PH 422: Quantum Mechanics II
Tutorial Sheet 2: Solution

This tutorial sheet contains problems related to the Clebsch-Gordon series, tensor operators, and the Wigner-Eckart theorem.

1. By use of the unitary condition for the D matrices and the orthogonality condition of the CGCs, derive from the Clebsch-Gordon series the result

$$\sum_{m_2'} \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle D^{(j_2)}_{m_2' m_2}(R) = \sum_{m_1 m} D^{(j_3)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle D^{(j_1)*}_{m_1' m_1}(R).$$

Soln: The Clebsch-Gordon series is

$$D^{(j_1)}_{m_1' m_1}(R) D^{(j_2)}_{m_2' m_2}(R) = \sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m,m'} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m' \rangle D^{(j)}_{m' m}(R).$$

Multiplying on both the sides by $\langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle$ and summing over m_1' and m_2'

$$\sum_{m_1', m_2'} D^{(j_1)}_{m_1' m_1}(R) D^{(j_2)}_{m_2' m_2}(R) \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle =$$
$$\sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m,m'} D^{(j)}_{m' m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$$
$$\times \sum_{m_1', m_2'} \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m' \rangle$$

Using the fact that $\sum_{m_1', m_2'} \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m' \rangle = \delta_{j, j_3} \delta_{m', m_3}$, we obtain

$$\sum_{m_1', m_2'} D^{(j_1)}_{m_1' m_1}(R) D^{(j_2)}_{m_2' m_2}(R) \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle =$$
$$\sum_{m} D^{(j)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle$$

Multiplying on both the sides by $D^{(j_1)*}_{l m_1}$, summing over m_1, and using the fact that

$\sum_{m_1} D^{(j_1)}_{lm_1} D^{(j_1)*}_{m_1' m_1} = \delta_{lm_1'}$, we have

$$\sum_{m_1', m_2'} \left(\sum_{m_1} D^{(j_1)}_{m_1' m_1}(R) D^{(j_1)*}_{lm_1}(R) \right) D^{(j_2)}_{m_2' m_2}(R) \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle =$$
$$\sum_{m_1, m} D^{(j)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle D^{(j_1)*}_{lm_1}(R)$$
$$\Longrightarrow \sum_{m_1', m_2'} \left(\delta_{lm_1'} \right) D^{(j_2)}_{m_2' m_2}(R) \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle =$$
$$\sum_{m_1, m} D^{(j)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle D^{(j_1)*}_{lm_1}(R)$$
$$\Longrightarrow \sum_{m_2'} \langle j_1 j_2 l m_2' | j_1 j_2 j_3 m_3 \rangle D^{(j_2)}_{m_2' m_2}(R) = \sum_{m_1 m} D^{(j_3)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle D^{(j_1)*}_{lm_1}(R)$$

on replacing $l \to m_1'$ we get the desired result

$$\sum_{m_2'} \langle j_1 j_2 m_1' m_2' | j_1 j_2 j_3 m_3 \rangle D^{(j_2)}_{m_2' m_2}(R) = \sum_{m_1 m} D^{(j_3)}_{m_3 m}(R) \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_3 m \rangle D^{(j_1)*}_{m_1' m_1}(R).$$

2. Prove

$$D^{(j)}_{mm'}(R) = \sum_{m_1, m_1', m_2, m_2'} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle D^{(j_1)}_{m_1 m_1'}(R) D^{(j_2)}_{m_2, m_2'}(R) \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m' \rangle.$$

Verify that this result holds for $j_1 = 1/2$, $j_2 = 1$, $j = 3/2$, when R denotes a rotation by an angle θ about the z axis.
Soln: We have

$$D^{(j)}_{mm'}(R) = \langle jm | e^{-\frac{i\mathbf{J}\cdot\hat{\mathbf{n}}\theta}{\hbar}} | jm' \rangle.$$

When j is obtained by coupling two angular momenta j_1 and j_2, then

$$|jm\rangle = |j_1 j_2 j m\rangle$$
$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$$
$$\sum_{m_1, m_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2| = I.$$

Using these above

$$\begin{aligned} D^{(j)}_{mm'}(R) &= \langle j_1 j_2 j m | e^{-\frac{i\mathbf{J}_1\cdot\hat{\mathbf{n}}\theta}{\hbar}} e^{-\frac{i\mathbf{J}_2\cdot\hat{\mathbf{n}}\theta}{\hbar}} | j_1 j_2 j m' \rangle \\ &= \sum_{\substack{m_1, m_2 \\ m_1', m_2'}} \langle j_1 j_2 j m | j_1 j_2 m_1 m_2 \rangle \langle j_1 j_2 m_1 m_2 | e^{-\frac{i\mathbf{J}_1\cdot\hat{\mathbf{n}}\theta}{\hbar}} e^{-\frac{i\mathbf{J}_2\cdot\hat{\mathbf{n}}\theta}{\hbar}} | j_1 j_2 m_1' m_2' \rangle \\ &\times \langle j_1 j_2 m_1' m_2' | j_1 j_2 j m' \rangle. \end{aligned}$$

Using the fact

$$\langle j_1 j_2 m_1 m_2| e^{-\frac{i\mathbf{J}_1\cdot\hat{\mathbf{n}}\theta}{\hbar}} e^{-\frac{i\mathbf{J}_2\cdot\hat{\mathbf{n}}\theta}{\hbar}} |j_1 j_2 m_1^{'} m_2^{'}\rangle = \langle j_1 m_1| e^{-\frac{i\mathbf{J}_1\cdot\hat{\mathbf{n}}\theta}{\hbar}} |j_1 m_1^{'}\rangle \times \langle j_2 m_2| e^{-\frac{i\mathbf{J}_2\cdot\hat{\mathbf{n}}\theta}{\hbar}} |j_2 m_2^{'}\rangle = D^{(j_1)}_{m_1 m_1^{'}}(R) D^{(j_2)}_{m_2, m_2^{'}}.$$

