

1. (a) Normalize $R_{2,0}$ for hydrogen and construct the wavefunction $\psi_{2,0,0}$.

From Griffiths Eq. 4.82,

$$R_{2,0} = \frac{c_0}{2a} \left(1 - \frac{r}{2a}\right) \exp\left[-\frac{r}{2a}\right],$$

where c_0 is the normalization constant. Then,

$$\begin{aligned} 1 &= \int_0^\infty |R_{2,0}|^2 r^2 dr \\ &= \left(\frac{c_0}{2a}\right)^2 \int_0^\infty \left(1 - \frac{r}{2a}\right)^2 \exp\left[-\frac{r}{a}\right] r^2 dr \\ &= \left(\frac{c_0}{2a}\right)^2 \left(\int_0^\infty r^2 e^{-r/a} dr - \frac{1}{a} \int_0^\infty r^3 e^{-r/a} dr + \frac{1}{4a^2} \int_0^\infty r^4 e^{-r/a} dr \right), \end{aligned}$$

where all three integrals are of the form of integral (7) from the provided integral table; that is,

$$\int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}} \Rightarrow \int_0^\infty r^n e^{-r/a} dr = n! a^{n+1}.$$

Then,

$$\begin{aligned} 1 &= \left(\frac{c_0}{2a}\right)^2 \left(2!a^3 - \frac{1}{a}3!a^4 + \frac{1}{4a^2}4!a^5\right) \\ &= \left(\frac{c_0}{2a}\right)^2 (2a^3 - 6a^3 + 6a^3) \\ &= c_0^2 \frac{1}{4a^2} 2a^3 \\ &= c_0^2 \frac{a}{2}, \end{aligned}$$

which is satisfied for

$$c_0 = \sqrt{\frac{2}{a}}.$$

Thus,

$$R_{2,0} = \frac{a^{-3/2}}{\sqrt{2}} \left(1 - \frac{r}{2a}\right) \exp\left[-\frac{r}{2a}\right].$$

The wavefunction, $\psi_{2,0,0}$, is given by

$$\psi_{2,0,0} = R_{2,0} Y_0^0,$$

where Y_0^0 is given by Griffiths Table 4.3 as

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}.$$

Thus,

$$\psi_{2,0,0} = \frac{a^{-3/2}}{\sqrt{8\pi}} \left(1 - \frac{r}{2a}\right) \exp\left[-\frac{r}{2a}\right].$$

(b) Normalize $R_{2,1}$ for hydrogen and construct the wavefunction $\psi_{2,1,1}$, $\psi_{2,1,0}$, and $\psi_{2,1,-1}$.

From Griffiths Eq. 4.83,

$$R_{2,1} = \frac{c_0}{4a^2} r \exp\left[-\frac{r}{2a}\right],$$

where c_0 is the normalization constant. Then,

$$\begin{aligned} 1 &= \int_0^\infty |R_{2,1}|^2 r^2 dr \\ &= \left(\frac{c_0}{4a^2}\right)^2 \int_0^\infty r^4 \exp\left[-\frac{r}{a}\right] dr, \end{aligned}$$

which is an integral of the same form as in part (a). Thus,

$$\begin{aligned} 1 &= \left(\frac{c_0}{4a^2}\right)^2 4!a^5 \\ &= c_0^2 a \frac{3}{2}, \end{aligned}$$

which is satisfied for

$$c_0 = \sqrt{\frac{2}{3a}}.$$

Thus,

$$R_{2,1} = \frac{a^{-5/2}}{\sqrt{24}} r \exp\left[-\frac{r}{2a}\right].$$

The wavefunctions, $\psi_{2,1,1}$, $\psi_{2,1,0}$, and $\psi_{2,1,-1}$ are given by

$$\begin{aligned} \psi_{2,1,1} &= R_{2,1} Y_1^1, \\ \psi_{2,1,0} &= R_{2,1} Y_1^0, \\ \psi_{2,1,-1} &= R_{2,1} Y_1^{-1}. \end{aligned}$$

The angular components of the wavefunctions, Y_1^1 , Y_1^0 , and Y_1^{-1} , are given by Griffiths Table 4.3 as

$$\begin{aligned} Y_1^1 &= -\sqrt{\frac{3}{8\pi}} \sin[\theta] \exp[i\phi], \\ Y_1^0 &= \sqrt{\frac{3}{4\pi}} \cos[\theta], \\ Y_1^{-1} &= \sqrt{\frac{3}{8\pi}} \sin[\theta] \exp[-i\phi]. \end{aligned}$$

Then,

$$\begin{aligned} \psi_{2,1,1} &= -\frac{a^{-5/3}}{\sqrt{64\pi}} r \exp\left[i\phi - \frac{r}{2a}\right] \sin[\theta], \\ \psi_{2,1,0} &= \frac{a^{-5/3}}{\sqrt{32\pi}} r \exp\left[-\frac{r}{2a}\right] \cos[\theta], \\ \psi_{2,1,-1} &= \frac{a^{-5/3}}{\sqrt{64\pi}} r \exp\left[-\left(i\phi + \frac{r}{2a}\right)\right] \sin[\theta]. \end{aligned}$$

2. (a) Determine $\langle r \rangle$ and $\langle r^2 \rangle$ for an electron in the ground state of the hydrogen atom. Express solutions in terms of the Bohr radius, a .

