Problem 1

[35 pts] Hydrogen radial wavefunctions: the hydrogen potential is $V(r) = -Zk_e e^2/r$.

Part a

Using the Lapacian ∇^2 in spherical coordinates, show that

$$\hat{T} = \frac{-\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\hat{L}^2}{2\mu r^2}$$

where the second term represents rotational kinetic energy, with

$$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$

Write Schrödinger's equation for $\psi(r,\theta,\phi)$ of the hydrogen atom using this form of \hat{T} .

Similar to problem (2) part (a) in homework set #6, we start with the multi-dimensional time-independent Schrödinger's equation and substitute in the Lapacian in spherical coordinates:

$$\begin{aligned} \dot{H}\psi &= E\psi\\ \hat{T}\psi + \hat{V}\psi &= E\psi\\ -\frac{\hbar^2}{2\mu}\nabla^2\psi + \hat{V}\psi &= E\psi\\ -\frac{\hbar^2}{2\mu}\nabla^2\psi + \hat{V}\psi &= E\psi \end{aligned}$$

So now we must show that $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) = \frac{1}{r}\frac{\partial^2}{\partial r^2}r$, so:

$$\begin{aligned} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) &= \frac{1}{r} \frac{\partial^2}{\partial r^2} r \\ \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) f\left(r \right) &= \frac{1}{r} \frac{\partial^2}{\partial r^2} r f\left(r \right) \\ \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) f\left(r \right) &= \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{\partial}{\partial r} r f\left(r \right) \right) \\ \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) f\left(r \right) &= \frac{1}{r} \frac{\partial}{\partial r} \left(r f'\left(r \right) + f\left(r \right) \right) \\ \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) f\left(r \right) &= \frac{1}{r} \left(r f''\left(r \right) + f'\left(r \right) + f'\left(r \right) \right) \\ \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) f\left(r \right) &= f''\left(r \right) + \frac{2}{r} f'\left(r \right) \\ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} &= \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \end{aligned}$$

So, we can replace $\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$ with $\frac{1}{r} \frac{\partial^2}{\partial r^2} r$.

$$-\frac{\hbar^2}{2\mu} \left(\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \right) \psi + \hat{V}\psi = E\psi$$

$$\left(\frac{-\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{-\hbar^2}{2\mu r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \right) \psi + \hat{V}\psi = E\psi$$

If $\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$, then we have:

$$\frac{-\hbar^2}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{\dot{L}^2}{2\mu r^2} \psi + \dot{V}\psi = E\psi$$
$$\hat{T}\psi + \dot{V}\psi = E\psi$$

Schrödinger's equation is, then:

$$\left(\frac{-\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2}\right)\psi\left(r,\theta,\phi\right) + \hat{V}\psi\left(r,\theta,\phi\right) = E\psi\left(r,\theta,\phi\right)$$

But $\hat{V} = V(r) = -Zk_ee^2/r$, so

$$\left(\frac{-\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2}\right)\psi\left(r,\theta,\phi\right) - \frac{Zk_e e^2}{r}\psi\left(r,\theta,\phi\right) = E\psi\left(r,\theta,\phi\right)$$

Part b

Make the substitution $\psi(r, \theta, \phi) = \frac{1}{r}u(r)Y_{lm}(\theta, \phi)$. The factor $\frac{1}{r}$ takes into account the spreading out of the wave function as it gets farther from the origin. Use the eigenvalue of Y_{lm} ,

$$\hat{L}^2 Y_{lm} = \hbar^2 l \left(l + 1 \right) Y_{lm}$$

to simplify the equation.

We start with:

$$\left(\frac{-\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2}\right)\psi\left(r,\theta,\phi\right) - \frac{Zk_e e^2}{r}\psi\left(r,\theta,\phi\right) = E\psi\left(r,\theta,\phi\right)$$

Substituting in $\psi(r,\theta,\phi) = \frac{1}{r}u(r)Y_{lm}(\theta,\phi)$, we get:

$$\begin{split} E\frac{1}{r}u(r)Y_{lm}(\theta,\phi) &= \left(\frac{-\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2}\right)\frac{1}{r}u(r)Y_{lm}(\theta,\phi) - \frac{Zk_ee^2}{r}\frac{1}{r}u(r)Y_{lm}(\theta,\phi) \\ &= \frac{-\hbar^2}{2\mu}\frac{1}{r}Y_{lm}(\theta,\phi)\frac{\partial^2}{\partial r^2}\frac{r}{r}u(r) + \frac{u(r)}{2\mu r^3}\hat{L}^2Y_{lm}(\theta,\phi) - \frac{Zk_ee^2}{r}\frac{1}{r}u(r)Y_{lm}(\theta,\phi) \\ &= \frac{-\hbar^2}{2\mu}\frac{1}{r}Y_{lm}(\theta,\phi)\frac{\partial^2}{\partial r^2}u(r) + \frac{u(r)}{2\mu r^3}\hbar^2l(l+1)Y_{lm}(\theta,\phi) - \frac{Zk_ee^2}{r}\frac{1}{r}u(r)Y_{lm}(\theta,\phi) \\ E\frac{1}{r}u(r) &= \frac{-\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}u(r) + \frac{u(r)}{2\mu r^3}\hbar^2l(l+1) - \frac{Zk_ee^2}{r}\frac{1}{r}u(r) \\ Eu(r) &= \frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u(r) + \frac{u(r)}{2\mu r^2}\hbar^2l(l+1) - \frac{Zk_ee^2}{r}u(r) \end{split}$$

Part c

Show that the result looks like the Schrödinger equation for u(r) in one dimension with a centrifugal potential $V_c(r) = \hbar^2 l (l+1) / 2\mu r^2$ in addition to the Colomb potential. Compare with the potential of the centrifugal force $F = ma_c = mv^2/r$ using L = mvr.

If $V_c(r) = \hbar^2 l \left(l+1
ight) / 2 \mu r^2$, then we can replace $\hbar^2 l \left(l+1
ight) / 2 \mu r^2$:

$$Eu(r) = \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} u(r) + V_c(r) u(r) - \frac{Zk_e e^2}{r} u(r)$$

If $V_c(r) = \hbar^2 l \left(l+1 \right) / 2\mu r^2$, then we should be able to find $F = -\frac{d}{dr} \left(\hbar^2 l \left(l+1 \right) / 2\mu r^2 \right)$. So:

$$F = -\frac{d}{dr} \left(\frac{\hbar^2 l \left(l+1 \right)}{2\mu r^2} \right)$$

$$F = -\frac{\hbar^2 l \left(l+1 \right)}{2\mu} \frac{d}{dr} \left(r^{-2} \right)$$

$$F = -\frac{\hbar^2 l \left(l+1 \right)}{2\mu} - 2r^{-3}$$

$$F = \frac{\hbar^2 l \left(l+1 \right)}{\mu} r^{-3}$$

$$F = \frac{L^2}{\mu r^3}$$

$$F = \frac{L^2}{\mu r^3}$$

$$F = \frac{\mu v^2}{r}$$

So, we can see that the derivative of $V_{c}\left(r
ight)$ gives us an apparent centrifugal force.

