Solutions:
Homework Set 10

Due November 6, 2020

1. (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 $T^{(1)}_{\pm 1,0}$ in terms of $U_{x,y,z}$ and $V_{x,y,z}$.

One can construct a spherical tensor out of products of other spherical tensors according to

$$T^k_q = \sum_{q_1,q_2} X^{k_1}_{q_1} Y^{k_1}_{q_1} \langle k_1 q_1; k_2 q_2 | kq \rangle \tag{1}$$

In this case we have two rank-1 tensors, which can be written in the spherical basis as

$$U_0 = U_z, \quad V_0 = V_z \tag{2}$$

$$U_\pm = \mp \frac{1}{\sqrt{2}}(U_x \pm iU_y), \quad V_\pm = \mp \frac{1}{\sqrt{2}}(V_x \pm iV_y) \tag{3}$$

The simplest spherical tensor made from U and V is a simple product (note that one can also make more complicated tensors from higher order products UUV, $UUVV$, etc.):

$$T^k_q = \sum_{q_1 q_2} U_{q_1} V_{q_2} \langle 1 q_1; 1 q_2 | kq \rangle, \tag{4}$$

recalling that the only non-zero terms in the sum have $q_1 + q_2 = q$.

For $k = 1$:

$$T_{\pm 1}^{1} = \sum_{q_1} U_{q_1} V_{q_1 \pm 1} \langle 1 q_1; 1, q_1 \pm 1 | 1, \pm 1 \rangle \tag{5}$$

$$= U_{\pm 1} V_0 \langle 1, \pm 1; 1, 0 | 1, \pm 1 \rangle + U_0 V_{\pm 1} \langle 1, 0; 1, \pm 1 | 1, \pm 1 \rangle \tag{6}$$

$$= \pm \frac{1}{\sqrt{2}} \left(U_{\pm 1} V_0 - U_0 V_{\pm 1} \right) \tag{7}$$

and

$$T_0^1 = \sum_{q_1} U_{q_1} V_{-q_1} \langle 1 q_1; 1, -q_1 | 1, \pm 1 \rangle \tag{8}$$

$$= U_1 V_{-1} \langle 1, 1; 1, -1 | 1, 0 \rangle + U_{-1} V_1 \langle 1, -1; 1, 1 | 1, 0 \rangle \tag{9}$$

$$= \frac{1}{\sqrt{2}} \left(U_1 V_{-1} - U_{-1} V_1 \right) \tag{10}$$

Written in terms of Cartesian components, we have:

$$T_{\pm 1}^{1} = \frac{1}{2} \Big\{ (U_x \pm i U_y) V_z - U_z (V_x \pm i V_y) \Big\} \tag{11}$$

$$T_0^1 = -\frac{1}{2\sqrt{2}} \Big\{ (U_x + i U_y)(V_x - i V_y) - (U_x - i U_y)(V_x + i V_y) \Big\} \tag{12}$$

$$= \frac{i}{\sqrt{2}} \Big\{ U_x V_y - U_y V_x \Big\} \tag{13}$$

(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 $V_{x,y,z}$.

For $k = 2$ we have

$$T_q^2 = \sum_{q_1} U_{q_1} V_{q - q_1} \langle 1 q_1; 1, q - q_1 | 2 q \rangle \tag{14}$$

and for each component q:

$$T^2_{\pm 2} = U_{\pm 1}V_{\pm 1} \tag{15}$$

$$T^2_{\pm 1} = \frac{1}{\sqrt{2}}\Big(U_{\pm 1}V_0 + U_0V_{\pm 1}\Big) \tag{16}$$

$$T^2_0 = \frac{1}{\sqrt{6}}\Big(U_1V_{-1} + 4U_0V_0 + U_{-1}V_1\Big). \tag{17}$$

In terms of Cartesian tensors:

$$T^2_{\pm 2} = \frac{1}{2}(U_x \pm iU_y)(V_x \pm iV_y) \tag{18}$$

$$T^2_{\pm 1} = \mp\frac{1}{2}\Big((U_x \pm iU_y)V_z + U_z(V_x \pm iV_y)\Big) \tag{19}$$

$$T^2_0 = -\frac{1}{2\sqrt{6}}\Big((U_x + iU_y)(V_x - iV_y) - 4U_zV_z + (U_x - iU_y)(V_x + iV_y)\Big) \tag{20}$$

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

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

$$\langle n', l', m'| \mp \frac{1}{\sqrt{2}}(x \pm iy)|n, l, m\rangle \tag{21}$$

and

$$\langle n', l', m'|z|n, l, m\rangle \tag{22}$$

using *only* the Wigner-Eckart theorem. Make sure to state under what conditions the matrix elements are nonvanishing.

