\mathbf{r}} + \boldsymbol{\xi} \times \hat{\mathbf{r}}, \quad \xi_0 = \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \quad \boldsymbol{\xi} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}, \quad (19.70)$$

$$\hat{\mathbf{s}} = \xi'_0 \hat{\mathbf{p}} + \boldsymbol{\xi}' \times \hat{\mathbf{p}}, \quad \xi'_0 = \hat{\mathbf{p}} \cdot \hat{\mathbf{s}}, \quad \boldsymbol{\xi}' = \hat{\mathbf{p}} \times \hat{\mathbf{s}}. \quad (19.71)$$

Substituting (19.70) into (19.71) gives:

$$\begin{aligned} \hat{\mathbf{s}} &= \xi'_0 (\xi_0 \hat{\mathbf{r}} + \boldsymbol{\xi} \times \hat{\mathbf{r}}) + \boldsymbol{\xi}' \times (\xi_0 \hat{\mathbf{r}} + \boldsymbol{\xi} \times \hat{\mathbf{r}}) \\ &= \xi''_0 \hat{\mathbf{r}} + \boldsymbol{\xi}'' \times \hat{\mathbf{r}}, \end{aligned} \quad (19.72)$$

where

$$\begin{aligned} \xi''_0 &= \xi'_0 \xi_0 - \boldsymbol{\xi}' \cdot \boldsymbol{\xi}, \\ \boldsymbol{\xi}'' &= \xi_0 \boldsymbol{\xi}' + \xi'_0 \boldsymbol{\xi} + \boldsymbol{\xi}' \times \boldsymbol{\xi}. \end{aligned} \quad (19.73)$$

Now since $\hat{\mathbf{r}} \cdot \boldsymbol{\xi}'' = 0$, we find from (19.72) that

$$\hat{\mathbf{r}} \cdot \hat{\mathbf{s}} = \cos(\theta''/2), \quad \hat{\mathbf{r}} \times \hat{\mathbf{s}} = \hat{\mathbf{n}}'' \sin(\theta''/2), \quad (19.74)$$

which means that the set of all turns form a group, with a composition rule.

Exercise 51. Show that (19.73) follows from (19.72). Show also that $\hat{\mathbf{r}} \cdot \boldsymbol{\xi}'' = 0$.

Cayley [13] noticed that the composition rule, Eq. (19.73), is the same rule for multiplication of two quaternions. That is, if we define

$$\hat{\boldsymbol{\xi}} = \xi_0 \hat{\mathbf{1}} + \xi_1 \hat{\mathbf{i}} + \xi_2 \hat{\mathbf{j}} + \xi_3 \hat{\mathbf{k}} = \xi_0 \hat{\mathbf{1}} + \boldsymbol{\xi}, \quad (19.75)$$

where the quaternion multiplication rules are:⁵

$$\hat{\mathbf{i}}\hat{\mathbf{j}} = -\hat{\mathbf{j}}\hat{\mathbf{i}} = \hat{\mathbf{k}}, \quad \hat{\mathbf{j}}\hat{\mathbf{k}} = -\hat{\mathbf{k}}\hat{\mathbf{j}} = \hat{\mathbf{i}}, \quad \hat{\mathbf{k}}\hat{\mathbf{i}} = -\hat{\mathbf{i}}\hat{\mathbf{k}} = \hat{\mathbf{j}}, \quad \hat{\mathbf{1}}^2 = \hat{\mathbf{1}}, \quad \hat{\mathbf{i}}^2 = \hat{\mathbf{j}}^2 = \hat{\mathbf{k}}^2 = -\hat{\mathbf{1}}, \quad (19.76)$$

⁵One should think of quaternions as an extension of the complex numbers. They form what is called a **division algebra**.

then it is easy to show that *quaternion* multiplication reproduces the composition rule:

$$\hat{\xi}'' = \hat{\xi}' \hat{\xi}. \quad (19.77)$$

So it is natural to use the algebra of quaternions to describe rotations.

Exercise 52. Show that Eq. (19.77) reproduces the composition rule (19.73) using the quaternion multiplication rules of Eq. (19.76).

The adjoint quaternion $\hat{\xi}^\dagger$ is defined by:

$$\hat{\xi}^\dagger = \xi_0 \hat{1} - \xi_1 \hat{i} - \xi_2 \hat{j} - \xi_3 \hat{k} = \xi_0 \hat{1} - \boldsymbol{\xi}, \quad (19.78)$$

so that the length of $\hat{\xi}$ is given by:

$$\hat{\xi}^\dagger \hat{\xi} = \xi_0^2 + \boldsymbol{\xi}^2 = 1. \quad (19.79)$$

We next have to show how a position (x_1, x_2, x_3) on the unit sphere is transformed by a turn $(\xi_0, \boldsymbol{\xi})$. To this end, we define a quaternion \hat{x} by the definition:

$$\hat{x} = x_1 \hat{i} + x_2 \hat{j} + x_3 \hat{k}, \quad \text{with} \quad x_0 = 0. \quad (19.80)$$

Then a rotation of the coordinates by a turn $\hat{\xi}$ is given by the quaternion product:

$$\hat{x}' = \hat{\xi} \hat{x} \hat{\xi}^\dagger. \quad (19.81)$$

To prove this statement, we note that

$$\begin{aligned} \hat{x}' &= \hat{\xi} \hat{x} \hat{\xi}^\dagger = (\xi_0 \hat{1} + \xi_1 \hat{i} + \xi_2 \hat{j} + \xi_3 \hat{k}) (x_1 \hat{i} + x_2 \hat{j} + x_3 \hat{k}) (\xi_0 \hat{1} - \xi_1 \hat{i} - \xi_2 \hat{j} - \xi_3 \hat{k}) \\ &= 0 \hat{1} + x'_1 \hat{i} + x'_2 \hat{j} + x'_3 \hat{k}, \end{aligned} \quad (19.82)$$

where, after some algebra, we find:

$$\begin{aligned} x'_1 &= \xi_0 (\xi_0 x_1 + \xi_2 x_3 - \xi_3 x_2) + \xi_1 (\xi_1 x_1 + \xi_2 x_2 + \xi_3 x_3) + \xi_2 (\xi_0 x_3 + \xi_1 x_2 - \xi_2 x_1) \\ &\quad - \xi_3 (\xi_0 x_2 - \xi_1 x_3 + \xi_3 x_1) \\ &= x_1 \cos^2(\theta/2) + (n_2 x_3 - n_3 x_2 + n_2 x_3 - n_3 x_2) \sin(\theta/2) \cos(\theta/2) \\ &\quad + (n_1^2 x_1 + n_1 n_2 x_2 + n_1 n_3 x_3 + n_2 n_1 x_2 - n_2^2 x_1 + n_3 n_1 x_3 - n_3^2 x_1) \sin^2(\theta/2) \\ &= x_1 \cos^2(\theta/2) + (2 n_2 x_3 - 2 n_3 x_2) \sin(\theta/2) \cos(\theta/2) \\ &\quad + (2 n_1^2 x_1 - x_1 + 2 n_1 n_2 x_2 + 2 n_1 n_3 x_3) \sin^2(\theta/2) \\ &= x_1 \cos(\theta) + (n_2 x_3 - n_3 x_2) \sin(\theta) \\ &\quad + (n_1^2 x_1 + n_1 n_2 x_2 + n_1 n_3 x_3) (1 - \cos(\theta)) \\ &= n_1 (n_1 x_1 + n_2 x_2 + n_3 x_3) \\ &\quad + (x_1 - n_1^2 (n_1 x_1 + n_2 x_2 + n_3 x_3)) \cos(\theta) + (n_2 x_3 - n_3 x_2) \sin(\theta) \\ &= (\hat{\mathbf{n}} \cdot \mathbf{r}) n_1 + (\mathbf{n} \times (\mathbf{r} \times \mathbf{n}))_1 \cos(\theta) - (\mathbf{r} \times \hat{\mathbf{n}})_1 \sin(\theta), \end{aligned} \quad (19.83)$$

with similar results for x'_2 and x'_3 , so in vector form, we find:

$$\mathbf{r}' = (\hat{\mathbf{n}} \cdot \mathbf{r}) \mathbf{n} + (\mathbf{n} \times (\mathbf{r} \times \mathbf{n})) \cos(\theta) - (\mathbf{r} \times \hat{\mathbf{n}}) \sin(\theta), \quad (19.84)$$

which is a rotation of a *vector*. So the quaternion product (19.81) does describe the rotation of coordinate systems generated by a turn.

Rather than using quaternions, physicists prefer to use the Pauli matrices to represent turns. That is, if we make the identification,

$$\hat{i} \mapsto 1, \quad \hat{j} \mapsto \sigma_x, \quad \hat{k} \mapsto \sigma_y, \quad \hat{l} \mapsto \sigma_z, \quad (19.85)$$

so that a turn is represented by the *unitary* 2×2 matrix:

$$\xi \equiv D(R) = \begin{pmatrix} \xi_0 + \xi_3 & \xi_1 - i\xi_2 \\ \xi_1 + i\xi_2 & \xi_0 - \xi_3 \end{pmatrix} = \xi_0 + \boldsymbol{\xi} \cdot \boldsymbol{\sigma} = \cos(\theta/2) + i \hat{\mathbf{n}} \cdot \boldsymbol{\sigma} \sin(\theta/2). \quad (19.86)$$

Here the composition rule is represented by *matrix* multiplication, $D(R'') \equiv D(R'R) = D(R')D(R)$. A point P on the unit sphere in frame Σ is represented by the 2×2 matrix function of coordinates $V(\mathbf{r})$, given by:

$$V(\hat{\mathbf{r}}) = \hat{\mathbf{r}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix}, \quad (19.87)$$

with a similar expression for $V(\hat{\mathbf{r}}') = \hat{\mathbf{r}}' \cdot \boldsymbol{\sigma}$ with $x'_i = R_{ij}x_j$. The matrix version of the quaternion product (19.81) for the rotation of the coordinates is given in the next theorem.

Theorem 34. *The matrices $V(\hat{\mathbf{r}})$ and $V(\hat{\mathbf{r}}')$ are related by:*

$$V(\hat{\mathbf{r}}') = D(R) V(\hat{\mathbf{r}}) D^\dagger(R), \quad (19.88)$$

where the unitary matrix $D(R)$ is given by:

$$D(\hat{\mathbf{n}}, \theta) = e^{i \hat{\mathbf{n}} \cdot \boldsymbol{\sigma} \theta/2} = \cos(\theta/2) + i (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \sin(\theta/2), \quad (19.89)$$

in terms of an axis and angle of rotation $(\hat{\mathbf{n}}, \theta)$,

$$D(a, b, c, d) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (19.90)$$

in terms of the Cayley-Klein parameters (a, b, c, d) which satisfy:

$$|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1, \quad ca^* + db^* = 0. \quad (19.91)$$

and

$$D(\gamma, \beta, \alpha) = \begin{pmatrix} e^{i(+\gamma+\alpha)/2} \cos(\beta/2) & e^{i(+\gamma-\alpha)/2} \sin(\beta/2) \\ -e^{i(-\gamma+\alpha)/2} \sin(\beta/2) & e^{i(-\gamma-\alpha)/2} \cos(\beta/2) \end{pmatrix}, \quad (19.92)$$

in terms of the Euler angles (α, β, γ) .

Proof. We will prove this using the axis and angle of rotation parameters. We first consider a basis transformation of the σ matrices of the form:

$$\begin{aligned} D(\hat{\mathbf{n}}, \theta) \boldsymbol{\sigma} D^\dagger(\hat{\mathbf{n}}, \theta) &= [\cos(\theta/2) + i (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \sin(\theta/2)] \boldsymbol{\sigma} [\cos(\theta/2) - i (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \sin(\theta/2)] \\ &= \boldsymbol{\sigma} \cos^2(\theta/2) - i [\boldsymbol{\sigma}, (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})] \sin(\theta/2) \cos(\theta/2) + (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \boldsymbol{\sigma} (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \sin^2(\theta/2) \end{aligned} \quad (19.93)$$

Now using

$$\begin{aligned} [\boldsymbol{\sigma}, (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma})] &= 2i (\hat{\mathbf{n}} \times \boldsymbol{\sigma}), \\ (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \boldsymbol{\sigma} (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) &= \boldsymbol{\sigma} + 2i (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) (\hat{\mathbf{n}} \times \boldsymbol{\sigma}) = 2 (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \hat{\mathbf{n}} - \boldsymbol{\sigma}, \end{aligned} \quad (19.94)$$

Eq. (19.93) becomes:

$$\begin{aligned} D(\hat{\mathbf{n}}, \theta) \boldsymbol{\sigma} D^\dagger(\hat{\mathbf{n}}, \theta) &= \boldsymbol{\sigma} \cos(\theta) - (\boldsymbol{\sigma} \times \hat{\mathbf{n}}) \sin(\theta) + (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \hat{\mathbf{n}} (1 - \cos(\theta)) \\ &= (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \hat{\mathbf{n}} + \hat{\mathbf{n}} \times (\boldsymbol{\sigma} \times \hat{\mathbf{n}}) \cos(\theta) - (\boldsymbol{\sigma} \times \hat{\mathbf{n}}) \sin(\theta). \end{aligned} \quad (19.95)$$

Then, in the adjoint representation, the rotation of coordinates is expressed as:

$$\begin{aligned}
D(\hat{\mathbf{n}}, \theta) V(\hat{\mathbf{r}}) D^\dagger(\hat{\mathbf{n}}, \theta) &= D(\hat{\mathbf{n}}, \theta) \hat{\mathbf{r}} \cdot \boldsymbol{\sigma} D^\dagger(\hat{\mathbf{n}}, \theta) \\
&= (\hat{\mathbf{n}} \cdot \hat{\mathbf{r}}) (\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) + \hat{\mathbf{r}} \cdot \hat{\mathbf{n}} \times (\boldsymbol{\sigma} \times \hat{\mathbf{n}}) \cos(\theta) - \hat{\mathbf{r}} \cdot (\boldsymbol{\sigma} \times \hat{\mathbf{n}}) \sin(\theta) \\
&= [(\hat{\mathbf{n}} \cdot \hat{\mathbf{r}}) \hat{\mathbf{n}} + \hat{\mathbf{n}} \times (\hat{\mathbf{r}} \times \hat{\mathbf{n}}) \cos(\theta) + (\hat{\mathbf{r}} \times \hat{\mathbf{n}}) \sin(\theta)] \cdot \boldsymbol{\sigma} \\
&= \hat{\mathbf{r}}' \cdot \boldsymbol{\sigma} = V(\hat{\mathbf{r}}'),
\end{aligned} \tag{19.96}$$

where the vector $\hat{\mathbf{r}}'$ is given by Eq. (19.59), with $x'_i = R_{ij}(\hat{\mathbf{n}}, \theta) x_j$. This completes the proof. \square

But Eq. (19.88) is not the only way to describe a rotation, here. We can also use the transformation properties of spinors which are eigenvectors of the operator $V(\hat{\mathbf{r}})$. There are *two* such spinors. From Theorem 27 in Chapter 13, the eigenvalue equation for the operator $V(\hat{\mathbf{r}}) = \hat{\mathbf{r}} \cdot \boldsymbol{\sigma}$ is given by:

$$\hat{\mathbf{r}} \cdot \boldsymbol{\sigma} \chi_{\pm}(\theta, \phi) = \pm \chi_{\pm}(\theta, \phi). \tag{19.97}$$

The eigenvectors, written in a number of different ways, are given by:

$$\begin{aligned}
\chi_+(\theta, \phi) &= \begin{pmatrix} \chi_{+,+}(\theta, \phi) \\ \chi_{+,-}(\theta, \phi) \end{pmatrix} = \begin{pmatrix} e^{-i\phi/2} \cos(\theta/2) \\ e^{+i\phi/2} \sin(\theta/2) \end{pmatrix} \\
&= \frac{e^{-i\phi/2}}{2 \cos(\theta/2)} \begin{pmatrix} 2 \cos^2(\theta/2) \\ e^{+i\phi} \sin(\theta/2) \cos(\theta/2)/2 \end{pmatrix} = \frac{e^{-i\phi/2}}{2 \cos(\theta/2)} \begin{pmatrix} 1 + x_3 \\ x_1 + ix_2 \end{pmatrix}, \\
&= \frac{e^{+i\phi/2}}{2 \sin(\theta/2)} \begin{pmatrix} e^{-i\phi} \sin(\theta/2) \cos(\theta/2)/2 \\ 2 \sin^2(\theta/2) \end{pmatrix} = \frac{e^{-i\phi/2}}{2 \sin(\theta/2)} \begin{pmatrix} x_1 - ix_2 \\ 1 - x_3 \end{pmatrix},
\end{aligned} \tag{19.98}$$

and

$$\begin{aligned}
\chi_-(\theta, \phi) &= \begin{pmatrix} \chi_{-,+}(\theta, \phi) \\ \chi_{-,-}(\theta, \phi) \end{pmatrix} = \begin{pmatrix} -e^{-i\phi/2} \sin(\theta/2) \\ e^{+i\phi/2} \cos(\theta/2) \end{pmatrix} \\
&= \frac{e^{+i\phi/2}}{2 \cos(\theta/2)} \begin{pmatrix} -e^{-i\phi} \sin(\theta/2) \cos(\theta/2)/2 \\ 2 \cos^2(\theta/2) \end{pmatrix} = \frac{e^{+i\phi/2}}{2 \cos(\theta/2)} \begin{pmatrix} -x_1 + ix_2 \\ 1 + x_3 \end{pmatrix}, \\
&= \frac{e^{-i\phi/2}}{2 \sin(\theta/2)} \begin{pmatrix} -2 \sin^2(\theta/2) \\ e^{+i\phi} \sin(\theta/2) \cos(\theta/2)/2 \end{pmatrix} = \frac{e^{-i\phi/2}}{2 \sin(\theta/2)} \begin{pmatrix} x_3 - 1 \\ x_1 + ix_2 \end{pmatrix},
\end{aligned} \tag{19.99}$$

where

$$x_1 = \sin \theta \cos \phi, \quad x_2 = \sin \theta \sin \phi, \quad x_3 = \cos \theta. \tag{19.100}$$

We define the *ratio* of the complex conjugates of the upper to lower components of these spinors by:

$$z_{\pm} = \frac{\chi_{\pm,+}^*(\theta, \phi)}{\chi_{\pm,-}^*(\theta, \phi)}. \tag{19.101}$$