Part d

Make the substitutions

$$\begin{split} u(r) &= U(\rho) \text{ where } \rho = \frac{2r}{r_n} \\ r_n &= \frac{na_0}{Z} \text{ where } a_0 = \frac{\hbar^2}{\mu k_e e^2} \\ E_n &= \frac{-Z^2 E_0}{n^2} \text{ where } E_0 = \frac{\mu k_e^2 e^4}{2\hbar^2} \end{split}$$

to obtain the dimensionless equation

$$\left(\frac{\partial^2}{\partial\rho^2} - \frac{l\left(l+1\right)}{\rho^2} + \frac{n}{\rho} - \frac{1}{4}\right)U(\rho) = 0$$

Starting with:

$$Eu(r) = \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} u(r) + \frac{u(r)}{2\mu r^2} \hbar^2 l(l+1) - \frac{Zk_e e^2}{r} u(r)$$

and substituting in $u(r) = U(\rho)$, where $\rho = \frac{2r}{r_n}$, and recognizing that $r = \rho r_n/2$, we get:

$$EU(\rho) = \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} U(\rho) + \frac{U(\rho)}{2\mu r^2} \hbar^2 l(l+1) - \frac{Zk_e e^2}{r} U(\rho)$$
$$= \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} U(\rho) + \frac{U(\rho)}{2\mu \left(\frac{\rho r_n}{2}\right)^2} \hbar^2 l(l+1) - \frac{2Zk_e e^2}{\rho r_n} U(\rho)$$

$$= \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} U(\rho) + \frac{U(\rho)}{2\mu \left(\frac{\rho r_n}{2}\right)^2} \hbar^2 l(l+1) - \frac{2Zk_e e^2}{\rho r_n} U(\rho)$$
$$= \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} U(\rho) + \frac{2U(\rho)}{\mu \left(\rho r_n\right)^2} \hbar^2 l(l+1) - \frac{2Zk_e e^2}{\rho r_n} U(\rho)$$

We also have that $\frac{\partial \rho}{\partial r} \frac{\partial}{\partial \rho} = \frac{\partial}{\partial r}$, and that

$$\frac{\partial^2}{\partial r^2} = \frac{\partial}{\partial r} \left(\frac{\partial \rho}{\partial r} \frac{\partial}{\partial \rho} \right)$$

But, we know that $\frac{\partial \rho}{\partial r} = \frac{\partial}{\partial r} \left(\frac{2r}{r_n} \right) = \frac{2}{r_n}$, so this becomes:

$$\begin{aligned} \frac{\partial^2}{\partial r^2} &= \frac{\partial}{\partial r} \left(\frac{2}{r_n} \frac{\partial}{\partial \rho} \right) \\ &= \frac{2}{r_n} \frac{\partial}{\partial r} \left(\frac{\partial}{\partial \rho} \right) \\ &= \frac{2}{r_n} \left(\frac{\partial \rho}{\partial r} \frac{\partial}{\partial \rho} \right) \left(\frac{\partial}{\partial \rho} \right) \\ &= \left(\frac{2}{r_n} \right)^2 \frac{\partial^2}{\partial \rho^2} \\ &= \frac{4}{r_n^2} \frac{\partial^2}{\partial \rho^2} \end{aligned}$$

So, substituting this in, we get:

$$EU(\rho) = \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} U(\rho) + \frac{2U(\rho)}{\mu(\rho r_n)^2} \hbar^2 l(l+1) - \frac{2Zk_e e^2}{\rho r_n} U(\rho)$$
$$= \frac{-\hbar^2}{2\mu} \frac{4}{r_n^2} \frac{\partial^2}{\partial \rho^2} U(\rho) + \frac{2U(\rho)}{\mu(\rho r_n)^2} \hbar^2 l(l+1) - \frac{2Zk_e e^2}{\rho r_n} U(\rho)$$

Now, since $r_n = \frac{na_0}{Z}$, $a_0 = \frac{\hbar^2}{\mu k_e e^2}$, $E_n = \frac{-Z^2 E_0}{n^2}$, and $E_0 = \frac{\mu k_e^2 e^4}{2\hbar^2}$.

$$\begin{split} EU\left(\rho\right) &= \frac{-\hbar^{2}}{2\mu} \frac{4}{r_{n}^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{2U\left(\rho\right)}{\mu\left(\rho r_{n}\right)^{2}} \hbar^{2}l\left(l+1\right) - \frac{2Zk_{e}e^{2}}{\rho r_{n}} U\left(\rho\right) \\ &= \frac{-\hbar^{2}}{2\mu} \frac{4}{\left(\frac{na_{0}}{a_{0}}\right)^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{2U\left(\rho\right)}{\mu\left(\rho\frac{na_{0}}{Z}\right)^{2}} \hbar^{2}l\left(l+1\right) - \frac{2Zk_{e}e^{2}}{\rho\frac{na_{0}}{Z}} U\left(\rho\right) \\ &= \frac{-\hbar^{2}}{2\mu} \frac{Z^{2}4}{\left(na_{0}\right)^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{2ZU\left(\rho\right)}{\mu\left(\rho na_{0}\right)^{2}} \hbar^{2}l\left(l+1\right) - \frac{2Z^{2}k_{e}e^{2}}{\rho na_{0}} U\left(\rho\right) \\ &= \frac{-\hbar^{2}}{2\mu} \frac{Z^{2}4}{\left(n\frac{\hbar^{2}}{\mu k_{e}e^{2}}\right)^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{2Z^{2}U\left(\rho\right)}{\mu\left(\rho n\frac{\hbar^{2}}{\mu k_{e}e^{2}}\right)^{2}} \hbar^{2}l\left(l+1\right) - \frac{2Z^{2}k_{e}e^{2}}{\rho n\frac{\hbar^{2}}{a}} U\left(\rho\right) \\ &= \frac{-\hbar^{2}}{2\mu} \frac{\left(\mu k_{e}e^{2}\right)^{2}Z^{2}4}{\left(n\hbar^{2}\right)^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{\left(\mu k_{e}e^{2}\right)^{2}2ZU\left(\rho\right)}{\mu\left(\rho n\hbar^{2}\right)^{2}} \hbar^{2}l\left(l+1\right) - \frac{2\mu e^{2}Z^{2}k_{e}^{2}e^{2}}{\rho n\hbar^{2}} U\left(\rho\right) \\ &= \frac{-\hbar^{2}}{2\mu} \frac{\mu^{2}k_{e}^{2}e^{4}Z^{2}4}{n^{2}\hbar^{4}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{\mu^{2}k_{e}^{2}e^{4}2Z^{2}U\left(\rho\right)}{\mu\rho^{2}n^{2}\hbar^{4}} \hbar^{2}l\left(l+1\right) - \frac{2\mu k_{e}^{2}e^{4}Z^{2}}{\rho n\hbar^{2}} U\left(\rho\right) \\ &= \frac{-1}{2} \frac{\mu k_{e}^{2}e^{4}Z^{2}4}{n^{2}\hbar^{2}} \frac{\partial^{2}}{\partial \rho^{2}} U\left(\rho\right) + \frac{\mu k_{e}^{2}e^{4}Z^{2}U\left(\rho\right)}{2\rho^{2}n^{2}\hbar^{2}} l\left(l+1\right) - \frac{4\mu k_{e}^{2}e^{4}Z^{2}}{\rho n\hbar^{2}} U\left(\rho\right) \end{split}$$