Using this above, we obtain the desired result

$$D^{(j)}_{mm'}(R) = \sum_{m_1, m_1^{'}, m_2, m_2^{'}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle D^{(j_1)}_{m_1 m_1^{'}}(R) D^{(j_2)}_{m_2, m_2^{'}}(R) \langle j_1 j_2 m_1^{'} m_2^{'} | j_1 j_2 j m^{'}\rangle. \tag{1}$$

For a rotation of angle θ about the z-axis, for angular momentum j, we have

$$D^{(j)}_{mm'}(\theta) = \langle jm| e^{-\frac{iJ_z\theta}{\hbar}} |jm^{'}\rangle = e^{-im\theta}\delta_{m,m'}.$$

Using this on the RHS of Eq. 1, we have

$$\sum_{m_1, m_1^{'}, m_2, m_2^{'}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle \langle j_1 j_2 m_1^{'} m_2^{'} | j_1 j_2 j m^{'}\rangle e^{-im_1\theta}\delta_{m_1, m_1^{'}} e^{-im_2\theta}\delta_{m_2, m_2^{'}}$$
$$= \sum_{m_1, m_2} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m^{'}\rangle e^{-im_1\theta} e^{-im_2\theta}$$

If we take, $m_1 = j_1$, $m_2 = j_2$, $m = m^{'} = j$, the CGC's involved are both 1, and on both the LHS and RHS we obtain $e^{-im\theta} = e^{-i(m_1+m_2)\theta}$. For other values of angular momenta, one will have to use the CGCs to verify the result.

3. Using the spherical harmonics $Y_l^m(\theta, \phi)$, establish the connection between components of a Cartesian tensor of rank 2 defined as $T_{ij} = x_i x_j$, and the corresponding spherical tensor $T^q_{k=2}$. Here x_i denotes the i-th Cartesian component of the position vector.
Soln: Let us express the components of Y_2^m in Cartesian coordinates. For $m = \pm 2$

$$\begin{aligned}
Y_2^{\pm 2}(\theta, \phi) &= \sqrt{\frac{15}{32\pi}} e^{\pm i2\phi} \sin^2\theta \\
&= \sqrt{\frac{15}{32\pi}} (\cos 2\phi \pm i \sin 2\phi) \sin^2\theta \\
&= \sqrt{\frac{15}{32\pi}} \left(\cos^2\phi - \sin^2\phi \pm 2i \sin\phi\cos\phi\right) \sin^2\theta \\
&= \sqrt{\frac{15}{32\pi}} \frac{(x^2 - y^2 \pm 2ixy)}{r^2} = \sqrt{\frac{15}{32\pi}} \frac{(x \pm iy)^2}{r^2} \\
&= \sqrt{\frac{15}{32\pi}} \frac{(T_{xx} - T_{yy} \pm 2iT_{xy})}{r^2}
\end{aligned}$$

For $m = \pm 1$

$$\begin{aligned}
Y_2^{\pm 1}(\theta, \phi) &= \mp\sqrt{\frac{15}{8\pi}} e^{\pm i\phi} \sin\theta\cos\theta \\
&= \mp\sqrt{\frac{15}{8\pi}} (\sin\theta\cos\phi \pm i\sin\theta\sin\phi)\cos\theta \\
&= \mp\sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2} \\
&= \mp\sqrt{\frac{15}{8\pi}} \frac{(T_{xz} \pm iT_{yz})}{r^2}
\end{aligned}$$

For $m = 0$

$$\begin{aligned}
Y_2^0(\theta, \phi) &= \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) \\
&= \sqrt{\frac{5}{16\pi}} \frac{(3z^2 - r^2)}{r^2} \\
&= \sqrt{\frac{5}{16\pi}} \frac{(2z^2 - x^2 - y^2)}{r^2} \\
&= \sqrt{\frac{5}{16\pi}} \frac{(2T_{zz} - T_{xx} - T_{yy})}{r^2}
\end{aligned}$$

So we can define various components of T_2^q tensor as follows

$$\begin{aligned}
T_2^{\pm 2} &= T_{xx} - T_{yy} \pm 2iT_{xy} \\
T_2^{\pm 1} &= \mp 2(T_{xz} \pm iT_{yz}) \\
T_2^0 &= \sqrt{\frac{2}{3}} (2T_{zz} - T_{xx} - T_{yy})
\end{aligned}$$

Additionally, we also will have to define the scalar $T_0^0 = r^2 = (x^2 + y^2 + z^2) = T_{xx} + T_{yy} + T_{zz}$, to completely determine the spherical tensors.

4. If $|nlm\rangle$ denotes an eigenfunction of the hydrogen atom (without considering its spin), and we define

$$\chi = \langle n^{'} = 3, l^{'} = 2, m^{'} = 2|xy|n = 3, l = 0, m = 0\rangle.$$

Compute, as a function of χ, the matrix elements

$$\langle n^{'} = 3, l^{'} = 2, m^{'}|T_{ij}|n = 3, l = 0, m = 0\rangle,$$

where T_{ij} is defined in the previous problem.
Soln: To solve this problem, we will be extensively using the Wigner-Eckart theorem

$$\begin{aligned}
\langle\alpha' j' m'|T_k^q|\alpha jm\rangle = \langle jkmq|jkj'm'\rangle \\
\langle\alpha' j'||T_k||\alpha j\rangle,
\end{aligned} \tag{2}$$

