Physics 449 hw#2

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Due Date: 2/9 W3F

```
<< "http://www.physics.wisc.edu/~tgwalker/448defs.m"
```

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1)

(The main work is on the paper copy.)

```
Integrate[Sin[θ]^7 Cos[θ]^2 Sin[3 ϕ] 3/8 Sqrt[35/π] e^(-3 i ϕ), {θ, 0, π}]
```

$$\frac{4\, e^{-3 i \phi} \operatorname{Sin}[3\,\phi]}{3\sqrt{35\,\pi}}$$

```
Integrate[(4 e^(-3 i ϕ) Sin[3 ϕ])/(3 Sqrt[35 π]), {ϕ, 0, 2 π}]
```

$$-\frac{4}{3}\, i \sqrt{\frac{\pi}{35}}$$

---

3)

(The main work is on the paper copy.)

$c_{1,0}$ for f_1:

```
2 π * Integrate[-1/16 Sqrt[3^3/π^3 5] (Cos[θ]^2 Sin[θ] - Cos[θ]^4 Sin[θ]), {θ, 0, π}]
```

$$-\frac{1}{2}\sqrt{\frac{3}{5\,\pi}}$$

$c_{3,0}$ for f_1:

```
Integrate[-3/(8 π) √5 (Cos[θ] - Cos[θ]^3) 1/4 Sqrt[7/π] (5 Cos[θ]^3 - 3 Cos[θ]) Sin[θ], {θ, 0, π}]
```

$$\frac{3}{4\sqrt{35}\,\pi^{3/2}}$$

$c_{3,0}$ for f_2:

```
Integrate[√35/(16 π) (5 Cos[θ]^3 - 3 Cos[θ])
  (3 Cos[θ]^2 - 1) 1/4 Sqrt[7/π] (5 Cos[θ]^3 - 3 Cos[θ]) Sin[θ], {θ, 0, π}]
```

$$\frac{1}{3\sqrt{5}\,\pi^{3/2}}$$

```
Integrate[1/(3 √5 π^(3/2)), {ϕ, 0, 2 π}]
```

$$\frac{2}{3\sqrt{5}\,\sqrt{\pi}}$$

$c_{1,0}$ for f_2:

```
Integrate[√35/(16 π) (5 Cos[θ]^3 - 3 Cos[θ]) (3 Cos[θ]^2 - 1) (1/2 Sqrt[3/π] Cos[θ]) Sin[θ], {θ, 0, π}]
```

$$\frac{3\sqrt{\frac{3}{35}}}{4\,\pi^{3/2}}$$

```
Integrate[(3 Sqrt[3/35])/(4 π^(3/2)), {ϕ, 0, 2 π}]
```

$$\frac{3}{2}\sqrt{\frac{3}{35\,\pi}}$$

4) Find the lowest 8 energy levels (and their degeneracies) for the potential $V = b\,r$