So from (19.98), we find:

$$\begin{aligned}
z_+^* &= \frac{1 + x_3}{x_1 + ix_2} = \frac{x_1 - ix_2}{1 - x_3}, \\
z_-^* &= \frac{-x_1 + ix_2}{1 + x_3} = \frac{x_3 - 1}{x_1 + ix_2} = -\frac{1}{z_+}.
\end{aligned} \tag{19.102}$$

But now we recognize z_+ as the stereographic projection mapping discovered by Klein and Cayley given in Eq. (19.66) from the unit sphere to the complex plane:

$$z_+ = x + iy = \frac{x_1 + ix_2}{1 - x_3} = \frac{1 + x_3}{x_1 - ix_2}. \tag{19.103}$$

z_-^* is the negative reciprocal of this mapping. So except for a normalization factor, components of the spinor $\chi_+(\theta, \phi)$ are fixed by the stereographic projection mapping. We now need to find out how spinors transform under rotations of the coordinate system. We can deduce this transformation from Eq. (19.88). Since

$$(\hat{\mathbf{r}}' \cdot \boldsymbol{\sigma}) D(R) = D(R) (\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}), \quad (19.104)$$

we see that when this equation operates on a spinor $\chi_{\pm}(\theta, \phi)$, we find:

$$(\hat{\mathbf{r}}' \cdot \boldsymbol{\sigma}) \{ D(R) \chi_{\pm}(\theta, \phi) \} = \pm \{ D(R) \chi_{\pm}(\theta, \phi) \}, \quad (19.105)$$

so $\{ D(R) \chi_{\pm}(\theta, \phi) \}$ is an eigenvector of $(\hat{\mathbf{r}}' \cdot \boldsymbol{\sigma})$ with eigenvalue ± 1 . That is, the transformation rule for spinors is:

$$\chi_{\pm}(\theta', \phi') = D(R) \chi_{\pm}(\theta, \phi). \quad (19.106)$$

Writing this out explicitly for χ_+ , we have:

$$\begin{pmatrix} \chi'_{+,+} \\ \chi'_{+,-} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \chi_{+,+} \\ \chi_{+,-} \end{pmatrix} = \begin{pmatrix} a \chi_{+,+} + b \chi_{+,-} \\ c \chi_{+,+} + d \chi_{+,-} \end{pmatrix}. \quad (19.107)$$

So z_+^* , defined by Eq. (19.101), transforms under rotation of the coordinate system as:

$$z_+^{\prime*} = \frac{a z_+^* + b}{c z_+^* + d}, \quad (19.108)$$

in agreement with linear fractional transformation we claimed in Eq. (19.67). It is remarkable that Kline and Cayley discovered this two-dimensional representation of rotations using quaternions in the nineteenth century, long before quantum mechanics was invented.

Remark 32. Given a 2×2 unitary operator $D(R)$, and the Cartan mapping (19.87), we can find the rotation matrix R associated with $D(R)$ by noting:

$$x'_i = \frac{1}{2} \text{Tr}[\sigma_i V(\mathbf{r}')] = \frac{1}{2} \text{Tr}[\sigma_i D(R) V(\mathbf{r}) D^\dagger(R)] = \frac{1}{2} \text{Tr}[\sigma_i D(R) \sigma_j D^\dagger(R)] x_j = R_{ij} x_j, \quad (19.109)$$

where

$$R_{ij} = \frac{1}{2} \text{Tr}[\sigma_i D(R) \sigma_j D^\dagger(R)]. \quad (19.110)$$

Schwinger [14] used (19.110) to show that for every $D(R) \in SU(2)$, $R \in SO(3)$.

Remark 33. We have just shown that

$$D(R) x_j \sigma_j D^\dagger(R) = x'_i \sigma_i = R_{ij} x_j \sigma_i, \quad (19.111)$$

for arbitrary x_i . So

$$D(R) \sigma_j D^\dagger(R) = \sigma_i R_{ij}. \quad (19.112)$$

Inverting this expression gives:

$$D^\dagger(R) \sigma_i D(R) = R_{ij} \sigma_j. \quad (19.113)$$

That is, the matrices σ_i are rotated in the reverse way by the transformation.

Remark 34. We have show here that we can equally use these two-dimensional unitary, unimodular matrices to describe the relative orientation of two coordinate systems. The set of all such matrices $U(R)$ form a group called $SU(2)$, the special group of two-dimensional unitary matrices. Theorem 34 demonstrates that for every rotation matrix R , there is a unitary matrix $U(R)$ that provides the same relation between components of vectors in the two systems. The two groups, $O^+(3)$ and $SU(2)$, are said to be isomorphic: $O^+(3) \sim SU(2)$. We emphasize again that the above discussion is completely classical.

Exercise 53. Compute $\det[V(\mathbf{r})]$ and show that $\det[V(\mathbf{r}')] = \det[V(\mathbf{r})]$.

Exercise 54. Using the definition (19.89) for $D(R)$, show that $D(R')D(R) = D(R'R)$.

Exercise 55. Show that for the Euler angle parameterization, the $D(R)$ matrix is given by:

$$\begin{aligned} D(\gamma, \beta, \alpha) &= D_z(\gamma) D_y(\beta) D_z(\alpha) = e^{i\sigma_z\gamma/2} e^{i\sigma_y\beta/2} e^{i\sigma_z\alpha/2} \\ &= \begin{pmatrix} e^{i(+\gamma+\alpha)/2} \cos(\beta/2) & e^{i(+\gamma-\alpha)/2} \sin(\beta/2) \\ -e^{i(-\gamma+\alpha)/2} \sin(\beta/2) & e^{i(-\gamma-\alpha)/2} \cos(\beta/2) \end{pmatrix}, \end{aligned} \quad (19.114)$$

as stated in Eq. (19.92).

Exercise 56. Using the sequential matrix construction for $D(\gamma, \beta, \alpha)$ given in Exercise 55, and the Euler angle rotation matrix $R(\gamma, \beta, \alpha) = R_z(\gamma) R_y(\beta) R_z(\alpha)$, prove (19.113) directly, and thus Theorem 34 for the Euler angle representation of rotations.

19.3 Rotations in quantum mechanics

In quantum mechanics, symmetry transformations, such as rotations of the coordinate system, are represented by unitary transformations of vectors in the Hilbert space. Unitary representations of the rotation group are faithful representations. This means that the composition rule, $R'' = R'R$ of the group is preserved by the unitary representation, *without any phase factors*.⁶ That is: $U(R'') = U(R')U(R)$. We also have $U(1) = 1$ and $U^{-1}(R) = U^\dagger(R) = U(R^{-1})$. For infinitesimal rotations, we write the classical rotational matrix as in Eq. (19.52):

$$R_{ij}(\hat{\mathbf{n}}, \Delta\theta) = \delta_{ij} + \epsilon_{ijk} \hat{n}_k \Delta\theta + \dots, \quad (19.115)$$

which we abbreviate as $R = 1 + \Delta\theta + \dots$. We write the infinitesimal unitary transformation as:

$$U_{\mathbf{J}}(1 + \Delta\theta) = 1 + i n_i J_i \Delta\theta / \hbar + \dots, \quad (19.116)$$

where J_i is the Hermitian generator of the transformation. We will show in this section that the set of generators J_i , for $i = 1, 2, 3$, transform under rotations in quantum mechanics as a pseudo-vector and that it obeys the commutation relations we assumed in Eq. (19.1) at the beginning of this chapter. The factor of \hbar is inserted here so that J_i can have units of classical angular momentum, and is the *only* way that makes $U_{\mathbf{J}}(R)$ into a quantum operator. Now let us consider the combined transformation:

$$U_{\mathbf{J}}^\dagger(R) U_{\mathbf{J}}(1 + \Delta\theta') U_{\mathbf{J}}(R) = U_{\mathbf{J}}(R^{-1}) U_{\mathbf{J}}(1 + \Delta\theta') U_{\mathbf{J}}(R) = U_{\mathbf{J}}(R^{-1} (1 + \Delta\theta') R) = U_{\mathbf{J}}(1 + \Delta\theta''). \quad (19.117)$$

We first work out the classical transformation:

$$1 + \Delta\theta'' + \dots = R^{-1} (1 + \Delta\theta') R = 1 + R^{-1} \Delta\theta' R + \dots \quad (19.118)$$

That is

$$\epsilon_{ijk} \hat{n}_k \Delta\theta'' = \epsilon_{i'j'k'} R_{i'i} R_{j'j} \hat{n}_{k'} \Delta\theta'. \quad (19.119)$$

Now using the relation:

$$\det[R] \epsilon_{ijk} = \epsilon_{i'j'k'} R_{i'i} R_{j'j} R_{k'k}, \quad \text{or} \quad \det[R] \epsilon_{ijk} R_{k'k} = \epsilon_{i'j'k'} R_{i'i} R_{j'j}. \quad (19.120)$$

Inserting this result into (19.119) gives the relation:

$$\hat{n}_k \Delta\theta'' = \det[R] R_{k'k} \hat{n}_{k'} \Delta\theta' \quad (19.121)$$

⁶This is not the case for the full Galilean group, where there is a phase factor involved (see Chapter 7 and particularly Section 7.5).

So from (19.117), we find:

$$\begin{aligned} 1 + i \hat{n}_j J_j \Delta\theta''/\hbar + \cdots &= U_{\mathbf{J}}^\dagger(R) \left\{ 1 + i \hat{n}_i J_i \Delta\theta'/\hbar + \cdots \right\} U_{\mathbf{J}}(R) \\ &= 1 + i U_{\mathbf{J}}^\dagger(R) J_i U_{\mathbf{J}}(R) \hat{n}_i \Delta\theta'/\hbar + \cdots, \end{aligned} \quad (19.122)$$

or

$$U_{\mathbf{J}}^\dagger(R) J_i U_{\mathbf{J}}(R) \hat{n}_i \Delta\theta' = \hat{n}_j J_j \Delta\theta' = \det[R] R_{ij} J_j \hat{n}_i \Delta\theta'. \quad (19.123)$$

Comparing coefficients of $\hat{n}_i \Delta\theta'$ on both sides of this equation, we find:

$$U_{\mathbf{J}}^\dagger(R) J_i U_{\mathbf{J}}(R) = \det[R] R_{ij} J_j, \quad (19.124)$$

showing that under rotations, the generators of rotations J_i transform as pseudo-vectors. For ordinary rotations $\det[R] = +1$; whereas for Parity or mirror inversions of the coordinate system $\det[R] = -1$. We restrict ourselves here to ordinary rotations. Iterating the infinitesimal rotation operator (19.118) gives the finite unitary transformation:

$$U_{\mathbf{J}}(\hat{\mathbf{n}}, \theta) = e^{i \hat{\mathbf{n}} \cdot \mathbf{J} \theta / \hbar}, \quad R \mapsto (\hat{\mathbf{n}}, \theta). \quad (19.125)$$

Further expansion of $U(R)$ in Eq. (19.124) for infinitesimal $R = 1 + \Delta\theta + \cdots$ gives:

$$\left\{ 1 - i \hat{n}_j J_j \Delta\theta/\hbar + \cdots \right\} J_i \left\{ 1 + i \hat{n}_j J_j \Delta\theta/\hbar + \cdots \right\} = \left\{ \delta_{ij} + \epsilon_{ijk} \hat{n}_k \Delta\theta + \cdots \right\} J_j. \quad (19.126)$$

Comparing coefficients of $\hat{n}_j \Delta\theta$ on both sides of this equation gives the commutation relations for the angular momentum generators:

$$[J_i, J_j] = i \hbar \epsilon_{ijk} J_k. \quad (19.127)$$

This derivation of the properties of the unitary transformations and generators of the rotation group parallels that of the properties of the full Galilean group done in Chapter 7.

Remark 35. When $j = 1/2$ we can put $\mathbf{J} = \mathbf{S} = \hbar \boldsymbol{\sigma}/2$, so that the unitary rotation operator is given by:

$$U_{\mathbf{S}}(\hat{\mathbf{n}}, \theta) = e^{i \hat{\mathbf{n}} \cdot \mathbf{S} / \hbar} = e^{i \hat{\mathbf{n}} \cdot \boldsymbol{\sigma} / 2}, \quad (19.128)$$

which is the same as the unitary operator, Eq. (G.131), which we used to describe classical rotations in the adjoint representation.

Exercise 57. Suppose the composition rule for the unitary representation of the rotation group is of the form:

$$U(R') U(R) = e^{i \phi(R', R)} U(R' R), \quad (19.129)$$

where $\phi(R', R)$ is a phase which may depend on R and R' . Using Bargmann's method (see Section 7.2.1), show that the phase $\phi(R', R)$ is a trivial phase, and can be absorbed into the overall phase of the unitary transformation. This exercise shows that the unitary representation of the rotation group is faithful.

Now we want to find relations between eigenvectors $|j, m\rangle$ angular momentum in two frames related by a rotation. So let $|j, m\rangle$ be eigenvectors of J^2 and J_z in the Σ frame and $|j, m'\rangle$ be eigenvectors of J^2 and J_z in the Σ' frame. We first note that the square of the total angular momentum vector is invariant under rotations:

$$U_{\mathbf{J}}^\dagger(R) J^2 U_{\mathbf{J}}(R) = J^2, \quad (19.130)$$

so the total angular momentum quantum numbers for the eigenvectors must be the same in each frame, $j' = j$. From (19.124), J_i transforms as follows (in the following, we consider the case when $\det[R] = +1$):

$$U_{\mathbf{J}}^\dagger(R) J_i U_{\mathbf{J}}(R) = R_{i,j} J_j = J'_i, \quad (19.131)$$

So multiplying (19.131) on the left by $U_{\mathbf{J}}^{\dagger}(R)$, setting $i = z$, and operating on the eigenvector $|j, m\rangle$ defined in frame Σ , we find:

$$J_{z'} \{ U_{\mathbf{J}}^{\dagger}(R) |j, m\rangle \} = U_{\mathbf{J}}^{\dagger}(R) J_z |j, m\rangle = \hbar m \{ U_{\mathbf{J}}^{\dagger}(R) |j, m\rangle \}, \quad (19.132)$$

from which we conclude that $U_{\mathbf{J}}^{\dagger}(R) |j, m\rangle$ is an eigenvector of $J_{z'}$ with eigenvalue $\hbar m$. That is:

$$|j, m\rangle' = U_{\mathbf{J}}^{\dagger}(R) |j, m\rangle = \sum_{m'=-j}^{+j} |j, m'\rangle \langle j, m' | U_{\mathbf{J}}^{\dagger}(R) |j, m\rangle = \sum_{m'=-j}^{+j} D_{m, m'}^{(j)*}(R) |j, m'\rangle, \quad (19.133)$$

where we have defined the D -functions, which are angular momentum matrix elements of the rotation operator, by:

Definition 36 (D -functions). The D -functions are the matrix elements of the rotation operator, and are defined by:

$$D_{m, m'}^{(j)}(R) = \langle j, m | U_{\mathbf{J}}(R) |j, m'\rangle = \langle j, m | j, m'\rangle = \langle j, m | U_{\mathbf{J}}(R) |j, m'\rangle'. \quad (19.134)$$

The D -function can be computed in either the Σ or Σ' frames. Eq. (19.133) relates eigenvectors of the angular momentum in frame Σ' to those in Σ . Note that the matrix $D_{m, m'}^{(j)}(R)$ is the overlap between the state $|j, m\rangle'$ in the Σ' frame and $|j, m\rangle$ in the Σ frame. The *row's* of this matrix are the adjoint eigenvectors of J'_z in the Σ frame, so that the *columns* of the adjoint matrix, $D_{m', m}^{(j)*}(R)$ are the eigenvectors of J'_z in the Σ frame.

For infinitesimal rotations, the D -function is given by:

$$\begin{aligned} D_{m, m'}^{(j)}(\hat{\mathbf{n}}, \Delta\theta) &= \langle j, m | U_{\mathbf{J}}(\hat{\mathbf{n}}, \Delta\theta) |j, m'\rangle = \langle j, m | \{ 1 + \frac{i}{\hbar} \hat{\mathbf{n}} \cdot \mathbf{J} \Delta\theta + \dots \} |j, m'\rangle \\ &= \delta_{m, m'} + \frac{i}{\hbar} \langle j, m | \hat{\mathbf{n}} \cdot \mathbf{J} |j, m'\rangle \Delta\theta + \dots \end{aligned} \quad (19.135)$$

Exercise 58. Find the first order matrix elements of $D_{m, m'}^{(j)}(\hat{\mathbf{n}}, \Delta\theta)$ for $\hat{\mathbf{n}} = \hat{\mathbf{e}}_z$ and $\hat{\mathbf{n}} = \hat{\mathbf{e}}_x \pm i\hat{\mathbf{e}}_y$.