$$= -\frac{E_0 Z^2 4}{n^2} \frac{\partial^2}{\partial \rho^2} U(\rho) + \frac{E_0 Z^2 4 U(\rho)}{\rho^2 n^2} l(l+1) - \frac{4E_0 Z^2 n}{\rho n^2} U(\rho)$$

$$= 4E_n \frac{\partial^2}{\partial \rho^2} U(\rho) - 4E_n \frac{U(\rho)}{\rho^2} l(l+1) + 4E_n \frac{n}{\rho} U(\rho)$$

Here, we know that $E = E_n$, so we have E_n cancelling:

$$\begin{split} E_n U(\rho) &= 4E_n \frac{\partial^2}{\partial \rho^2} U(\rho) - 4E_n \frac{U(\rho)}{\rho^2} l(l+1) + 4E_n \frac{n}{\rho} U(\rho) \\ U(\rho) &= 4\frac{\partial^2}{\partial \rho^2} U(\rho) - 4\frac{U(\rho)}{\rho^2} l(l+1) + 4\frac{n}{\rho} U(\rho) \\ 0 &= 4\frac{\partial^2}{\partial \rho^2} U(\rho) - 4\frac{U(\rho)}{\rho^2} l(l+1) + 4\frac{n}{\rho} U(\rho) - U(\rho) \\ 0 &= \frac{\partial^2}{\partial \rho^2} U(\rho) - \frac{U(\rho)}{\rho^2} l(l+1) + \frac{n}{\rho} U(\rho) - \frac{U(\rho)}{4} \\ 0 &= \left(\frac{\partial^2}{\partial \rho^2} - \frac{l(l+1)}{\rho^2} + \frac{n}{\rho} - \frac{1}{4}\right) U(\rho) \end{split}$$

Part e

Use repeated product rules to show that

$$(fgh)'' = f''gh + fg''h + fgh'' + 2f'g'h + 2f'gh' + 2fg'h'$$

Use this and the substitution $U(\rho)=e^{-p/2}\rho^l L(\rho)$ to obtain Laguerre's differential equation

 $\rho L'' + (2l + 2 - \rho) L' + (n - l - 1) L = 0$

The solutions are associated Laguerre polynomials $L_{n-l-1}^{(2l+1)}(\rho).$

Assuming that these are all functions in x, we get:

$$\begin{aligned} \frac{\partial}{\partial x} fgh &= \frac{\partial}{\partial x} f(gh) \\ &= f \frac{\partial}{\partial x} gh + f'gh \\ &= f(gh' + g'h) + f'gh \\ &= fgh' + fg'h + f'gh \end{aligned}$$

and:

$$\begin{aligned} \frac{\partial^2}{\partial x^2} fgh &= \frac{\partial}{\partial x} \left(fgh' + fg'h + f'gh \right) \\ &= \frac{\partial}{\partial x} fgh' + \frac{\partial}{\partial x} fg'h + \frac{\partial}{\partial x} f'gh \\ &= \frac{\partial}{\partial x} f(gh') + \frac{\partial}{\partial x} f(g'h) + \frac{\partial}{\partial x} f'(gh) \\ &= f\frac{\partial}{\partial x} (gh') + f'(gh') + f\frac{\partial}{\partial x} (g'h) + f'(gh) + f'\frac{\partial}{\partial x} (gh) + f''(gh) \\ &= f(gh'' + g'h') + f'gh' + f(g'h' + g''h) + f'g'h + f'(gh' + g'h) + f''gh \\ &= fgh'' + fg'h' + f'gh' + fg'h' + fg''h + f'g'h + f'gh' + f'g'h + f''gh \end{aligned}$$

Here, it becomes necessary to change the given function, $U(\rho)$ by multiplying through by a factor ρ , so we get $\rho U(\rho) = e^{-p/2}\rho^{l+1}L(\rho)$. Doing this, we get:

$$\begin{array}{lll} 0 & = & \left(\frac{\partial^2}{\partial\rho^2} - \frac{l\left(l+1\right)}{\rho^2} + \frac{n}{\rho} - \frac{1}{4}\right)\rho U\left(\rho\right) \\ 0 & = & \frac{\partial^2}{\partial\rho^2}\rho U\left(\rho\right) - \frac{l\left(l+1\right)}{\rho^2}\rho U\left(\rho\right) + \frac{n}{\rho}\rho U\left(\rho\right) - \frac{1}{4}\rho U\left(\rho\right) \\ 0 & = & \frac{\partial^2}{\partial\rho^2}\rho U\left(\rho\right) - \frac{l\left(l+1\right)}{\rho^2}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) + \frac{n}{\rho}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) - \frac{1}{4}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) \\ 0 & = & \frac{\partial^2}{\partial\rho^2}\rho U\left(\rho\right) - \frac{l\left(l+1\right)}{\rho^2}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) + \frac{n}{\rho}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) - \frac{1}{4}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) \end{array}$$

Now, using the triple product rule from above, we can calculate the second derivative. But first, we find f', g', h', f'', g'', h'', with $f(\rho) = e^{-\rho/2}$, $g(\rho) = \rho^{l+1}$, $h(\rho) = L(\rho)$:

$$\begin{aligned} f' &= -\frac{1}{2}e^{-\rho/2} \\ g' &= (l+1)\,\rho^l \\ h' &= L'\,(\rho) \\ f'' &= \frac{1}{4}e^{-\rho/2} \\ g'' &= l\,(l+1)\,\rho^{l-1} \\ h'' &= L''\,(\rho) \end{aligned}$$