From the results of the previous problem

$$xy = T_{xy} = \frac{i}{4}\left(T_2^{-2} - T_2^2\right).$$

Thus

$$\chi = \langle 322|T_{xy}|300\rangle = \frac{i}{4}\langle 322|\left(T_2^{-2} - T_2^2\right)|300\rangle$$

on using the Wigner-Eckart theorem, the first term vanishes due to m selection rule

$$\chi = -\frac{i}{4}\langle 0202|0222\rangle\langle 32||T_2||30\rangle = -\frac{i}{4}\lambda. \tag{3}$$

Above we used the fact that $\langle 0202|0222\rangle = 1$, and $\lambda = \langle 32||T_2||30\rangle$ is the reduced matrix element. We obtain $\lambda = 4i\chi$. Now

$$\langle 32-2|T_{xy}|300\rangle = \frac{i}{4}\langle 32-2|\left(T_2^{-2} - T_2^2\right)|300\rangle = \frac{i}{4}\langle 32-2|T_2^{-2}|300\rangle = \frac{i}{4}\lambda = -\chi.$$

The rest of the matrix elements of T_{xy} are zero. Next, we compute T_{xz}

$$\begin{aligned}
\langle 32m^{'}|T_{xz}|300\rangle &= \frac{1}{4}\langle 32m^{'}|T_2^{-1} - T_2^1|300\rangle \\
&= \frac{1}{4}\left\{\langle 32m^{'}|T_2^{-1}|300\rangle - \langle 32m^{'}|T_2^1|300\rangle\right\} \\
&= \frac{1}{4}\left\{\langle 020-1|022m^{'}\rangle - \langle 0201|022m^{'}\rangle\right\}\langle 32||T_2||30\rangle \\
&= \frac{1}{4}\left\{\langle 020-1|022-1\rangle\delta_{m^{'}-1} - \langle 0201|0221\rangle\delta_{m^{'}1}\right\}\lambda \\
&= i\chi\left(\delta_{m^{'}-1} - \delta_{m^{'}1}\right)
\end{aligned}$$

All other matrix elements of T_{xz} vanish. For T_{yz}

$$\begin{aligned}
\langle 32m^{'}|T_{yz}|300\rangle &= \frac{i}{4}\langle 32m^{'}|T_2^{-1} + T_2^1|300\rangle \\
&= \frac{i}{4}\left\{\langle 32m^{'}|T_2^{-1}|300\rangle + \langle 32m^{'}|T_2^1|300\rangle\right\} \\
&= \frac{i}{4}\left\{\langle 020-1|022m^{'}\rangle + \langle 0201|022m^{'}\rangle\right\}\langle 32||T_2||30\rangle \\
&= \frac{i}{4}\left\{\langle 020-1|022-1\rangle\delta_{m^{'}-1} + \langle 0201|0221\rangle\delta_{m^{'}1}\right\}\lambda \\
&= -\chi\left(\delta_{m^{'}-1} + \delta_{m^{'}1}\right),
\end{aligned}$$

while rest of the components of T_{yz} vanish. Next, we compute the diagonal components.

For T_{zz}, we have

$$
\begin{aligned}
\langle 32m^{'}|T_{zz}|300\rangle &= \langle 32m^{'}|\frac{1}{3}T_0^0 + \frac{1}{\sqrt{6}}T_2^0|300\rangle \\
&= \frac{1}{3}\langle 32m^{'}|T_0^0|300\rangle + \frac{1}{\sqrt{6}}\langle 32m^{'}|T_2^0|300\rangle \\
&= \frac{1}{3}\langle 0000|002m^{'}\rangle\langle 32||T_0^0||30\rangle + \frac{1}{\sqrt{6}}\langle 0200|022m^{'}\rangle\lambda \\
&= \frac{1}{\sqrt{6}}\langle 0200|0220\rangle\lambda\delta_{m'0} \\
&= \frac{4i\chi}{\sqrt{6}}\delta_{m'0}.
\end{aligned}
$$

The first term above vanished because the CGC involved violates the triangular inequality. Rest of the matrix elements will be zero. For T_{xx}, we have

$$
\begin{aligned}
\langle 32m^{'}|T_{xx}|300\rangle &= \langle 32m^{'}|\frac{1}{3}T_0^0 - \frac{1}{2\sqrt{6}}T_2^0 + \frac{1}{4}\left(T_2^2 + T_2^{-2}\right)|300\rangle \\
&= \frac{1}{3}\langle 32m^{'}|T_0^0|300\rangle - \frac{1}{2\sqrt{6}}\langle 32m^{'}|T_2^0|300\rangle \\
&+ \frac{1}{4}\langle 32m^{'}|T_2^2|300\rangle + \frac{1}{4}\langle 32m^{'}|T_2^{-2}|300\rangle \\
&= \frac{1}{3}\langle 0000|002m^{'}\rangle\langle 32||T_0^0||30\rangle - \frac{1}{2\sqrt{6}}\langle 0200|022m^{'}\rangle\lambda \\
&+ \frac{1}{4}\langle 0202|022m^{'}\rangle\lambda + \frac{1}{4}\langle 020-2|022m^{'}\rangle\lambda \\
&= -\frac{1}{2\sqrt{6}}\lambda\delta_{m'0} + \frac{1}{4}\lambda\delta_{m'2} + \frac{1}{4}\lambda\delta_{m'-2} \\
&= i\chi\left(-\frac{2}{\sqrt{6}}\delta_{m'0} + \delta_{m'2} + \delta_{m'-2}\right).
\end{aligned}
$$

