Physics 220
Homework #5
Spring 2017
Due Wednesday, 5/10/17

** Note this assignment has been updated from the original one. **

1. Griffith's 4.11

   a. From equation 4.82 we have $R_{20} = \frac{c}{2a}(1-\frac{r}{2a})e^{-\frac{r}{2a}}$. Applying the normalization condition (and evaluating the integral on Mathematica) and determining the wave function we have:

$$1 = \frac{c^2}{4a^2}\int_0^\infty (1-\frac{r}{2a})^2 e^{-\frac{r}{a}} r^2\, dr = \frac{c^2}{4a^2}\left(2a^3\right) \rightarrow c = \sqrt{\frac{2}{a}}$$

$$\therefore \left|\psi_{200}\right\rangle = R_{20}Y_0^0 = \sqrt{\frac{2}{a}}\frac{1}{2a}(1-\frac{r}{2a})e^{-\frac{r}{2a}}\frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{8\pi a^3}}(1-\frac{r}{2a})e^{-\frac{r}{2a}}.$$

   b. From equation 4.83 we have $R_{21} = \frac{c}{4a^2} r e^{-\frac{r}{2a}}$. Applying the normalization condition (evaluating the integral on Mathematica) and determining the wave function we have:

$$1 = \frac{c^2}{16a^4}\int_0^\infty r^2 e^{-\frac{r}{a}} r^2\, dr = \frac{c^2}{16a4}\left(24a^5\right) \rightarrow c = \sqrt{\frac{2}{3a}}$$

$$\therefore \left|\psi_{210}\right\rangle = R_{21}Y_1^0 = \sqrt{\frac{2}{3a}}\frac{1}{4a^2} r e^{-\frac{r}{2a}}\left(\sqrt{\frac{3}{4\pi}}\cos\theta\right) = \frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2} r e^{-\frac{r}{2a}}\cos\theta \quad .$$

$$\therefore \left|\psi_{211}\right\rangle = R_{21}Y_1^1 = \sqrt{\frac{2}{3a}}\frac{1}{4a^2} r e^{-\frac{r}{2a}}\left(-\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}\right) = -\frac{1}{\sqrt{\pi a}}\frac{1}{8a^2} r e^{-\frac{r}{2a}}\sin\theta e^{i\phi}$$

$$\therefore \left|\psi_{21-1}\right\rangle = R_{21}Y_1^{-} = \sqrt{\frac{2}{3a}}\frac{1}{4a^2} r e^{-\frac{r}{2a}}\left(\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi}\right) = \frac{1}{\sqrt{\pi a}}\frac{1}{8a^2} r e^{-\frac{r}{2a}}\sin\theta e^{-i\phi}$$

2. Griffith's 4.14

   The probability is: $P=\int_0^\infty |R|^2 r^2\,dr\int_0^\pi |\Theta|^2 \sin\theta\, d\theta \int_0^{2\pi} |\Phi|^2\, d\phi$ and for the ground state of hydrogen we have $|\psi_{100}\rangle = R_{10}Y_0^0 = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$. Thus we have

   $P=\int_0^\infty \left|\frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}\right|^2 r^2\,dr \int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi = \int_0^\infty \frac{4\pi}{\pi a^3} e^{-\frac{2r}{a}} r^2\, dr$, so that the probability density is

   $\frac{dP}{dr} = 4\pi r^2 |R(r)|^2 = \frac{4\pi r^2}{\pi a^3} e^{-\frac{2r}{a}}$.

   To find a maximum we set the derivative of the radial probability density equal to zero and solve for the r-coordinate. We have:

   $\frac{d}{dr}\left(\frac{dP}{dr}\right) = \frac{d}{dr}\left(\frac{4}{a^3} e^{-\frac{2r}{a}} r^2\right) = 0 \rightarrow \left(2re^{-\frac{2r}{a}} - \frac{2}{a} r^2 e^{-\frac{2r}{a}}\right) = 0 \rightarrow r = a$.