19.3.1 Rotations using Euler angles

Consider the sequential rotations $\Sigma \rightarrow \Sigma' \rightarrow \Sigma'' \rightarrow \Sigma'''$, described by the Euler angles defined in Section 19.2.3. The unitary operator in quantum mechanics for this classical transformation is then given by the composition rule:

$$U_{\mathbf{J}}(\gamma, \beta, \alpha) = U_{\mathbf{J}}(\hat{\mathbf{e}}_z, \gamma) U_{\mathbf{J}}(\hat{\mathbf{e}}_y, \beta) U_{\mathbf{J}}(\hat{\mathbf{e}}_z, \alpha) = e^{iJ_z\gamma/\hbar} e^{iJ_y\beta/\hbar} e^{iJ_z\alpha/\hbar}. \quad (19.136)$$

So the angular momentum operator J_i transforms according to ($\det[R] = 1$):

$$U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) J_i U_{\mathbf{J}}(\gamma, \beta, \alpha) = R_{z i j}(\gamma) R_{y j k}(\beta) R_{z k l}(\alpha) J_l = R_{il}(\gamma, \beta, \alpha) J_l \equiv J_i''', \quad (19.137)$$

where $R_{il}(\gamma, \beta, \alpha)$ is given by Eq. (19.63). Again, multiplying on the right by $U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha)$, setting $i = z$, and operating on the eigenvector $|j, m\rangle$ defined in frame Σ , we find:

$$J_{z'''} \{ U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) |j, m\rangle \} = U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) J_z |j, m\rangle = \hbar m \{ U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) |j, m\rangle \}. \quad (19.138)$$

So we conclude here that $U_{\mathbf{J}}^{\dagger}(\alpha, \beta, \gamma) |j, m\rangle$ is an eigenvector of $J_{z''}$ with eigenvalue $\hbar m$. That is:

$$\begin{aligned} |j, m\rangle''' &= U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) |j, m\rangle \\ &= \sum_{m'=-j}^{+j} |j, m'\rangle \langle j, m' | U_{\mathbf{J}}^{\dagger}(\gamma, \beta, \alpha) |j, m\rangle = \sum_{m'=-j}^{+j} D_{m, m'}^{(j)*}(\gamma, \beta, \alpha) |j, m'\rangle. \end{aligned} \quad (19.139)$$

where the D -matrix is defined by:

$$D_{m,m'}^{(j)}(\gamma, \beta, \alpha) = \langle j, m | U_{\mathbf{J}}(\gamma, \beta, \alpha) | j, m' \rangle = \langle j, m | e^{iJ_z\gamma/\hbar} e^{iJ_y\beta/\hbar} e^{iJ_z\alpha/\hbar} | j, m' \rangle \quad (19.140)$$

We warn the reader that there is a great deal of confusion, especially in the early literature, concerning Euler angles and representation of rotations in quantum mechanics. From our point of view, all we need is the matrix representation provided by Eq. (19.63) and the composition rule for unitary representation of the rotation group. Our definition of the D -matrices, Eq. (19.140), agrees with the 1996 printing of Edmonds[2][Eq. (4.1.9) on p. 55]. Earlier printings of Edmonds were in error. (See the articles by Bouten [15] and Wolf [16].)

19.3.2 Properties of D -functions

Matrix elements of the rotation operator using Euler angles to define the rotation are given by:

$$D_{m,m'}^{(j)}(\gamma, \beta, \alpha) = \langle jm | U_{\mathbf{J}}(\gamma, \beta, \alpha) | jm' \rangle = e^{i(m\gamma+m'\alpha)} d_{m,m'}^{(j)}(\beta), \quad (19.141)$$

where $d_{m,m'}^{(j)}(\beta)$ is *real* and given by:⁷

$$d_{m,m'}^{(j)}(\beta) = \langle jm | e^{i\beta J_y/\hbar} | jm' \rangle.$$

We derive an explicit formula for the D -matrices in Theorem 58 in Section G.5 using Schwinger's methods, where we find:

$$D_{m,m'}^{(j)}(R) = \sqrt{(j+m)!(j-m)!(j+m')(j-m')} \\ \times \sum_{s=0}^{j+m} \sum_{r=0}^{j-m} \delta_{s-r,m-m'} \frac{(D_{+,+}(R))^{j+m-s} (D_{+,-}(R))^s (D_{-,+}(R))^r (D_{-,-}(R))^{j-m-r}}{s!(j+m-s)!r!(j-m-r)!}, \quad (19.142)$$

where elements of the matrix $D(R)$, with rows and columns labeled by \pm , are given by any of the parameterizations:

$$D(R) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \cos(\theta/2) + i(\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}) \sin(\theta/2) \\ = \begin{pmatrix} e^{i(+\gamma+\alpha)/2} \cos(\beta/2) & e^{i(+\gamma-\alpha)/2} \sin(\beta/2) \\ -e^{i(-\gamma+\alpha)/2} \sin(\beta/2) & e^{i(-\gamma-\alpha)/2} \cos(\beta/2) \end{pmatrix}. \quad (19.143)$$

Using Euler angles, this gives the formula:

$$d_{m,m'}^{(j)}(\beta) = \sqrt{(j+m)!(j-m)!(j+m')(j-m')} \\ \times \sum_{\sigma} \frac{(-)^{j-\sigma-m} (\cos(\beta/2))^{2\sigma+m+m'} (\sin(\beta/2))^{2j-2\sigma-m-m'}}{\sigma!(j-\sigma-m)!(j-\sigma-m')!(\sigma+m+m')!}. \quad (19.144)$$

From this, it is easy to show that:

$$d_{m,m'}^{(j)}(\beta) = d_{m,m'}^{(j)*}(\beta) = d_{m',m}^{(j)}(-\beta) = (-)^{m-m'} d_{-m,-m'}^{(j)}(\beta) = (-)^{m-m'} d_{m',m}^{(j)}(\beta). \quad (19.145)$$

In particular, in Section G.5, we show that:

$$d_{m,m'}^{(j)}(\pi) = (-)^{j-m} \delta_{m,-m'}, \quad \text{and} \quad d_{m,m'}^{(j)}(-\pi) = (-)^{j+m} \delta_{m,-m'}. \quad (19.146)$$

⁷This is the reason in quantum mechanics for choosing the second rotation to be about the y -axis rather than the x -axis.

The D -matrix for the inverse transformation is given by:

$$D_{m,m'}^{(j)}(R^{-1}) = D_{m',m}^{(j)*}(R) = (-)^{m-m'} D_{-m,-m'}^{(j)}(R) \quad (19.147)$$

For Euler angles, since $d_{m,m'}^{(j)}(\beta)$ is real, this means that:

$$D_{m,m'}^{(j)*}(\alpha, \beta, \gamma) = D_{m',m}^{(j)}(-\gamma, -\beta, -\alpha) = D_{m,m'}^{(j)}(-\alpha, \beta, -\gamma) = (-)^{m-m'} D_{-m,-m'}^{(j)}(\alpha, \beta, \gamma). \quad (19.148)$$

Exercise 59. Show that the matrix $d^{(1)}(\beta)$ for $j = 1/2$, is given by:

$$d^{(1/2)}(\beta) = e^{i\beta\sigma_y/2} = \cos(\beta/2) + i\sigma_y \sin(\beta/2) = \begin{pmatrix} \cos(\beta/2) & \sin(\beta/2) \\ -\sin(\beta/2) & \cos(\beta/2) \end{pmatrix},$$

so that

$$D^{(1/2)}(\gamma, \beta, \alpha) = \begin{pmatrix} e^{i(\gamma+\alpha)/2} \cos(\beta/2) & e^{i(\gamma-\alpha)/2} \sin(\beta/2) \\ -e^{i(-\gamma+\alpha)/2} \sin(\beta/2) & e^{i(-\gamma-\alpha)/2} \cos(\beta/2) \end{pmatrix}, \quad (19.149)$$

which agrees with Eq. (13.13) if we put $\gamma = 0$, $\beta = \theta$, and $\alpha = \phi$.

Exercise 60. Show that the matrix $d^{(1)}(\beta)$ for $j = 1$, is given by:

$$d^{(1)}(\beta) = e^{i\beta S_y} = \begin{pmatrix} (1 + \cos \beta)/2 & \sin \beta/\sqrt{2} & (1 - \cos \beta)/2 \\ -\sin \beta/\sqrt{2} & \cos \beta & \sin \beta/\sqrt{2} \\ (1 - \cos \beta)/2 & -\sin \beta/\sqrt{2} & (1 + \cos \beta)/2 \end{pmatrix}. \quad (19.150)$$

Use the results for S_y in Eq. (19.10) and expand the exponent in a power series in $i\beta S_y$ for a few terms (about four or five terms should do) in order to deduce the result directly.

Remark 36. From the results in Eq. (19.150), we note that:

$$Y_{1,m}(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \begin{cases} -\sin \theta e^{+i\phi}/\sqrt{2}, & \text{for } m = +1, \\ \cos \theta, & \text{for } m = 0, \\ +\sin \theta e^{-i\phi}/\sqrt{2}, & \text{for } m = -1. \end{cases} \quad (19.151)$$

so

$$D_{0,m}^{(1)}(\gamma, \beta, \alpha) = \sqrt{\frac{4\pi}{3}} Y_{1,m}(\beta, \alpha), \quad \text{and} \quad D_{m,0}^{(1)}(\gamma, \beta, \alpha) = (-)^m \sqrt{\frac{4\pi}{3}} Y_{1,m}(\beta, \gamma), \quad (19.152)$$

in agreement with Eqs. (19.162) and (19.163).

19.3.3 Rotation of orbital angular momentum

When the angular momentum has a coordinate representation so that $\mathbf{J} = \mathbf{L} = \mathbf{R} \times \mathbf{P}$,

$$U_{\mathbf{L}}^\dagger(\gamma, \beta, \alpha) X_i U_{\mathbf{L}}(\gamma, \beta, \alpha) = R_{ij}(\gamma, \beta, \alpha) X_j = X_i''', \quad (19.153)$$

or

$$X_i U_{\mathbf{L}}(\gamma, \beta, \alpha) = U_{\mathbf{L}}(\gamma, \beta, \alpha) X_i''', \quad (19.154)$$

so that:

$$X_i \{ U_{\mathbf{L}}(\gamma, \beta, \alpha) | \mathbf{r} \rangle \} = U_{\mathbf{L}}(\gamma, \beta, \alpha) X_i''' | \mathbf{r} \rangle = x_i''' \{ U_{\mathbf{L}}(\gamma, \beta, \alpha) | \mathbf{r} \rangle \}, \quad (19.155)$$

which means that $U_{\mathbf{L}}(\gamma, \beta, \alpha) | \mathbf{r} \rangle$ is an eigenvector of X_i with eigenvalue $x_i''' = R_{ij}(\gamma, \beta, \alpha) x_j$. That is:

$$| \mathbf{r}''' \rangle = U_{\mathbf{L}}(\gamma, \beta, \alpha) | \mathbf{r} \rangle. \quad (19.156)$$

The spherical harmonics of Section 19.1.2 are defined by:

$$Y_{\ell,m}(\theta, \phi) = \langle \hat{\mathbf{r}} | \ell, m \rangle = \langle \theta, \phi | \ell, m \rangle. \quad (19.157)$$

Now let the point P be on the unit circle so that the coordinates of this point is described by the polar angles (θ, ϕ) in frame Σ and the polar angles (θ', ϕ') in the rotated frame Σ' . So on this unit circle,

$$\begin{aligned} Y_{\ell,m}(\theta, \phi) &= \langle \theta, \phi | \ell, m \rangle = \langle \theta''', \phi''' | U_{\mathbf{L}}(\gamma, \beta, \alpha) | \ell, m \rangle = \langle \theta''', \phi''' | \ell, m \rangle''' = Y_{\ell,m}'''(\theta''', \phi''') \\ &= \sum_{m'=-\ell}^{+\ell} \langle \theta''', \phi''' | \ell, m' \rangle \langle \ell, m' | U_{\mathbf{L}}(\gamma, \beta, \alpha) | \ell, m \rangle = \sum_{m'=-\ell}^{+\ell} Y_{\ell,m'}(\theta''', \phi''') D_{m',m}^{(\ell)}(\gamma, \beta, \alpha), \end{aligned} \quad (19.158)$$

where

$$D_{m,m'}^{(\ell)}(\gamma, \beta, \alpha) = \langle \ell, m | U_{\mathbf{L}}(\gamma, \beta, \alpha) | \ell, m' \rangle. \quad (19.159)$$

As a special case, let us evaluate Eq. (19.158) at a point $P_0 = (x''', y''', z''') = (0, 0, 1)$ on the unit circle on the z''' -axis in the Σ''' , or $\theta''' = 0$. However Eq. (19.23) states that:

$$Y_{\ell,m'}(0, \phi''') = \sqrt{\frac{2\ell+1}{4\pi}} \delta_{m',0}, \quad (19.160)$$

so only the $m' = 0$ term in Eq. (19.158) contributes to the sum and so evaluated at point P_0 , Eq. (19.158) becomes:

$$Y_{\ell,m}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} D_{0,m}^{(\ell)}(\gamma, \beta, \alpha). \quad (19.161)$$

The point P in the Σ frame is given by Eqs. (19.65). So for this point, the polar angles of point P in the Σ frame are: $\theta = \beta$ and $\phi = \alpha$, and Eq. (19.161) gives the result:

$$D_{0,m}^{(\ell)}(\gamma, \beta, \alpha) = \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell,m}(\beta, \alpha) = C_{\ell,m}(\beta, \alpha). \quad (19.162)$$

By taking the complex conjugate of this expression and using properties of the spherical harmonics, we also find:

$$D_{m,0}^{(\ell)}(\gamma, \beta, \alpha) = (-)^m \sqrt{\frac{4\pi}{2\ell+1}} Y_{\ell,m}(\beta, \alpha) = C_{\ell,-m}^*(\beta, \alpha). \quad (19.163)$$

As a special case, we find:

$$D_{0,0}^{(\ell)}(\gamma, \beta, \alpha) = P_{\ell}(\cos \beta), \quad (19.164)$$

where $P_{\ell}(\cos \beta)$ is the Lagrendre polynomial of order ℓ .

Exercise 61. Prove Eq. (19.163).

19.3.4 Sequential rotations

From the general properties of the rotation group, we know that $U(R'R) = U(R')U(R)$. If we describe the rotations by Euler angles, we write the combined rotation as:

$$R(\gamma'', \beta'', \alpha'') = R(\gamma', \beta', \alpha') R(\gamma, \beta, \alpha). \quad (19.165)$$

The unitary operator for this sequential transformation is then given by:

$$U_{\mathbf{J}}(\gamma'', \beta'', \alpha'') = U_{\mathbf{J}}(\gamma', \beta', \alpha') U_{\mathbf{J}}(\gamma, \beta, \alpha). \quad (19.166)$$

So the D -functions for this sequential rotation is given by matrix elements of this expression:

$$D_{m,m''}^{(j)}(\gamma'', \beta'', \alpha'') = \sum_{m'=-j}^{+j} D_{m,m'}^{(j)}(\gamma', \beta', \alpha') D_{m',m''}^{(j)}(\gamma, \beta, \alpha). \quad (19.167)$$

We can derive the addition theorem for spherical harmonics by considering the sequence of transformations given by:

$$R(\gamma'', \beta'', \alpha'') = R(\gamma', \beta', \alpha') R^{-1}(\gamma, \beta, \alpha) = R(\gamma', \beta', \alpha') R(-\alpha, -\beta, -\gamma). \quad (19.168)$$

The D -functions for this sequential rotation for integer $j = \ell$, is given by:

$$D_{m,m''}^{(\ell)}(\gamma'', \beta'', \alpha'') = \sum_{m'=-\ell}^{+\ell} D_{m,m'}^{(\ell)}(\gamma', \beta', \alpha') D_{m',m''}^{(\ell)}(-\alpha, -\beta, -\gamma). \quad (19.169)$$

Next, we evaluate Eq. (19.169) for $m = m'' = 0$. Using Eqs. (19.162), (19.163), and (19.164), we find:

$$P_\ell(\cos \beta'') = \frac{4\pi}{2\ell + 1} \sum_{m'=-\ell}^{+\ell} Y_{\ell,m}(\beta', \alpha') Y_{\ell,m}^*(\beta, \alpha). \quad (19.170)$$

Here (β, α) and (β', α') are the polar angles of two points on the unit circle in a *fixed* coordinate frame. In order to find $\cos \beta''$, we need to multiply out the rotation matrices given in Eq. (19.168). Let us first set $(\beta, \alpha) = (\theta, \phi)$ and $(\beta', \alpha') = (\theta', \phi')$, and set γ and γ' to zero. Then we find:

$$\begin{aligned} R(\gamma'', \beta'', \alpha'') &= R_y(\theta') R_z(\phi') R_z(-\phi) R_y(-\theta) = R_y(\theta') R_z(\phi' - \phi) R_y(-\theta) \\ &= \begin{pmatrix} \cos \theta' & 0 & -\sin \theta' \\ 0 & 1 & 0 \\ \sin \theta' & 0 & \cos \theta' \end{pmatrix} \begin{pmatrix} \cos \phi' & \sin \phi' & 0 \\ -\sin \phi' & \cos \phi' & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix} \\ &= \begin{pmatrix} \sin \theta \sin \theta' + \cos \theta \cos \theta' \cos \phi' & \cos \theta' \sin \phi' & -\sin \theta' \cos \theta + \cos \theta' \cos \theta \cos \phi' \\ -\cos \theta \sin \phi' & \cos \phi' & -\sin \theta \sin \phi' \\ -\cos \theta' \sin \theta + \sin \theta' \cos \theta \cos \phi' & \sin \theta' \sin \phi' & \cos \theta' \cos \theta + \sin \theta' \sin \theta \cos \phi' \end{pmatrix}. \end{aligned} \quad (19.171)$$

where we have set $\phi'' = \phi' - \phi$. We compare this with the general form of the rotation matrix given in Eq. (19.63):

$$R(\gamma'', \beta'', \alpha'') = \begin{pmatrix} \cos \gamma'' \cos \beta'' \cos \alpha'' - \sin \gamma'' \sin \alpha'', & \cos \gamma'' \cos \beta'' \sin \alpha'' + \sin \gamma'' \sin \alpha'', & -\cos \gamma'' \sin \beta'' \\ -\sin \gamma'' \cos \beta'' \cos \alpha'' - \cos \gamma'' \sin \alpha'', & -\sin \gamma'' \cos \beta'' \sin \alpha'' + \cos \gamma'' \cos \alpha'', & \sin \gamma'' \sin \beta'' \\ \sin \beta'' \cos \alpha'', & \sin \beta'' \sin \alpha'', & \cos \beta'' \end{pmatrix}. \quad (19.172)$$

Comparing this with Eq. (19.171), we see that the (3,3) component requires that:

$$\cos \beta'' = \cos \theta' \cos \theta + \sin \theta' \sin \theta \cos \phi'. \quad (19.173)$$

It is not easy to find the values of α'' and γ'' . We leave this problem to the interested reader.

Exercise 62. Find α'' and γ'' by comparing Eqs. (19.171) and (19.172), using the result (19.173).

So Eq. (19.170) becomes:

$$P_\ell(\cos \gamma) = \frac{4\pi}{2\ell + 1} \sum_{m=-\ell}^{+\ell} Y_{\ell,m}(\theta', \phi') Y_{\ell,m}^*(\theta, \phi), \quad (19.174)$$

where $\cos \gamma = \cos \theta' \cos \theta + \sin \theta' \sin \theta \cos(\phi' - \phi)$. Eq. (19.174) is called the addition theorem of spherical harmonics.

