QUANTUM MECHANICS
Hwk Solution Set 7
Calculations For the Hydrogen Atom

Solution to Problem 4.10

The general formulas we need are

$$R_{n,l}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho), \quad \rho = r/(an) \quad (a = \text{Bohr radius}) \tag{1}$$

$$v(\rho) = \sum_{j=0}^{j_{\max}} a_j \rho^j \tag{2}$$

$$a_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}a_j \tag{3}$$

$$j_{\max} = n-l-1 \tag{4}$$

$R_{n=3,l=0}$

$$j_{\max} = 2 \tag{5}$$

$$R_{3,0}(r) = \frac{1}{r}\rho e^{-\rho}(a_0 + a_1\rho + a_2\rho^2) \tag{6}$$

$$a_1 = -2a_0 \tag{7}$$

$$a_2 = 2a_0/3 \tag{8}$$

$$a_{3+k} = 0, \quad k \in (0,1,2,3\ldots) \tag{9}$$

$$\Rightarrow R_{3,0}(r) = \frac{1}{r}\frac{r}{3a}e^{-\frac{r}{3a}}\left(a_0 - 2a_0\frac{r}{3a} + \frac{2a_0}{3}\left(\frac{r}{3a}\right)^2\right) \tag{10}$$

$$\Rightarrow R_{3,0}(r) = \frac{a_0}{3a}e^{-\frac{r}{3a}}\left(1 - \frac{2}{3}\left(\frac{r}{a}\right) + \frac{2}{3^3}\left(\frac{r}{a}\right)^2\right). \tag{11}$$

$R_{n=3,l=1}$

$$\begin{aligned}
j_{\max} &= 1 && (12)\\
R_{3,1}(r) &= \frac{1}{r}\rho^2 e^{-\rho}(a_0 + a_1\rho) && (13)\\
a_1 &= -\frac{1}{2}a_0 && (14)\\
a_{2+k} &= 0, \quad k \in (0,1,2,3\ldots) && (15)\\
\Rightarrow R_{3,1}(r) &= \frac{1}{r}\left(\frac{r}{3a}\right)^2 e^{-\frac{r}{3a}}\left(a_0 - \frac{1}{2}a_0\frac{r}{3a}\right) && (16)\\
\Rightarrow R_{3,1}(r) &= \left(\frac{a_0}{3^2a^2}\right) e^{-\frac{r}{3a}} r\left(1 - \frac{1}{6}\left(\frac{r}{a}\right)\right). && (17)
\end{aligned}$$

$R_{n=3,l=2}$

$$\begin{aligned}
j_{\max} &= 0 && (18)\\
R_{3,2}(r) &= \frac{1}{r}\rho^3 e^{-\rho}(a_0) && (19)\\
a_{1+k} &= 0, \quad k \in (0,1,2,3\ldots) && (20)\\
\Rightarrow R_{3,2}(r) &= \frac{1}{r}\left(\frac{r}{3a}\right)^3 e^{-\frac{r}{3a}} a_0 && (21)\\
\Rightarrow R_{3,2}(r) &= \left(\frac{a_0}{3^3a^3}\right) r^2 e^{-\frac{r}{3a}}. && (22)
\end{aligned}$$

Note we have not normalized.

Solution to Problem 4.13

Part (a)

We want the expectation value of

$$\langle r\rangle = \int_V r|\psi|^2 dV. \tag{23}$$

The ground state wavefunction is

$$\psi = \psi_{1,0,0} = Ne^{-r/a}, \quad N = \frac{1}{(\pi a^3)^{1/2}}, \quad dV = r^2 dr \sin\theta d\theta d\phi \to 4\pi r^2 dr. \tag{24}$$

Thus we get

$$\langle r\rangle = 4\pi\int_V r|\psi|^2 r^2 dr = N^2 4\pi\int_0^\infty e^{-2r/a} r^3 dr = \frac{4}{a^3}\int_0^\infty e^{-2r/a} r^3 dr. \tag{25}$$

Similarly

$$\langle r^2 \rangle = 4\pi^2 \int_V r^2 |\psi|^2 r^2 dr = \frac{4}{a^3} \int_0^\infty e^{-2r/a} r^4 dr. \tag{26}$$

We can derive this integral similarly to what was done in previous hwks. At this point however you may wish to recall:

$$\int_0^\infty e^{-kr} r^n dr = k^{-1-n} n! \quad Re(n) > -1 \quad and \quad Re(k) > 0. \tag{27}$$

Then with $k = 2/a$

$$\langle r \rangle = \frac{4}{a^3} \int_0^\infty e^{-k} r^3 dr = \frac{4}{a^3} \frac{6}{k^4} = \frac{4}{a^3} \frac{3a^4}{8} = \frac{3}{2} a. \tag{28}$$

Likewise,

$$\langle r^2 \rangle = \frac{4}{a^3} \int_0^\infty e^{-kr} r^4 dr = \frac{4}{a^3} \frac{24}{k^5} = \frac{4}{a^3} \frac{3a^5}{4} = 3a^2. \tag{29}$$

Part (b)

$\langle x \rangle = 0$ (use $x = r \sin\theta \cos\phi$ and note the integral over ϕ from 0 to 2π gives zero). Also by symmetry $\langle x^2 \rangle = \langle r^2 \rangle / 3 = a^2$.

Part (c)

Using the tables in Griffiths, you should be able to construct (R_{21} normalized and then multiply by Y_1^1)

$$\psi_{2,1,1} = -\frac{1}{(\pi a)^{1/2}} \frac{1}{8a^2} r e^{-\frac{r}{2a}} \sin\theta e^{i\phi}. \tag{30}$$

Then using $x^2 = (r \sin\theta \cos\phi)^2$

$$\begin{aligned} \langle x^2 \rangle &= \frac{1}{64\pi a^5} \int_0^\infty r^6 e^{-r/a} dr \int_0^\pi \sin^5\theta d\theta \int_0^{2\pi} \cos^2\phi d\phi & (31) \\ &= \frac{1}{64\pi a^5} * \frac{6!}{(1/a)^7} * (16/15) * (\pi) = 12a^2. & (32) \end{aligned}$$

Solution to Problem 4.43

Part (a)

Using the tables in Griffiths, you should be able to construct (R_{32} normalized and then multiply by Y_1^2)

$$\psi_{3,2,1} = -\frac{1}{(81\pi^{1/2})a^{7/2}} r^2 e^{-\frac{r}{3a}} \sin\theta \cos\theta e^{i\phi}. \quad (33)$$

Part (b)

To normalize (in this case check) we integrate as usual

$$\int_V |\psi_{3,2,1}|^2 dV = \frac{1}{(81^2\pi)a^7} \int_0^\infty r^6 e^{-\frac{2r}{3a}} dr \int_0^\pi \sin^3\theta \cos^2\theta d\theta \int_0^{2\pi} d\phi \quad (34)$$

$$= \frac{1}{(81^2\pi)a^7} * \frac{6!}{(2/(3a))^7} * (4/15) * (2\pi) = 1. \quad (35)$$

Part (c)

Using equation (27) and the r dependancy of the integral in Part (b), it is obvious the solution is proportional to $n! = (6+s)!$, where $Re(n) > -1$ is given in equation (27). Thus, the result is finite only if $s > -7$ where s is assumed to be real.