These quantities are matrix elements of a rank-1 spherical tensor operator

$$\langle n', l', m'|T^k_q|n, l, m\rangle \tag{23}$$

with $k = 1$ and

$$T_0^{(1)} = z \tag{24}$$

$$T_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}}(x \pm iy) \tag{25}$$

The Wigner-Eckart theorem says

$$\langle n', l', m' | T_q^{(1)} | n, l, m \rangle = \langle n' l' || T^{(1)} || nl \rangle \langle l' m' | lm; 1q \rangle \tag{26}$$

From the Clebsch-Gordan coefficient on the right, we can use the selection rules to note that the matrix element is nonzero only when $m' = m + q$ and $l' = |l \pm 1|$ or $l' = l$.

We haven't yet discussed discrete symmetries, but the operator $T_q^{(1)}$ is odd under parity (a reflection through the origin, $x \to -x, y \to -1, z \to -z$), $\pi^{-1} T_q^{(1)} \pi = -T_q^{(1)}$. The kets are also eigenstates of parity

$$\pi | n, l, m \rangle = (-1)^l | n, l, m \rangle \tag{27}$$

Using this information, we can determine that the matrix element vanishes unless the bra and ket have opposite parity, and so we know the $l' = l$ matrix elements actually vanish.

Since the reduced matrix element does not depend on m or m', it cancels in ratios of the form

$$\frac{\langle n', l', m'_1 | T_{q_1}^{(1)} | n, l, m_1 \rangle}{\langle n', l', m'_2 | T_{q_2}^{(1)} | n, l, m_2 \rangle} = \frac{\langle l' m'_1 | lm; 1q_1 \rangle}{\langle l' m'_2 | lm; 1q_2 \rangle} \tag{28}$$

(b) Do the same problem using wave functions

$$\psi(\mathbf{x}) = R_{nl}(r) Y_l^m(\theta, \phi) \tag{29}$$

In configuration space, note that

$$T_q^{(1)}(\mathbf{x}) \equiv \langle \mathbf{x} | T_q^{(1)} | \mathbf{x} \rangle = r \sqrt{\frac{4\pi}{3}} Y_1^q \tag{30}$$

With these wavefunctions, the matrix elements become

$$\langle n', l', m' | T_q^{(1)} | n, l, m \rangle = \int d^3x R_{n'l'}^*(r) R_{nl}(r) Y_{l'}^{m'*}(\Omega) Y_l^m(\Omega) T_q^{(1)}(\mathbf{x}) \tag{31}$$

$$= \sqrt{\frac{4\pi}{3}} \int dr r^3 R_{n'l'}^*(r) R_{nl}(r) \int d\Omega Y_{l'}^{m'*} Y_l^m Y_1^q \tag{32}$$

The angular integral can be related to Clebsch-Gordan coefficients using the identity

$$\int d\Omega Y_l^{m*} Y_{l_1}^{m_1} Y_{l_2}^{m_2} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \langle lm | l_1 m_1; l_2 m_2 \rangle \langle l_1 0; l_2 0 | l 0 \rangle \tag{33}$$

$$\implies \int d\Omega Y_{l'}^{m'*} Y_l^m Y_1^q = \sqrt{\frac{(2l+1)(2+1)}{4\pi(2l'+1)}} \langle l'm' | lm; 1q \rangle \langle l0; 10 | l'0 \rangle \tag{34}$$

The first Clebsch-Gordan coefficient makes it clear that non-zero matrix elements must have $m' = m + q$, which we can also see directly

$$\int d\phi Y_l^{m*} Y_{l_1}^{m_1} Y_{l_2}^{m_2} \propto \int d\phi e^{i(m+q-m')}, \tag{35}$$

and also that we must have $l' = |l \pm 1|, l$.

The second Clebsch-Gordan coefficient makes it clear that $l' = l$ is not allowed.

Again we can consider the ratio

$$\frac{\langle n', l', m_1' | T_{q_1}^{(1)} | n, l, m_1 \rangle}{\langle n', l', m_2' | T_{q_2}^{(1)} | n, l, m_2 \rangle} = \frac{\langle l'm_1' | lm; 1q_1 \rangle}{\langle l'm_2' | lm; 1q_2 \rangle}, \tag{36}$$

in agreement with the previous result.

