449 Homework #2

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In[86]:=
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<< "http://www.physics.wisc.edu/~tgwalker/448defs.m"
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1) Write f = $\mathrm{Sin}(\theta)^3$ $\mathrm{Cos}(\theta)$ $\mathrm{Sin}(3\,\phi)$ as a series of spherical harmonics.

In[57]:=
```
Clear[Y1, θ, ϕ]

Y1  =  SphericalHarmonicY[3, 3, θ, ϕ] *  SphericalHarmonicY[1, 0, θ, ϕ];
Y1 // ExpToTrig // FullSimplify
```

Out[59]=
$$-\frac{\sqrt{105}\; e^{3\,i\,\phi}\,\mathrm{Cos}[\theta]\,\mathrm{Sin}[\theta]^3}{16\,\pi}$$

$$\mathbf{f} = Y_{10} Y_{33}\left(\frac{-16\,\pi}{\sqrt{105}}\right)$$

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2) Write z = r $\mathrm{Cos}(\theta)$ in terms of spherical harmonics. Likewise for x. Show how to get the same result by applying a rotation operator about the y axis.

z = r $\mathrm{Cos}(\theta)$, x = r $\mathrm{Sin}(\theta)\mathrm{Cos}(\phi)$

Look up table of spherical harmonics on Wikipedia to find the ones that are of the form that we need:

In[56]:=
```
Y10 = SphericalHarmonicY[1, 0, θ, ϕ]
```

Out[56]=
$$\frac{1}{2}\sqrt{\frac{3}{\pi}}\ \mathrm{Cos}[\theta]$$

$z = r\,\mathrm{Cos}(\theta)$ $\mathrm{Cos}(\theta) = 2*\mathrm{Sqrt}\left[\frac{\pi}{3}\right] Y_{10}$ $\mathbf{Z = 2\,r\,Sqrt\left[\frac{\pi}{3}\right] Y_{10}}$

In[62]:=
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SphericalHarmonicY[1, -1, θ, ϕ] - SphericalHarmonicY[1, 1, θ, ϕ] // FullSimplify
```

Out[62]=
$$\sqrt{\frac{3}{2\pi}}\ \mathrm{Cos}[\phi]\ \mathrm{Sin}[\theta]$$

$x = r\ \mathrm{Sin}(\theta)\mathrm{Cos}(\phi)$ $\mathrm{Sin}(\theta)\mathrm{Cos}(\phi) = \mathrm{Sqrt}\left[\frac{2\pi}{3}\right] Y_{1,1} - Y_{1,-1}$

$\mathbf{X = r\,Sqrt\left[\frac{2\pi}{3}\right] Y_{1,1} - Y_{1,-1}}$

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3) Calculate: $\int Y_{1,-1}(\theta,\ \phi)\ Y_{2,1}(\theta,\ \phi)\ Y_{3,0}(\theta,\ \phi)\ Y_{2,0}(\theta,\ \phi)\ d\Omega$ by expanding each pair of Y’s as a series of Spherical Harmonics and using the orthogonality of the Y’s.

We know that is the m’s sum to not be zero than the integral is 0 but our sum to zero so that means it will be a nonzero value. The l values for the first two are 1, 2, 3 and the l values for the second two are 1, 2, 3, 4, 5.

In[67]:=
```
Integrate[SphericalHarmonicY[1, -1, θ, ϕ] *
  SphericalHarmonicY[2, 1, θ, ϕ] * Sin[θ] * SphericalHarmonicY[3, 0, θ, ϕ] *
  SphericalHarmonicY[2, 0, θ, ϕ], {ϕ, 0, 2 π}, {θ, 0, π}]
```

Out[67]=
$$-\frac{1}{4\sqrt{7}\,\pi}$$

$$\mathbf{-\frac{1}{4\sqrt{7}\,\pi}}$$

4) Find the 8 lowest energy levels (and their degeneracies) for the potential v= b*r

In[63]:=

In[64]:=

5) For, $l_1 = 0$

$S\,(n_2,\; l_2,\; n_1,\; l_1) =$

$\sum_{m_1, m_2, i} \langle n_2\, l_2\, m_2 |\; r_i \;| n_1\, l_1\, m_1 \rangle \langle n_1\, l_1\, m_1 |\; r_i \;| n_2\, l_2\, m_2 \rangle =$

$\left(\_\_ \int_0^\infty r\, P_{n_2 l_2}\, P_{n_1 l_1}\, r\, dr \right)^2$

$$S\,(n_2,\; l_2,\; n_1,\; l_1) = \sum_{m_1, m_2, i} \langle n_2\, l_2\, m_2 |\; r_i \;| n_1\, l_1\, m_1 \rangle \langle n_1\, l_1\, m_1 |\; r_i \;| n_2\, l_2\, m_2 \rangle$$

$$=$$

$$\int \psi_{n_2 l_2 m_2}{}^{*}\; r\; \psi_{n_1 l_1 m_1}\, d^3 r \;=\; \int dr\, d\Omega\, P_{n_2 l_2}\, Y_{l_2 m_2}\, r\, P_{n_1 l_1}\, Y_{l_1 m_1}$$

$$= \left(\int Y_{l_2 m_2}\, Y_{l_1 m_1}\; \mathrm{Sin}[\theta]\; d\theta\, d\phi \int P_{n_2 l_2}\, r\, P_{n_1 l_1}\, dr \right)^2$$

$$= \left(\int Y_{10}\, Y_{00}\; \mathrm{Sin}[\theta]\; d\theta\, d\phi \int P_{n_2 l_2}\, r\, P_{n_1 l_1}\, dr \right)^2$$

In[89]:=

