Spin Orbit Spectra Calculations

```
(%i1) kill(all);
(%o0) done
```

1 Define operators

```
(%i1) assume(h[bar]>0, m>0, a[0]>0, b>0, Z>0);
(%o1) [h_bar>0,m>0,a_0>0,b>0,Z>0]
```

```
(%i2) /* Norm of radial function */
      N(f) := (integrate(conjugate(f)*f*r^2, r, 0, inf));
(%o2) N(f):=∫_0^∞ conjugate(f) f r^2 dr
```

```
(%i3) /* Norm of spherical function */
      NY(f) := integrate(integrate(conjugate(f)*f*sin(theta), theta, 0, %pi
(%o3) NY(f):=∫_0^(2 π) ∫_0^π conjugate(f) f sin(θ) dθ dϕ
```

```
(%i4) /* Norm of 3d function */
      N3(f) := integrate(integrate(integrate(conjugate(f)*f*sin(theta), the
      phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o4) N3(f):=∫_0^∞ ∫_0^(2 π) ∫_0^π conjugate(f) f sin(θ) dθ dϕ r^2 dr
```

```
(%i5) /* Expectation value of radial function */
      Ex(f,op) := (integrate(conjugate(f)*op*f*r^2, r, 0, inf));
(%o5) Ex(f,op):=∫_0^∞ conjugate(f) op f r^2 dr
```

```
(%i6) /* Expectation value of 3D wave function */
      Ex3(f,op) := integrate(integrate(integrate(conjugate(f)*op*f*sin(thet
      phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o6) Ex3(f,op):=∫_0^∞ ∫_0^(2 π) ∫_0^π conjugate(f) op f sin(θ) dθ dϕ r^2 dr
```

```
(%i7) /* Integral of two 3D wave functions */
      Ex32(f1,op,f2) := integrate(integrate(integrate(conjugate(f1)*op*f2*s
      phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o7) Ex32(f1,op,f2):=∫_0^∞ ∫_0^(2 π) ∫_0^π conjugate(f1) op f2 sin(θ) dθ dϕ r^2 dr
```

Define energy levels of Hydrogen

2 Define Radial Eigenfunctions

```
(%i8) rhon: 2*Z*r/(n*a[0]);
```

$$(\%o8)\ \frac{2\,r\,Z}{a_0\,n}$$

1s radial function

```
(%i9) rho: ev(rhon, [n=1]);
```

$$(\%o9)\ \frac{2\,r\,Z}{a_0}$$

```
(%i10) R[0]: 2*(Z/a[0])^(3/2)*exp(-rho/2);
```

$$(\%o10)\ \frac{2\,Z^{3/2}\,\%e^{-\frac{r\,Z}{a_0}}}{a_0^{3/2}}$$

2s radial function

```
(%i11) rho: ev(rhon, [n=2]);
```

$$(\%o11)\ \frac{r\,Z}{a_0}$$

```
(%i12) R[1]: 1/(2*sqrt(2))*(Z/a[0])^(3/2)*(2-rho)*exp(-rho/2);
```

$$(\%o12)\ \frac{Z^{3/2}\left(2-\frac{r\,Z}{a_0}\right)\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{3/2}\,a_0^{3/2}}$$

2p radial function

```
(%i13) R[2]: 1/(2*sqrt(6))*(Z/a[0])^(3/2)*(rho)*exp(-rho/2);
```

$$(\%o13)\ \frac{r\,Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2\sqrt{6}\,a_0^{5/2}}$$

3s radial function

```
(%i14) rho: ev(rhon, [n=3]);
```

$$(\%o14)\ \frac{2\,r\,Z}{3\,a_0}$$

```
(%i15) R[3]: 1/(sqrt(243))*(Z/a[0])^(3/2)*(6-6*rho+rho^2)*exp(-rho/2);
```

$$(\%o15)\ \frac{Z^{3/2}\left(\frac{4\,r^2\,Z^2}{9\,a_0^2}-\frac{4\,r\,Z}{a_0}+6\right)\%e^{-\frac{r\,Z}{3\,a_0}}}{3^{5/2}\,a_0^{3/2}}$$

