Physics 741 – Graduate Quantum Mechanics 1

Solution Set U

1. [20] Our goal in this problem is to find every non-vanishing matrix element for Hydrogen of the form

$$\langle 41m|\mathbf{Q}|42m'\rangle\,;$$

that is, all matrix elements between 4d and 2p states.

(a) [4] Find the matrix element $\langle 410|Q_0|420\rangle$. It may be helpful to use the Maple routines that I have put online that allow you to calculate the radial integrals efficiently.

The matrix element in question is

$$\langle 410|Q_0|420\rangle = \langle 410|Q_z|420\rangle = \iiint d^3\mathbf{r}\,\psi^*_{410}(r,\theta,\phi)(r\cos\theta)\psi_{420}(r,\theta,\phi)$$

$$= \left[\int_0^\infty r^3 R_{41}(r)R_{42}(r)\,dr\right]\left[\int_0^{2\pi} d\phi\right]\left[\int_0^\pi \sin\theta\cos\theta\, Y_1^0(\theta,\phi)Y_2^0(\theta,\phi)\,d\theta\right]$$

We now let Maple do the work for us:

```
> integrate(r^3*radial(4,1)*radial(4,2),r=0..infinity);
> integrate(sin(theta)*cos(theta)*spherharm(2,0)*
spherharm(1,0),theta=0..Pi);
```

$$\langle 410|Q_0|420\rangle = \left[-12a_0\sqrt{3}\right]\left[2\pi\right]\left[1\big/\pi\sqrt{15}\right] = -24a_0\big/\sqrt{5}$$

(b) [4] Find the reduced matrix element $\langle 41\|\mathbf{Q}\|42\rangle$

By the Wigner-Eckart theorem, these matrix elements can be found from

$$\langle 41m|Q_q|42m'\rangle = \frac{\langle 41\|\mathbf{Q}\|42\rangle}{\sqrt{2\cdot 1+1}}\langle 1m|21;m'q\rangle = \langle 21;m'q|1m\rangle\langle 41\|\mathbf{Q}\|42\rangle\big/\sqrt{3}$$

Letting $m = m' = q = 0$, we then find

$$\langle 41\|\mathbf{Q}\|42\rangle = \frac{\sqrt{3}\langle 410|Q_0|420\rangle}{\langle 10|21;00\rangle} = \frac{\sqrt{3}\left(-24a_0\big/\sqrt{5}\right)}{-\sqrt{2/5}} = 12\sqrt{6}a_0$$

What we'll actually use in our equations is $\langle 41\|\mathbf{Q}\|42\rangle\big/\sqrt{3} = 12\sqrt{2}a_0$. We found the Clebsch with the help of Maple:

```
> clebsch(2,1,0,0,1,0);
```

(c) [8] Find all non-zero components of $\langle 41m|Q_q|42m'\rangle$. There should be nine non-zero ones (one of which you have from part (a)).

The non-zero ones are simply those with $m = q + m'$. In each case, we can simply calculate the Clebsch-Gordan coefficients using my online routine.

```
> for m from 1 to -1 by -1 do for q from 1 to -1 by -1 do
print(clebsch(2,1,m-q,q,1,m)) end do; end do;
```

$$\langle 411|R_1|420\rangle = \langle 21;01|11\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{1/10}\left(12\sqrt{2}a_0\right) = 12a_0/\sqrt{5},$$

$$\langle 411|R_0|421\rangle = \langle 21;10|11\rangle\langle 41\|R\|42\rangle/\sqrt{3} = -\sqrt{3/10}\left(12\sqrt{2}a_0\right) = -12a_0\sqrt{3/5},$$

$$\langle 411|R_{-1}|422\rangle = \langle 21;2,-1|11\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{3/5}\left(12\sqrt{2}a_0\right) = 12a_0\sqrt{6/5},$$

$$\langle 410|R_1|42,-1\rangle = \langle 21;-1,1|10\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{3/10}\left(12\sqrt{2}a_0\right) = 12a_0\sqrt{3/5},$$

$$\langle 410|R_0|420\rangle = \langle 21;00|10\rangle\langle 41\|R\|42\rangle/\sqrt{3} = -\sqrt{2/5}\left(12\sqrt{2}a_0\right) = -24a_0/\sqrt{5},$$

$$\langle 410|R_{-1}|421\rangle = \langle 21;1,-1|10\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{3/10}\left(12\sqrt{2}a_0\right) = 12a_0\sqrt{3/5},$$

