

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.

Since the ground state wavefunction is spherically symmetric,

$$\langle x \rangle = \langle y \rangle = \langle z \rangle = 0.$$

Likewise,

$$\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle,$$

and,

$$\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 3 \langle x^2 \rangle.$$

Thus,

$$\langle x^2 \rangle = a^2.$$

Which makes sense if indeed a is the radius of this wavefunction that $\langle x \rangle$ would be equally likely to be found at $\pm a$, the square of $\langle x \rangle$ would be a^2 .

- (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:

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

Using notation from Griffiths Eq. 4.97,

$$[L_z, x] = [xp_y - yp_x, x] = [xp_y, x] - [yp_x, x],$$

we notice p_y and x will commute while p_x and x will not. We also notice that the y term in the right-most term will commute with both p_x and x . Thus,

$$[L_z, x] = 0 - y[p_x, x] = y[x, p_x] = i\hbar y.$$

Similarly,

$$[L_z, y] = [xp_y - yp_x, y] = [xp_y, y] + [y, yp_x] = -x(i\hbar) + 0 = -i\hbar x.$$

Not so similarly,

$$[L_z, z] = [xp_y - yp_x, z] = [xp_y, z] - [yp_x, z].$$

Here, z commutes with x, y, p_x , and p_y . Thus,

$$[L_z, z] = 0 - 0 = 0.$$

The momentum terms will interact just like the position terms.

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

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

$$\begin{aligned} [L_z, L_x] &= [xp_y - yp_x, yp_z - zp_y] \\ &= [xp_y, yp_z] - [xp_y, zp_y] - [yp_x, yp_z] + [yp_x, zp_y], \end{aligned}$$

where here the middle two terms commute and so equal 0. Then,

$$\begin{aligned} [L_z, L_x] &= [xp_y, yp_z] + [yp_x, zp_y] \\ &= xp_z [p_y, y] + p_x z [y, p_y] \\ &= xp_z (-i\hbar) + p_x z (i\hbar) \\ &= i\hbar (-xp_z + p_x z) \\ &= i\hbar (p_x z - xp_z) \\ &= i\hbar (zp_x - xp_z) \\ &= i\hbar L_y. \end{aligned}$$

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

We begin by exploiting Griffiths Eq. 3.65;

$$\begin{aligned} [L_z, r^2] &= [L_z, x^2] + [L_z, y^2] + [L_z, z^2] \\ &= [L_z, x] x + x [L_z, x] + [L_z, y] y + y [L_z, y] + 0. \end{aligned}$$

Then by the results from part (a),

$$[L_z, r^2] = i\hbar yx + i\hbar xy - i\hbar xy - i\hbar xy = 0.$$

We appeal to identical arguments for $[L_z, p^2]$. Eq. 3.65 holds, the commutator relations from part (a) are of the same form, and thus

$$[L_z, p^2] = 0.$$

(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 .

Let L be an arbitrary component of angular momentum. The result from part (c) may exploit similar arguments to show $[L_x, p^2] = 0$ and $[L_y, p^2] = 0$. Then,

$$[L, H] = \frac{1}{2m} [L, p^2] + [L, V] = 0 + [L, V],$$

where V is a function only of r . Thus,

$$[L, H] = [L, r].$$

Let L be a particular component of orbital angular momentum by Eq. 4.96,

$$L = L_z = xp_y - yp_x = x i \hbar \frac{\partial}{\partial y} - y i \hbar \frac{\partial}{\partial x}.$$

Then, we evaluate $[L_z, r]$ with a test function, $v(r)$,

$$\begin{aligned} [L_z, r] v &= i \hbar \left[x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}, r \right] v \\ &= i \hbar \left[x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}, r \right] v \\ &= i \hbar \left(\left[x \frac{\partial}{\partial y}, r \right] v - \left[y \frac{\partial}{\partial x}, r \right] v \right), \end{aligned}$$

where

$$r = \sqrt{x^2 + y^2 + z^2}.$$

Then,

$$\begin{aligned} [L_z, r] v &= i \hbar \left(x \frac{\partial r v}{\partial y} - r x \frac{\partial v}{\partial y} - y \frac{\partial r v}{\partial x} + r y \frac{\partial v}{\partial x} \right) \\ &= i \hbar \left(x v \frac{1}{2} r^{-1} 2y - 0 - y v \frac{1}{2} r^{-1} 2x + 0 \right) \\ &= i \hbar v \left(\frac{xy}{r} - \frac{xy}{r} \right) \\ &= 0. \end{aligned}$$

By inspection, we see that any choice of L , L_x , L_y , or L_z , will interact with the test function, $v(r)$, and r similarly, and thus will commute.