For T_{yy}

$$\begin{aligned}
\langle 32m^{'}|T_{yy}|300\rangle &= \langle 32m^{'}|\frac{1}{3}T_0^0 - \frac{1}{2\sqrt{6}}T_2^0 - \frac{1}{4}\left(T_2^2 + T_2^{-2}\right)|300\rangle \\
&= \frac{1}{3}\langle 32m^{'}|T_0^0|300\rangle - \frac{1}{2\sqrt{6}}\langle 32m^{'}|T_2^0|300\rangle \\
&- \frac{1}{4}\langle 32m^{'}|T_2^2|300\rangle - \frac{1}{4}\langle 32m^{'}|T_2^{-2}|300\rangle \\
&= \frac{1}{3}\langle 0000|002m^{'}\rangle\langle 32||T_0^0||30\rangle - \frac{1}{2\sqrt{6}}\langle 0200|022m^{'}\rangle\lambda \\
&- \frac{1}{4}\langle 0202|022m^{'}\rangle\lambda - \frac{1}{4}\langle 020-2|022m^{'}\rangle\lambda \\
&= -\frac{1}{2\sqrt{6}}\lambda\delta_{m'0} - \frac{1}{4}\lambda\delta_{m'2} - \frac{1}{4}\lambda\delta_{m'-2} \\
&= -i\chi\left(\frac{2}{\sqrt{6}}\delta_{m'0} + \delta_{m'2} + \delta_{m'-2}\right).
\end{aligned}$$

5. Directly compute the matrix elements

$$\langle j=1, m^{'}|J^q|j=1, m\rangle,$$

where J^q denotes the q-th spherical component of the angular momentum operator. Verify that these matrix elements satisfy Wigner-Eckart theorem, and deduce the corresponding reduced matrix elements from them.

Soln: (i) Let $J^q = J^0 = J_z$, then, using the fact that $J_z|jm\rangle = m\hbar|jm\rangle$, and $\langle jm'|jm\rangle = \delta_{m'm}$, we obtain

$$\langle j=1, m^{'}|J_z|j=1, m\rangle = m\hbar\delta_{m'm}. \tag{4}$$

Using Wigner-Eckart theorem, we have

$$\begin{aligned}
&\langle j=1, m^{'}|J_z|j=1, m\rangle = \langle j=1, m^{'}|J_1^0|j=1, m\rangle \\
&= \langle 11m0|111m^{'}\rangle\langle j=1||J_1|j=1\rangle \\
&= \langle 11m0|111m\rangle\lambda\delta_{mm'} \qquad ; m = 1, 0, -1,
\end{aligned} \tag{5}$$

where $\lambda = \langle j=1||J_1|j=1\rangle$ is the reduced matrix element. From the table of CGCs', we have

$$\begin{aligned}
\langle 11m0|111m\rangle &= \frac{1}{\sqrt{2}}; \quad \text{for } m = 1 \\
&= 0; \quad \text{for } m = 0 \\
&= -\frac{1}{\sqrt{2}}; \quad \text{for } m = -1 \\
&= \frac{m}{\sqrt{2}}
\end{aligned} \tag{6}$$

Substituting Eq. 6 in Eq. 5, we obtain from Wigner-Eckart theorem

$$\langle j=1,m^{'}|J_z|j=1,m\rangle = \lambda\frac{m}{\sqrt{2}}\delta_{mm'} \tag{7}$$

On comparing Eqs. 4 and 7, we conclude that the two equations agree with each other if the reduced matrix element is given by $\lambda = \hbar\sqrt{2}$. Let us check this for the other two spherical components. First by Wigner-Eckart theorem

$$\begin{aligned}
\langle j=1,m^{'}|J_1^{\pm1}|j=1,m\rangle &= \langle 11m\pm1|111m^{'}\rangle\langle j=1||J_1|j=1\rangle \\
&= \langle 11m\pm1|111m^{'}\rangle\lambda \\
&= \langle 1,1,m,\pm1|1,1,1,m\pm1\rangle\lambda\delta_{m'm\pm1} \\
\Longrightarrow \langle j=1,m^{'}|J_1^{1}|j=1,m\rangle &= 0 \qquad \text{for } m=1 \\
&= -\frac{1}{\sqrt{2}}\lambda\delta_{m'm+1} \quad m=0,-1 \\
\text{and} \\
\langle j=1,m^{'}|J_1^{-1}|j=1,m\rangle &= 0 \qquad \text{for } m=-1 \\
&= \frac{1}{\sqrt{2}}\lambda\delta_{m'm+1} \quad m=0,1
\end{aligned}$$

Evaluating the same matrix element directly

$$\begin{aligned}
\langle j=1,m^{'}|J_1^{\pm1}|j=1,m\rangle &= \mp\frac{1}{\sqrt{2}}\langle j=1,m^{'}|J_{\pm}|j=1,m\rangle \\
&= \mp\frac{1}{\sqrt{2}}\sqrt{(1\mp m)(2\pm m)}\hbar\delta_{m'm\pm1} \\
\Longrightarrow \langle j=1,m^{'}|J_1^{1}|j=1,m\rangle &= 0 \text{ for } m=1 \\
&= -\hbar\delta_{m'm+1} \quad m=0,-1 \\
\text{and} \\
\langle j=1,m^{'}|J_1^{-1}|j=1,m\rangle &= 0 \text{ for } m=-1 \\
&= \hbar\delta_{m'm-1} \text{ for } m=0,1
\end{aligned}$$

Both sets of values are consistent with each other and the fact that $\lambda = \hbar\sqrt{2}$. Thus, these matrix elements are consistent with Wigner-Eckart theorem.

6. Evaluate

$$\sum_{m=-j}^{j} |D_{mm'}^{(j)}(\beta)|^2 m$$

for any j (integer or half-integer), then check your answer for $j=\frac{1}{2}$.