So, substituting these into the second derivative formula, we get:

$$(fgh)'' = \frac{1}{4} e^{-\rho/2} \rho^{l+1} L(\rho) + e^{-\rho/2} l(l+1) \rho^{l-1} L(\rho) + e^{-\rho/2} \rho^{l+1} L''(\rho) - 2\frac{1}{2} e^{-\rho/2} (l+1) \rho^{l} L(\rho) - 2\frac{1}{2} e^{-\rho/2} \rho^{l+1} L'(\rho) + 2e^{-\rho/2} (l+1) \rho^{l} L'(\rho)$$

Then, substituting this into the results from part (d), we get:

$$\begin{array}{lll} 0 &=& \frac{1}{4}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) + e^{-\rho/2}l\left(l+1\right)\rho^{l-1}L\left(\rho\right) + e^{-\rho/2}\rho^{l+1}L''\left(\rho\right) \\ &\quad -2\frac{1}{2}e^{-\rho/2}\left(l+1\right)\rho^{l}L\left(\rho\right) - 2\frac{1}{2}e^{-\rho/2}\rho^{l+1}L'\left(\rho\right) + 2e^{-\rho/2}\left(l+1\right)\rho^{l}L'\left(\rho\right) \\ &\quad -\frac{l\left(l+1\right)}{\rho^{2}}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) + \frac{n}{\rho}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) - \frac{1}{4}e^{-\rho/2}\rho^{l+1}L\left(\rho\right) \\ &=& \frac{1}{4}\rho^{l+1}L\left(\rho\right) + l\left(l+1\right)\rho^{l-1}L\left(\rho\right) + \rho^{l+1}L''\left(\rho\right) - \left(l+1\right)\rho^{l}L\left(\rho\right) - \rho^{l+1}L'\left(\rho\right) + 2\left(l+1\right)\rho^{l}L'\left(\rho\right) \\ &\quad -\frac{l\left(l+1\right)}{\rho^{2}}\rho^{l+1}L\left(\rho\right) + \frac{n}{\rho}\rho^{l+1}L\left(\rho\right) - \frac{1}{4}\rho^{l+1}L\left(\rho\right) \\ &=& \frac{1}{4}\rho^{1}L\left(\rho\right) + l\left(l+1\right)\rho^{-1}L\left(\rho\right) + \rho^{1}L''\left(\rho\right) - \left(l+1\right)L\left(\rho\right) - \rho^{1}L'\left(\rho\right) + 2\left(l+1\right)L'\left(\rho\right) \\ &\quad -\frac{l\left(l+1\right)}{\rho^{2}}\rho^{1}L\left(\rho\right) + \frac{n}{\rho}\rho^{1}L\left(\rho\right) - \frac{1}{4}\rho^{1}L\left(\rho\right) \\ &=& l\left(l+1\right)\rho^{-1}L\left(\rho\right) + \rhoL''\left(\rho\right) - \left(l+1\right)L\left(\rho\right) - \rhoL'\left(\rho\right) + 2\left(l+1\right)L'\left(\rho\right) \\ &\quad -l\left(l+1\right)P^{-1}L\left(\rho\right) + \frac{n}{\rho}\rhoL\left(\rho\right) \\ &=& \rhoL''\left(\rho\right) - \left(l+1\right)L\left(\rho\right) - \rhoL'\left(\rho\right) + nL\left(\rho\right) - \left(l+1\right)L\left(\rho\right) \\ &=& \rhoL''\left(\rho\right) + (2l+2-\rho)L'\left(\rho\right) + \left(n-l+1\right)L\left(\rho\right) \end{array}$$

$$\rho L'' + (2l+2-\rho) L' + (n-l-1) L = 0$$

Part f

Using the values of $L_{\kappa}^{(\alpha)}$ from http://mathworld.wolfram.com/LaguerrePolynomial.html, Eqs. 32-35, substitute back to find the radial wave functions $R_{nl}(r)$ for n = 1, 2, and 3. Compare your answers with table 7-2 in the text. What is the physical significance of κ ?

Equations 32 through 35 $L_{\kappa}^{(\alpha)}$ are:

Now we can substitute these back into $U_{\kappa}(\rho) = e^{-p/2} \rho^l L_{\kappa}^{(\alpha)}(\rho)$, using $\rho = \frac{2r}{r_n}$ and $r_n = \frac{na_0}{Z} = na_0$:

$$U_{0}(\rho) = e^{-p/2}\rho^{l}(1)$$

$$U_{1}(\rho) = e^{-p/2}\rho^{l}(-\rho + \alpha + 1)$$

$$U_{2}(\rho) = e^{-p/2}\rho^{l}\left(\frac{1}{2}\left[\rho^{2} - 2(\alpha + 2)\rho + (\alpha + 1)(\alpha + 2)\right]\right)$$

$$U_{0}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l}$$

$$U_{1}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l} \left(-\frac{2r}{na_{0}} + \alpha + 1\right)$$

$$U_{2}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l} \left(\frac{1}{2}\left[\left(\frac{2r}{na_{0}}\right)^{2} - 2\left(\alpha + 2\right)\left(\frac{2r}{na_{0}}\right) + (\alpha + 1)\left(\alpha + 2\right)\right]\right)$$

For n = 1, l = 0 (with $\alpha = 2l + 1 = 1$, and $\kappa = n - l - 1 = 0$), we get:

$$U_0(\frac{2r}{na_0}) = e^{-\frac{2r}{2na_0}} \left(\frac{2r}{na_0}\right)^l$$
$$U_0(\frac{2r}{a_0}) = e^{-\frac{2r}{2a_0}}$$
$$U_0(\frac{2r}{a_0}) = e^{-\frac{r}{a_0}}$$

For n=2, l=0 (with $\alpha=2l+1=1$, and $\kappa=n-l-1=1$), we get:

$$U_{1}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l} \left(-\frac{2r}{na_{0}} + \alpha + 1\right)$$
$$U_{1}\left(\frac{r}{a_{0}}\right) = e^{-\frac{2r}{4a_{0}}} \left(-\frac{2r}{2a_{0}} + 1 + 1\right)$$
$$U_{1}\left(\frac{r}{a_{0}}\right) = e^{-\frac{r}{2a_{0}}} \left(2 - \frac{r}{a_{0}}\right)$$
$$U_{1}\left(\frac{r}{a_{0}}\right) = 2e^{-\frac{r}{2a_{0}}} \left(1 - \frac{r}{2a_{0}}\right)$$