3. Griffith's 4.39

   We start with the radial wave equation $\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2m}{\hbar^2}(V-E)R = l(l+1)R$ and use the change of variables $u = rR$ to write the radial wave equation as

   $\frac{d^2u}{dr^2} - \frac{2m}{\hbar^2}\left(\frac{m\omega^2}{2} r^2 - E + \frac{\hbar^2}{2m} l(l+1)\right)u = 0$. (This derivation was done in class.)

   Distributing the constant term through the parenthesis we have

   $\frac{d^2u}{dr^2} + \left(-\frac{m^2\omega^2}{\hbar^2} r^2 + \frac{2mE}{\hbar^2} - \frac{l(l+1)}{r^2}\right)u = 0$. Defining $k^2 = \frac{2mE}{\hbar^2}$ and $\rho = \sqrt{\frac{m\omega}{\hbar}} r = \alpha r$, we have $d\rho = \alpha dr$. Using this the radial differential equation becomes a dimensionless differential equation

   $\alpha^2 \frac{d^2u}{d\rho^2} + \left(-\alpha^2\rho^2 + k^2 - \frac{\alpha^2 l(l+1)}{\rho^2}\right)u \rightarrow \frac{d^2u}{d\rho^2} + \left(-\rho^2 + \frac{k^2}{\alpha^2} - \frac{l(l+1)}{\rho^2}\right)u = 0$ where

   $\frac{k^2}{\alpha^2} = \frac{2E}{\hbar\omega}$.

   Next we need to determine the approximate form of the solution for large and small ρ and then couple the solutions together.

   As $\rho \rightarrow \infty$, $u \rightarrow 0$ and the dimensionless differential equation takes the approximate form $\frac{d^2u}{d\rho^2} - \rho^2 u \sim 0 \rightarrow u = Ae^{-\frac{\rho^2}{2}} + Be^{\frac{\rho^2}{2}}$. As $\rho \rightarrow \infty$, $u \rightarrow 0$ and

   $u = 0 = Ae^{-\infty} + Be^{\infty} \rightarrow B = 0$. Thus $u \approx Ae^{-\frac{\rho^2}{2}}$.

As $\rho \to 0$, $u \to 0$ and the dimensionless differential equation takes the approximate form $\frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2} \sim 0 \to u = C\rho^{-l} + D\rho^{l+1}$. As $\rho \to 0$, $u \to 0$ and $u = 0 = \frac{C}{0} + D(0) \to C = 0$. Thus $u \approx D\rho^{l+1}$.

Thus for any ρ we assume that $u(\rho) = e^{-\frac{\rho^2}{2}}\rho^{l+1}v(\rho)$ where we absorb the constants into the function $v(\rho)$, which we need to determine. To determine $v(\rho)$ we substitute this solution for $u(\rho)$ into the dimensionless form of the differential equation. Doing this we have:

$\frac{d^2u}{dr^2} = e^{-\frac{\rho^2}{2}}\rho^{l-1}\left[\left\{l(l+1) - 3\rho^2 - 2l\rho^2 + \rho^4\right\}v + 2\rho\left(l+1-\rho^2\right)\frac{dv}{d\rho} + \rho^2\frac{d^2v}{d\rho^2}\right]$. The derivatives were taken on Mathematica. The code is below. Now we take this equation and multiply and divide the right-hand-side by ρ^2.

$$\frac{d^2u}{dr^2} = \frac{\rho^2}{\rho^2}\left[e^{-\frac{\rho^2}{2}}\rho^{l-1}\left[\left\{l(l+1) - 3\rho^2 - 2l\rho^2 + \rho^4\right\}v + 2\rho\left(l+1-\rho^2\right)\frac{dv}{d\rho} + \rho^2\frac{d^2v}{d\rho^2}\right]\right]$$

$$\frac{d^2u}{dr^2} = e^{-\frac{\rho^2}{2}}\rho^{l+1}\left[\left\{\frac{l(l+1)}{\rho^2} - 3 - 2l + \rho^2\right\}v + 2\left(\frac{l+1}{\rho} - \rho\right)\frac{dv}{d\rho} + \frac{d^2v}{d\rho^2}\right]$$