(Continuation of the work on the paper copy.)

```
(* l=0 *)

ds = 0.01; s = Range[ds, 10 - ds, ds]; num = Length[s] ;
ones[n_] := 1 + 0 Range[n];

psq = 1/ds^2 (2 DiagonalMatrix[ones[num]] -
      DiagonalMatrix[ones[num - 1], 1] - DiagonalMatrix[ones[num - 1], -1]);
{eval0, evec0} = Eigensystem[1/2 psq + DiagonalMatrix[s]];
in0 = Ordering[eval0]; eval0 = eval0[[in]]; evec0 = evec0[[in0]];

eval0[[ ;; 10]]
```

```
{1.85575, 3.24457, 4.38161, 5.38652,
 6.30513, 7.16113, 7.96919, 8.74473, 9.52541, 10.3742}
```

```
(* l=1 *)

{eval1, evec1} = Eigensystem[1/2 psq + DiagonalMatrix[1/s^2 + s]];
in1 = Ordering[eval1]; eval1 = eval1[[in1]]; evec1 = evec1[[in1]];

eval1[[ ;; 10]]
```

```
{2.66782, 3.87676, 4.92694, 5.8778, 6.75843, 7.58583, 8.37273, 9.14213, 9.94772, 10.8471}
```

```
(* l=2 *)

{eval2, evec2} = Eigensystem[1/2 psq + DiagonalMatrix[3/s^2 + s]];
in2 = Ordering[eval2]; eval2 = eval2[[in2]]; evec2 = evec2[[in2]];

eval2[[ ;; 10]]
```

```
{3.37178, 4.46828, 5.45179, 6.35723,
 7.20433, 8.00599, 8.77659, 9.55296, 10.3975, 11.3511}
```

```
(* l=3 *)

{eval3, evec3} = Eigensystem[1/2 psq + DiagonalMatrix[6/s^2 + s]];
in3 = Ordering[eval3]; eval3 = eval3[[in3]]; evec3 = evec3[[in3]];

eval3[[ ;; 10]]
```

```
{4.00892, 5.02579, 5.9564, 6.82347, 7.64116, 8.42067, 9.1836, 9.98242, 10.8748, 11.883}
```

```
(* l=4 *)

{eval4, evec4} = Eigensystem[1/2 psq + DiagonalMatrix[15/s^2 + s]];
in4 = Ordering[eval4]; eval4 = eval4[[in4]]; evec4 = evec4[[in4]];

eval4[[ ;; 10]]
```

```
{5.15351, 6.06145, 6.91249, 7.71824, 8.48823, 9.24177, 10.0291, 10.909, 11.9056, 13.0192}
```

```
eval0[[ ;; 10]]
eval1[[ ;; 10]]
eval2[[ ;; 10]]
eval3[[ ;; 10]]
eval4[[ ;; 10]]
```

```
{1.85575, 3.24457, 4.38161, 5.38652,
 6.30513, 7.16113, 7.96919, 8.74473, 9.52541, 10.3742}
```

```
{2.66782, 3.87676, 4.92694, 5.8778, 6.75843, 7.58583, 8.37273, 9.14213, 9.94772, 10.8471}
```

```
{3.37178, 4.46828, 5.45179, 6.35723,
 7.20433, 8.00599, 8.77659, 9.55296, 10.3975, 11.3511}
```

```
{4.00892, 5.02579, 5.9564, 6.82347, 7.64116, 8.42067, 9.1836, 9.98242, 10.8748, 11.883}
```

```
{5.15351, 6.06145, 6.91249, 7.71824, 8.48823, 9.24177, 10.0291, 10.909, 11.9056, 13.0192}
```

The lowest 8 energy levels are as following:

n	1	1	2	3	2	1	3	2
l	0	1	0	2	1	3	0	2
Energies	1.85575	2.66782	3.24457	3.37178	3.87676	4.00892	4.38161	4.46828
Degeneracies	1	3	1	5	3	7	1	5

5) -

(Continuation of the work on the paper copy.)

```
Y11 = SphericalHarmonicY[1, 1, θ, ϕ];
Y1m1 = SphericalHarmonicY[1, -1, θ, ϕ];
Y10 = SphericalHarmonicY[1, 0, θ, ϕ];
Y00 = SphericalHarmonicY[0, 0, θ, ϕ];

A = {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]};

thInt1a = Integrate[Sin[θ] Y11 * Y00 * A[[1]], {θ, 0, π}] (* Y1,1 *)
thInt1b = Integrate[Sin[θ] Y10 * Y00 * A[[1]], {θ, 0, π}] (* Y1,0 *)
thInt1c = Integrate[Sin[θ] Y1m1 * Y00 * A[[1]], {θ, 0, π}] (* Y1,-1 *)
```

$$-\frac{1+e^{2 i \phi}}{2\sqrt{6}\,\pi}$$

0

$$\frac{e^{-i \phi}\,\mathrm{Cos}[\phi]}{\sqrt{6}\,\pi}$$

```
sqPhiInt1a = (Integrate[thInt1a, {ϕ, 0, 2 π}])^2
sqPhiInt1b = (Integrate[thInt1b, {ϕ, 0, 2 π}])^2
sqPhiInt1c = (Integrate[thInt1c, {ϕ, 0, 2 π}])^2
```

$$\frac{1}{6}$$

0

$$\frac{1}{6}$$

$\sum_{l=1,m=-1}^{m=1}\left(\int_0^{2\pi}\int_0^{\pi}\mathrm{Sin}[\theta]\,d\theta\,d\phi\,Y_{n_2 l_2}\,Y_{n_1 l_1}\,A_2\right)^2=\frac{1}{3}$

```
thInt2a = Integrate[Sin[θ] Y11 * Y00 * A[[2]], {θ, 0, π}] (* Y1,1 *)
thInt2b = Integrate[Sin[θ] Y10 * Y00 * A[[2]], {θ, 0, π}] (* Y1,0 *)
thInt2c = Integrate[Sin[θ] Y1m1 * Y00 * A[[2]], {θ, 0, π}] (* Y1,-1 *)
```