For n = 3, l = 0 (with $\alpha = 2l + 1 = 1$, and $\kappa = n - l - 1 = 2$), we get:

$$\begin{aligned} U_2(\frac{2r}{na_0}) &= e^{-\frac{2r}{2na_0}} \left(\frac{2r}{na_0}\right)^l \left(\frac{1}{2} \left[\left(\frac{2r}{na_0}\right)^2 - 2\left(\alpha + 2\right)\left(\frac{2r}{na_0}\right) + \left(\alpha + 1\right)\left(\alpha + 2\right)\right]\right) \\ U_2(\frac{2r}{3a_0}) &= e^{-\frac{2r}{6a_0}} \left(\frac{1}{2} \left[\left(\frac{2r}{3a_0}\right)^2 - 2\left(1 + 2\right)\left(\frac{2r}{3a_0}\right) + \left(1 + 1\right)\left(1 + 2\right)\right]\right) \\ U_2(\frac{2r}{3a_0}) &= e^{-\frac{r}{3a_0}} \left(\frac{1}{2} \left[\frac{4r^2}{9a_0^2} - 6\left(\frac{2r}{3a_0}\right) + 6\right]\right) \\ U_2(\frac{2r}{3a_0}) &= 3e^{-\frac{r}{3a_0}} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right) \end{aligned}$$

Next, we do n = 2, l = 1 (with $\alpha = 2l + 1 = 3$, and $\kappa = n - l - 1 = 0$), and we get:

$$U_0(\frac{2r}{na_0}) = e^{-\frac{2r}{2na_0}} \left(\frac{2r}{na_0}\right)^l$$
$$U_0(\frac{r}{a_0}) = e^{-\frac{2r}{2a_0}} \left(\frac{2r}{2a_0}\right)$$
$$U_0(\frac{r}{a_0}) = e^{-\frac{r}{a_0}} \frac{r}{a_0}$$

Next, we do n = 3, l = 1 (with $\alpha = 2l + 1 = 3$, and $\kappa = n - l - 1 = 1$), and we get:

$$U_{1}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l} \left(-\frac{2r}{na_{0}} + \alpha + 1\right)$$
$$U_{1}\left(\frac{2r}{3a_{0}}\right) = e^{-\frac{2r}{6a_{0}}} \left(\frac{2r}{3a_{0}}\right) \left(-\frac{2r}{3a_{0}} + 3 + 1\right)$$
$$U_{1}\left(\frac{2r}{3a_{0}}\right) = e^{-\frac{r}{3a_{0}}} \left(\frac{2}{3}\right) \left(\frac{r}{a_{0}}\right) \left(4 - \frac{2r}{3a_{0}}\right)$$
$$U_{1}\left(\frac{2r}{3a_{0}}\right) = e^{-\frac{r}{3a_{0}}} \left(\frac{8}{3}\right) \left(\frac{r}{a_{0}}\right) \left(1 - \frac{r}{6a_{0}}\right)$$

Finally, we do n = 3, l = 2 (with $\alpha = 2l + 1 = 5$, and $\kappa = n - l - 1 = 0$), and we get:

$$U_{0}\left(\frac{2r}{na_{0}}\right) = e^{-\frac{2r}{2na_{0}}} \left(\frac{2r}{na_{0}}\right)^{l}$$
$$U_{0}\left(\frac{2r}{3a_{0}}\right) = e^{-\frac{2r}{6a_{0}}} \left(\frac{2r}{3a_{0}}\right)^{2}$$
$$U_{0}\left(\frac{2r}{3a_{0}}\right) = e^{-\frac{r}{3a_{0}}} \left(\frac{4}{9}\right) \left(\frac{r^{2}}{a_{0}^{2}}\right)$$

After looking at many pictures, it appears as though κ corresponds to the number of radial lobes (plus one) in the probability distribution for the electron orbitals.

Part g

Show that the ground-state wave function is normalized:

$$\int d^3r \left| \psi_{100}(r,\theta,\phi) \right|^2 = 1$$

We know that $\psi_{100}(r,\theta,\phi) = C_{nlm}R_{21}(r)Y_{00}(\theta,\phi)$ [Tipler & Llewellyn, p. 7-30]. We know that $R_{21}(r) = \frac{2}{\sqrt{a_0^3}}e^{-r/a_0}$ and $Y_{00}(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$ Using the integral above, and substituting the spherical Jacobian for d^3r , we get:

$$\begin{split} \int d^3 r \left| \psi_{100}(r,\theta,\phi) \right|^2 &= 1 \\ \int_0^\infty \int_0^\pi \int_0^{2\pi} |C_{nlm} R_{21}(r) Y_{00}(\theta,\phi)|^2 r^2 \sin \theta \, d\phi d\theta dr &= 1 \\ \int_0^\infty \int_0^\pi \int_0^{2\pi} \left| C_{nlm} \frac{2}{\sqrt{a_0^2}} e^{-r/a_0} \sqrt{\frac{1}{4\pi}} \right|^2 r^2 \sin \theta \, d\phi d\theta dr &= 1 \\ \int_0^\infty \left| C_{nlm} \frac{2}{\sqrt{a_0^2}} e^{-r/a_0} \sqrt{\frac{1}{4\pi}} \right|^2 r^2 dr \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi &= 1 \\ 2\pi \int_0^\infty \left| C_{nlm} \frac{2}{\sqrt{a_0^2}} e^{-r/a_0} \sqrt{\frac{1}{4\pi}} \right|^2 r^2 dr \int_0^\pi \sin \theta \, d\theta = 1 \\ 2\pi \left(-\cos \theta \right|_0^\pi \right) \int_0^\infty \left| C_{nlm} \frac{2}{\sqrt{a_0^2}} e^{-r/a_0} \sqrt{\frac{1}{4\pi}} \right|^2 r^2 dr &= 1 \\ 4\pi \int_0^\infty \frac{1}{4\pi} \frac{4}{a_0^2} C_{nlm}^2 e^{-2r/a_0} r^2 dr &= 1 \\ \frac{4}{a_0^2} C_{nlm}^2 \left(-\frac{a_0}{2} e^{-2r/a_0} r^2 \right) \right|_0^\infty + a_0 \left(-\frac{a_0}{2} e^{-2r/a_0} r \right) \right|_0^\infty = 1 \\ \frac{4}{a_0^2} C_{nlm}^2 \left(-\frac{a_0}{2} e^{-2r/a_0} r^2 \right) \right|_0^\infty + a_0 \left(-\frac{a_0}{2} e^{-2r/a_0} r \right) \right) = 1 \\ \frac{4}{a_0^2} C_{nlm}^2 \left(-\frac{a_0}{2} e^{-2r/a_0} r^2 + a_0 \left(-\frac{a_0}{2} e^{-2r/a_0} r \right) \right) \right|_0^\infty = 1 \\ \frac{4}{a_0^2} C_{nlm}^2 \left(-\frac{a_0}{2} e^{-2r/a_0} r^2 + a_0 \left(-\frac{a_0}{2} r^2 - \frac{a_0^2}{4} r^2 - \frac{a_0^2}{4} r^2 \right) \right) \right|_0^\infty = 1 \\ \frac{4}{a_0^2} C_{nlm}^2 e^{-2r/a_0} \left(-\frac{a_0}{2} r^2 - \frac{a_0^2}{2} r - \frac{a_0^2}{4} r^2 \right) \right|_0^\infty = 1 \\ e^{-2r/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) \right|_0^\infty = 1 \\ e^{-2r/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) \right|_0^\infty = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) - e^{-20/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) \right|_0^\infty = 1 \\ e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = \frac{1}{C_{nlm}^2} e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) + 1 = \frac{1}{C_{nlm}^2} e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) = 1 \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2} r^2 - \frac{2}{a_0} r - 1 \right) \\ \frac{e^{-2m/a_0} \left(-\frac{2}{a_0^2$$