Soln: We can write

$$\sum_{m=-j}^{j} |D^{(j)}_{mm'}(\beta)|^2 m = \sum_{m=-j}^{j} D^{(j)*}_{mm'}(\beta) D^{(j)}_{mm'}(\beta) m$$

$$= \sum_{m=-j}^{j} D^{(j)\dagger}_{m'm}(\beta) D^{(j)}_{mm'}(\beta) m.$$

using the definition $D^{(j)}_{mm'}(\beta) = \langle jm|e^{-\frac{iJ_y\beta}{\hbar}}|jm'\rangle,$ we have

$$= \sum_{m=-j}^{j} \langle jm'|e^{\frac{iJ_y\beta}{\hbar}} m|jm\rangle\langle jm|e^{-\frac{iJ_y\beta}{\hbar}}|jm'\rangle$$

using $J_z|jm\rangle = m\hbar|jm\rangle,$ we have

$$\frac{1}{\hbar}\sum_{m=-j}^{j} \langle jm'|e^{\frac{iJ_y\beta}{\hbar}} J_z|jm\rangle\langle jm|e^{-\frac{iJ_y\beta}{\hbar}}|jm'\rangle,$$

using resolution of identity $\sum_{m=-j}^{j} |jm\rangle\langle jm| = I,$ we obtain

$$\frac{1}{\hbar}\langle jm'|e^{\frac{iJ_y\beta}{\hbar}} J_z e^{-\frac{iJ_y\beta}{\hbar}}|jm'\rangle.$$

Given the fact that operation $e^{\frac{iJ_y\beta}{\hbar}} J_z e^{-\frac{iJ_y\beta}{\hbar}}$ represents a rotation by angle β about the $y-$axis, we will have $e^{\frac{iJ_y\beta}{\hbar}} J_z e^{-\frac{iJ_y\beta}{\hbar}} = J_z\cos\beta - J_x\sin\beta$, so that

$$\sum_{m=-j}^{j} |D^{(j)}_{mm'}(\beta)|^2 m = \frac{1}{\hbar}\langle jm'|J_z\cos\beta - J_x\sin\beta|jm'\rangle$$

$$= m'\cos\beta.$$

Above we used $\langle jm'|J_z|jm'\rangle = m'\hbar$ and $\langle jm'|J_x|jm'\rangle = 0$. Let us verify this for $j = \frac{1}{2}$, for which

$$D^{(\frac{1}{2})}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}.$$

With this we have for $m' = \frac{1}{2}$

$$\sum_{m=-j}^{j} |D^{(j)}_{mm'}(\beta)|^2 m = \frac{1}{2}\cos^2\frac{\beta}{2} - \frac{1}{2}\sin^2\frac{\beta}{2} = \frac{1}{2}\cos\beta,$$

and for $m' = -\frac{1}{2}$

$$\sum_{m=-j}^{j} |D^{(j)}_{mm'}(\beta)|^2 m = \frac{1}{2}\sin^2\frac{\beta}{2} - \frac{1}{2}\cos^2\frac{\beta}{2} = -\frac{1}{2}\cos\beta.$$

Thus the result has been verified

7. Prove the following results for $j = 1$, using the corresponding representation of J_y

(a)

$$e^{-\frac{iJ_y\beta}{\hbar}} = I - i\left(\frac{J_y}{\hbar}\right)\sin\beta - \left(\frac{J_y}{\hbar}\right)^2(1-\cos\beta)$$

Soln: Using the expressions for the matrix elements of the ladder operators $J_\pm$

$$\langle jm'|J_\pm|jm\rangle = \sqrt{(j\mp m)(j\pm m+1)}\hbar\delta_{m',m\pm1},$$

and then

$$J_x = \frac{1}{2}(J_+ + J_-)$$
$$J_y = \frac{1}{2i}(J_+ - J_-),$$

along with the fact that $j = 1$ and $m = 0, \pm 1$, we obtain

$$J_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

For even powers of J_y we have

$$J_y^2 = \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} = \frac{h^2}{2}A$$

It is easy to verify that

$$A^2 = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}^2 = 2\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix} = 2A$$

$$\implies J_y^4 = \left(\frac{\hbar^2}{2}\right)^2 A^2 = \left(\frac{\hbar^2}{2}\right)^2 2A = \hbar^2 J_y^2$$

$$\implies J_y^6 = J_y^4 J_y^2 = \hbar^2 J_y^2 J_y^2 = \hbar^2 J_y^4 = \hbar^4 J_y^2$$

$$\implies J_y^{2m} = \hbar^{2m-2} J_y^2 \tag{8}$$

For odd powers of J_y

$$J_y^3 = \left(\frac{\hbar}{\sqrt{2}}\right)^3 \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}^3 = \left(\frac{\hbar}{\sqrt{2}}\right)^3 2\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \hbar^2 J_y$$

$$\implies J_y^5 = J_y^3 J_y^2 = \hbar^2 J_y^3 = \hbar^4 J_y$$

$$\implies J_y^{2m+1} = \hbar^{2m} J_y. \tag{9}$$

Now

$$e^{-i\frac{J_y\beta}{\hbar}} = \sum_{n=0}^{\infty}\left(-i\frac{J_y\beta}{n!\hbar}\right)^n$$
$$= I + \sum_{m=0}^{\infty}\frac{(-i\beta)^{2m+1}}{(2m+1)!}\frac{J_y^{2m+1}}{\hbar^{2m+1}} + \sum_{m=1}^{\infty}\frac{(-i\beta)^{2m}}{(2m)!}\frac{J_y^{2m}}{\hbar^{2m}}$$

Using equations 8 and 9 along with $(-i)^{2m} = (-1)^m$, we obtain

$$e^{-i\frac{J_y\beta}{\hbar}} = I - i\left(\beta - \frac{\beta^3}{3!} + \frac{\beta^5}{5!} + \cdots\right)\left(\frac{J_y}{\hbar}\right) - \left(\frac{\beta^2}{2!} - \frac{\beta^4}{4!} + \frac{\beta^6}{6!}\cdots\right)\left(\frac{J_y}{\hbar}\right)^2$$
$$= I - i\sin\beta\left(\frac{J_y}{\hbar}\right) - (1-\cos\beta)\left(\frac{J_y}{\hbar}\right)^2$$

