Physics 742 – Graduate Quantum Mechanics 1

Solutions to Chapter 13

2. [15] Complete the computation of the spin-orbit splitting for hydrogen for the 2*p*, 3*p*, and 3*d* states of hydrogen. Write your answers as multiples of $\alpha^2 |E_n|$, where α is the fine structure constant and $|E_n|$ is the unperturbed binding energy of this state.

Starting from equation (13.8) in the class notes, we have

$$\Delta E = \frac{\hbar^2 (2l+1)}{4m^2c^2} \int_0^\infty r^2 dr \left(\frac{1}{r} \frac{dV_c(r)}{dr} \right) R_{nl}^2(r) = \frac{\hbar^2 (2l+1) k_e e^2}{4m^2c^2} \int_0^\infty \frac{dr}{r} R_{nl}^2(r).$$

Recalling that the energy of the *n*'th state is $|E_n| = k_e e^2 / 2n^2 a_0$, this can be rewritten as

$$\Delta E = |E_n| \frac{\hbar^2 (2l+1) a_0 n^2}{2m^2c^2} \int_0^\infty \frac{dr}{r} R_{nl}^2(r) = |E_n| \frac{\hbar^2 (2l+1) n^2}{2m^2c^2 a_0^2} \int_0^\infty \frac{dr}{r} a_0^3 R_{nl}^2(r).$$

Substituting $a_0 = \hbar^2 / k_e e^2 m$, and then using $\alpha = k_e e^2 / \hbar c$, this can be rewritten as

$$\Delta E = |E_n| \frac{k_e^2 e^4 (2l+1) n^2}{2c^2\hbar^2} \int_0^\infty \frac{dr}{r} a_0^3 R_{nl}^2(r) = \tfrac{1}{2}\alpha^2 |E_n| n^2 (2l+1) \int_0^\infty \frac{dr}{r} a_0^3 R_{nl}^2(r).$$

Only the final integral remains. We find

$$\int_0^\infty \frac{dr}{r} a_0^3 R_{21}^2(r) = \frac{1}{a_0^2} \int_0^\infty \frac{dr}{r} \frac{r^2}{24} e^{-r/a_0} = \frac{1}{24} \int_0^\infty x e^{-x} dx = \frac{1}{24},$$

$$\int_0^\infty \frac{dr}{r} a_0^3 R_{31}^2(r) = \frac{1}{a_0^2} \int_0^\infty \frac{dr}{r} \frac{2^5 r^2}{3^7} \left(1 - \frac{r}{6a_0}\right)^2 e^{-2r/3a_0} = \frac{2^5}{3^7} \left(\frac{3}{2}\right)^2 \int_0^\infty x \left(1 - \frac{x}{4}\right)^2 e^{-x} dx$$
$$= \frac{8}{243} \cdot \left(1 - \frac{2 \cdot 2}{4} + \frac{6}{16}\right) = \frac{1}{81},$$

$$\int_0^\infty \frac{dr}{r} a_0^3 R_{32}^2(r) = \frac{1}{a_0^4} \int_0^\infty \frac{dr}{r} \frac{2^3 r^4}{3^9 \cdot 5} e^{-2r/3a_0} = \frac{2^3}{3^9 \cdot 5} \left(\frac{3}{2}\right)^4 \int_0^\infty x^3 e^{-x} dx = \frac{6}{3^5 \cdot 10} = \frac{1}{405}.$$

We now just substitute these numbers into our previous equations, to find

$$\Delta E_{2p} = \frac{1}{2}\alpha^2 |E_2| 2^2 (3) \frac{1}{24} = \frac{1}{4}\alpha^2 |E_2|,$$

$$\Delta E_{3p} = \frac{1}{2}\alpha^2 |E_3| 3^2 (3) \frac{1}{81} = \frac{1}{6}\alpha^2 |E_3|,$$

$$\Delta E_{3d} = \frac{1}{2}\alpha^2 |E_3| 3^2 (5) \frac{1}{405} = \frac{1}{18}\alpha^2 |E_3|.$$

3. **[5] Prove, as asserted in section C, that** $\int\left(3\hat{r}_j\hat{r}_k-\delta_{jk}\right)d\Omega=0$**. This is actually nine formulas, but only six of them are independent.**

We simply write $\hat{\mathbf{r}}=\mathbf{r}/r=\left(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta\right)$ and work out all the components. We'll do it as a matrix for fun.

$$\int\left(3\hat{r}_j\hat{r}_k-\delta_{jk}\right)d\Omega=\int\begin{pmatrix}3\sin^2\theta\cos^2\phi-1 & 3\sin^2\theta\cos\phi\sin\phi & 3\sin\theta\cos\theta\cos\phi\\ 3\sin^2\theta\cos\phi\sin\phi & 3\sin^2\theta\sin^2\phi-1 & 3\sin\theta\cos\theta\sin\phi\\ 3\sin\theta\cos\theta\cos\phi & 3\sin\theta\cos\theta\sin\phi & 3\cos^2\theta-1\end{pmatrix}d\Omega$$

We start with the integral over ϕ. It is easy to see that the integral of $\cos\phi$ or $\sin\phi$ is just zero, and since $\cos\phi\sin\phi=\frac{1}{2}\sin\left(2\phi\right)$, this can be seen to integrate to zero. The integral of 1 is trivial, and we can use Carlson's rule on the $\cos^2\phi$ and $\sin^2\phi$ (they are each half of the size of the interval), so we have

$$\int\left(3\hat{r}_j\hat{r}_k-\delta_{jk}\right)d\Omega=2\pi\int_0^\pi\begin{pmatrix}\frac{3}{2}\sin^2\theta-1 & 0 & 0\\ 0 & \frac{3}{2}\sin^2\theta-1 & 0\\ 0 & 0 & 3\cos^2\theta-1\end{pmatrix}\sin\theta d\theta$$

$$=\begin{pmatrix}\pi & 0 & 0\\ 0 & \pi & 0\\ 0 & 0 & -2\pi\end{pmatrix}\int_{-1}^{1}\left(1-3\cos^2\theta\right)d\left(\cos\theta\right)=0.$$