But, by L'Hopital's rule, we know that $e^{-2\infty/a_0}\left(-\frac{2}{a_0^2}\infty^2-\frac{2}{a_0}\infty-1\right)=0$, so we have that:

$$0 = \frac{1}{C_{nlm}^2} - 1$$

1

But, this is only true if $C_{nlm}^2 = 1$, which tells us that $\psi(r, \theta, \phi)$ was already normalized.

Problem 7.26

Show that an electron in the n = 2, l = 1 state of hydrogen is most likely to be found at $r = 4a_0$.

Generally, ψ_{nlm} is defined by $\psi_{nlm}(r,\theta,\phi) = C_{nlm}R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi) = C_{nlm}R_{nl}(r)Y_{lm}(\theta,\phi)$. We also know that:

$$\int \psi^* \psi d\tau = 1$$
$$\int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^* \psi r^2 \sin \theta \, d\phi d\theta dr = 1$$

And, we know that

$$R_{21}(r) = \frac{1}{2\sqrt{6a_0^3}} \frac{r}{a_0} e^{-r/2a_0}$$
$$Y_{10}(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta$$
$$Y_{1\pm 1}(\theta, \phi) = \pm \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$$

If we recognize that $R_{21}(r)$ does not depend at all upon either θ or ϕ , and that neither $Y_{10}(\theta, \phi)$ nor $Y_{1\pm 1}(\theta, \phi)$ depend on r, we can rewrite the integral from above:

$$\int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} \psi^{*} \psi r^{2} \sin \theta \, d\phi d\theta dr = 1$$
$$\int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} C_{21m}^{*} R_{21}^{*} Y_{1m}^{*} C_{nlm} R_{21} Y_{1m} r^{2} \sin \theta \, d\phi d\theta dr = 1$$
$$\int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} C_{21m}^{*} C_{21m} R_{21}^{2} Y_{1m}^{*} Y_{1m} r^{2} \sin \theta \, d\phi d\theta dr = 1$$
$$C_{21m}^{*} C_{21m} \int_{0}^{\infty} R_{21}^{2} r^{2} dr \int_{0}^{\pi} \int_{0}^{2\pi} Y_{1m}^{*} Y_{1m} \sin \theta \, d\phi d\theta = 1$$

Strictly speaking, the next two steps are not required. $Y(\theta, \phi)$ will only scale the value of the function at $r = 4a_0$, but it will not change that $r = 4a_0$ is where the maximal occurs. However, since it is instructive to see these integrals, and since the work has already been done, they are included. We can now find $\int_0^{\pi} \int_0^{2\pi} Y_{1m}^* Y_{1m} \sin \theta \, d\phi d\theta$ for both m = 0 and $m = \pm 1$. For m = 0, we have:

$$\int_0^{\pi} \int_0^{2\pi} Y_{10}^* Y_{10} \sin \theta \, d\phi d\theta = \int_0^{\pi} \int_0^{2\pi} Y_{10}^2 \sin \theta \, d\phi d\theta$$
$$= \int_0^{\pi} \int_0^{2\pi} \left(\sqrt{\frac{3}{4\pi}} \cos \theta \right)^2 \sin \theta \, d\phi d\theta$$
$$= \int_0^{\pi} \int_0^{2\pi} \frac{3}{4\pi} \cos^2 \theta \sin \theta \, d\phi d\theta$$
$$= \frac{3}{4\pi} \int_0^{\pi} \int_0^{2\pi} \cos^2 \theta \sin \theta \, d\phi d\theta$$
$$= \frac{3}{4\pi} \int_0^{\pi} \cos^2 \theta \sin \theta \, d\theta \int_0^{2\pi} d\phi$$

$$= \frac{3}{4\pi} (2\pi) \int_0^\pi \cos^2 \theta \sin \theta \, d\theta$$
$$= \frac{3}{2} \int_0^\pi \cos^2 \theta \sin \theta \, d\theta$$
$$= \frac{3}{2} \left(-\frac{1}{3} \cos^3 \theta \Big|_{\theta=0}^\pi \right)$$
$$= \frac{1}{2} \left(-(-1-1) \right)$$
$$= 1$$

For $m = \pm 1$ we have:

$$\begin{split} \int_{0}^{\pi} \int_{0}^{2\pi} Y_{1\pm 1}^{*} Y_{1\pm 1} \sin \theta \, d\phi d\theta &= \int_{0}^{\pi} \int_{0}^{2\pi} \left(\pm \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{-i\phi} \right) \left(\pm \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{i\phi} \right) \sin \theta \, d\phi d\theta \\ &= \int_{0}^{\pi} \int_{0}^{2\pi} \frac{3}{8\pi} \sin^{3} \theta \left(e^{-i\phi} \right) \left(e^{i\phi} \right) \sin \theta \, d\phi d\theta \\ &= \int_{0}^{\pi} \int_{0}^{2\pi} \frac{3}{8\pi} \sin^{3} \theta \left(e^{-i\phi+i\phi} \right) \, d\phi d\theta \\ &= \frac{3}{8\pi} \int_{0}^{\pi} \sin^{3} \theta \, d\theta \, d\theta \\ &= \frac{3}{8\pi} \int_{0}^{\pi} \sin^{3} \theta \, d\theta \int_{0}^{2\pi} d\phi \\ &= \frac{3}{4} \int_{0}^{\pi} \left(1 - \cos^{2} \theta \right) \sin \theta \, d\theta \\ &= \frac{3}{4} \left(\int_{0}^{\pi} \sin \theta \, d\theta - \int_{0}^{\pi} \cos^{2} \theta \sin \theta \, d\theta \right) \\ &= \frac{3}{4} \left(\cos^{3} \theta - 3 \cos \theta \right) \Big|_{\theta=0}^{\pi} \\ &= \frac{1}{4} \left((\cos^{3} \pi - 3 \cos \pi) - (\cos^{3} 0 - 3 \cos 0) \right) \\ &= \frac{1}{4} \left(-1 - 3 \left(-1 \right) - 1 + 3 \left(1 \right) \right) \\ &= \frac{1}{4} \left(-1 + 3 - 1 + 3 \right) \\ &= 1 \end{split}$$