(b) **Soln:** On the RHS of the equation

$$e^{-i\frac{J_y\beta}{\hbar}} = I - i\sin\beta\left(\frac{J_y}{\hbar}\right) - (1-\cos\beta)\left(\frac{J_y}{\hbar}\right)^2,$$

we substitute

$$1 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\frac{J_y}{\hbar} \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$
$$\left(\frac{J_y}{\hbar}\right)^2 \equiv \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

to obtain the desired result

$$D^{(j=1)}(\beta) = \begin{pmatrix} \left(\frac{1}{2}\right)(1+\cos\beta) & -\left(\frac{1}{\sqrt{2}}\right)\sin\beta & \left(\frac{1}{2}\right)(1-\cos\beta) \\ \left(\frac{1}{\sqrt{2}}\right)\sin\beta & \cos\beta & -\left(\frac{1}{\sqrt{2}}\right)\sin\beta \\ \left(\frac{1}{2}\right)(1-\cos\beta) & \left(\frac{1}{\sqrt{2}}\right)\sin\beta & \left(\frac{1}{2}\right)(1+\cos\beta) \end{pmatrix}$$

8. Consider a spherical tensor of rank 1 (that is, a vector)

$$V_1^{\pm 1} = \mp\frac{V_x \pm iV_y}{\sqrt{2}}, \qquad V_1^0 = V_z.$$

Using the expression for $D^{(j=1)}(\beta)$ given in the previous problem, evaluate

$$\sum_{q'} D^{(1)}_{qq'}(\beta)V_1^{q'},$$

and show that your results are just what you expect from the transformation properties of $V_{x,y,z}$, under rotation about the y-axis.
Soln: Let

$$\mathbf{V} = \begin{pmatrix} -\frac{V_x+iV_y}{\sqrt{2}} \\ V_z \\ \frac{V_x-iV_y}{\sqrt{2}} \end{pmatrix},$$

then expression $\sum_{q'} D^{(1)}_{qq'}(\beta)V_1^{q'}$ implies matrix multiplication of the column vector $\mathbf{V}$ by $D^{(1)}(\beta)$ matrix of the previous problem

$$\begin{pmatrix} \left(\frac{1}{2}\right)(1+\cos\beta) & -\left(\frac{1}{\sqrt{2}}\right)\sin\beta & \left(\frac{1}{2}\right)(1-\cos\beta) \\ \left(\frac{1}{\sqrt{2}}\right)\sin\beta & \cos\beta & -\left(\frac{1}{\sqrt{2}}\right)\sin\beta \\ \left(\frac{1}{2}\right)(1-\cos\beta) & \left(\frac{1}{\sqrt{2}}\right)\sin\beta & \left(\frac{1}{2}\right)(1+\cos\beta) \end{pmatrix} \begin{pmatrix} -\frac{V_x+iV_y}{\sqrt{2}} \\ V_z \\ \frac{V_x-iV_y}{\sqrt{2}} \end{pmatrix}$$
$$= \begin{pmatrix} -\frac{(V_x\cos\beta+V_z\sin\beta)+iV_y}{\sqrt{2}} \\ V_z\cos\beta - V_x\sin\beta \\ \frac{(V_x\cos\beta+V_z\sin\beta)-iV_y}{\sqrt{2}} \end{pmatrix}.$$

From the RHS it is obvious that under the transformation

$$\begin{aligned} V_x &\to V_x^{'} = V_x\cos\beta + V_z\sin\beta \\ V_y &\to V_y^{'} = V_y \\ V_z &\to V_z^{'} = V_z\cos\beta - V_x\sin\beta, \end{aligned}$$

which can be written as

$$\begin{pmatrix} V_x^{'} \\ V_y^{'} \\ V_z^{'} \end{pmatrix} = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}.$$

This is precisely how the Cartesian components of a vector will transform under a rotation by angle β about the y axis.

9. (a) Construct a spherical tensor of rank 1 out of two different vectors $\mathbf{U} = (U_x, U_y, U_z)$ and $\mathbf{V} = (V_x, V_y, V_z)$. Explicitly write $T_1^{\pm1,0}$, in terms of $U_{x,y,z}$ and $V_{x,y,z}$.
Soln: A vector which is bilinear in $\mathbf{U}$ and $\mathbf{V}$ the cross product of two vectors

$$\begin{aligned} \mathbf{W} &= \mathbf{U}\times\mathbf{V} \\ &= (U_yV_z - U_zV_y)\hat{\imath} + (U_zV_x - U_xV_z)\hat{\jmath} + (U_xV_y - U_yV_x)\hat{k} \\ &= W_x\hat{\imath} + W_y\hat{\jmath} + W_z\hat{k}. \end{aligned}$$

Spherical vector components will be

$$T_1^{\pm 1} = \mp \frac{(W_x \pm iW_y)}{\sqrt{2}}$$
$$= \mp \frac{(U_y V_z - U_z V_y) \pm i(U_z V_x - U_x V_z)}{\sqrt{2}}$$

and

$$T_1^0 = W_z = (U_x V_y - U_y V_x)$$

(b) Construct a spherical tensor of rank 2 out of two different vectors **U** and **V**. Write down explicitly $T_2^{\pm 2, \pm 1, 0}$, in terms of $U_{x,y,z}$ and $V_{x,y,z}$.
Soln: Defining $U_1^{\pm 1} = \mp \frac{(U_x \pm iU_y)}{\sqrt{2}}$, $U_1^0 = U_z$, $V_1^{\pm 1} = \mp \frac{(V_x \pm iV_y)}{\sqrt{2}}$, $V_1^0 = V_z$, we have

$$T_2^{\pm 2} = U^{\pm 1} V^{\pm 1}$$
$$T_2^{\pm 1} = \frac{U^{\pm 1} V^0 + U^0 V^{\pm 1}}{\sqrt{2}}$$
$$T_2^0 = \frac{U^{+1} V^{-1} + U^{-1} V^{+1} + 2U^0 V^0}{\sqrt{6}}$$

The expressions in terms of $U_{x,y,z}$ and $V_{x,y,z}$ can be obtained by substituting the expressions for the components of spherical vectors U_1^q and V_1^q given above.