$$-\frac{e^{i\phi}\,\mathrm{Sin}[\phi]}{\sqrt{6}\,\pi}$$

0

$$\frac{e^{-i\phi}\,\mathrm{Sin}[\phi]}{\sqrt{6}\,\pi}$$

```
sqPhiInt2a = Abs[(Integrate[thInt2a, {ϕ, 0, 2 π}])^2]
sqPhiInt2b = Abs[(Integrate[thInt2b, {ϕ, 0, 2 π}])^2]
sqPhiInt2c = Abs[(Integrate[thInt2c, {ϕ, 0, 2 π}])^2]
```

$$\frac{1}{6}$$

0

$$\frac{1}{6}$$

$\sum_{l=1,m=-1}^{m=1}\left(\int_0^{2\pi}\int_0^{\pi}\mathrm{Sin}[\theta]\,d\theta\,d\phi\,Y_{n_2 l_2}\,Y_{n_1 l_1}\,A_2\right)^2=\frac{1}{3}$

```
thInt3a = Integrate[Sin[θ] Y11 * Y00 * A[[3]], {θ, 0, π}] (* Y1,1 *)
thInt3b = Integrate[Sin[θ] Y10 * Y00 * A[[3]], {θ, 0, π}] (* Y1,0 *)
thInt3c = Integrate[Sin[θ] Y1m1 * Y00 * A[[3]], {θ, 0, π}] (* Y1,-1 *)
```

0

$$\frac{1}{2\sqrt{3}\,\pi}$$

0

```
sqPhiInt3a = (Integrate[thInt3a, {ϕ, 0, 2 π}])^2
sqPhiInt3b = (Integrate[thInt3b, {ϕ, 0, 2 π}])^2
sqPhiInt3c = (Integrate[thInt3c, {ϕ, 0, 2 π}])^2
```

0

$\frac{1}{3}$

0

$\sum_{l=1,m=-1}^{m=1}\left(\int_0^{2\pi}\int_0^{\pi}\mathrm{Sin}[\theta]\,d\theta\,d\phi\,Y_{n_2 l_2}\,Y_{n_1 l_1}\,A_3\right)^2=\frac{1}{3}$

$\sum_{i=1}^{3}\sum_{l=1,m=-1}^{m=1}\left(\int_0^{2\pi}\int_0^{\pi}\mathrm{Sin}[\theta]\,d\theta\,d\phi\,Y_{n_2 l_2}\,Y_{n_1 l_1}\,A_i\right)^2=1$

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

6-7) Exercises 5&6 in the Supersymmetry handout: Write a Mathematica function to calculate $P_{n\,l}$ using supersymmetry. Verify its correctness for $P_{7\,d}$.

```
W1_ := 1/(l+1) - (l+1)/s;
A†1_@f_ := -∂s f + W1 f
```

```
grdϰ = s^n e^(-s/n);
Pnl[n_, l_] := Do[A†lb@grdϰ, {lb, n-2, l, -1}];
```

Verify its correctness for $P_{7\,d}$:

```
W2
P7d = A†2@A†3@A†4@A†5@grdϰ // Simplify
```

$\frac{1}{3}-\frac{3}{s}$

$\frac{1}{360\,n^4}e^{-\frac{s}{n}}(6+n)\,s^{-4+n}\left(360\,n^7+n^6\,(2160-342\,s)+60\,s^4+n\,s^3\,(-1080+47\,s)+n^4\,s\,(-8316+1309\,s-18\,s^2)+6\,n^2\,s^2\,(870-141\,s+2\,s^2)+n^5\,(2880-3078\,s+119\,s^2)+n^3\,s\,(-6300+4626\,s-216\,s^2+s^3)\right)$

```
P7dN = 1/(360 × 1^4) e^(-s/1) (6+1) s^(-4+1) (360 × 1^7 + 1^6 (2160 - 342 s) + 60 s^4 +
   1 * s^3 (-1080 + 47 s) + 1^4 s (-8316 + 1309 s - 18 s^2) + 6 × 1^2 s^2 (870 - 141 s + 2 s^2) +
   1^5 (2880 - 3078 s + 119 s^2) + 1^3 s (-6300 + 4626 s - 216 s^2 + s^3)) // Simplify
```