Inserting this expression into the dimensionless form of the differential equation and dividing out the common $e^{-\frac{\rho^2}{2}}\rho^{l+1}$ terms, we arrive at

$\frac{d^2v}{d\rho^2} + 2\left(\frac{l+1}{\rho} - \rho\right)\frac{dv}{d\rho} + \left(\frac{k^2}{\alpha^2} - 3 - 2l\right)v = 0$ which is a 2nd order differential equation with non-constant coefficients and we assume a polynomial series solution given by $v(\rho) = \sum_{j=0}^{\infty} c_j\rho^j$. Taking the derivatives we have:

$\frac{dv}{d\rho} = \sum_{j=1}^{\infty} c_j j\rho^{j-1}$ and $\frac{2(l+1)}{\rho}\frac{dv}{d\rho} = 2(l+1)\sum_{j=1}^{\infty} c_j j\frac{\rho^{j-1}}{\rho} = 2(l+1)\sum_{j=1}^{\infty} c_j j\rho^{j-2}$. Re-indexing we have $2(l+1)\sum_{q=-1}^{\infty} c_{q+2}(q+2)\rho^q$ and there is no $q = -1$ term. Thus the add terms involving a_1 must be zero. Further, $-2\rho\frac{dv}{d\rho} = -2\sum_{j=1}^{\infty} c_j j\rho^j$ and re-indexing $-2\rho\frac{dv}{d\rho} = -2\sum_{q=1}^{\infty} c_q q\rho^q$. The second derivative term becomes $\frac{d^2v}{d\rho^2} = \sum_{j=2}^{\infty} c_j j(j-1)\rho^{j-2}$

and re-indexing $\frac{d^2v}{d\rho^2}=\sum_{q=0}^{\infty}c_{q+2}(q+2)(q+1)\rho^q$. The differential equation for $v(\rho)$ becomes

$$\frac{d^2v}{d\rho^2}+2\left(\frac{l+1}{\rho}-\rho\right)\frac{dv}{d\rho}+\left(\frac{k^2}{\alpha^2}-3-2l\right)v=0$$

$$\sum_{q=0}^{\infty}\left[c_{q+2}(q+2)(q+1)-2c_q q+\left(\frac{k^2}{\alpha^2}-3-2l\right)c_q\right]\rho^q=0$$

The only way this infinite sum can vanish is if coefficients all vanish. This leads us to a recursion relation that we can use to determine the energy associated with the system. Thus $c_{q+2}(q+2)(q+1)-2c_q q+\left(\frac{k^2}{\alpha^2}-3-2l\right)c_q=0$. The recursion relation is $c_{q+2}=\left[\frac{2q-\left(\frac{k^2}{\alpha^2}-3-2l\right)}{(q+2)(q+1)}\right]c_q$. The index q increases and at some c_q, c_{q+2} approximates to zero and thus the numerator has to vanish. We have $2q-\left(\frac{k^2}{\alpha^2}-3-2l\right)=0\rightarrow 2q=\left(\frac{k^2}{\alpha^2}-3-2l\right)\rightarrow\frac{k^2}{\alpha^2}=\frac{2E}{\hbar\omega}=2q+2l+3$. Solving for the energy we have, defining $n=q+l$, $E=\left(n+\frac{3}{2}\right)\hbar\omega$.

```
In[37]:= Clear[v, u, p, l, x]
         v[p_]
         u = (p^(m+1)) * Exp[-p^2/2] * v[p]
         Simplify[D[D[u, p], p]]

Out[38]= v[p_]

Out[39]= e^(-p^2/2) p^(1+m) v[p]

Out[40]= e^(-p^2/2) p^(-1+m) ((m + m^2 - 3 p^2 - 2 m p^2 + p^4) v[p] + p (2 (1 + m - p^2) v'[p] + p v''[p]))
```