19.4 Addition of angular momentum

If a number of angular momentum vectors commute, the eigenvectors of the combined system can be written as a direct product consisting of the vectors of each system:

$$|j_1, m_1, j_2, m_2, \dots, j_N, m_N\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle \otimes \cdots \otimes |j_N, m_N\rangle. \quad (19.175)$$

This vector is an eigenvector of J_i^2 and $J_{i,z}$ for $i = 1, 2, \dots, N$. It is also an eigenvector of the total z -component of angular momentum: $J_z |j_1, m_1, j_2, m_2, \dots, j_N, m_N\rangle = M |j_1, m_1, j_2, m_2, \dots, j_N, m_N\rangle$, where $M = m_1 + m_2 + \cdots + m_N$. It is *not*, however, an eigenvector of the total angular momentum J^2 , defined by

$$J^2 = \mathbf{J} \cdot \mathbf{J}, \quad \mathbf{J} = \sum_{i=1}^N \mathbf{J}_i. \quad (19.176)$$

We can find eigenvectors of the total angular momentum of any number of commuting angular momentum vectors by coupling them in a number of ways. This coupling is important in applications since very often the *total* angular momentum of a system is conserved. We show how to do this coupling in this section. We start with the coupling of the eigenvectors of two angular momentum vectors.

19.4.1 Coupling of two angular momenta

Let \mathbf{J}_1 and \mathbf{J}_2 be two commuting angular momentum vectors: $[J_{1i}, J_{2j}] = 0$, with $[J_{1i}, J_{1j}] = i\epsilon_{ijk}J_{1k}$ and $[J_{2i}, J_{2j}] = i\epsilon_{ijk}J_{2k}$. One set of four commuting operators for the combined system is the direct product set, given by: $(J_1^2, J_{1z}, J_2^2, J_{2z})$, and with eigenvectors:

$$|j_1, m_1, j_2, m_2\rangle. \quad (19.177)$$

However, we can find another set of four commuting operators by defining the total angular momentum operator:

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2, \quad (19.178)$$

which obeys the usual angular momentum commutation rules: $[J_i, J_j] = i\epsilon_{ijk}J_k$, with $[J^2, J_1^2] = [J^2, J_2^2] = 0$. So another set of four commuting operators for the combined system is: (J^2, J_1^2, J_2^2, J_z) , with eigenvectors:

$$|(j_1, j_2), j, m\rangle. \quad (19.179)$$

Either set of eigenvectors are equivalent descriptions of the combined angular momentum system, and so there is a unitary operator relating them. Matrix elements of this operator are called **Clebsch-Gordan coefficients**, or vector coupling coefficients, which we write as:

$$|(j_1, j_2), j, m\rangle = \sum_{m_1, m_2} |j_1, m_1, j_2, m_2\rangle \langle j_1, m_1, j_2, m_2 | (j_1, j_2), j, m\rangle, \quad (19.180)$$

or in the reverse direction:

$$|j_1, m_1, j_2, m_2\rangle = \sum_{j, m} |(j_1, j_2), j, m\rangle \langle (j_1, j_2), j, m | j_1, m_1, j_2, m_2\rangle. \quad (19.181)$$

Since the basis states are orthonormal and complete, Clebsch-Gordan coefficients satisfy:

$$\begin{aligned} \sum_{m_1, m_2} \langle (j_1, j_2), j, m | j_1, m_1, j_2, m_2\rangle \langle j_1, m_1, j_2, m_2 | (j_1, j_2), j', m'\rangle &= \delta_{j, j'} \delta_{m, m'}, \\ \sum_{j, m} \langle j_1, m_1, j_2, m_2 | (j_1, j_2), j, m\rangle \langle (j_1, j_2), j, m | j_1, m'_1, j_2, m'_2\rangle &= \delta_{m_1, m'_1} \delta_{m_2, m'_2}. \end{aligned} \quad (19.182)$$

In addition, a phase convention is adopted so that the phase of the Clebsch-Gordan coefficient $\langle j_1, j_1, j_2, j - j_1 | (j_1, j_2) j, m \rangle$ is taken to be zero, i.e. the argument is +1. With this convention, all Clebsch-Gordan coefficients are real.

Operating on (19.180) by $J_z = J_{1z} + J_{2z}$, gives

$$m |(j_1, j_2) j, m\rangle = \sum_{m_1, m_2} (m_1 + m_2) |j_1, m_1, j_2, m_2\rangle \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \rangle, \quad (19.183)$$

or

$$(m - m_1 - m_2) \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \rangle = 0, \quad (19.184)$$

so that Clebsch-Gordan coefficients vanish unless $m = m_1 + m_2$. Operating on (19.180) by $J_{\pm} = J_{1\pm} + J_{2\pm}$ gives two recursion relations:

$$A(j, \mp m) \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \pm 1 \rangle = A(j_1, \pm m_1) \langle j_1, m_1 \mp 1, j_2, m_2 | (j_1, j_2) j, m \rangle + A(j_2, \pm m_2) \langle j_1, m_1, j_2, m_2 \mp 1 | (j_1, j_2) j, m \rangle, \quad (19.185)$$

where $A(j, m) = \sqrt{(j+m)(j-m+1)} = A(j, 1 \mp m)$. The range of j is determined by noticing that $\langle j_1, m_1, j - j_1, m_2 | (j_1, j_2) j, m \rangle$ vanished unless $-j_2 \leq j - j_1 \leq j_2$ or $j_1 - j_2 \leq j \leq j_1 + j_2$. Similarly $\langle j_1, j - j_2, j_2, j_2 | (j_1, j_2) j, m \rangle$ vanished unless $-j_1 \leq j - j_2 \leq j_1$ or $j_2 - j_1 \leq j \leq j_1 + j_2$, from which we conclude that

$$|j_1 - j_2| \leq j \leq j_1 + j_2, \quad (19.186)$$

which is called the **triangle inequality**. One can find a closed form for the Clebsch-Gordan coefficients by solving the recurrence formula, Eq. (19.185). The result [5][p. 78], which is straightforward but tedious is:

$$\begin{aligned} & \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \rangle \\ &= \delta_{m, m_1 + m_2} \left[\frac{(2j+1)(j_1+j_2-j)!(j_1-m_1)!(j_2-m_2)!(j-m)!(j+m)!}{(j_1+j_2+j+1)!(j+j_1-j_2)!(j+j_2-j_1)!(j_1+m_1)!(j_2+m_2)!} \right]^{1/2} \\ & \quad \times \sum_t (-)^{j_1-m_1+t} \left[\frac{(j_1+m_1+t)!(j+j_2-m_1-t)!}{t!(j-m-t)!(j_1-m_1-t)!(j_2-j+m_1+t)!} \right]. \quad (19.187) \end{aligned}$$

This form for the Clebsch-Gordan coefficient is called ‘‘Racah’s first form.’’ A number of other forms of the equation can be obtained by substitution. For numerical calculations for small j , it is best to start with the vector for $m = -j$ and then apply J_+ to obtain vectors for the other m -values, or start with the vector for $m = +j$ and then apply J_- to obtain vectors for the rest of the m -values. Orthonormalization requirements between states with different value of j with the same value of m can be used to further fix the vectors. We illustrate this method in the next example.

Example 31. For $j_1 = j_2 = 1/2$, the total angular momentum can have the values $j = 0, 1$. For this example, let us simplify our notation and put $|1/2, m, 1/2, m'\rangle \mapsto |m, m'\rangle$ and $|(1/2, 1/2) j, m\rangle \mapsto |j, m\rangle$. Then for $j = 1$ and $m = 1$, we start with the unique state:

$$|1, 1\rangle = |1/2, 1/2\rangle. \quad (19.188)$$

Our convention is that the argument of this Clebsch-Gordan coefficient is +1. Apply J_- to this state:

$$J_- |1, 1\rangle = J_{1-} |1/2, 1/2\rangle + J_{2-} |1/2, 1/2\rangle, \quad (19.189)$$

from which we find:

$$|1, 0\rangle = \frac{1}{\sqrt{2}} (|-1/2, 1/2\rangle + |1/2, -1/2\rangle). \quad (19.190)$$

Applying J_- again to this state gives:

$$|1, -1\rangle = |-1/2, -1/2\rangle. \quad (19.191)$$

For the $j = 0$ case, we have:

$$|0, 0\rangle = \alpha |1/2, -1/2\rangle + \beta |-1/2, 1/2\rangle. \quad (19.192)$$

Applying J_- to this state gives zero on the left-hand-side, so we find that $\beta = -\alpha$. Since our convention is that the argument of α is $+1$, we find:

$$|0, 0\rangle = \frac{1}{\sqrt{2}} (|1/2, -1/2\rangle - |-1/2, 1/2\rangle). \quad (19.193)$$

As a check, we note that (19.193) is orthogonal to (19.190). We summarize these familiar results as follows:

$$|j, m\rangle = \begin{cases} (|1/2, -1/2\rangle - |-1/2, 1/2\rangle)/\sqrt{2}, & \text{for } j = m = 0, \\ |1/2, 1/2\rangle, & \text{for } j = 1, m = +1, \\ (|1/2, -1/2\rangle + |-1/2, 1/2\rangle)/\sqrt{2}, & \text{for } j = 1, m = 0, \\ |-1/2, -1/2\rangle, & \text{for } j = 1, m = -1. \end{cases} \quad (19.194)$$

Exercise 63. Work out the Clebsch-Gordan coefficients for the case when $j_1 = 1/2$ and $j_2 = 1$.

Tables of Clebsch-Gordan coefficients can be found on the internet. We reproduce one of them from the Particle Data group in Table 19.1.⁸ More extensive tables can be found in the book by Rotenberg, et.al. [17], and computer programs for numerically calculating Clebsch-Gordan coefficients, 3j-, 6j-, and 9j-symbols are also available. Important symmetry relations for Clebsch-Gordan coefficients are the following:

1. Interchange of the order of (j_1, j_2) coupling:

$$\langle j_2, m_2, j_1, m_1 | (j_2, j_1) j_3, m_3 \rangle = (-)^{j_1+j_2-j_3} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j_3, m_3 \rangle. \quad (19.195)$$

2. Cyclic permutation of the coupling $[(j_1, j_2) j_3]$:

$$\langle j_2, m_2, j_3, m_3 | (j_2, j_3) j_1, m_1 \rangle = (-)^{j_2-m_2} \sqrt{\frac{2j_1+1}{2j_3+1}} \langle j_1, m_1, j_2, -m_2 | (j_1, j_2) j_3, m_3 \rangle, \quad (19.196)$$

$$\langle j_3, m_3, j_1, m_1 | (j_3, j_1) j_2, m_2 \rangle = (-)^{j_1+m_1} \sqrt{\frac{2j_2+1}{2j_3+1}} \langle j_1, -m_1, j_2, m_2 | (j_1, j_2) j_3, m_3 \rangle. \quad (19.197)$$

3. Reversal of all m values:

$$\langle j_1, -m_1, j_2, -m_2 | (j_1, j_2) j_3, -m_3 \rangle = (-)^{j_1+j_2-j_3} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j_3, m_3 \rangle. \quad (19.198)$$

Some special values of the Clebsch-Gordan coefficients are useful to know:

$$\langle j, m, 0, 0 | (j, 0) j, m \rangle = 1, \quad \langle j, m, j, m' | (j, j) 0, 0 \rangle = \delta_{m, -m'} \frac{(-)^{j-m}}{\sqrt{2j+1}}. \quad (19.199)$$

The symmetry relations are most easily obtained from the simpler symmetry relations for 3j-symbols, which are defined below, and proved in Section G.6 using Schwinger's methods.

⁸The sign conventions for the d -functions in this table are those of Rose[6], who uses an active rotation. To convert them to our conventions put $\beta \rightarrow -\beta$.

34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

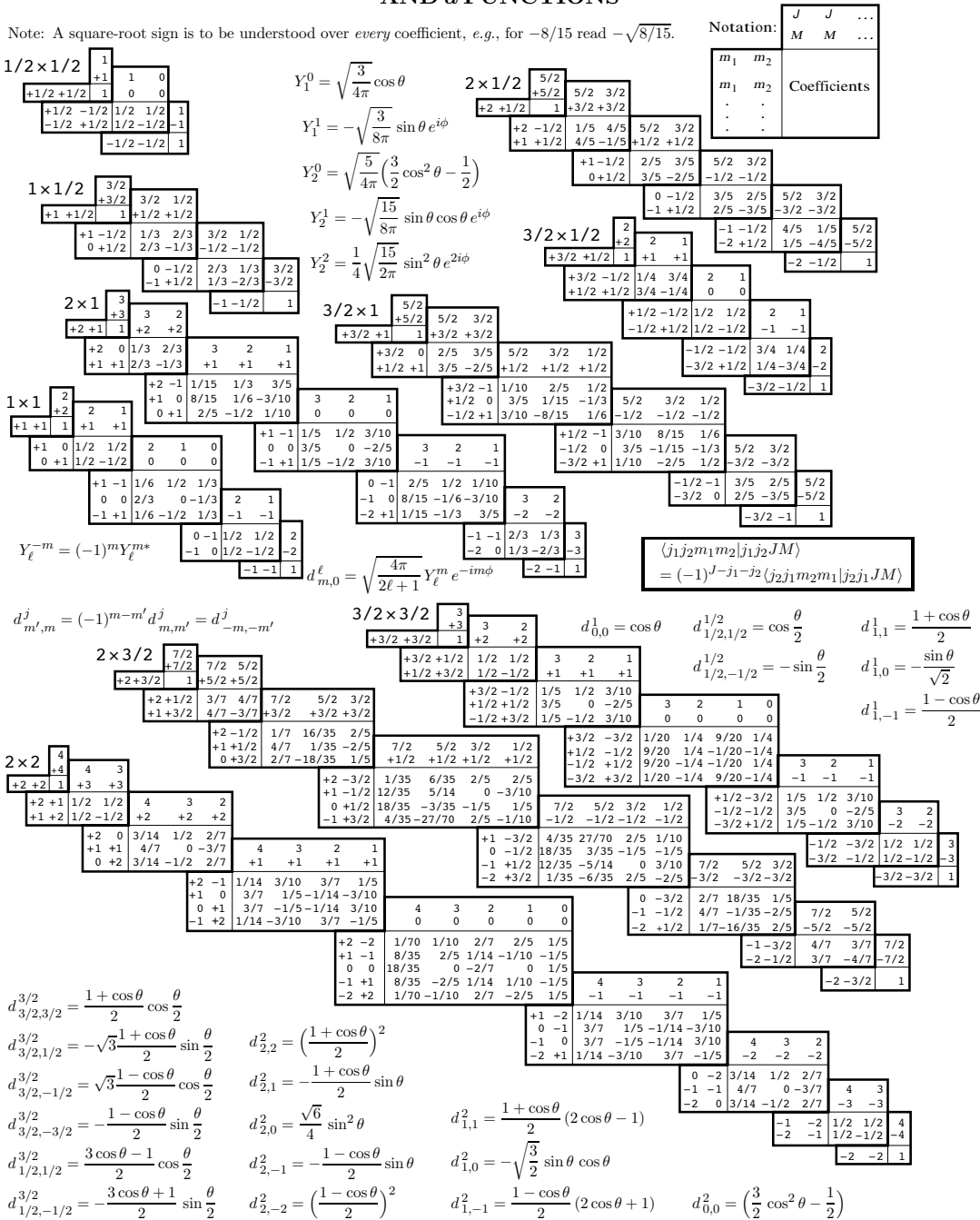


Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Table 19.1: Table of Clebsch-Gordan coefficients, spherical harmonics, and d -functions.

3j symbols

Clebsch-Gordan coefficients do not possess simple symmetry relations upon exchange of the angular momentum quantum numbers. 3-j symbols which are related to Clebsch-Gordan coefficients, have better symmetry properties. They are defined by (Edmonds [2]):

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \frac{(-)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j_3, -m_3 \rangle. \quad (19.200)$$

In terms of 3j-symbols, the orthogonality relations (19.182) become:

$$\begin{aligned} (2j_3+1) \sum_{m_1, m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} &= \delta_{j_3, j'_3} \delta_{m_3, m'_3}, \\ \sum_{j_3, m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m_3 \end{pmatrix} &= \delta_{m_1, m'_1} \delta_{m_2, m'_2}. \end{aligned} \quad (19.201)$$

Symmetry properties of the 3j-symbols are particularly simple. They are:

1. The 3j-symbols are invariant under even (cyclic) permutation of the columns:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}. \quad (19.202)$$

and are multiplied by a phase for odd permutations:

$$\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} = \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} = (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (19.203)$$

2. For reversal of all m values:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}. \quad (19.204)$$

The 3j-symbols vanish unless $m_1 + m_2 + m_3 = 0$. For $j_3 = 0$, the 3j-symbol is:

$$\begin{pmatrix} j & j & 0 \\ m & m' & 0 \end{pmatrix} = \delta_{m, -m'} \frac{(-)^{j-m}}{\sqrt{2j+1}}. \quad (19.205)$$

A few useful 3j-symbols are given in Table 19.2. More can be found in Edmonds [2][Table 2, p. 125] and Brink and Satchler [18][Table 3, p. 36].

19.4.2 Coupling of three and four angular momenta

We write the direct product eigenvector for three angular momenta as:

$$|j_1, m_1, j_2, m_2, j_3, m_3\rangle = |j_1, m_1\rangle \otimes |j_2, m_2\rangle \otimes |j_3, m_3\rangle. \quad (19.206)$$

This state is an eigenvector of J_1^2, J_{1z} , J_2^2, J_{2z} , and J_3^2, J_{3z} . If we want to construct eigenvectors of total angular momentum J^2 and J_z , where

$$J^2 = \mathbf{J} \cdot \mathbf{J}, \quad \mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3, \quad (19.207)$$

there are three ways to do this: (1) couple \mathbf{J}_1 to \mathbf{J}_2 to get an intermediate vector \mathbf{J}_{12} and then couple this intermediate vector to \mathbf{J}_3 to get an eigenvector of \mathbf{J} , (2) couple \mathbf{J}_2 to \mathbf{J}_3 to get \mathbf{J}_{23} and then couple \mathbf{J}_1 to

$$\begin{aligned}
\begin{pmatrix} j & j+1/2 & 1/2 \\ m & -m-1/2 & 1/2 \end{pmatrix} &= (-)^{j-m-1} \sqrt{\frac{j+m+1}{(2j+1)(2j+2)}} \\
\begin{pmatrix} j & j & 1 \\ m & -m-1 & 1 \end{pmatrix} &= (-)^{j-m} \sqrt{\frac{2(j-m)(j+m+1)}{2j(2j+1)(2j+2)}} \\
\begin{pmatrix} j & j & 1 \\ m & -m & 0 \end{pmatrix} &= (-)^{j-m} \frac{m}{\sqrt{j(j+1)(2j+1)}} \\
\begin{pmatrix} j & j+1 & 1 \\ m & -m-1 & 1 \end{pmatrix} &= (-)^{j-m} \sqrt{\frac{(j+m+1)(j+m+2)}{(2j+1)(2j+2)(2j+3)}} \\
\begin{pmatrix} j & j+1 & 1 \\ m & -m & 0 \end{pmatrix} &= (-)^{j-m-1} \sqrt{\frac{2(j-m+1)(j+m+1)}{(2j+1)(2j+2)(2j+3)}}
\end{aligned}$$

Table 19.2: Algebraic formulas for some $3j$ -symbols.