```
Clear[θ, ϕ]
Integrate[SphericalHarmonicY[1, 0, θ, ϕ]* *
  SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ]* *
  SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ], {ϕ, 0, 2 π}, {θ, 0, π}]
```

Out[90]=

$$\frac{1}{4\,\pi}$$

$$\mathbf{S\,(n_2,\; l_2,\; n_1,\; l_1) = \left(\frac{1}{4\,\pi} \int_0^\infty r\, P_{n_2 l_2}\, P_{n_1 l_1}\, r\, dr \right)^2}$$

6) & 7)

In[20]:=

8) Hydrogen: S(3p, 2s) = ?

From before:

$$S\,(n_2,\ l_2,\ n_1,\ l_1)\ =\ \left(\int Y_{l_2\,m_2}\,Y_{l_1\,m_1}\ \mathrm{Sin}[\theta]\ d\theta\ d\phi\ \int P_{n_2\,l_2}\ r\ P_{n_1\,l_1}\ dr\right)^2$$

$$S\,(3,\ 1,\ 2,\ 0)\ =\ \left(\int Y_{l_2\,m_2}\,Y_{l_1\,m_1}\ \mathrm{Sin}[\theta]\ d\theta\ d\phi\ \int P_{n_2\,l_2}\ r\ P_{n_1\,l_1}\ dr\right)^2$$

In[96]:=

```
Clear[θ, ϕ]
Integrate[SphericalHarmonicY[1, 0, θ, ϕ]* *
   SphericalHarmonicY[1, 0, θ, ϕ] * SphericalHarmonicY[0, 0, θ, ϕ]* *
   SphericalHarmonicY[0, 0, θ, ϕ] * Sin[θ], {ϕ, 0, 2 π}, {θ, 0, π}]

Integrate[
 r * (1/(2 * Sqrt[2 * π]) (1 - r/2) e^(-r/2)) * (1/(81 * Sqrt[3 * π]) (27 - 18 * r + 2 r^2) e^(-r/3)), {r, 0, ∞}]
```

Out[97]=

$$\frac{1}{4\,\pi}$$

Integrate: Invalid integration variable or limit(s) in $\left\{\sqrt{x^2+z^2},\ 0,\ \infty\right\}$.

Out[98]=

$$\int_0^{\infty} \frac{1}{162\,\sqrt{6}\,\pi}\,e^{-\frac{5}{6}\sqrt{x^2+z^2}}\,\sqrt{x^2+z^2}\,\left(1-\frac{1}{2}\sqrt{x^2+z^2}\right)\left(27-18\sqrt{x^2+z^2}+2\left(x^2+z^2\right)\right)d\sqrt{x^2+z^2}$$

9) How many radial zero crossings are there for the 5p m=1 state of Hydrogen?

For the p states there are p-2 zero crossings, so **the 5p m=1 state has 3 zero crossings.**

In[34]:=

```
psipsi[r_, n_, l_, Z_] :=
 (Factorial[(n - l - 1)]/(Factorial[n + l] * 2 n) (2 Z/(n * a))^3)^(1/2) (2 (Z * r)/(n * a))^l LaguerreL[n - l - 1, 2 l + 1, 2 (Z * r)/(n * a)] e^(-Z*r/(n*a))
psipsi[r, 5, 1, 1] * SphericalHarmonicY[1, 1, θ, ϕ]
```

Out[35]=

$$-\frac{1}{46\,875\,a\,\sqrt{5\,\pi}}\left(\frac{1}{a^3}\right)^{3/2} e^{-\frac{r}{5\,a}+i\,\phi}\ r\left(3750\,a^3-1125\,a^2\,r+90\,a\,r^2-2\,r^3\right)\mathrm{Sin}[\theta]$$

In[77]:=

```
a = 1;
r = √(x² + y² + z²);
θ = ArcTan[√(x² + y²)/z];
ϕ = ArcCos[y/x];
y = 0;
```

In[82]:=

$$-\frac{1}{46875\, a \sqrt{5\pi}} \left(\frac{1}{a^3}\right)^{3/2} e^{-\frac{r}{5a} - i\phi}\, r \left(3750\, a^3 - 1125\, a^2\, r + 90\, a\, r^2 - 2\, r^3\right) \mathrm{Sin}[\theta] * -\frac{1}{46875\, a \sqrt{5\pi}} \left(\frac{1}{a^3}\right)^{3/2} e^{-\frac{r}{5a} + i\phi}\, r \left(3750\, a^3 - 1125\, a^2\, r + 90\, a\, r^2 - 2\, r^3\right) \mathrm{Sin}[\theta]$$

Out[82]=

$$\left(e^{-\frac{2}{5}\sqrt{x^2+z^2}}\, x^2 \left(x^2+z^2\right) \left(3750 - 1125\sqrt{x^2+z^2} + 90\left(x^2+z^2\right) - 2\left(x^2+z^2\right)^{3/2}\right)^2\right) \Big/ \left(10986328125\, \pi \left(1 + \frac{x^2}{z^2}\right) z^2\right)$$

In[84]:=

$$\text{ContourPlot}\left[\left(e^{-\frac{2}{5}\sqrt{x^2+z^2}}\, x^2 \left(x^2+z^2\right)\left(3750 - 1125\sqrt{x^2+z^2} + 90\left(x^2+z^2\right) - 2\left(x^2+z^2\right)^{3/2}\right)^2\right) \Big/ \left(10\,986\,328\,125\,\pi\left(1+\frac{x^2}{z^2}\right) z^2\right), \{x, -30, 30\}, \{z, -30, 30\}, \text{ImageSize} \to \text{Large}, \text{Contours} \to \text{Automatic}\right]$$

Out[84]=