$$\langle 41,-1|R_1|42,-2\rangle = \langle 21;-2,1|1,-1\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{3/5}\left(12\sqrt{2}a_0\right) = 12a_0\sqrt{6/5},$$

$$\langle 41,-1|R_0|42,-1\rangle = \langle 21;-1,0|1,-1\rangle\langle 41\|R\|42\rangle/\sqrt{3} = -\sqrt{3/10}\left(12\sqrt{2}a_0\right) = -12a_0\sqrt{3/5},$$

$$\langle 41,-1|R_{-1}|420\rangle = \langle 21;0,-1|1,-1\rangle\langle 41\|R\|42\rangle/\sqrt{3} = \sqrt{1/10}\left(12\sqrt{2}a_0\right) = 12a_0/\sqrt{5}.$$

The one right in the middle we already had from part (a).

(d) [4] To show that you understand how to do it, find $\langle 410|Q_x|421\rangle$.

The point is simply that $R_{-1} - R_{+1} = \sqrt{2}Q_x$, so we have

$$\langle 410|Q_x|421\rangle = \tfrac{1}{\sqrt{2}}\left(\langle 410|R_{-1}|421\rangle - \langle 410|R_{+1}|421\rangle\right) = \tfrac{1}{\sqrt{2}}\left(12a_0\sqrt{3/5} - 0\right) = 6a_0\sqrt{6/5}.$$

2. [10] The quadrupole operators are spherical tensors of rank 2; that is, a spherical tensor with *k* = 2. Its components are:

$$T_{\pm2}^{(2)} = \tfrac{1}{2}\left(Q_x \pm iQ_y\right)^2, \quad T_{\pm1}^{(2)} = \mp Q_xQ_z - iQ_yQ_z, \; T_0^{(2)} = \sqrt{\tfrac{1}{6}}\left(2Q_z^2 - Q_x^2 - Q_y^2\right)$$

(a) [2] Show that these operators either commute or anti-commute with parity, Π.

Parity anti-commutes with the operators Q_x, Q_y, and Q_z, so we have, for example

$$\Pi T_{\pm1}^{(2)} = \Pi\left(\mp Q_xQ_z - iQ_yQ_z\right) = \pm Q_x\Pi Q_z + iQ_y\Pi Q_z = \left(\mp Q_xQ_z - iQ_yQ_z\right)\Pi = T_{\pm1}^{(2)}\Pi.$$

It is clear this method generalizes to any of the five operators, so $\Pi T_q^{(2)} = T_q^{(2)}\Pi$.

(b) [3] To calculate electric quadrupole radiation, it is necessary to calculate matrix elements of the form

$$\left\langle \alpha lm \middle| T_q^{(2)} \middle| \alpha' l' m' \right\rangle$$

Based on the Wigner Eckart theorem, what constraints can we put on *m’*, *m*, and *q*? What constraints can we put on *l* and *l’*?

The Wigner-Eckart theorem tells us that $m = m' + q$ and *l* lies in the range $\left|l' - 2\right| \le l \le l' + 2$.

(c) [2] Based on parity, what constraints can we put on *l* and *l’*?

Take our equation showing that parity commutes with the electric quadrupole moments, and sandwich it between two states, and we have

$$\left\langle \alpha lm \middle| \Pi T_q^{(2)} \middle| \alpha' l' m' \right\rangle = \left\langle \alpha lm \middle| T_q^{(2)} \Pi \middle| \alpha' l' m' \right\rangle,$$

$$\left(-1\right)^l \left\langle \alpha lm \middle| T_q^{(2)} \middle| \alpha' l' m' \right\rangle = \left(-1\right)^{l'} \left\langle \alpha lm \middle| T_q^{(2)} \middle| \alpha' l' m' \right\rangle.$$

Assuming the matrix elements don’t vanish, this can happen only if *l* and *l’* have the same parity, that is, they are both odd or both even.

(d)[3] Given *l’*, what values of *l* are acceptable? List all acceptable values of *l* for *l’* = 0, 1, 2, 3, 4, 5.

Well, since *l* is in the range $\left|l' - 2\right| \le l \le l' + 2$, then if *l’* is two or bigger, then this becomes $l' - 2 \le l \le l' + 2$. With the additional constraint that they be of the same parity, the only possible *l* values are *l’* – 2, *l’*, and *l’* + 2. However, when *l’* is 1, the restriction becomes that *l* = 1 or 3, and for *l’* = 0, then only *l* = 2 is allowed. The table at right summarizes this in several cases.

l'	l
0	2
1	1,3
2	0,2,4
3	1,3,5
4	2,4,6
5	3,5,7