4. Griffith's 4.44 parts a and b only.
   a. The wave function $|\psi_{433}\rangle$ can be generated by hand, but we can construct it from the tables given in Griffiths. We need R_{43} and Y_3^3. From page 139 $Y_3^3=-\sqrt{\frac{35}{64\pi}}\sin^3\theta e^{3i\phi}$ and from page 154, $R_{43}=\frac{1}{768\sqrt{35}}a^{-\frac{3}{2}}\left(\frac{r}{a}\right)^3 e^{-\frac{r}{4a}}$.

   Therefore $|\psi_{433}\rangle=R_{43}Y_3^3=-\frac{1}{768\sqrt{35}}\sqrt{\frac{35}{64\pi}}a^{-\frac{3}{2}}\left(\frac{r}{a}\right)^3 e^{-\frac{r}{4a}}\sin^3\theta e^{3i\phi}$.

b. The expectation value of the radial coordinate is given by

$$\langle r\rangle=\langle\psi_{433}|r\psi_{433}\rangle=\left(\frac{1}{768\sqrt{35}}\sqrt{\frac{35}{64\pi}}\right)^2\frac{1}{a^9}\int_0^\infty r\left(r^6e^{-\frac{r}{2a}}\right)r^2\,dr\int_0^\pi \sin^6\sin\theta\,d\theta\int_0^{2\pi}d\phi$$

$$\langle r\rangle=\frac{1}{118591000a^9}\left(371589120a^{10}\right)\left(\frac{32}{35}\right)(2\pi)$$

$$\langle r\rangle=18a$$

The integrals were done on Mathematica. The code is below.

```
In[5]:= Integrate[r^9*Exp[-r/(2*a)], {r, 0, Infinity}]
Out[5]= ConditionalExpression[371 589 120 a^10, Re[a] > 0]

In[3]:= Integrate[Sin[t]^7, {t, 0, Pi}]
Out[3]= 32/35

In[6]:= Integrate[1, {phi, 0, 2*Pi}]
Out[6]= 2 π

In[4]:= 768*768*64*3.14159
Out[4]= 1.18591 × 10^8
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5. Griffith's 4.45

a. The ground state of hydrogen is given by $|\psi_{100}\rangle=R_{10}Y_0^0=\frac{1}{\sqrt{\pi a^3}}e^{-\frac{r}{a}}$.

The probability of finding the electron in the nucleus is given by

$$P=\langle\psi_{100}|\psi_{100}\rangle=\frac{1}{\pi a^3}\int_0^b e^{-\frac{2r}{a}}r^2\,dr\int_0^\pi\sin\theta\,d\theta\int_0^{2\pi}d\phi=\frac{4\pi}{\pi a^3}\left[\frac{a}{4}\left(a^2-\left(a^2+2ab+2b^2\right)e^{-\frac{2b}{a}}\right)\right]$$

$$P=\frac{4}{a^3}\frac{a}{4}a^2\left(1-\left(1+2\frac{b}{a}+2\frac{b^2}{a^2}\right)e^{-\frac{2b}{a}}\right)$$

$$P=1-\left(1+2\frac{b}{a}+2\frac{b^2}{a^2}\right)e^{-\frac{2b}{a}}$$

The integrals were evaluated on Mathematica. The code is below.

```
      Integrate[r^2*Exp[-2*r/a], {r, 0, b}]
Out[11]= 1/4 a (a^2 - (a^2 + 2 a b + 2 b^2) e^(-2b/a))

In[12]:= Integrate[Sin[theta], {theta, 0, Pi}]
         Integrate[1, {phi, 0, 2*Pi}]
Out[12]= 2