3p radial function

```
(%i16) R[4]: 1/(sqrt(486))*(Z/a[0])^(3/2)*(4-rho)*rho*exp(-rho/2);
```

$$(\%o16)\ \frac{2\,r\,Z^{5/2}\left(4-\frac{2\,r\,Z}{3\,a_0}\right)\%e^{-\frac{r\,Z}{3\,a_0}}}{27\sqrt{6}\,a_0^{5/2}}$$

3d radial function

```
(%i17) R[5]: 1/(sqrt(2430))*(Z/a[0])^(3/2)*(rho^2)*exp(-rho/2);
```

$$(\%o17)\ \frac{4\,r^2\,Z^{7/2}\,\%e^{-\frac{r\,Z}{3\,a_0}}}{81\sqrt{30}\,a_0^{7/2}}$$

Normalization check

```
(%i18) for i: 0 thru 5 do (
       print (i, "  N(R): ", N(R[i]))
       );
0   N(R):  1
1   N(R):  1
2   N(R):  1
3   N(R):  1
4   N(R):  1
5   N(R):  1
(%o18) done
```

3 Spherial Harmonics

Define Eigenfunctions

Y(0,0)

```
(%i19) Y[0]: 1/(2*sqrt(%pi));
```

$$(\%o19)\ \frac{1}{2\sqrt{\pi}}$$

Y(1,0)

```
(%i20) Y[1]: 1/2*sqrt(3/%pi)*cos(theta);
```

$$(\%o20)\ \frac{\sqrt{3}\cos(\theta)}{2\sqrt{\pi}}$$

Y(1,1)

(%i21) `Y[2]: -1/2*sqrt(3/(2*%pi))*sin(theta)*exp(%i*phi);`

(%o21) $$-\frac{\sqrt{3}\,\%e^{\%i\,\phi}\sin(\theta)}{2^{3/2}\sqrt{\pi}}$$

`Y(2,0)`

(%i22) `Y[3]: 1/4*sqrt(5/%pi)*(3*cos(theta)^2-1);`

(%o22) $$\frac{\sqrt{5}\,(3\cos(\theta)^2-1)}{4\sqrt{\pi}}$$

`Y(2,1)`

(%i23) `Y[4]: -1/2*sqrt(15/(2*%pi))*sin(theta)*cos(theta)*exp(%i*phi);`

(%o23) $$-\frac{\sqrt{15}\,\%e^{\%i\,\phi}\cos(\theta)\sin(\theta)}{2^{3/2}\sqrt{\pi}}$$

`Y(2,2)`

(%i24) `Y[5]: 1/4*sqrt(15/(2*%pi))*sin(theta)^2*exp(2*%i*phi);`

(%o24) $$\frac{\sqrt{15}\,\%e^{2\,\%i\,\phi}\sin(\theta)^2}{2^{5/2}\sqrt{\pi}}$$

`Y(3,0)`

(%i25) `Y[6]: 1/4*sqrt(7/%pi)*(5*cos(theta)^3-3*cos(theta));`

(%o25) $$\frac{\sqrt{7}\,(5\cos(\theta)^3-3\cos(\theta))}{4\sqrt{\pi}}$$

`Y(3,1)`

(%i26) `Y[7]: -1/8*sqrt(21/(%pi))*sin(theta)*(5*cos(theta)^2-1)*exp(%i*phi);`

(%o26) $$-\frac{\sqrt{21}\,\%e^{\%i\,\phi}\,(5\cos(\theta)^2-1)\sin(\theta)}{8\sqrt{\pi}}$$

`Y(3,2)`

(%i27) `Y[8]: 1/4*sqrt(105/(2*%pi))*sin(theta)^2*cos(theta)*exp(2*%i*phi);`

(%o27) $$\frac{\sqrt{105}\,\%e^{2\,\%i\,\phi}\cos(\theta)\sin(\theta)^2}{2^{5/2}\sqrt{\pi}}$$

`Y(3,3)`

(%i28) Y[9]: -1/8*sqrt(35/(%pi))*sin(theta)^3*exp(3*%i*phi);