\mathbf{J}_{23} to get \mathbf{J} , or (3) couple \mathbf{J}_1 to \mathbf{J}_3 to get \mathbf{J}_{13} and then couple \mathbf{J}_2 to \mathbf{J}_{13} to get \mathbf{J} . Keeping in mind that the *order* of the coupling of two vectors is just a phase and not a different coupling scheme, it turns out that this last coupling is just a combined transformation of the first two (see Eq. (19.214) below). So the first two coupling schemes can be written as:

$$\begin{aligned}
|(j_1, j_2) j_{12}, j_3, j, m\rangle &= \sum_{\substack{m_1, m_2, m_3 \\ m_{12}}} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j_{12}, m_{12} \rangle \langle j_{12}, m_{12}, j_3, m_3 | (j_{12}, j_3) j, m \rangle \\
&\quad \times |j_1, m_1, j_2, m_2, j_3, m_3\rangle, \\
|j_1 (j_2, j_3) j_{23}, j, m\rangle &= \sum_{\substack{m_1, m_2, m_3 \\ m_{23}}} \langle j_2, m_2, j_3, m_3 | (j_2, j_3) j_{23}, m_{23} \rangle \langle j_1, m_1, j_{23}, m_{23} | (j_1, j_{23}) j, m \rangle \\
&\quad \times |j_1, m_1, j_2, m_2, j_3, m_3\rangle.
\end{aligned} \tag{19.208}$$

The overlap between these two coupling vectors is independent of m and is proportional to the $6j$ -symbol:

$$\begin{aligned}
\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} &= \frac{(-)^{j_1+j_2+j_3+j}}{\sqrt{(2j_{12}+1)(2j_{23}+1)}} \langle (j_1, j_2) j_{12}, j_3, j, m | j_1 (j_2, j_3) j_{23}, j, m \rangle \\
&= \frac{(-)^{j_1+j_2+j_3+j}}{\sqrt{(2j_{12}+1)(2j_{23}+1)}} \sum_{\substack{m_1, m_2, m_3 \\ m_{12}, m_{23}}} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j_{12}, m_{12} \rangle \\
&\quad \times \langle j_{12}, m_{12}, j_3, m_3 | (j_{12}, j_3) j, m \rangle \langle j_2, m_2, j_3, m_3 | (j_2, j_3) j_{23}, m_{23} \rangle \langle j_1, m_1, j_{23}, m_{23} | (j_1, j_{23}) j, m \rangle
\end{aligned} \tag{19.209}$$

Here $m = m_1 + m_2 + m_3$. The $6j$ -symbols vanish unless (j_1, j_2, j_{12}) , (j_2, j_3, j_{23}) , (j_{12}, j_3, j) , and (j_1, j_{23}, j) all satisfy triangle inequalities. In terms of $3j$ -symbols, the $6j$ -symbol is given by the symmetric expression:

$$\begin{aligned}
\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} &= \sum_{\text{all } m} (-)^{\sum_{\text{all}} (j+m)} \\
&\quad \times \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ -m_1 & m_5 & -m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ -m_4 & -m_2 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ m_4 & -m_5 & -m_3 \end{pmatrix}.
\end{aligned} \tag{19.210}$$

Here, the sums over all m 's are restricted because the $3j$ -symbols vanish unless their m -values add to zero. A number of useful relations between $3j$ and $6j$ -symbols follow from Eq. (19.210), and are tabulated by Brink and Satchler [18][Appendix II, p. 141]. One of these which we will use later is:

$$\sqrt{(2\ell+1)(2\ell'+1)} \begin{Bmatrix} \ell & \ell' & k \\ j' & j & 1/2 \end{Bmatrix} \begin{pmatrix} \ell & \ell' & k \\ 0 & 0 & 0 \end{pmatrix} = (-)^{j+\ell+j'+\ell'+1} \begin{pmatrix} \ell' & \ell & k \\ -1/2 & 1/2 & 0 \end{pmatrix} \delta(\ell, \ell', k), \tag{19.211}$$

$$\begin{aligned} \begin{Bmatrix} j_1 & j_2 & j_3 \\ 0 & j_3 & j_2 \end{Bmatrix} &= \frac{(-)^{j_1+j_2+j_3}}{\sqrt{(2j_2+1)(2j_3+1)}}, \\ \begin{Bmatrix} j_1 & j_2 & j_3 \\ 1/2 & j_3-1/2 & j_2+1/2 \end{Bmatrix} &= (-)^{j_1+j_2+j_3} \sqrt{\frac{(j_1+j_3-j_2)(j_1+j_2-j_3+1)}{(2j_2+1)(2j_2+2)2j_3(2j_3+1)}}, \\ \begin{Bmatrix} j_1 & j_2 & j_3 \\ 1/2 & j_3-1/2 & j_2-1/2 \end{Bmatrix} &= (-)^{j_1+j_2+j_3} \sqrt{\frac{(j_2+j_3-j_1)(j_1+j_2+j_3+1)}{2j_2(2j_2+1)2j_3(2j_3+1)}}, \\ \begin{Bmatrix} j_1 & j_2 & j_3 \\ 1 & j_3 & j_2 \end{Bmatrix} &= 2(-)^{j_1+j_2+j_3} \frac{j_1(j_1+1) - j_2(j_2+1) - j_3(j_3+1)}{\sqrt{2j_2(2j_2+1)(2j_2+2)2j_3(2j_3+1)(2j_3+2)}}, \end{aligned}$$

Table 19.3: Algebraic formulas for some 6j-symbols.

where $\delta(\ell, \ell', k) = 1$ if $\ell + \ell' + k$ is even and (ℓ, ℓ', k) satisfy the triangle inequality, otherwise it is zero. The 6j-symbol is designed so as to maximize the symmetries of the coupling coefficient, as in the 3j-symbol. For example, the 6j-symbol is invariant under any permutation of columns:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_3 & j_1 \\ j_5 & j_6 & j_4 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_1 & j_2 \\ j_6 & j_4 & j_5 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_3 & j_2 \\ j_4 & j_6 & j_5 \end{Bmatrix} = \begin{Bmatrix} j_3 & j_2 & j_1 \\ j_6 & j_5 & j_4 \end{Bmatrix}.$$

It is also invariant under exchange of the upper and lower elements of any two columns:

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_4 & j_5 & j_3 \\ j_1 & j_2 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_4 & j_2 & j_6 \\ j_1 & j_5 & j_3 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_5 & j_6 \\ j_4 & j_2 & j_3 \end{Bmatrix}.$$

Some particular 6j-symbols are given in Table 19.3 Additional tables of 6j-symbols for values of $j = 1$ and 2 can be found in Edmonds [2][Table 5, p. 130]. Several relations between 6j-symbols are obtained by consideration of the recoupling matrix elements. For example, since:

$$\sum_{j_{12}} \langle j_1(j_2, j_3)j_{23}, j | (j_1, j_2)j_{12}, j_3, j \rangle \langle (j_1, j_2)j_{12}, j_3, j | j_1(j_2, j_3)j'_{23}, j \rangle = \delta_{j_{23}, j'_{23}}, \quad (19.212)$$

we have:

$$\sum_{j_{12}} (2j_{12} + 1)(2j_{23} + 1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j'_{23} \end{Bmatrix} = \delta_{j_{23}, j'_{23}}. \quad (19.213)$$

A similar consideration of

$$\begin{aligned} \sum_{j_{23}} \langle (j_1, j_2)j_{12}, j_3, j | j_1(j_2, j_3)j_{23}, j \rangle \langle j_1(j_2, j_3)j_{23}, j | j_2(j_3, j_1)j_{31}, j \rangle \\ = \langle (j_1, j_2)j_{12}, j_3, j | j_2(j_3, j_1)j_{31}, j \rangle, \end{aligned} \quad (19.214)$$

gives:

$$\sum_{j_{23}} (-)^{j_{23}+j_{31}+j_{12}} (2j_{23} + 1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} \begin{Bmatrix} j_2 & j_3 & j_{23} \\ j_1 & j & j_{31} \end{Bmatrix} = \begin{Bmatrix} j_3 & j_1 & j_{31} \\ j_2 & j & j_{12} \end{Bmatrix}. \quad (19.215)$$

Other important formula involving 6j-symbols can be found in standard references.

The coupling of four angular momenta is done in a similar way. Let us take the special case of two particles with orbital angular momentum ℓ_1 and ℓ_2 and spin s_1 and s_2 . Two important ways of coupling these four angular momentum are the j - j coupling scheme:

$$\begin{aligned} |(\ell_1, s_1)j_1, (\ell_2, s_2)j_2, j, m \rangle = \\ \sum_{\substack{m_{\ell_1}, m_{s_1}, m_{\ell_2}, m_{s_2} \\ m_{j_1}, m_{j_2}}} \langle \ell_1, m_{\ell_1}, s_1, m_{s_1} | (\ell_1, s_1)j_1, m_1 \rangle \langle \ell_2, m_{\ell_2}, s_2, m_{s_2} | (\ell_2, s_2)j_2, m_2 \rangle \langle j_1, m_1, j_2, m_2 | (j_1, j_2)j, m \rangle, \end{aligned} \quad (19.216)$$

and the ℓ - s coupling scheme:

$$|(\ell_1, \ell_2) \ell, (s_1, s_2) s, j, m\rangle = \sum_{\substack{m_{\ell_1}, m_{\ell_2}, m_{s_1}, m_{s_2} \\ m_{\ell}, m_s}} \langle \ell_1, m_{\ell_1}, \ell_2, m_{\ell_2} | (\ell_1, \ell_2) \ell, m_{\ell} \rangle \langle s_1, m_{s_1}, s_2, m_{s_2} | (s_1, s_2) s, m_s \rangle \langle \ell, m_{\ell}, s, m_s | (\ell, s) j, m \rangle, \quad (19.217)$$

The overlap between these two coupling schemes define the $9j$ -symbol:

$$\left\{ \begin{array}{ccc} \ell_1 & s_1 & j_1 \\ \ell_2 & s_2 & j_2 \\ \ell & s & j \end{array} \right\} = \frac{\langle (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j, m | (\ell_1, \ell_2) \ell, (s_1, s_2) s, j, m \rangle}{\sqrt{(2j_1 + 1)(2j_2 + 1)(2\ell + 1)(2s + 1)}} \quad (19.218)$$

and is independent of the value of m . The rows and columns of the $9j$ -symbol must satisfy the triangle inequality. From Eqs. (19.216) and (19.217), the $9j$ -symbol can be written in terms of sums over $6j$ -symbols or $3j$ -symbols:

$$\begin{aligned} \left\{ \begin{array}{ccc} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{array} \right\} &= \sum_j (-)^{2j} (2j + 1) \left\{ \begin{array}{ccc} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & j \end{array} \right\} \left\{ \begin{array}{ccc} j_{12} & j_{22} & j_{32} \\ j_{21} & j & j_{23} \end{array} \right\} \left\{ \begin{array}{ccc} j_{13} & j_{23} & j_{33} \\ j & j_{11} & j_{12} \end{array} \right\} \\ &= \sum_{\text{all } m} \begin{pmatrix} j_{11} & j_{12} & j_{13} \\ m_{11} & m_{12} & m_{13} \end{pmatrix} \begin{pmatrix} j_{21} & j_{22} & j_{23} \\ m_{21} & m_{22} & m_{23} \end{pmatrix} \begin{pmatrix} j_{31} & j_{32} & j_{33} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \\ &\quad \times \begin{pmatrix} j_{11} & j_{21} & j_{31} \\ m_{11} & m_{21} & m_{31} \end{pmatrix} \begin{pmatrix} j_{12} & j_{22} & j_{32} \\ m_{12} & m_{22} & m_{32} \end{pmatrix} \begin{pmatrix} j_{13} & j_{23} & j_{33} \\ m_{13} & m_{23} & m_{33} \end{pmatrix}. \quad (19.219) \end{aligned}$$

From Eq. (19.219), we see that an even permutation of rows or columns or a transposition of rows and columns leave the $9j$ -symbol invariant, whereas an odd permutation of rows or columns produces a sign change given by:

$$(-)^{j_{11}+j_{12}+j_{13}+j_{21}+j_{22}+j_{23}+j_{31}+j_{32}+j_{33}}.$$

Orthogonal relations of $9j$ -symbols are obtained in the same way as with the $3j$ -symbols. We find:

$$\sum_{j_{12}, j_{34}} (2j_{12} + 1)(2j_{34} + 1)(2j_{13} + 1)(2j_{24} + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j'_{13} & j'_{24} & j \end{array} \right\} = \delta_{j_{13}, j'_{13}} \delta_{j_{24}, j'_{24}}, \quad (19.220)$$

and

$$\begin{aligned} \sum_{j_{13}, j_{24}} (-)^{2j_3+j_{24}+j_{23}-j_{34}} (2j_{13} + 1)(2j_{24} + 1) &\left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_3 & j_{13} \\ j_4 & j_2 & j_{24} \\ j_{14} & j_{23} & j \end{array} \right\} \\ &= \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_4 & j_3 & j_{34} \\ j_{14} & j_{23} & j \end{array} \right\}. \quad (19.221) \end{aligned}$$

Relations between $6j$ - and $9j$ -symbols are obtained from orthogonality relations and recoupling vectors. One which we will have occasion to use is:

$$\sum_{j_{12}} (2j_{12} + 1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_{34} & j & j' \end{array} \right\} = (-)^{2j'} \left\{ \begin{array}{ccc} j_3 & j_4 & j_{34} \\ j_2 & j' & j_{24} \end{array} \right\} \left\{ \begin{array}{ccc} j_{13} & j_{24} & j \\ j' & j_1 & j_3 \end{array} \right\}. \quad (19.222)$$

The $9j$ -symbol with one of the j 's zero is proportional to a $6j$ -symbol:

$$\left\{ \begin{matrix} j_1 & j_2 & j \\ j_3 & j_4 & j \\ j' & j' & 0 \end{matrix} \right\} = \frac{(-)^{j_2+j_3+j+j'}}{\sqrt{(2j+1)(2j'+1)}} \left\{ \begin{matrix} j_1 & j_2 & j \\ j_4 & j_3 & j' \end{matrix} \right\}. \quad (19.223)$$

Algebraic formulas for the the commonly occurring $9j$ -symbol:

$$\left\{ \begin{matrix} \ell & \ell' & L \\ j & j' & J \\ 1/2 & 1/2 & S \end{matrix} \right\}, \quad (19.224)$$

for $S = 0, 1$ are given by Matsunobu and Takebe [19]. Values of other special $9j$ -symbols can be found in Edmonds [2], Brink and Satchler [18], or Rotenberg, Bivins, Metropolis, and Wooten [17]. The coupling of five and more angular momenta can be done in similar ways as described in this section, but the recoupling coefficients are not used as much in the literature, so we stop here in our discussion of angular momentum coupling.

19.4.3 Rotation of coupled vectors

The relation between eigenvectors of angular momentum for a coupled system described in two coordinate frames Σ and Σ' is given by a rotation operator $U(R)$ for the combined system, $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$. Since \mathbf{J}_1 and \mathbf{J}_2 commute, the rotation operator can be written in two ways:

$$U_{\mathbf{J}}(R) = e^{i\hat{\mathbf{n}} \cdot \mathbf{J}\theta/\hbar} = e^{i\hat{\mathbf{n}} \cdot \mathbf{J}_1\theta/\hbar} e^{i\hat{\mathbf{n}} \cdot \mathbf{J}_2\theta/\hbar} = U_{\mathbf{J}_1}(R) U_{\mathbf{J}_2}(R). \quad (19.225)$$

Operating with on (19.180) with $U_{\mathbf{J}}(R)$ and multiplying on the left by the adjoint of Eq. (19.180) gives:

$$\begin{aligned} \langle (j_1, j_2) j, m | U_{\mathbf{J}}(R) | (j_1, j_2) j, m' \rangle &= \sum_{m_1, m_2, m'_1, m'_2} \langle j_1, m_1 | U_{\mathbf{J}_1}(R) | j_1, m'_1 \rangle \langle j_2, m_2 | U_{\mathbf{J}_2}(R) | j_2, m'_2 \rangle \\ &\times \langle (j_1, j_2) j, m | j_1, m_1, j_2, m_2 \rangle \langle j_1, m'_1, j_2, m'_2 | (j_1, j_2) j, m' \rangle. \end{aligned} \quad (19.226)$$

Here we have used the fact that the matrix elements of the rotation operator is diagonal in the total angular momentum quantum number j . But from Definition 36, matrix elements of the rotation operator are just the D -functions, so (19.226) becomes:

$$D_{m, m'}^{(j)}(R) = \sum_{m_1, m_2, m'_1, m'_2} D_{m_1, m'_1}^{(j_1)}(R) D_{m_2, m'_2}^{(j_2)}(R) \langle (j_1, j_2) j, m | j_1, m_1, j_2, m_2 \rangle \langle j_1, m'_1, j_2, m'_2 | (j_1, j_2) j, m' \rangle. \quad (19.227)$$

Eq. (19.227) is called the **Clebsch-Gordan series**.⁹ Another form of it is found by multiplying (19.227) through by another Clebsch-Gordan coefficient and using relations (19.182):

$$\begin{aligned} \sum_m \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \rangle D_{m, m'}^{(j)}(R) \\ = \sum_{m'_1, m'_2} D_{m_1, m'_1}^{(j_1)}(R) D_{m_2, m'_2}^{(j_2)}(R) \langle j_1, m'_1, j_2, m'_2 | (j_1, j_2) j, m' \rangle. \end{aligned} \quad (19.228)$$

⁹According to Rotenberg, et. al. [17], A. Clebsch and P. Gordan had little to do with what physicists call the Clebsch-Gordan series.