Out[13]= 2 π
```

b. Let $\varepsilon = \frac{2b}{a}$ and we have

$$P = 1 - \left(1 + \varepsilon + \frac{\varepsilon^2}{2}\right)e^{-\varepsilon} = 1 - \left(1 + \varepsilon + \frac{\varepsilon^2}{2}\right)\left(1 - \varepsilon + \frac{\varepsilon^2}{2!} - \frac{\varepsilon^3}{3!} + \ldots\right)$$

$$P = 1 - \left[1 - \varepsilon + \frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{6} + \varepsilon - \varepsilon^2 + \frac{\varepsilon^3}{2} - \frac{\varepsilon^4}{6} + \frac{\varepsilon^2}{2} - \frac{\varepsilon^3}{2} + \ldots\right] \quad .$$

$$P \sim \frac{\varepsilon^3}{6} = \frac{1}{6}\left(\frac{2b}{a}\right)^3 = \frac{4}{3}\frac{b^3}{a^3}$$

c. Let $P = \frac{4}{3}\pi b^3 \left|\psi_{100}(r)\right|^2 = \frac{4}{3}\pi b^3 \left(\frac{1}{\pi a^3} e^{-\frac{2r}{a}}\right)$. At $r = 0$,

$$P = \frac{4}{3}\pi b^3 \left|\psi_{100}(r = 0)\right|^2 = \frac{4}{3}\pi b^3 \left(\frac{1}{\pi a^3}\right) = \frac{4}{3}\frac{b^3}{a^3}.$$

d. For $a = 0.5 \times 10^{-10}\,m$ and $b = 1 \times 10^{-15}\,m$,

$$P = \frac{4}{3}\frac{b^3}{a^3} = \frac{4}{3}\left(\frac{1 \times 10^{-15}\,m}{0.5 \times 10^{-10}\,m}\right)^3 = 1.1 \times 10^{-14}.$$

6. Radial Probability density for hydrogen

a. Calculate the location at which the radial probability density is a maximum for the $n = 2, l = 1$ state of the hydrogen atom.

The radial probability density is $\frac{dP}{dr} = 4\pi r^2 \left|R_{21}(r)\right|^2$,

where $R_{21} = \sqrt{\frac{2}{3a}}\left(\frac{1}{4a^2}\right) r e^{-\frac{r}{2a}} = \sqrt{\frac{1}{24a^5}}\, r e^{-\frac{r}{2a}}$. To find the maximum, we set the derivative of the radial probability density equal to zero and solve for the radial coordinate. We have

$$\frac{d}{dr}\left(\frac{dP}{dr}\right) = \frac{d}{dr}\left(4\pi r^2 \left|R_{21}(r)\right|^2\right) = \frac{d}{dr}\left(4\pi r^2 \left|\sqrt{\frac{1}{24a^5}}\, r e^{-\frac{r}{2a}}\right|^2\right) = \frac{d}{dr}\left(\frac{4\pi r^4}{24a^5} e^{-\frac{r}{a}}\right) = 0$$

$$4r^3 e^{-\frac{r}{a}} - \frac{r^4}{a} e^{-\frac{r}{a}} = 0$$

$$\therefore r = 4a$$

b. Calculate the expectation value of the radial coordinate in this state.

The expectation value of the radial coordinate is given by:

$$\langle r \rangle = \langle R_{21} | r R_{21} \rangle = \int_0^\infty \left|\sqrt{\frac{1}{24a^5}}\, r e^{-\frac{r}{2a}}\right|^2 r r^2\, dr = \frac{1}{24a^5}\int_0^\infty r^5 e^{-\frac{r}{a}}\, dr = \frac{1}{24a^5}\left(120a^6\right) = 5a.$$

The integral was evaluated on mathematica. The code is below.

In[14]:=

```
Integrate[r^5*Exp[-r/a], {r, 0, Infinity}]
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Out[14]= ConditionalExpression[$120\,a^6$, Re[a] > 0]

c. Are the answers to parts a and b the same? If they are, what is the physical significance for the fact that they are? If they are not, what is the physical significance for the fact that they are not.

These two values are not the same. The physical reason that they are not the same is that for the expectation value of the radial coordinate the wave function extends to infinity.