$$\frac{7\, e^{-s}\left(900-3006\, s+1879\, s^{2}-360\, s^{3}+20\, s^{4}\right)}{60\, s^{3}}$$

```
SE = -1/2 ∂_{s,s} P7dN + (2 * 3)/(2 s^2) P7dN // Simplify
```

$$-\frac{7\, e^{-s}\left(5400+5400\, s-18\,640\, s^{2}+2912\, s^{3}+1759\, s^{4}-400\, s^{5}+20\, s^{6}\right)}{120\, s^{5}}$$

The result approaches to zero → This formulation can be verified on P_{7d}.

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

```
a0 = 0.529 Å; Z = 1;
R31 = (4 √2)/9 (Z/(3 a0))^(3/2) (Z r)/a0 (1 - (Z r)/(6 a0)) e^(-Z r/(3 a0));
R20 = 2 (Z/(2 a0))^(3/2) (1 - (Z r)/(2 a0)) e^(-Z r/(2 a0));
(Integrate[r * R31 * R20, {r, 0, ∞}])^2
```

$$\text{ConditionalExpression}\left[\frac{0.000499606}{\text{Å}^{2}},\ \text{Re}[\text{Å}]>0\right]$$

9) How many radial zero crossings are there for the 5p m=1 state of hydrogen? Plot the probability distribution in the x-z plane. (Use ContourPlot)

```
P5p = A†₁@A†₂@A†₃@grdϰ // Simplify
```

$$-\frac{1}{24\, n^{3}} e^{-\frac{s}{n}}\,(4+n)\, s^{-3+n}\left(24\, n^{5}+n^{4}\,(48-26\, s)+n\,(54-5\, s)\, s^{2}-6\, s^{3}+n^{3}\, s\,(-104+9\, s)-n^{2}\, s\left(90-45\, s+s^{2}\right)\right)$$

```
ψ5p = P5p * SphericalHarmonicY[1, 1, θ, ϕ]
```

$$\frac{1}{16\, n^3 \sqrt{6\pi}} e^{-\frac{s}{n}+i\phi} (4+n)\, s^{-3+n} \left(24 n^5 + n^4 (48 - 26 s) + n (54 - 5 s) s^2 - 6 s^3 + n^3 s (-104 + 9 s) - n^2 s (90 - 45 s + s^2)\right) \text{Sin}[\theta]$$

```
n = 5;
ψ5pSq = ψ5p* ψ5p // Simplify
```

$$\frac{1}{500\,000\,\pi} 1323\, e^{-\frac{s}{5}+i\phi-\frac{\text{Conjugate}[s]}{5}-i\,\text{Conjugate}[\phi]}\, s^2 \left(-3750 + 1125 s - 90 s^2 + 2 s^3\right) \text{Conjugate}[s]^2 \left(-3750 + 1125\,\text{Conjugate}[s] - 90\,\text{Conjugate}[s]^2 + 2\,\text{Conjugate}[s]^3\right) \text{Conjugate}[\text{Sin}[\theta]]\, \text{Sin}[\theta]$$

Plug in $s = \sqrt{x^2+z^2}$, gives: $-\dfrac{e^{-\frac{2}{5}\sqrt{x^2+z^2}} \sqrt{x^2+z^2} \left(3750-1125\sqrt{x^2+z^2}+90\left(x^2+z^2\right)+2\left(x^2+z^2\right)^{3/2}\right)}{10\,986\,328\,125\,\pi \Big/ \left(\frac{1}{\sqrt{1-\frac{z^2}{x^2+z^2}}}\right)}$

$$\text{ContourPlot}\left[\left(\sqrt{1-\frac{z^2}{x^2+z^2}}\right)\frac{1}{10\,986\,328\,125\,\pi}\, e^{-\frac{2}{5}\sqrt{x^2+z^2}}\sqrt{x^2+z^2}\left(3750-1125\sqrt{x^2+z^2}+90\left(x^2+z^2\right)+2\left(x^2+z^2\right)^{3/2}\right),\right.$$
$$\left.\{x,-25,25\},\{z,-25,25\},\text{ImageSize}\to\text{Large},\text{Contours}\to\text{Automatic}\right]$$