Exercise 64. Using the infinitesimal expansions:

$$\begin{aligned} D_{m,m'}^{(j)}(\hat{\mathbf{n}}_z, \Delta\theta) &= \delta_{m,m'} + i m \delta_{m,m'} \Delta\theta + \dots \\ D_{m,m'}^{(j)}(\hat{\mathbf{n}}_{\pm}, \Delta\theta) &= \delta_{m,m'} + i A(j, \mp m') \delta_{m,m' \pm 1} \Delta\theta + \dots, \end{aligned} \quad (19.229)$$

evaluate the Clebsch-Gordan series, Eq. (19.228), for infinitesimal values of θ and for $\hat{\mathbf{n}} = \hat{\mathbf{n}}_z$ and $\hat{\mathbf{n}}_{\pm}$ to show that Clebsch-Gordan series reproduces Eqs. (19.184) and (19.185). That is, the Clebsch-Gordan series *determines* the Clebsch-Gordan coefficients.

Multiplication of Eq. (19.228) again by a Clebsch-Gordan coefficient and summing over j and m' gives a third relation between D -functions:

$$\begin{aligned} D_{m_1, m_1'}^{(j_1)}(R) D_{m_2, m_2'}^{(j_2)}(R) \\ = \sum_{j, m, m'} \langle j_1, m_1, j_2, m_2 | (j_1, j_2) j, m \rangle \langle j_1, m_1', j_2, m_2' | (j_1, j_2) j, m' \rangle D_{m, m'}^{(j)}(R). \end{aligned} \quad (19.230)$$

In terms of $3j$ -symbols, (19.230) becomes:

$$D_{m_1, m_1'}^{(j_1)}(R) D_{m_2, m_2'}^{(j_2)}(R) = \sum_{j, m, m'} (2j+1) \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j \\ m_1' & m_2' & m' \end{pmatrix} D_{m, m'}^{(j)*}(R). \quad (19.231)$$

For integer values of $j_1 = \ell_1$ and $j_2 = \ell_2$ and $m_1 = m_2 = 0$, (19.231) reduces to:

$$C_{\ell_1, m_1}(\Omega) C_{\ell_2, m_2}(\Omega) = \sum_{\ell, m} (2\ell+1) \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ m_1 & m_2 & m \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell \\ 0 & 0 & 0 \end{pmatrix} C_{\ell, m}^*(\Omega). \quad (19.232)$$

Using the orthogonality of the spherical harmonics, Eq. (19.232) can be used to find the integral over three spherical harmonics:

$$\int d\Omega C_{\ell_1, m_1}(\Omega) C_{\ell_2, m_2}(\Omega) C_{\ell_3, m_3}(\Omega) = 4\pi \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & \ell_3 \\ 0 & 0 & 0 \end{pmatrix}. \quad (19.233)$$

19.5 Tensor operators

The key to problems involving angular momentum matrix elements of operators is to write the operators in terms of tensor operators, and then use powerful theorems regarding the matrix elements of these tensors. The most important theorem is the Wigner-Eckart theorem, which will be discussed in the next section. Others are discussed in the next section where we also give several examples of the use of these theorems.

19.5.1 Tensor operators and the Wigner-Eckart theorem

Definition 37 (tensor operator). An irreducible tensor operator $T_{k,q}$ of **rank** k and **component** q , with $-k \leq q \leq +k$, is defined so that under rotation of the coordinate system, it transforms as:

$$U_{\mathbf{J}}(R) T_{k,q} U_{\mathbf{J}}^\dagger(R) = \sum_{q'=-k}^{+k} T_{k,q'} D_{q',q}^{(k)}(R). \quad (19.234)$$

where $D_{q,q'}^{(k)}(R)$ is the rotation matrix. The infinitesimal version of (19.234) is:

$$[J_i, T_{k,q}] = \sum_{q'=-k}^{+k} T_{k,q'} \langle k, q' | J_i | k, q \rangle, \quad (19.235)$$

which gives the equations:

$$[J_{\pm}, T_{k,q}] = \hbar A(k, \mp q) T_{k,q\pm 1}, \quad [J_z, T_{k,q}] = \hbar q T_{k,q}. \quad (19.236)$$

Definition 38 (Hermitian tensor operator). The usual definition of a Hermitian tensor operator for integer rank k , and the one we will adopt here, is:

$$T_{k,q}^{\dagger} = (-)^q T_{k,-q}. \quad (19.237)$$

$R_{1,q}$ and $J_{1,q}$, defined above, and the spherical harmonics satisfies this definition and are Hermitian operators. A second definition, which preserves the Hermitian property for tensor products (see Theorem 36 below) is:

$$T_{k,q}^{\dagger} = (-)^{k-q} T_{k,-q}. \quad (19.238)$$

The only difference between the two definitions is a factor of i^k .

The adjoint operator $T_{k,q}^{\dagger}$ transforms according to:

$$U(R) T_{k,q}^{\dagger} U^{\dagger}(R) = \sum_{q'=-k}^{+k} T_{k,q'}^{\dagger} D_{q',q}^{(k)*}(R) = \sum_{q'=-k}^{+k} T_{k,q'}^{\dagger} D_{q,q'}^{(k)}(R^{-1}). \quad (19.239)$$

Or putting $R \rightarrow R^{-1}$, this can be written as:

$$U^{\dagger}(R) T_{k,q}^{\dagger} U(R) = \sum_{q'=-k}^{+k} T_{k,q'}^{\dagger} D_{q,q'}^{(k)}(R). \quad (19.240)$$

For tensors of half-integer rank, the definition of a Hermitian tensor operator does not work since, for this case, the Hermitian adjoint, taken twice, does not reproduce the same tensor. So a definition of Hermitian is not possible for half-integer operators.

Example 32. The operator made up of the components of the angular momentum operator and defined by:

$$J_{1,q} = \begin{cases} -(J_x + i J_y)/\sqrt{2}, & \text{for } q = +1, \\ J_z, & \text{for } q = 0, \\ +(J_x - i J_y)/\sqrt{2}, & \text{for } q = -1, \end{cases} \quad (19.241)$$

is a tensor operator of rank one. Since (J_x, J_y, J_z) are Hermitian operators, $J_{1,q}$ satisfies $J_{1,q}^{\dagger} = (-)^q J_{1,-q}$, and therefore is a Hermitian tensor operator.

Example 33. The spherical harmonics $Y_{k,q}(\Omega)$, considered as operators in coordinate space, are tensor operators. Eqs. (19.18) mean that:

$$[J_{\pm}, Y_{k,q}(\Omega)] = \hbar A(k, \mp q) Y_{k,q\pm 1}(\Omega), \quad [J_z, Y_{k,q}(\Omega)] = \hbar q Y_{k,q}(\Omega), \quad (19.242)$$

The reduced spherical harmonics $C_{k,q}(\Omega)$, given in Definition 34, are also tensor operators of rank k component q .

Example 34. The operator $R_{1,q}$ made up of components of the coordinate vector (X, Y, Z) and defined by:

$$R_{1,q} = \begin{cases} -(X + i Y)/\sqrt{2}, & \text{for } q = +1, \\ Z, & \text{for } q = 0, \\ +(X - i Y)/\sqrt{2}, & \text{for } q = -1. \end{cases} \quad (19.243)$$

where X, Y , and Z are coordinate operators, is a tensor operator of rank one. Using $[X_i, L_j] = i\hbar \epsilon_{ijk} X_k$, one can easily check that Eq. (19.236) is satisfied. Note that since (X, Y, Z) are all Hermitian operators, $R_{1,q}$ satisfies $R_{1,q}^{\dagger} = (-)^q R_{1,-q}$ and so $R_{1,q}$ is a Hermitian tensor operator.

The tensor operator $R_{1,q}$ is a special case of a solid harmonic, defined by:

Definition 39 (solid harmonic). A solid harmonic $R_{k,q}$ is defined by:

$$R_{k,q} = R^k C_{k,q}(\Omega). \quad (19.244)$$

Solid harmonics, like the reduced spherical harmonics, are tensor operators of rank k component q .

Finally let us define spherical unit vectors $\hat{\mathbf{e}}_q$ by:

$$\hat{\mathbf{e}}_q = \begin{cases} -(\hat{\mathbf{e}}_x + i\hat{\mathbf{e}}_y)/\sqrt{2}, & \text{for } q = +1, \\ \hat{\mathbf{e}}_z, & \text{for } q = 0, \\ +(\hat{\mathbf{e}}_x - i\hat{\mathbf{e}}_y)/\sqrt{2}, & \text{for } q = -1. \end{cases} \quad (19.245)$$

These spherical unit vectors are *not* operators. The complex conjugate satisfies: $\hat{\mathbf{e}}_q^* = (-)^q \hat{\mathbf{e}}_{-q}$. They also obey the orthogonality and completeness relations:

$$\hat{\mathbf{e}}_q \cdot \hat{\mathbf{e}}_{q'}^* = \delta_{q,q'}, \quad \sum_q \hat{\mathbf{e}}_q \hat{\mathbf{e}}_q^* = \sum_q (-)^q \hat{\mathbf{e}}_q \hat{\mathbf{e}}_{-q} = \mathbf{1}. \quad (19.246)$$

where $\mathbf{1} = \hat{\mathbf{e}}_x \hat{\mathbf{e}}_x + \hat{\mathbf{e}}_y \hat{\mathbf{e}}_y + \hat{\mathbf{e}}_z \hat{\mathbf{e}}_z$ is the unit dyadic. Any vector operator can be expanded in terms of spherical tensors using these spherical unit vectors. For example, the vector operator \mathbf{R} can be written as:

$$\mathbf{R} = \sum_q (-)^q R_{1,q} \hat{\mathbf{e}}_{-q}, \quad \text{where} \quad R_{1,q} = \mathbf{R} \cdot \hat{\mathbf{e}}_q. \quad (19.247)$$

Exercise 65 (Edmonds). Let us define a vector operator $\mathbf{S} = \mathbf{e}_x S_x + \mathbf{e}_y S_y + \mathbf{e}_z S_z$, which operates on vectors, by:

$$S_i = i\hbar \hat{\mathbf{e}}_i \times, \quad \text{for } i = (x, y, z). \quad (19.248)$$

Show that:

$$S^2 \hat{\mathbf{e}}_q = \hbar^2 2 \hat{\mathbf{e}}_q, \quad S_z \hat{\mathbf{e}}_q = \hbar q \hat{\mathbf{e}}_q. \quad (19.249)$$

That is, \mathbf{S} is vector operator for spin one.

Angular momentum matrix elements of irreducible tensor operators with respect to angular momentum eigenvectors are proportional to a Clebsch-Gordan coefficient, or $3j$ -symbol, which greatly simplifies calculation of these quantities. The Wigner-Eckart theorem [20, 21], which we now prove, states that fact:

Theorem 35 (Wigner-Eckart). *Angular momentum matrix elements of an irreducible tensor operator $T(k, q)$ is given by:*

$$\begin{aligned} \langle j, m | T_{k,q} | j', m' \rangle &= (-)^{j'-m'} \frac{\langle j, m, j', -m' | (j, j') k, q \rangle}{\sqrt{2k+1}} \langle j || T_k || j' \rangle, \\ &= (-)^{j-m} \begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix} \langle j || T_k || j' \rangle. \end{aligned} \quad (19.250)$$

Here $\langle j || T_k || j' \rangle$ is called the **reduced** matrix element, and is independent of m, m' , and q , which is the whole point of the theorem.

Proof. Eq. (19.234) can be written as:

$$U(R) T_{k,q'} U^\dagger(R) = \sum_{q=-k}^{+k} T_{k,q}^\dagger D_{q,q'}^{(k)}(R). \quad (19.251)$$

Matrix elements of this equation gives:

$$\begin{aligned} \sum_{q=-k}^{+k} \langle j, m | T_{k,q} | j', m' \rangle D_{q,q'}^{(j)}(R) &= \sum_{m'', m'''} D_{m, m''}^{(j)}(R) D_{m', m'''}^{(j)*}(R) \langle j, m'' | T_{k,q} | j', m''' \rangle \\ &= \sum_{m'', m'''} (-)^{m' - m'''} D_{m, m''}^{(j)}(R) D_{-m', -m'''}^{(j)}(R) \langle j, m'' | T_{k,q} | j', m''' \rangle \end{aligned} \quad (19.252)$$

Now let $m' \rightarrow -m'$ and $m''' \rightarrow -m'''$, so that (19.252) becomes:

$$\begin{aligned} \sum_{q=-k}^{+k} \langle j, m | T_{k,q} | j', -m' \rangle D_{q,q'}^{(j)}(R) \\ = \sum_{m'', m'''} (-)^{m' - m'''} D_{m, m''}^{(j)}(R) D_{m', m'''}^{(j')}(R) \langle j, m'' | T_{k,q} | j', -m''' \rangle \end{aligned} \quad (19.253)$$

Comparison with Eq. (19.228) gives:

$$\langle j, m | T_{k,q} | j', -m' \rangle = (-)^{j' + m'} \langle j, m, j', m' | (j, j') k, q \rangle f(j, j', k), \quad (19.254)$$

where $f(j, j', k)$ is some function of j, j' , and k , and independent of m, m' , and q . Choosing $f(j, j', k)$ to be:

$$f(j, j', k) = \frac{\langle j \| T_k \| j' \rangle}{\sqrt{2k+1}}, \quad (19.255)$$

proves the theorem as stated. \square

Definition 40 (tensor product). Let $T_{k_1, q_1}(1)$ and $T_{k_2, q_2}(2)$ be tensor operators satisfying Definition 37. Then the tensor product of these two operators is defined by:

$$[T_{k_1}(1) \otimes T_{k_2}(2)]_{k,q} = \sum_{q_1, q_2} \langle k_1, q_1, k_2, q_2 | (k_1, k_2) k, q \rangle T_{k_1, q_1}(1) T_{k_2, q_2}(2). \quad (19.256)$$

Theorem 36. *The tensor product of Definition 40 is a tensor operator also.*

Proof. The proof relies on the Clebsch-Gordan series, and is left to the reader. \square

Theorem 36 means that the Wigner-Eckart theorem applies equally well to tensor products. The Hermitian property for tensor products is preserved if we use the second definition, Eq. (19.238); it is *not* preserved with the usual definition, Eq. (19.237).

Example 35. The tensor product of two commuting vectors

$$[R_1(1) \otimes R_1(2)]_{k,q} = \sum_{q_1, q_2} \langle 1, q_1, 1, q_2 | (1, 1) k, q \rangle R_{1, q_1}(1) R_{1, q_2}(2), \quad (19.257)$$

where $R_{1, q_1}(1)$ and $R_{1, q_2}(2)$ are tensor operators of rank one defined by Eq. (19.243), gives tensor operators of rank $k = 0, 1$ and 2 . For $k = 0$, the tensor product is:

$$\begin{aligned} [R_1(1) \otimes R_1(2)]_{0,0} &= \sum_{q_1, q_2} \langle 1, q_1, 1, q_2 | (1, 1) 0, 0 \rangle R_{1, q_1}(1) R_{1, q_2}(2) \\ &= \frac{-1}{\sqrt{3}} \sum_q (-)^q R_{1, q}(1) R_{1, -q}(2) = \frac{-1}{\sqrt{3}} \mathbf{R}(1) \cdot \mathbf{R}(2), \end{aligned} \quad (19.258)$$

which is a scalar under rotations. For $k = 1$, the tensor product is:

$$[R_1(1) \otimes R_1(2)]_{1,q} = \sum_{q_1, q_2} \langle 1, q_1, 1, q_2 | (1, 1) 1, q \rangle R_{1, q_1}(1) R_{1, q_2}(2), \quad (19.259)$$

so that using Table 19.1, for $q = +1$, we find:

$$\begin{aligned} [R_1(1) \otimes R_1(2)]_{1,1} &= \frac{1}{\sqrt{2}} (R_{1,1}(1)R_{1,0}(2) - R_{1,0}(1)R_{1,1}(2)) \\ &= \frac{-i}{2} ((Y(1)Z(2) - Z(1)Y(2)) + i(Z(1)X(2) - X(2)Z(1))) = \frac{i}{\sqrt{2}} [\mathbf{R}(1) \times \mathbf{R}(2)]_{1,1}, \end{aligned} \quad (19.260)$$

with similar expressions for $q = 0, -1$. So for $q = 1, 0, -1$, we find:

$$[R_1(1) \otimes R_1(2)]_{1,q} = \frac{i}{\sqrt{2}} [\mathbf{R}(1) \times \mathbf{R}(2)]_{1,q}, \quad (19.261)$$

which is a pseudovector under rotations. For $k = 2$, the five q components are given by,

$$\begin{aligned} [R_1(1) \otimes R_1(2)]_{2,\pm 2} &= R_{1,\pm 1}(1) R_{1,\pm 1}(2), \\ [R_1(1) \otimes R_1(2)]_{2,\pm 1} &= \frac{1}{\sqrt{2}} (R_{1,\pm 1}(1) R_{1,0}(2) + R_{1,0}(1) R_{1,\pm 1}(2)), \\ [R_1(1) \otimes R_1(2)]_{2,0} &= \frac{1}{\sqrt{6}} (R_{1,1}(1) R_{1,-1}(2) + 2 R_{1,0}(1) R_{1,0}(2) + R_{1,-1}(1) R_{1,1}(2)), \end{aligned} \quad (19.262)$$

which can be written in terms of the Cartesian components of the traceless symmetric tensor:

$$R_{ij}(1, 2) = \frac{1}{2} (R_i(1)R_j(2) + R_j(1)R_i(2)) - \frac{1}{3} \delta_{ij} (\mathbf{R}(1) \cdot \mathbf{R}(2)). \quad (19.263)$$

Definition 41 (Scalar product). For the zero rank tensor product of two rank one tensors, it is useful to have a special definition, called the **scalar product**, so that it agrees with the usual dot product of vectors. So we define:

$$\begin{aligned} [T_k(1) \odot T_k(2)] &= \sum_q (-)^q T_{k,q}(1) T_{k,-q}(2) = \sum_q T_{k,q}(1) T_{k,q}^\dagger(2) = \sum_q T_{k,q}^\dagger(1) T_{k,q}(2) \\ &= \sqrt{2k+1} (-)^k [T_k(1) \otimes T_k(2)]_{0,0}. \end{aligned} \quad (19.264)$$

Example 36. The scalar product of two vectors is just the vector dot product. We find:

$$[R_1(1) \odot R_1(2)] = \sum_q (-)^q R_{1,q}(1) R_{1,-q}(2) = \mathbf{R}(1) \cdot \mathbf{R}(2). \quad (19.265)$$

Example 37. An important example of a scalar product is given by writing the addition theorem for spherical harmonics, Eq. (19.174), as a tensor product:

$$P_k(\cos \gamma) = \frac{4\pi}{2\ell+1} \sum_{q=-k}^{+k} Y_{k,q}(\Omega) Y_{k,q}^*(\Omega') = \sum_{q=-k}^{+k} C_{k,q}(\Omega) C_{k,q}^*(\Omega') = [C_k(\Omega) \odot C_k(\Omega')]. \quad (19.266)$$

19.5.2 Reduced matrix elements

The Wigner-Eckart theorem enables us to calculate matrix elements of any operator for different values of (m, m', q) if we know the reduced matrix element, so it is useful to have a table of reduced matrix elements for operators that enter into calculations. In order to find the reduced matrix element, we only have to

compute the full matrix element for certain values of (m, m', q) , usually $q = 0$, and then use the tables of Clebsch-Gordan coefficients or $3j$ -symbols.