So, we now know that $Y_{1m}\left(\theta,\phi\right)=1.$ So we're left with:

$$C_{21m}^* C_{21m} \int_0^\infty R_{21}^2 r^2 dr = 1$$

However, looking ahead, we know that we will be finding where the derivative of some function is zero, and a constant factor will not change where the derivative is zero, just the magnitude of the function at that point. So, we have $\int_0^\infty C_{21m}^* C_{21m} R_{21}^2 r^2 dr = 1$,

which looks like a probability distribution integration, of the form $\int_0^\infty P(r) dr = 1$. So, let's let $P(r) dr = C_{21m}^* C_{21m} R_{21}^2 r^2 dr$, so $P(r) = C_{21m}^* C_{21m} R_{21}^2 r^2$, and the maximum probability will occur at $\frac{dP}{dr} = 0$. This is:

$$\frac{d}{dr}P(r) = 0$$

$$\frac{d}{dr}(C_{21m}^*C_{21m}R_{21}^2r^2) = 0$$

$$C_{21m}^*C_{21m}\frac{d}{dr}\left(\left(\frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0}e^{-r/2a_o}\right)^2r^2\right) = 0$$

$$C_{21m}^*C_{21m}\frac{d}{dr}\left(\left(\frac{1}{2a_0\sqrt{6a_0^3}}\right)^2r^2e^{-r/a_o}r^2\right) = 0$$

$$C_{21m}^*C_{21m}\left(\frac{1}{2a_0\sqrt{6a_0^3}}\right)^2\frac{d}{dr}\left(r^4e^{-r/a_o}\right) = 0$$

$$C_{21m}^*C_{21m}\left(\frac{1}{2a_0\sqrt{6a_0^3}}\right)^2\left(r^4\left(-\frac{1}{a_0}\right)e^{-r/a_0}+4r^3e^{-r/a_0}\right) = 0$$

$$C_{21m}^*C_{21m}\left(\frac{1}{2a_0\sqrt{6a_0^3}}\right)^2r^3e^{-r/a_0}\left(-\frac{r}{a_0}+4\right) = 0$$

Since e^{-r/a_0} is never zero, and since r = 0 is impossible because l = 1 so the electron must have angular momentum which would not happen at r = 0, we have:

$$\frac{r}{a_0} + 4 = 0$$

$$-\frac{r}{a_0} = -4$$

$$r = -4(-a_0)$$

$$r = 4a_0$$

Problem 7.29

If a classical system does not have a constant charge-to-mass ratio throughout the system, the magnetic moment can be written

$$\mu = g \frac{Q}{2M} L$$

where Q is the total charge, M is the total mass, and $g \neq 1.$

Part a

Show that g = 2 for a solid cylinder $(I = \frac{1}{2}MR^2)$ that spins about its axis and has a uniform charge on its cylindrical surface.

We know that $\mu = iA$. We also know, in this case, that the area of the loop about which the charge is circulating is $A = \pi R^2$. To find *i*, we must recognize that current is equal to charge times the frequency, or i = Qf, that $f = \frac{\omega}{2\pi}$, and that $L = I\omega$. This gives us:

$$\mu = iA$$

$$= Qf\pi R^{2}$$

$$= Q\frac{\omega}{2\pi}\pi R^{2}$$

$$= Q\frac{1}{2}\left(\frac{L}{I}\right)R^{2}$$

$$= Q\frac{1}{2}\left(\frac{L}{\frac{1}{2}MR^{2}}\right)R^{2}$$

$$= Q\left(\frac{L}{M}\right)$$

$$= 2\frac{Q}{2M}L$$

So,
$$g = 2$$
.

Part b

Show that g = 2.5 for a solid sphere ($I = 2MR^2/5$) that has a ring of charge on the surface at the equator, as shown in Figure 7-33 [Tipler & Llewellyn, p. 309].

In this case, practically everything is identical to part (a) except for the moment of inertia. So we have:

$$\mu = iA$$

$$= Qf\pi R^{2}$$

$$= Q\frac{\omega}{2\pi}\pi R^{2}$$

$$= Q\frac{1}{2}\left(\frac{L}{I}\right)R^{2}$$

$$= Q\frac{1}{2}\left(\frac{L}{\frac{2}{5}MR^{2}}\right)R^{2}$$

$$= \frac{5}{4}Q\left(\frac{L}{M}\right)$$

$$= \frac{5}{2}\cdot\frac{Q}{2M}L$$

So, $g = \frac{5}{2} = 2.5$.

Problem 7.39

Consider a system of two electrons, each with l = 1 and $s = \frac{1}{2}$.

Part a

What are the possible values of the quantum number for the total orbital angular momentum $\vec{L} = \vec{L}_1 + \vec{L}_2$?

The quantum number, L, for \vec{L} has possible values $l_1 + l_2, l_1 + l_2 - 1, \ldots, |l_1 - l_2|$, where l_1 and l_2 are the total orbital angular momentum quantum numbers for \vec{L}_1 and \vec{L}_2 respectively. These are both 1, so, we have that L = 2, L = 1, or L = 0.

Part b

What are the possible values of the quantum number S for the total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$?

Similarly to the above, we have quantum numbers, s_1 and s_2 equal to $\frac{1}{2}$, so we have the total spin quantum number as S = 1 or S = 0.

Part c

Using the results of parts (a) and (b), find the possible quantum numbers j for the combination $\vec{J} = \vec{L} + \vec{S}$.

The possible quantum numbers for j can be either j = L + S or j = |L - S|. Since we have multiple possibilities for L and S, we try each combination to find all possible quantum numbers. So, for j we have: 2 + 1 = 3, 2 - 1 = 1, 2 + 0 = 2, 2 - 0 = 2, 1 + 1 = 2, 1 - 1 = 0, 1 + 0 = 1, 1 - 0 = 0, 0 + 1 = 1, |0 - 1| = 1, 0 + 0 = 0, 0 - 0 = 0. So, j can equal: 3, 2, 1, or 0.

Part d

What are the possible quantum numbers j_1 and j_2 for the total angular momentum of each particle?

Since $l_1 = l_2 = 1$ and $s_1 = s_2 = \frac{1}{2}$, both j_1 and j_2 have the same possible quantum numbers. These are given, as in part (c), by $j_1 = l_1 + s_1$ or $j_1 = |l_1 - s_1|$. So, we get the possible quantum numbers for $j_1 = j_2$ to be 1.5 or 0.5.

Part e

Use the results of part (d) to calculate the possible values of j from the combinations of j_1 and j_2 . Are these the same as in part (c)?