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

We can create a spherical tensor of rank 2 from the position vector $\mathbf{x}$ by first writing the vector in a spherical basis

$$X_0 = z \tag{37}$$

$$X_{\pm 1} = \mp \frac{1}{\sqrt{2}}(x \pm iy), \tag{38}$$

and using the decomposition formula

$$T_q^k = \sum_{q_1,q_2} X_{q_1}^{k_1} Y_{q_1}^{k_1} \langle k_1 q_1; k_2 q_2 | kq \rangle \tag{39}$$

$$\implies T_q^{(2)} = \sum_{q_1,q_2} X_{q_1} X_{q_1} \langle 1 q_1; 1 q_2 | 2q \rangle \tag{40}$$

So we have (see the results from problem 1b)

$$T_{\pm 2}^{(2)} = X_{\pm 1}^2 = \frac{1}{2}(x \pm iy)^2 = \frac{1}{2}x^2 - \frac{1}{2}y^2 \pm 2ixy \tag{41}$$

$$\implies x^2 - y^2 = T_2^{(2)} + T_{-2}^{(2)} \tag{42}$$

$$xy = \frac{1}{4i}\left[T_2^{(2)} - T_{-2}^{(2)}\right] \tag{43}$$

$$\tag{44}$$

$$T_{\pm 1}^{(2)} = \mp 2(x \pm iy)z = \mp 2xz + 2yz \tag{45}$$

$$\implies xz = \frac{-1}{4}\left[T_1^{(2)} - T_{-1}^{(2)}\right] \tag{46}$$

(b) The expectation value

$$Q \equiv e\langle \alpha, j, m = j | (3z^2 - r^2) | \alpha, j, m = j \rangle \tag{47}$$

is known as the *quadrupole moment*. Evaluate

$$e\langle \alpha, j, m' | (x^2 - y^2) | \alpha, j, m = j \rangle \tag{48}$$

where $m' = j, j-1, j-2, \ldots$, in terms of Q and appropriate Clebsch-Gordan coefficients

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The last component of the $k = 2$ tensor is

$$T_0^{(2)} = -\frac{1}{\sqrt{6}}\Big((x+iy)(x-iy) - 2z^2\Big) = \frac{1}{\sqrt{6}}\Big(3z^2 - r^2\Big) \tag{49}$$

so in terms of the spherical tensor,

$$Q = \frac{e}{\sqrt{6}} \langle \alpha, j, j | T_0^{(2)} | \alpha, j, j \rangle \tag{50}$$

and the matrix element we want to obtain is

$$e\langle \alpha, j, m' | (x^2 - y^2) | \alpha, j, j \rangle = e\langle \alpha, j, m' | \left[T_2^{(2)} + T_{-2}^{(2)} \right] | \alpha, j, j \rangle \tag{51}$$

We can use the Wigner-Eckart theorem to relate both of these to the same reduced matrix element.

$$\langle n', l', m' | T_q^{(2)} | n, l, m \rangle = \langle n'l' || T^{(2)} || nl \rangle \langle l'm' | lm; 2q \rangle \tag{52}$$

$$\implies Q = \frac{e}{\sqrt{6}} \langle \alpha, j, j | T_0^{(2)} | \alpha, j, j \rangle = \frac{e}{\sqrt{6}} \langle \alpha j || T^{(2)} || \alpha j \rangle \langle jj | jj; 20 \rangle \tag{53}$$

$$\implies \langle \alpha j || T^{(2)} || \alpha j \rangle = \frac{Q\sqrt{6}}{e \langle jj | jj; 20 \rangle} \tag{54}$$

and so the matrix element in terms of Q is

$$e\langle \alpha, j, m' | \left[T_2^{(2)} + T_{-2}^{(2)} \right] | \alpha, j, j \rangle = e\langle \alpha j || T^{(2)} || \alpha j \rangle \left[\langle jm' | jj; 22 \rangle + \langle jm' | jj; 2, -2 \rangle \right] \tag{55}$$

$$= \frac{Q\sqrt{6}}{\langle jj | jj; 20 \rangle} \left[\langle jm' | jj; 22 \rangle + \langle jm' | jj; 2, -2 \rangle \right] \tag{56}$$

$$= Q 2\sqrt{6} \frac{\langle jm' | jj; 22 \rangle}{\langle jj | jj; 20 \rangle} \tag{57}$$