10. Consider a spinless particle bound to a fixed center by a central force potential.

(a) Relate, as much as possible, the matrix elements

$$\langle n', l', m' | \mp \frac{1}{\sqrt{2}} (x \pm iy) | n, l, m \rangle \qquad \text{and } \langle n', l', m' | z | n, l, m \rangle$$

using only the Wigner-Eckart theorem. Make sure to state under what conditions the matrix elements are nonvanishing.
Soln: Let $X_1^{\pm 1} = \mp \frac{1}{\sqrt{2}} (x \pm iy)$ and $X_1^0 = z$, then using Wigner-Eckart theorem we have

$$\langle n', l', m' | - \frac{1}{\sqrt{2}} (x + iy) | n, l, m \rangle = \langle n', l', m' | X_1^1 | n, l, m \rangle = \langle l1m1 | l1l'm' \rangle \langle n'l' || X_1 | nl \rangle$$
$$\langle n', l', m' | \frac{1}{\sqrt{2}} (x - iy) | n, l, m \rangle = \langle n', l', m' | X_1^{-1} | n, l, m \rangle = \langle l1m-1 | l1l'm' \rangle \langle n'l' || X_1 | nl \rangle$$
$$\langle n', l', m' | z | n, l, m \rangle = \langle n', l', m' | X_1^0 | n, l, m \rangle = \langle l1m0 | l1l'm' \rangle \langle n'l' || X_1 | nl \rangle$$

Thus it is obvious that all the three matrix elements are proportional to the same reduced matrix element $\langle n'l' || X_1 | nl \rangle$. Additionally, in all the three cases the selection rule $|l - 1| \leq l' \leq l + 1$. Must be satisfied. However, m selection rules are different. They are: (a) $m' = m + 1$, (b) $m' = m - 1$, and (c) $m' = m$, respectively.

(b) Do the same problem using the wave function $\psi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_l^m(\theta, \phi)$.
Soln: We know

$$\langle n^{'}, l^{'}, m^{'}|X_1^q|n, l, m\rangle = \int d^3\mathbf{r}\psi^*_{n^{'}l^{'}m^{'}}(\mathbf{r})X_1^q\psi_{nlm}(\mathbf{r}).$$

On substituting the values of the wave functions, and using the fact that $X_1^q = \sqrt{\frac{4\pi}{3}}rY_1^q(\Omega)$, in spherical polar coordinates we obtain

$$\langle n^{'}, l^{'}, m^{'}|X_1^q|n, l, m\rangle = \left\{\sqrt{\frac{4\pi}{3}}\int_0^\infty r^3R^*_{n^{'}l^{'}}(r)R_{nl}(r)dr\right\}\left\{\int Y_{l^{'}}^{m^{'}*}(\Omega)Y_1^q(\Omega)Y_l^m(\Omega)d\Omega\right\}$$

In Eq. (17.74) of Merzbacher, the relevant angular integral is given

$$\int Y_{l_3}^{m_3*}(\Omega)Y_{l_2}^{m_2}(\Omega)Y_{l_1}^{m_1}(\Omega)d\Omega = N_{l_1l_2l_3}\langle l_1l_2m_1m_2|l_1l_2l_3m_3\rangle$$

$$\text{where } N_{l_1l_2l_3} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}}\langle l_1l_200|l_1l_2l_30\rangle.$$

Using this we get

$$\langle n^{'}, l^{'}, m^{'}|X_1^q|n, l, m\rangle = \langle l1mq|l1l^{'}m^{'}\rangle\left\{N_{l1l^{'}}\sqrt{\frac{4\pi}{3}}\int_0^\infty r^3R^*_{n^{'}l^{'}}(r)R_{nl}(r)dr\right\},$$

which is exactly of the same form as derived in part (a), using Wigner-Eckart theorem, with the reduced matrix element given by

$$\langle n^{'}l^{'}||X_1|nl\rangle = N_{l1l^{'}}\sqrt{\frac{4\pi}{3}}\int_0^\infty r^3R^*_{n^{'}l^{'}}(r)R_{nl}(r)dr.$$

11. (a) Write xy, xz, and $(x^2 - y^2)$ as components of a spherical (irreducible) tensor of rank 2.

(b) The expectation value

$$Q \equiv e\langle\alpha, j, m = j|(3z^2 - r^2)|\alpha, j, m = j\rangle$$

is known as *quadrupole moment.* Evaluate

$$e\langle\alpha, j, m^{'}|(x^2 - y^2)|\alpha, j, m = j\rangle,$$

(where $m^{'} = j, j-1, j-2, \ldots$) in terms of Q and appropriate C-G coefficients.

Soln: Both parts (a) and (b) of this problem are similar to problem 4, and can be solved using the same approach.

12. The magnetic moment of an atom is defined as

$$\boldsymbol{\mu} = -\frac{e}{2mc}\left(g_L\mathbf{L} + g_S\mathbf{S}\right),$$

where e is the electronic charge, m is the electronic mass, c is the speed of light, $\mathbf{L}$ is the total orbital angular momentum operator for the atom, $\mathbf{S}$ is total spin angular momentum operator of the atom, and g_L and g_S are, respectively, orbital and spin Lande g factors.

