Physics 741 – Graduate Quantum Mechanics 1

Solutions to Chapter 8

7. [10] Let V be any vector operator satisfying Eq. (8.22), and define V_q for $q=-1,0,1$ as given by Eq. (8.23). Show that this results in a tensor of rank 1; that is, that Eqs. (8.25) are satisfied by V_q with *k* = 1.

We'll simply work them all out

$$[J_z,V_0]=[J_z,V_z]=0\,,$$
$$[J_z,V_{\pm1}]=\sqrt{\tfrac{1}{2}}\left[J_z,\mp V_x-iV_y\right]=i\hbar\sqrt{\tfrac{1}{2}}\left(\mp V_y+iU_x\right)=\pm\hbar\sqrt{\tfrac{1}{2}}\left(\mp V_x-iV_y\right)=\hbar V_{\pm1}\,,$$
$$[J_\pm,V_0]=\left[J_x\pm iJ_y,V_z\right]=i\hbar\left(-V_y\pm iU_x\right)=\hbar\left(\mp V_x-iV_y\right)=\hbar\sqrt{2}V_{\pm1}\,,$$
$$[J_\pm,V_{\pm1}]=\sqrt{\tfrac{1}{2}}\left[J_x\pm iJ_y,\mp V_x-iV_y\right]=\sqrt{\tfrac{1}{2}}\left\{-i\left[J_x,V_y\right]-i\left[J_y,V_x\right]\right\}=\hbar\sqrt{\tfrac{1}{2}}\{V_z-V_z\}=0\,,$$
$$\left[J_\pm,V_{\mp1}\right]=\sqrt{\tfrac{1}{2}}\left[J_x\pm iJ_y,\pm V_x-iV_y\right]=\sqrt{\tfrac{1}{2}}\left\{-i\left[J_x,V_y\right]+i\left[J_y,V_x\right]\right\}=\hbar\sqrt{\tfrac{1}{2}}\{V_z+V_z\}=\hbar\sqrt{2}V_0\,.$$

They all worked out as they should.

8. [20] Our goal in this problem is to find every non-vanishing matrix element for Hydrogen of the form $\langle 41m|\mathbf{R}|42m'\rangle$; that is, all matrix elements between 4d and 4p states.

(a) [4] Find the matrix element $\langle 410|R_0|420\rangle$. 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

$$\langle 410|R_0|420\rangle=\langle 410|Z|420\rangle=\int d^3\mathbf{r}\,\psi^*_{410}(r,\theta,\phi)(r\cos\theta)\psi_{420}(r,\theta,\phi)$$
$$=\left[\int_0^\infty r^3R_{41}(r)R_{42}(r)\,dr\right]\left[\int_0^{2\pi}d\phi\right]\left[\int_0^\pi\sin\theta\cos\theta\,Y_1^0(\theta,\phi)Y_2^0(\theta,\phi)\,d\theta\right].$$

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);
```

$$\langle 410|R_0|420\rangle=\left[-12a_0\sqrt{3}\right]\left[2\pi\right]\left[1/\pi\sqrt{15}\right]=-24a_0/\sqrt{5}\,.$$

(b) [4] Find the reduced matrix element $\langle 41 \| R \| 42 \rangle$

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

$$\langle 41m | R_q | 42m' \rangle = \langle 41 \| \mathbf{R} \| 42 \rangle \langle 1m | 21; m'q \rangle / \sqrt{2 \cdot 1 + 1} = \langle 21; m'q | 1m \rangle \langle 41 \| \mathbf{R} \| 42 \rangle / \sqrt{3} .$$

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

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

so $\langle 41 \| \mathbf{R} \| 42 \rangle = 12\sqrt{6} a_0$. We found the Clebsch with the help of Maple:

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

(c) [8] Find all non-zero components of $\langle 41m | R_q | 42m' \rangle$. 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.

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

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

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

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

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

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

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

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

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

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

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

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

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