Two important ones are the angular momentum tensor J of rank one and the spherical harmonic tensor of rank k :

$$\langle j \| J \| j' \rangle = \hbar \delta_{j,j'} \sqrt{j(j+1)(2j+1)}. \quad (19.267)$$

$$\langle \ell \| Y_k \| \ell' \rangle = (-)^\ell \sqrt{\frac{(2\ell+1)(2\ell'+1)(2k+1)}{4\pi}} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix}. \quad (19.268)$$

Special cases are:

$$\langle \ell \| L \| \ell' \rangle = \hbar \delta_{\ell,\ell'} \sqrt{\ell(\ell+1)(2\ell+1)}, \quad \langle 1/2 \| \sigma \| 1/2 \rangle = \sqrt{6}, \quad (19.269)$$

$$\langle \ell \| C_k \| \ell' \rangle = (-)^\ell \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix}. \quad (19.270)$$

Exercise 66. Prove Eqs. (19.267) and (19.270). [Hint: The reduced matrix element of J can be found using Table 19.2. The reduced matrix elements of $C_k(\Omega)$ can be found in coordinate space using Eq. (19.233).]

The reduced matrix element of solid harmonics involve radial integrals, which we have ignored up to now. Adding radial quantum numbers to the matrix elements gives, for the solid harmonics:

$$\langle n, \ell \| R_k \| n', \ell' \rangle = (-)^\ell \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix} \int_0^\infty r^2 dr R_{n,\ell}(r) r^k R_{n',\ell'}(r), \quad (19.271)$$

where $R_{n,\ell}(r)$ are (real) radial wave functions for the state (n, ℓ) .

19.5.3 Angular momentum matrix elements of tensor operators

In this section, we give several theorems regarding angular momentum matrix elements of tensor operators. These theorems are the basis for calculating all matrix elements in coupled schemes. The theorems are from Edmonds [2][Chapter 7].

Theorem 37. Let $T_{k_1,q_1}(1)$ and $T_{k_2,q_2}(2)$ be two tensor operators which act on the same angular momentum system. Then

$$\begin{aligned} \langle j \| [T_{k_1}(1) \otimes T_{k_2}(2)]_k \| j' \rangle \\ = \sqrt{2k+1} (-)^{k+j+j'} \sum_{j''} \begin{Bmatrix} k_1 & k_2 & k \\ j' & j & j'' \end{Bmatrix} \langle j \| T_{k_1}(1) \| j'' \rangle \langle j'' \| T_{k_2}(2) \| j' \rangle. \end{aligned} \quad (19.272)$$

Proof. XXX □

Theorem 38. Let $T_{k_1,q_1}(1)$ and $T_{k_2,q_2}(2)$ be two tensor operators which act on parts one and two of a combined system, so that $[T_{k_1,q_1}(1), T_{k_2,q_2}(2)] = 0$. Then

$$\begin{aligned} \langle (j_1, j_2) j \| [T_{k_1}(1) \otimes T_{k_2}(2)]_k \| (j'_1, j'_2) j' \rangle \\ = \sqrt{(2k+1)(2j+1)(2j'+1)} \begin{Bmatrix} j_1 & j'_1 & k_1 \\ j_2 & j'_2 & k_2 \\ j & j' & k \end{Bmatrix} \langle j_1 \| T_{k_1}(1) \| j'_1 \rangle \langle j_2 \| T_{k_2}(2) \| j'_2 \rangle. \end{aligned} \quad (19.273)$$

Proof. XXX □

Theorem 39. Matrix elements of the scalar product of two tensor operators $T_{k,q}(1)$ and $T_{k,q}(2)$ which act on parts one and two of a coupled system is given by:

$$\begin{aligned} & \langle (j_1, j_2) j, m | [T_k(1) \odot T_k(2)] | (j'_1, j'_2) j', m' \rangle \\ &= \delta_{j,j'} \delta_{m,m'} (-)^{j'_1+j_2+j} \begin{Bmatrix} j & j_2 & j_1 \\ k & j'_1 & j'_2 \end{Bmatrix} \langle j_1 \| T_k(1) \| j'_1 \rangle \langle j_2 \| T_k(2) \| j'_2 \rangle. \end{aligned} \quad (19.274)$$

Proof. XXX □

Theorem 40. The reduced matrix element of a tensor operators $T_{k,q}(1)$ which acts only on part one of a coupled system is given by:

$$\begin{aligned} & \langle (j_1, j_2) j \| T_k(1) \| (j'_1, j'_2) j' \rangle \\ &= \delta_{j_2, j'_2} (-)^{j_1+j_2+j'+k} \sqrt{(2j+1)(2j'+1)} \begin{Bmatrix} j_1 & j & j'_2 \\ j' & j'_1 & k \end{Bmatrix} \langle j_1 \| T_k(1) \| j'_1 \rangle. \end{aligned} \quad (19.275)$$

Proof. XXX □

Theorem 41. The reduced matrix element of a tensor operators $T_2(k, q)$ which acts only on part two of a coupled system is given by:

$$\begin{aligned} & \langle (j_1, j_2) j \| T_k(2) \| (j'_1, j'_2) j' \rangle \\ &= \delta_{j_2, j'_2} (-)^{j'_1+j_2+j+k} \sqrt{(2j+1)(2j'+1)} \begin{Bmatrix} j_2 & j & j'_1 \\ j' & j'_2 & k \end{Bmatrix} \langle j_2 \| T_k(2) \| j'_2 \rangle. \end{aligned} \quad (19.276)$$

Proof. XXX □

19.6 Application to selected problems in atomic and nuclear physics

In this section, we give several examples of the use of tensor operators in atomic and nuclear physics.

19.6.1 Spin-orbit force in hydrogen

The spin-orbit force for the electron in a hydrogen atom in atomic units is given by a Hamiltonian of the form (see Section 20.3.2):

$$H_{so} = V(R) (\mathbf{L} \cdot \mathbf{S}) / \hbar^2. \quad (19.277)$$

Of course it is easy to calculate this in perturbation theory for the states $|n, (\ell, s) j, m_j\rangle$. Since $\mathbf{J} = \mathbf{L} + \mathbf{S}$, and squaring this expression, we find that we can write:

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2} (J^2 - L^2 - S^2), \quad (19.278)$$

so that we find:

$$\langle (\ell, s) j, m_j | \mathbf{L} \cdot \mathbf{S} | (\ell, s) j, m_j \rangle / \hbar^2 = \frac{1}{2} (j(j+1) - \ell(\ell+1) - 3/4). \quad (19.279)$$

Since $\mathbf{L} \cdot \mathbf{S} = [L \odot S]$, we can also find matrix elements of the spin-orbit force using Theorem 39. This gives:

$$\langle (\ell, s) j, m_j | [L \odot S] | (\ell, s) j, m_j \rangle / \hbar^2 = (-)^{j+\ell+s} \begin{Bmatrix} j & s & \ell \\ 1 & \ell & s \end{Bmatrix} \langle \ell \| L \| \ell \rangle \langle s \| S \| s \rangle / \hbar^2. \quad (19.280)$$

Now using the $6j$ -tables in Edmonds, we find:

$$\begin{aligned} \left\{ \begin{matrix} j & s & \ell \\ 1 & \ell & s \end{matrix} \right\} &= (-)^{j+\ell+s} \frac{2[j(j+1) - \ell(\ell+1) - s(s+1)]}{\sqrt{2\ell(2\ell+1)(2\ell+2)2s(2s+1)(2s+2)}}, \\ \langle \ell \| L \| \ell \rangle / \hbar &= \sqrt{2\ell(2\ell+1)(2\ell+2)/2}, \\ \langle s \| S \| s \rangle / \hbar &= \sqrt{2s(2s+1)(2s+2)/2}, \end{aligned} \quad (19.281)$$

so (19.280) becomes simply:

$$\langle (\ell, s) j, m_j | [L \odot S] | (\ell, s) j, m_j \rangle / \hbar^2 = \frac{1}{2} (j(j+1) - \ell(\ell+1) - 3/4). \quad (19.282)$$

in agreement with Eq. (20.62). Of course, using the fancy angular momentum theorems for tensor operators in this case is over-kill! Our point was to show that the theorems give the same result as the simple way. We will find in later examples that the *only* way to do the problem is to use the fancy theorems.

19.6.2 Transition rates for photon emission in Hydrogen

Omit?

19.6.3 Hyperfine splitting in Hydrogen

In this section, we show how to compute the hyperfine energy splitting in hydrogen due to the interaction between the magnetic moment of the proton and the electron. We derive the forces responsible for the splitting in Section 20.3.3 where, in atomic units, we found the Hamiltonian:

$$\bar{H}_{\text{hf}} = 2 \lambda_p \left(\frac{m}{M} \right) \alpha^2 \frac{\mathbf{K}_e \cdot \mathbf{S}_p / \hbar^2}{R^3}, \quad \mathbf{K}_e = \mathbf{L}_e - \mathbf{S}_e + 3(\mathbf{S}_e \cdot \hat{\mathbf{R}}) \hat{\mathbf{R}}, \quad (19.283)$$

where \mathbf{L}_e and \mathbf{S}_e are the angular momentum and spin operators for the electron, \mathbf{S}_p is the spin operator for the proton, and $\hat{\mathbf{r}}$ is the unit vector pointing from the proton to the electron. Here \mathbf{K}_e acts on the electron part and \mathbf{S}_e on the proton part. Both \mathbf{K}_e and \mathbf{S}_e are tensor operators of rank one. Using first order perturbation theory, we want to show that matrix elements of this Hamiltonian in the coupled states:

$$|n, (\ell, s_e) j, s_p, f, m_f \rangle, \quad (19.284)$$

are diagonal for states with the same value of j , and we want to find the splitting energy. We first want to write $\mathbf{S}_e - 3(\mathbf{S}_e \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}}$ as a tensor operator. We state the result of this derivation as the following theorem:

Theorem 42. *The vector $\mathbf{S}_e - 3(\mathbf{S}_e \cdot \hat{\mathbf{r}}) \hat{\mathbf{r}}$ can be written as a rank one tensor operator of the form:*

$$[\mathbf{S}_e - 3(\mathbf{S}_e \cdot \hat{\mathbf{R}}) \hat{\mathbf{R}}]_{1,q} = \sqrt{10} [C_2(\hat{\mathbf{R}}) \otimes S_1(\mathbf{e})]_{1,q}. \quad (19.285)$$

Proof. We start by writing:

$$[\mathbf{S}_e - 3(\mathbf{S}_e \cdot \hat{\mathbf{R}}) \hat{\mathbf{R}}]_{1,q} = \sum_{q_1} S_{1,q_1}(\mathbf{e}) \{ \delta_{q_1,q} - 3 C_{1,q_1}^*(\hat{\mathbf{R}}) C_{1,q}(\hat{\mathbf{R}}) \}. \quad (19.286)$$

Next, we have:

$$\begin{aligned} 3 C_{1,q_1}^*(\hat{\mathbf{R}}) C_{1,q}(\hat{\mathbf{R}}) &= 3 (-)^{q_1} \sum_{k,q_2} C_{k,q_2}(\hat{\mathbf{R}}) \langle 1, -q_1, 1, q | (1, 1) k, q \rangle \langle 1, 0, 1, 0 | (1, 1) k, 0 \rangle \\ &= \delta_{q_1,q} - \sqrt{10} \sum_{q_2} C_{2,q_2}(\hat{\mathbf{R}}) \langle 2, q_2, 1, q_1 | (1, 2) 1, q \rangle. \end{aligned} \quad (19.287)$$

Here we have used $\langle 1, 0, 1, 0 | (1, 1) k, 0 \rangle = -1/\sqrt{3}$, 0, and $+\sqrt{2/3}$ for $k = 0, 1$, and 2 respectively. Substitution of (19.287) into (19.286) gives:

$$[\mathbf{S}_e - 3(\mathbf{S}_e \cdot \hat{\mathbf{R}}) \hat{\mathbf{R}}]_{1,q} = \sqrt{10} \sum_{q_2} \langle 2, q_2, 1, q_1 | (1, 2) 1, q \rangle C_{2,q_2}(\hat{\mathbf{R}}) S_{1,q_1}(\mathbf{e}) = \sqrt{10} [C_2(\hat{\mathbf{R}}) \otimes S_1(\mathbf{e})]_{1,q}, \quad (19.288)$$

which proves the theorem. \square

We now want to find the matrix elements of the scalar product:

$$\langle n, (\ell, s_e) j, s_p, f, m_f | [K_1(\mathbf{e}) \odot S_1(\mathbf{p})] | n, (\ell', s_e) j, s_p, f', m_f' \rangle, \quad (19.289)$$

where $K_{1,q}(\mathbf{e})$ is the rank one tensor operator:

$$K_{1,q}(\mathbf{e}) = L_{1,q}(\mathbf{e}) - \sqrt{10} [C_2(\hat{\mathbf{R}}) \otimes S_1(\mathbf{e})]_{1,q}. \quad (19.290)$$

Here $K_1(\mathbf{e})$ only operates on the electron part (the first part of the coupled state) and $S_1(\mathbf{p})$ on the proton part (the second part of the coupled state). So using Theorem 39, we find:

$$\begin{aligned} & \langle n, (\ell, s_e) j, s_p, f, m_f | [K_1(\mathbf{e}) \odot S_1(\mathbf{p})] | n, (\ell', s_e) j, s_p, f', m_f' \rangle / \hbar^2 \\ &= \delta_{f,f'} \delta_{m_f,m_f'} (-)^{j+s_p+f} \begin{Bmatrix} f & s_p & j \\ 1 & j & s_p \end{Bmatrix} \langle (\ell, s_e) j \| K_1(\mathbf{e}) \| (\ell', s_e) j \rangle \langle s_p \| S_1(\mathbf{p}) \| s_p \rangle / \hbar^2 \\ &= \delta_{f,f'} \delta_{m_f,m_f'} (-)^{f+j+1/2} \sqrt{3/2} \begin{Bmatrix} f & 1/2 & j \\ 1 & j & 1/2 \end{Bmatrix} \langle (\ell, s_e) j \| K_1(\mathbf{e}) \| (\ell', s_e) j \rangle / \hbar \\ &= \delta_{f,f'} \delta_{m_f,m_f'} \frac{f(f+1) - j(j+1) - 3/4}{2\sqrt{j(j+1)(2j+1)}} \langle (\ell, s_e) j \| K_1(\mathbf{e}) \| (\ell', s_e) j \rangle / \hbar. \end{aligned} \quad (19.291)$$

Since $L_1(\mathbf{e})$ only operates on the first part of the coupled scheme $(\ell, s_e) j$, its reduced matrix elements can be found by application of Theorem 40, and we find:

$$\begin{aligned} \langle (\ell, s_e) j \| L_1(\mathbf{e}) \| (\ell', s_e) j \rangle / \hbar &= (-)^{\ell+j+3/2} (2j+1) \begin{Bmatrix} \ell & j & 1/2 \\ j & \ell' & 1 \end{Bmatrix} \langle \ell \| L_1(\mathbf{e}) \| \ell' \rangle / \hbar. \\ &= \delta_{\ell,\ell'} \frac{1}{2} \sqrt{2\ell(2\ell+1)(2\ell+2)} (-)^{\ell+j+3/2} (2j+1) \begin{Bmatrix} 1/2 & j & \ell \\ 1 & \ell & j \end{Bmatrix} \\ &= \delta_{\ell,\ell'} \frac{1}{2} \sqrt{\frac{2j+1}{j(j+1)}} \{ j(j+1) + \ell(\ell+1) - 3/4 \}, \end{aligned} \quad (19.292)$$

where we have used Table 19.3. Using Theorem 38 the reduced matrix element of $\sqrt{10} [C_2(\hat{\mathbf{r}}) \otimes S_1(\mathbf{e})]_1$ is given by

$$\begin{aligned} & \sqrt{10} \langle (\ell, s_e) j \| [C_2(\hat{\mathbf{R}}) \otimes S_1(\mathbf{e})]_1 \| (\ell', s_e) j \rangle / \hbar \\ &= \sqrt{30} (2j+1) \begin{Bmatrix} \ell & \ell' & 2 \\ s_e & s_e & 1 \\ j & j & 1 \end{Bmatrix} \langle \ell \| C_2(\hat{\mathbf{r}}) \| \ell' \rangle \langle s_e \| S_1(\mathbf{e}) \| s_e \rangle / \hbar \\ &= (-)^\ell 3\sqrt{5} (2j+1) \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & 2 & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell & \ell' & 2 \\ 1/2 & 1/2 & 1 \\ j & j & 1 \end{Bmatrix}. \end{aligned} \quad (19.293)$$