(a) Argue that the expectation value components $\langle\mu_i\rangle = \langle\alpha jj|\mu_i|\alpha jj\rangle$, are proportional to each other, where i denotes a Cartesian component

Soln: We know that the spherical components of $\boldsymbol{\mu}$ in terms of its Cartesian components are

$$\begin{aligned} \mu_1^{\pm 1} &= \mp\frac{(\mu_x \pm i\mu_y)}{\sqrt{2}} \\ \mu_1^0 &= \mu_z. \end{aligned} \tag{10}$$

From Wigner-Eckart theorem we have

$$\langle\alpha jj|\mu_1^q|\alpha jj\rangle = \langle j1jq|j1jj\rangle\langle\alpha j||\mu||\alpha j\rangle, \tag{11}$$

where $\langle\alpha j||\mu||\alpha j\rangle$ denotes the reduced matrix element $\langle\alpha j||\mu_1||\alpha j\rangle$. Thus, the expectation values of all the spherical components of μ_1^q is be proportional to the same reduced matrix element $\langle\alpha j||\mu||\alpha j\rangle$. Using Eq. 10, we can write the Cartesian components of $\boldsymbol{\mu}$ in terms of its spherical components

$$\begin{aligned} \mu_x &= -\tfrac{1}{\sqrt{2}}(\mu_1^1 - \mu_1^{-1}) \\ \mu_y &= \tfrac{i}{\sqrt{2}}(\mu_1^1 + \mu_1^{-1}) \\ \mu_z &= \mu_1^0 \end{aligned} \tag{12}$$

Using Eqs. 12 and 11, we conclude that various Cartesian components of $\langle\mu_i\rangle = \langle\alpha jj|\mu_i|\alpha jj\rangle$, are proportional to the same reduced matrix elements

$$\begin{aligned} \langle\mu_x\rangle &\propto \langle\alpha j||\mu||\alpha j\rangle \\ \langle\mu_y\rangle &\propto \langle\alpha j||\mu||\alpha j\rangle \\ \langle\mu_z\rangle &\propto \langle\alpha j||\mu||\alpha j\rangle, \end{aligned}$$

which is the desired result.

(b) Using the projection theorem, prove that if $g_L = 1$ and $g_S = 2$, $\mu = \langle\mu_z\rangle$ is given by

$$\mu = -\frac{e\hbar}{2mc}g_J J,$$

where

$$g_J = \left\{1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right\},$$

and S, L, and J, respectively denote the total spin, orbital angular momentum, and total angular momentum of the atom.
Soln: For $g_L = 1$ and $g_S = 2$, we have

$$\boldsymbol{\mu} = -\frac{e}{2mc}(\mathbf{L} + 2\mathbf{S}) = -\frac{e}{2mc}(\mathbf{J} + \mathbf{S}),$$

where $\mathbf{J} = \mathbf{L} + \mathbf{S}$, is the total angular momentum operator. The projection theorem for a spherical vector operator A^q (see Eq. 108 of chapter 1) is given by

$$\langle \alpha' jm' | A^q | \alpha jm \rangle = \frac{\langle \alpha' jm | \mathbf{J} \cdot \mathbf{A} | \alpha jm \rangle}{j(j+1)\hbar^2} \times \langle jm' | J^q | jm \rangle \tag{13}$$

Using this for $\mathbf{A} = \boldsymbol{\mu}$, and $q = 0$ (note that $A^0 = A_z$), we obtain

$$\mu = \langle \alpha jj | \mu_z | \alpha jj \rangle = \frac{\langle \alpha jj | \boldsymbol{\mu} \cdot \mathbf{J} | \alpha jj \rangle}{\hbar^2 J(J+1)} \langle jj | J_z | jj \rangle.$$

Above

$$\langle jj | J_z | jj \rangle = j\hbar,$$

and

$$\begin{aligned}
\boldsymbol{\mu} \cdot \mathbf{J} &= -\frac{e}{2mc}\left(\mathbf{J}^2 + \mathbf{S} \cdot \mathbf{J}\right) \\
\mathbf{S} \cdot \mathbf{J} &= \mathbf{S}^2 + \mathbf{L} \cdot \mathbf{S} \\
\mathbf{L} \cdot \mathbf{S} &= \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \\
\implies \boldsymbol{\mu} \cdot \mathbf{J} &= -\frac{e}{2mc}(\frac{3}{2}\mathbf{J}^2 + \frac{1}{2}\mathbf{S}^2 - \frac{1}{2}\mathbf{L}^2)
\end{aligned}$$

Using the fact that

$$\begin{aligned}
\mathbf{J}^2 | \alpha jj \rangle &= J(J+1)\hbar^2 | \alpha jj \rangle \\
\mathbf{S}^2 | \alpha jj \rangle &= S(S+1)\hbar^2 | \alpha jj \rangle \\
\mathbf{L}^2 | \alpha jj \rangle &= L(L+1)\hbar^2 | \alpha jj \rangle,
\end{aligned}$$

we have

$$\begin{aligned}
\langle \alpha jj | \boldsymbol{\mu} \cdot \mathbf{J} | \alpha jj \rangle &= -\frac{e}{2mc}(\frac{3}{2}J(J+1) + \frac{1}{2}S(S+1) - \frac{1}{2}L(L+1))\hbar^2 \\
\implies \mu = \langle \alpha jj | \mu_z | \alpha jj \rangle &= -\frac{e\hbar}{2mc} \frac{\left\{\frac{3}{2}J(J+1) + \frac{1}{2}S(S+1) - \frac{1}{2}L(L+1)\right\}}{J(J+1)} J \\
&= -\frac{e\hbar}{2mc}\left\{1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right\} J \\
\implies g_J &= \left\{1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right\}
\end{aligned}$$