We know that that the quantum number, j, for \vec{J} has possible values $j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|$, So, using the results from part (d), we see that the possible values for j are the integers between 1.5 + 1.5 = 3 and 1.5 - 1.5 = 0, or between 1.5 + 0.5 = 2 and 1.5 - 0.5 = 1, or between 0.5 + 1.5 = 2 and |0.5 - 1.5| = 1, or between 0.5 + 0.5 = 1 and 0.5 - 0.5 = 0. So, all the possible values are: 3, 2, 1, and 0. This is the same as in part (c).

Problem 7.44

Write the electron configuration of the following elements:

Part a

Carbon

Carbon has Z = 6, so its electron configuration is $1s^22s^22p^2$.

Part b

Oxygen

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Oxygen has Z = 8, so its electron configuration is 1s^2 2s^2 2p^4.
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Argon

Argon has Z = 18, so its electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^6$.

Problem 7.73

In the anomalous Zeeman effect, the external magnetic field is much weaker than the internal field seen by the electron as a result of its orbital motion. In the vector model (Figure 7-30 [www.whfreeman.com/tiplermodernphysics5e]) the vectors \vec{L} and \vec{S} precess rapidly around \vec{J} because of the internal field and \vec{J} precesses slowly around the external field. The energy splitting is found by first calculating the component of the magnetic moment μ_J in the direction of \vec{J} and then finding the component of \vec{B} .

Part a

Show that $\mu_J = \frac{\vec{\mu} \cdot \vec{J}}{I}$ can be written

$$\mu_J = -\frac{\mu_B}{\hbar J} \left(L^2 + 2S^2 + 3\vec{S} \cdot \vec{L} \right)$$

We can substitute $\vec{\mu} = \frac{-g_L \mu_B \vec{L}}{\hbar} + \frac{-g_S \mu_B \vec{S}}{\hbar} = -\frac{\mu_B}{\hbar} \left(g_L \vec{L} + g_S \vec{S} \right)$, where $g_L = 1$ and $g_S \approx 2$ ([Tipler & Llewellyn, p. 287]), and $\vec{J} = \vec{L} + \vec{S}$, and we get:

$$\begin{split} \mu_J &= \frac{\vec{\mu} \cdot \vec{J}}{J} \\ &= \frac{\left(-\frac{\mu_B(\vec{L}+2\vec{S})}{\hbar}\right) \cdot \left(\vec{L}+\vec{S}\right)}{J} \\ &= \frac{\left(-\frac{\mu_B}{\hbar}\right) \left(\left(\vec{L}+2\vec{S}\right) \cdot \left(\vec{L}+\vec{S}\right)\right)}{J} \\ &= \frac{-\mu_B}{\hbar J} \left(\left(\vec{L}+2\vec{S}\right) \cdot \left(\vec{L}+\vec{S}\right)\right) \\ &= \frac{-\mu_B}{\hbar J} \left(\vec{L} \cdot \left(\vec{L}+\vec{S}\right) + 2\vec{S} \cdot \left(\vec{L}+\vec{S}\right)\right) \\ &= \frac{-\mu_B}{\hbar J} \left(\left(\vec{L} \cdot \vec{L}+\vec{L} \cdot \vec{S}\right) + \left(2\vec{S} \cdot \vec{L}+2\vec{S} \cdot \vec{S}\right)\right) \\ &= \frac{-\mu_B}{\hbar J} \left(L^2 + \vec{L} \cdot \vec{S} + 2\vec{L} \cdot \vec{S} + 2S^2\right) \\ &= -\frac{\mu_B}{\hbar J} \left(L^2 + 2S^2 + 3\vec{L} \cdot \vec{S}\right) \end{split}$$

Part b

From $J^2 = \left(\vec{L} + \vec{S}\right) \cdot \left(\vec{L} + \vec{S}\right)$ show that $\vec{S} \cdot \vec{L} = \frac{1}{2} \left(J^2 - L^2 - S^2\right)$.

This is, easily:

$$J^{2} = \left(\vec{L} + \vec{S}\right) \cdot \left(\vec{L} + \vec{S}\right)$$
$$J^{2} = \left(\vec{L} \cdot \left(\vec{L} + \vec{S}\right) + \vec{S} \cdot \left(\vec{L} + \vec{S}\right)\right)$$

$$\begin{array}{rcl} J^2 &=& \vec{L} \cdot \vec{L} + \vec{L} \cdot \vec{S} + \vec{S} \cdot \vec{L} + \vec{S} \cdot \vec{S} \\ J^2 &=& \vec{L} \cdot \vec{L} + \vec{S} \cdot \vec{L} + \vec{S} \cdot \vec{L} + \vec{S} \cdot \vec{S} \\ J^2 &=& L^2 + 2\vec{S} \cdot \vec{L} + S^2 \\ \frac{1}{2} \left(J^2 - L^2 - S^2 \right) &=& \vec{S} \cdot \vec{L} \end{array}$$

Part c

Substitute your result in part (b) into that of part (a) to obtain

$$\mu_J = -\frac{\mu_B}{2\hbar J} \left(3J^2 + S^2 - L^2\right)$$

This becomes:

$$\begin{aligned} \mu_J &= -\frac{\mu_B}{\hbar J} \left(L^2 + 2S^2 + 3\vec{L} \cdot \vec{S} \right) \\ &= -\frac{\mu_B}{\hbar J} \left(L^2 + 2S^2 + 3\frac{1}{2} \left(J^2 - L^2 - S^2 \right) \right) \\ &= -\frac{\mu_B}{2\hbar J} \left(2L^2 + 4S^2 + 3J^2 - 3L^2 - 3S^2 \right) \\ &= -\frac{\mu_B}{2\hbar J} \left(3J^2 - L^2 + S^2 \right) \end{aligned}$$

Part d

Multiply your result by $J_{\boldsymbol{z}}/J$ to obtain

$$\mu_z = -\mu_B \left(1 + \frac{J^2 + S^2 - L^2}{2J^2} \right) \frac{J_z}{\hbar}$$

This becomes:

$$\begin{aligned} -\frac{\mu_B}{2\hbar J} \left(3J^2 - L^2 + S^2 \right) \left(\frac{J_z}{J} \right) &= -\frac{\mu_B J_z}{2\hbar J^2} \left(3J^2 - L^2 + S^2 \right) \\ &= -\frac{\mu_B J_z}{\hbar} \left(\frac{3J^2 - L^2 + S^2}{2J^2} \right) \\ &= -\mu_B \left(\frac{2J^2}{2J^2} + \frac{J^2 - L^2 + S^2}{2J^2} \right) \frac{J_z}{\hbar} \\ &= -\mu_B \left(1 + \frac{J^2 - L^2 + S^2}{2J^2} \right) \frac{J_z}{\hbar} \end{aligned}$$