The $6j$ -symbol vanished unless $\ell + \ell' + 2$ is even. But since we are only considering states with the same j values, this means that $\ell = \ell'$. From tables in Edmonds, we have:

$$\begin{pmatrix} \ell & 2 & \ell \\ 0 & 0 & 0 \end{pmatrix} = (-)^{\ell+1} \sqrt{\frac{\ell(\ell+1)}{(2\ell-1)(2\ell+1)(2\ell+3)}}, \quad (19.294)$$

and from tables in Matsunobu and Takebe [19], we have:

$$\left\{ \begin{array}{ccc} \ell & \ell & 2 \\ j & j & 1 \\ 1/2 & 1/2 & 1 \end{array} \right\} = \frac{1}{3\sqrt{5}(2j+1)(2\ell+1)} \begin{cases} (-)\sqrt{2\ell(2\ell-1)}, & \text{for } j = \ell + 1/2, \\ (+)\sqrt{(2\ell+1)(2\ell+3)}, & \text{for } j = \ell - 1/2. \end{cases} \quad (19.295)$$

Putting Eqs. (19.294) and (19.295) into Eq. (19.293) gives:

$$\begin{aligned} \sqrt{10} \langle (\ell, s_e) j \| [C_2(\hat{\mathbf{R}}) \otimes S_1(\mathbf{e})]_1 \| (\ell', s_e) j \rangle / \hbar \\ = \delta_{\ell, \ell'} \frac{1}{2} \sqrt{\frac{2j+1}{j(j+1)}} \times \begin{cases} \ell & \text{for } j = \ell + 1/2, \\ -(\ell+1) & \text{for } j = \ell - 1/2 \end{cases} \\ = \delta_{\ell, \ell'} \frac{1}{2} \sqrt{\frac{2j+1}{j(j+1)}} \{ j(j+1) - \ell(\ell+1) - 3/4 \}. \end{aligned} \quad (19.296)$$

So subtracting (19.296) from (19.292), we find the result:

$$\langle (\ell, s_e) j \| K_1(\mathbf{e}) \| (\ell', s_e) j \rangle / \hbar = \delta_{\ell, \ell'} \ell(\ell+1) \sqrt{\frac{2j+1}{j(j+1)}}. \quad (19.297)$$

Putting this into Eq. (19.291) gives:

$$\begin{aligned} \langle n, (\ell, s_e) j, s_p, f, m_f \| [K_1(\mathbf{e}) \odot S_1(\mathbf{p})] \| n, (\ell', s_e) j, s_p, f', m'_f \rangle / \hbar^2 \\ = \delta_{f, f'} \delta_{m_f, m'_f} \delta_{\ell, \ell'} \frac{\ell(\ell+1)}{2j(j+1)} \{ f(f+1) - j(j+1) - 3/4 \}. \end{aligned} \quad (19.298)$$

So we have shown that:

$$\langle n, (\ell, s_e) j, s_p, f, m_f | \bar{H}_{\text{hf}} | n, (\ell', s_e) j, s_p, f', m'_f \rangle = \delta_{f, f'} \delta_{m_f, m'_f} \delta_{\ell, \ell'} \Delta E_{n, \ell, j, f}, \quad (19.299)$$

where, in atomic units, the energy shift $\Delta \bar{E}_{n, \ell, j, f}$ is given by:

$$\Delta \bar{E}_{n, \ell, j, f} = 2\lambda_p \left(\frac{m}{M} \right) \alpha^2 \frac{f(f+1) - j(j+1) - 3/4}{n^3 j(j+1)(2\ell+1)}. \quad (19.300)$$

Here we have used:

$$\left\langle \frac{1}{R^3} \right\rangle_{n, \ell} = \frac{2}{n^3 \ell(\ell+1)(2\ell+1)}. \quad (19.301)$$

Eq. (19.300) is quoted in our discussion of the hyperfine structure of hydrogen in Section 20.3.3.

19.6.4 Zeeman effect in Hydrogen

The Hamiltonian for the Zeeman effect in Hydrogen is given by Eq. (20.91), where we found:

$$H_z = \mu_B (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{B} / \hbar, \quad \text{with} \quad \mu_B = \frac{e \hbar}{2mc}. \quad (19.302)$$

We shall find matrix elements within the hyperfine splitting levels. That is, taking the z -axis in the direction of the \mathbf{B} field,

$$\begin{aligned} \langle (\ell, s_e) j, s_p, f, m_f | H_z | (\ell, s_e) j, s_p, f', m'_f \rangle \\ = \mu_B B \langle (\ell, s_e) j, s_p, f, m_f | (L_z + 2S_z) | (\ell, s_e) j, s_p, f', m'_f \rangle / \hbar. \end{aligned} \quad (19.303)$$

Now both L_z and S_z are $q = 0$ components of tensor operators of rank $k = 1$. So using the Wigner-Eckart Theorem 35, and Theorems 40 and 41, we find:

$$\begin{aligned}
& \langle (\ell, s_e) j, s_p, f, m_f | L_{1,0}(e) | (\ell, s_e) j, s_p, f', m'_f \rangle / \hbar \\
&= (-)^{f-m_f} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \langle (\ell, s_e) j, s_p, f | L_1(e) | (\ell, s_e) j, s_p, f' \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+1} \sqrt{(2f+1)(2f'+1)} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \langle (\ell, s_e) j | L_1(e) | (\ell, s_e) j \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+j+\ell+1/2} (2j+1) \sqrt{(2f+1)(2f'+1)} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times \begin{Bmatrix} \ell & j & 1/2 \\ j & \ell & 1 \end{Bmatrix} \langle \ell | L_1(e) | \ell \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+j+\ell+1/2} (2j+1) \sqrt{(2f+1)(2f'+1)\ell(\ell+1)(2\ell+1)} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times \begin{Bmatrix} \ell & j & 1/2 \\ j & \ell & 1 \end{Bmatrix} \\
&= (-)^{f+f'-m_f+j-1/2} \frac{1}{2} \sqrt{\frac{(2j+1)(2f+1)(2f'+1)}{j(j+1)}} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times [j(j+1) + \ell(\ell+1) - 3/4] \quad (19.304)
\end{aligned}$$

and

$$\begin{aligned}
& \langle (\ell, s_e) j, s_p, f, m_f | S_{1,0}(e) | (\ell, s_e) j, s_p, f', m'_f \rangle / \hbar \\
&= (-)^{f-m_f} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \langle (\ell, s_e) j, s_p, f | S_1(e) | (\ell, s_e) j, s_p, f' \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+1} \sqrt{(2f+1)(2f'+1)} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \langle (\ell, s_e) j | S_1(e) | (\ell, s_e) j \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+j+\ell+1/2} (2j+1) \sqrt{(2f+1)(2f'+1)} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times \begin{Bmatrix} 1/2 & j & \ell \\ j & 1/2 & 1 \end{Bmatrix} \langle 1/2 | S_1(e) | 1/2 \rangle / \hbar \\
&= (-)^{f-m_f+j+1/2+f'+j+\ell+1/2} (2j+1) \sqrt{(2f+1)(2f'+1)3/2} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\times \begin{Bmatrix} 1/2 & j & \ell \\ j & 1/2 & 1 \end{Bmatrix} = (-)^{f+f'-m_f+j-1/2} \frac{1}{2} \sqrt{\frac{(2j+1)(2f+1)(2f'+1)}{j(j+1)}} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times [j(j+1) - \ell(\ell+1) + 3/4]. \quad (19.305)
\end{aligned}$$

So multiplying Eq. (19.305) by a factor of two and adding it to Eq. (19.304) gives:

$$\begin{aligned}
& \langle (\ell, s_e) j, s_p, f, m_f | H_z | (\ell, s_e) j, s_p, f', m'_f \rangle \\
&= \mu_B B (-)^{f+f'-m_f+j-1/2} \frac{1}{2} \sqrt{\frac{(2j+1)(2f+1)(2f'+1)}{j(j+1)}} \begin{pmatrix} f & 1 & f' \\ -m_f & 0 & m'_f \end{pmatrix} \begin{Bmatrix} j & f & 1/2 \\ f' & j & 1 \end{Bmatrix} \\
&\quad \times [3j(j+1) - \ell(\ell+1) + 3/4]. \quad (19.306)
\end{aligned}$$

The $3j$ -symbol vanishes unless $m'_f = m_f$, so the matrix element connects only states of the same m_f . Now if $f' = f$, we find the simple result:

$$\begin{aligned} & \langle (\ell, s_e) j, s_p, f, m_f | H_z | (\ell, s_e) j, s_p, f, m_f \rangle \\ &= (\mu_B B) m_f \frac{[f(f+1) + j(j+1) - 3/4] [3j(j+1) - \ell(\ell+1) + 3/4]}{4f(f+1)j(j+1)}. \end{aligned} \quad (19.307)$$

On the other hand, if $f' = f + 1$, we get:

$$\begin{aligned} & \langle (\ell, s_e) j, s_p, f, m_f | H_z | (\ell, s_e) j, s_p, f + 1, m_f \rangle \\ &= (\mu_B B) \frac{3j(j+1) - \ell(\ell+1) + 3/4}{j(j+1)(f+1)} \\ & \times \sqrt{\frac{(f - m_f + 1)(f + m_f + 1)(f + j + 5/2)(f + j + 1/2)(f - j + 3/2)(j - f + 1/2)}{(2f + 1)(2f + 3)}}. \end{aligned} \quad (19.308)$$

with an identical expression for the matrix elements of $\langle (\ell, s_e) j, s_p, f + 1, m_f | H_z | (\ell, s_e) j, s_p, f, m_f \rangle$. We use these results in Section 20.3.4.

19.6.5 Matrix elements of two-body nucleon-nucleon potentials

In the nuclear shell model, nucleons (protons and neutrons) with spin $s = 1/2$ are in $(\ell, s) j, m_j$ coupled orbitals with quantum numbers given by: $n(\ell)_j = 1s_{1/2}, 1p_{1/2}, 2s_{1/2}, 2p_{3/2}, \dots$. We leave it to a nuclear physics book to explain why this is often a good approximation (see, for example, the book *Nuclear Physics* by J. D. Walecka). The nucleon-nucleon interaction between nucleons in these orbitals give a splitting of the shell energies of the nucleus. One such interaction is the one-pion exchange interaction of the form:

$$V(\mathbf{r}_1, \mathbf{r}_2) = V_0 \frac{e^{-\mu r}}{r} \left\{ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \left[\frac{1}{(\mu r)^2} + \frac{1}{\mu r} + \frac{1}{3} \right] S_{1,2} \right\} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2, \quad (19.309)$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$ is the distance between the nucleons, $\mu = m_\pi c/\hbar$ the inverse pion Compton wavelength, $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ the spin operators, $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ the isospin operators for the two nucleons, and $S_{1,2}$ the tensor operator:

$$S_{1,2} = 3(\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}_1)(\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}_2) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2. \quad (19.310)$$

The nuclear state is given by the coupling:

$$|n_1, n_2; (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j, m\rangle \quad (19.311)$$

To find the nuclear energy levels, we will need to find matrix elements of the nuclear force between these states. The calculation of these matrix elements generally involve a great deal of angular momentum technology. The nucleon-nucleon force, given in Eq. (19.309), is only one example of a static nucleon-nucleon interaction. Other examples are the V_6 and V_{12} Argonne interactions. Matrix elements of these interactions have been worked out in the literature by B. Mihaila and J. Heisenberg [22]. We show how to compute some of these matrix elements here.

Scalar force

Let us first make a multipole expansion of a scalar potential. Let \mathbf{r}_1 and \mathbf{r}_2 be the location of nucleon 1 and nucleon 2 in the center of mass coordinate system of the nucleus. Then a scalar potential, which depends only on the magnitude of the distance between the particles is given by:

$$\begin{aligned} V_S(\mathbf{r}_1, \mathbf{r}_2) &= V_S(|\mathbf{r}_1 - \mathbf{r}_2|) = V(r_1, r_2, \cos \theta) \\ &= \sum_{k=0}^{\infty} V_k(r_1, r_2) P_k(\cos \theta) = \sum_{k=0}^{\infty} V_k(r_1, r_2) [C_k(\Omega_1) \odot C_k(\Omega_2)], \end{aligned} \quad (19.312)$$

where

$$V_k(r_1, r_2) = \frac{2k+1}{2} \int_{-1}^{+1} V(r_1, r_2, \cos \theta) P_k(\cos \theta) d(\cos \theta), \quad (19.313)$$

and where we have used Eq. (19.266). Eq. (19.312) is now in the form required for the j - j coupling state given in (19.311). So now applying Theorem 19.274, we find:

$$\begin{aligned} \Delta E &= \langle n_1, n_2; (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j, m | V(|\mathbf{r}_1 - \mathbf{r}_2|) | n_1, n_2; (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j', m' \rangle \\ &= \sum_{k=0}^{\infty} F_k(1, 2) \langle (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j, m | [C_k(\Omega_1) \odot C_k(\Omega_2)] | (\ell_1, s_1) j_1, (\ell_2, s_2) j_2, j, m \rangle \\ &= \delta_{j, j'} \delta_{m, m'} \sum_{k=0}^{\infty} F_k(1, 2) (-)^{j_1+j_2+j} \begin{Bmatrix} j & j_2 & j_1 \\ k & j_1 & j_2 \end{Bmatrix} \\ &\quad \times \langle (\ell_1, s_1) j_1 \| C_k(\Omega_1) \| (\ell_1, s_1) j_1 \rangle \langle (\ell_2, s_2) j_2 \| C_k(\Omega_2) \| (\ell_2, s_2) j_2 \rangle. \end{aligned} \quad (19.314)$$

Here

$$F_k(1, 2) = \int_0^{\infty} r_1^2 dr_1 \int_0^{\infty} r_2^2 dr_2 R_{n_1, \ell_1, j_1}^2(r_1) R_{n_2, \ell_2, j_2}^2(r_2) V_k(r_1, r_2) \quad (19.315)$$

are integrals over the radial wave functions for the nucleons in the orbitals $n_1(\ell_1)_{j_1}$ and $n_2(\ell_2)_{j_2}$. It is now a simple matter to compute the reduced matrix elements of $C_k(\Omega)$ using Theorem 40 and Eqs. (19.211) and (19.270). We find:

$$\begin{aligned} \langle (\ell, 1/2) j \| C_k(\Omega) \| (\ell', 1/2) j' \rangle &= (-)^{\ell+\ell'+j'+k} \sqrt{(2j+1)(2j'+1)} \begin{Bmatrix} \ell & j & 1/2 \\ j' & \ell' & k \end{Bmatrix} \langle \ell \| C_k \| \ell' \rangle \\ &= (-)^{\ell'+j'+k} \sqrt{(2j+1)(2j'+1)(2\ell+1)(2\ell'+1)} \begin{Bmatrix} \ell & j & 1/2 \\ j' & \ell' & k \end{Bmatrix} \begin{pmatrix} \ell & k & \ell' \\ 0 & 0 & 0 \end{pmatrix} \\ &= (-)^{k+j'-1/2} \sqrt{(2j+1)(2j'+1)} \begin{Bmatrix} j & j' & k \\ 1/2 & -1/2 & 0 \end{Bmatrix} \delta(\ell, \ell', k), \end{aligned} \quad (19.316)$$

where $\delta(\ell, \ell', k) = 1$ if $\ell + \ell' + k$ is even and (ℓ, ℓ', k) satisfy the triangle inequality, otherwise it is zero. Substitution into Eq. (19.314) gives $\Delta E = \delta_{j, j'} \delta_{m, m'} E_j$, where E_j is given by:

$$\begin{aligned} \Delta E_j &= \sum_{k=0}^{\infty} F_k(1, 2) (-)^{j+1} (2j_1+1)(2j_2+1) \\ &\quad \times \begin{Bmatrix} j & j_2 & j_1 \\ k & j_1 & j_2 \end{Bmatrix} \begin{Bmatrix} j_1 & j_1 & k \\ 1/2 & -1/2 & 0 \end{Bmatrix} \begin{Bmatrix} j_2 & j_2 & k \\ 1/2 & -1/2 & 0 \end{Bmatrix} \delta(\ell_1, \ell_1, k) \delta(\ell_2, \ell_2, k), \end{aligned} \quad (19.317)$$

which completes the calculation. Note that k has to be even.

Exercise 67. If $j_1 = j_2$ and all values of $F_k(1, 2)$ are negative corresponding to an attractive nucleon-nucleon potential, show that the expected nuclear spectra is like that shown in Fig. ?? [J. D. Walecka, p. 517].

Spin-exchange force

The nucleon-nucleon spin-exchange force is of the form:

$$V_{SE}(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = V_{SE}(|\mathbf{r}_1 - \mathbf{r}_2|) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = \sum_{k, \ell} (-)^{\ell+1-k} V_{\ell}(r_1, r_2) [T_{\ell, k}(1) \odot T_{\ell, k}(2)], \quad (19.318)$$

where

$$\begin{aligned} T_{(\ell, 1) k, q}(1) &= [C_{\ell}(\Omega_1) \otimes \sigma(1)]_{k, q}, \\ T_{(\ell, 1) k, q}(2) &= [C_{\ell}(\Omega_2) \otimes \sigma(2)]_{k, q}. \end{aligned} \quad (19.319)$$

This now is in a form suitable for calculation in j - j coupling.

Spin-orbit force

XXX

Tensor force

The tensor force is of the form:

$$\begin{aligned} V_T(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) &= V_T(|\mathbf{r}_1 - \mathbf{r}_2|) \{ (\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}}_{12}) (\boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}}_{12}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)/3 \} \\ &= V_T(|\mathbf{r}_1 - \mathbf{r}_2|) [L_2(1, 2) \odot S_2(1, 2)], \end{aligned} \quad (19.320)$$

where

$$\begin{aligned} S_{2,q}(1, 2) &= [\sigma_1(1) \otimes \sigma_1(2)]_{2,q}, \\ L_{2,q}(1, 2) &= [\hat{R}_1(1, 2) \otimes \hat{R}_1(1, 2)]_{2,q}, \end{aligned} \quad (19.321)$$

with $\hat{R}_1(1, 2)$ the spherical vector of components of the unit vector \mathbf{r}_{12} . We follow the method described by de-Shalit and Walecka [23] here. Expanding

$$V_T(|\mathbf{r}_1 - \mathbf{r}_2|) = \sum_{k=0}^{\infty} V_{T k}(r_1, r_2) [C_k(\Omega_1) \odot C_k(\Omega_2)], \quad (19.322)$$

After some work, we find:

$$V_T(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = \sum_{k,\ell} (-)^{\ell+1-k} V_{\ell}(r_1, r_2) [X_{\ell,k}(1) \odot X_{\ell,k}(2)], \quad (19.323)$$

where

19.6.6 Density matrix for the Deuteron**References**

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