The ground state wavefunction for hydrogen is given by $\psi_{1,0,0}$ where from Griffiths Table 4.3 and 4.7,

$$\psi_{1,0,0} = R_{1,0}Y_0^0 = 2a^{-3/2}e^{-r/a}\sqrt{\frac{1}{4\pi}} = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}.$$

Then,

$$\begin{aligned}\langle r^n \rangle &= \int_0^{2\pi} \int_0^\pi \int_0^\infty (\psi_{1,0,0}^* r^n \psi_{1,0,0}) r^2 \sin(\theta) dr d\theta d\phi \\ &= \frac{4\pi}{\pi a^3} \int_0^\infty r^{n+2} \exp\left[-2\frac{r}{a}\right] dr,\end{aligned}$$

where this integral is of the form of integral (7) from the provided integral table; that is,

$$\int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}} \Rightarrow \int_0^\infty r^{n+2} e^{-2r/a} dr = (n+3)! \left(\frac{a}{2}\right)^{n+2}.$$

Thus,

$$\langle r^n \rangle = \frac{a^n}{2^{(n+1)}}(n+2)!.$$

Therefore,

$$\begin{aligned}\langle r \rangle &= \frac{3}{2}a, \\ \langle r^2 \rangle &= 3a^2.\end{aligned}$$

- (b) Determine $\langle x \rangle$ and $\langle x^2 \rangle$ for an electron in the ground state of the hydrogen atom. If the symmetry of the ground state is exploited, there will not be any new integration for this calculation.

- (c) Determine $\langle x^2 \rangle$ for an electron in a hydrogen atom in the state $n = 2$, $l = 1$, $m = 1$. It is helpful to use the fact that $x = r \sin(\theta) \cos(\phi)$.

The wavefunction of this state is given by $\psi_{2,1,1}$ where from Griffiths Table 4.3 and 4.7

$$\psi_{2,1,1} = R_{1,0} Y_1^1 = -\frac{1}{2\sqrt{6}} a^{-3/2} \frac{r}{a} \exp\left[-\frac{r}{2a}\right] \sqrt{\frac{3}{8\pi}} \sin[\theta] \exp[i\phi].$$

Then,

$$\begin{aligned} \langle x^2 \rangle &= \int_0^{2\pi} \int_0^\pi \int_0^\infty (\psi_{2,1,1}^* x^2 \psi_{2,1,1}) r^2 \sin(\theta) dr d\theta d\phi \\ &= \int_0^{2\pi} \int_0^\pi \int_0^\infty (\psi_{2,1,1}^* \psi_{2,1,1}) r^2 (\sin(\theta))^2 (\cos(\theta))^2 r^2 \sin(\theta) dr d\theta d\phi \\ &= \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{1}{24a^3} \left(\frac{r}{a}\right)^2 e^{-r/a} \frac{3}{8\pi} r^4 (\sin[\theta])^5 (\cos[\theta])^2 dr d\theta d\phi \\ &= \frac{1}{64\pi a^5} \int_0^{2\pi} \int_0^\pi \int_0^\infty e^{-r/a} r^6 (\sin[\theta])^5 (\cos[\theta])^2 dr d\theta d\phi \\ &= \frac{1}{64\pi a^5} \int_0^{2\pi} (\cos[\phi])^2 d\phi \int_0^\pi (\sin[\theta])^5 d\theta \int_0^\infty r^6 \exp\left[-\frac{r}{a}\right] dr, \end{aligned}$$

where we have an integral of the form of integral (7) from the provided integral table; that is,

$$\int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}} \Rightarrow \int_0^\infty r^6 e^{-r/a} dr = 6! a^7.$$

Then,

$$\langle x^2 \rangle = \frac{45}{4\pi} a^2 \int_0^{2\pi} (\cos[\phi])^2 d\phi \int_0^\pi (\sin[\theta])^5 d\theta,$$

where the remaining integrals are of the form that Mathematica can solve¹.

Then,

$$\langle x^2 \rangle = \frac{45}{4\pi} a^2 \frac{16}{15} \pi = 12a^2.$$

¹I could too, but would rather not apply integration by parts many times over.

3. (a) Starting with $[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}$ and $[r_i, r_j] = [p_i, p_j] = 0$, where the index i stands for x, y , or z , and $r_x = x, r_y = y, r_z = z$, work out the following commutator relations:

$$\begin{aligned} [L_z, x] &= i\hbar y, & [L_z, y] &= i\hbar x, & [L_z, z] &= 0, \\ [L_z, p_x] &= i\hbar p_y, & [L_z, p_y] &= i\hbar p_x, & [L_z, p_z] &= 0. \end{aligned}$$

- (b) Use the results from part (a) and the definitions

$$L_x = yp_z - zp_y,$$

$$L_y = zp_x - xp_z,$$

$$L_z = xp_y - yp_x,$$

to obtain $[L_z, L_x] = i\hbar L_y$.

- (c) Evaluate the commutators $[L_z, r^2]$ and $[L_z, p^2]$, where $r^2 = x^2 + y^2 + z^2$ and $p^2 = p_x^2 + p_y^2 + p_z^2$.

- (d) Show that the Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V},$$

commutes with all three components of $\hat{\vec{L}}$ if \hat{V} depends only on r .