(%o28) $$-\frac{\sqrt{35}\,\%e^{3\,\%i\,\phi}\sin(\theta)^3}{8\sqrt{\pi}}$$

4 Wave functions psi(r,theta,phi)=R[n]*Y[l,m] and radial derivatives dpsi=dR[n]*Y[l,m]

psi[n=1, l=0, ml=0]

(%i29) qn[0]: "n=1, l=0, ml=0"$

(%i30) psi[0]: R[0]*Y[0]$

psi[n=2, l=0, ml=0]

(%i31) qn[1]: "n=2, l=0, ml=0"$

(%i32) psi[1]: R[1]*Y[0]$

psi[n=2, l=1, ml=0]

(%i33) qn[2]: "n=2, l=1, ml=0"$

(%i34) psi[2]: R[2]*Y[1]$

psi[n=2, l=1, ml=1]

(%i35) qn[3]: "n=2, l=1, ml=1"$

(%i36) psi[3]: R[2]*Y[2]$

psi[n=3, l=0, ml=0]

(%i37) qn[4]: "n=3, l=0, ml=0"$

(%i38) psi[4]: R[3]*Y[0]$

psi[n=3, l=1, ml=0]

(%i39) qn[5]: "n=3, l=1, ml=0"$

(%i40) psi[5]: R[4]*Y[1]$

psi[n=3, l=1, ml=1]

(%i41) qn[6]: "n=3, l=1, ml=1"$

```
(%i42) psi[6]:  R[4]*Y[2]$
```

```
 psi[n=3, l=2, ml=0]
```

```
(%i43) qn[7]: "n=3, l=2, ml=0"$
```

```
(%i44) psi[7]:  R[5]*Y[3]$
```

```
 psi[n=3, l=2, ml=1]
```

```
(%i45) qn[8]: "n=3, l=2, ml=1"$
```

```
(%i46) psi[8]:  R[5]*Y[4]$
```

```
 psi[n=3, l=2, ml=2]
```

```
(%i47) qn[9]: "n=3, l=2, ml=2"$
```

```
(%i48) psi[9]:  R[5]*Y[5]$
```

```
(%i49) for i: 0 thru 9 do (
           print (qn[i], ", psi: ", psi[i])
       );
```

$$n=1,\ l=0,\ ml=0,\ psi:\ \frac{Z^{3/2}\,\%e^{-\frac{r\,Z}{a_0}}}{\sqrt{\pi}\,a_0^{3/2}}$$

$$n=2,\ l=0,\ ml=0,\ psi:\ \frac{Z^{3/2}\left(2-\frac{r\,Z}{a_0}\right)\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{\pi}\,a_0^{3/2}}$$

$$n=2,\ l=1,\ ml=0,\ psi:\ \frac{\sqrt{3}\,r\cos(\theta)Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{4\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$n=2,\ l=1,\ ml=1,\ psi:\ -\frac{\sqrt{3}\,\%e^{\%i\,\phi}\,r\sin(\theta)Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$n=3,\ l=0,\ ml=0,\ psi:\ \frac{Z^{3/2}\left(\frac{4\,r^2\,Z^2}{9\,a_0^2}-\frac{4\,r\,Z}{a_0}+6\right)\%e^{-\frac{r\,Z}{3\,a_0}}}{2\,3^{5/2}\sqrt{\pi}\,a_0^{3/2}}$$

$$n=3,\ l=1,\ ml=0,\ psi:\ \frac{r\cos(\theta)Z^{5/2}\left(4-\frac{2\,r\,Z}{3\,a_0}\right)\%e^{-\frac{r\,Z}{3\,a_0}}}{3^{5/2}\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$n=3,\ l=1,\ ml=1,\ psi:\ -\frac{\%e^{\%i\,\phi}\,r\sin(\theta)Z^{5/2}\left(4-\frac{2\,r\,Z}{3\,a_0}\right)\%e^{-\frac{r\,Z}{3\,a_0}}}{\sqrt{2}\,3^{5/2}\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$n=3,\ l=2,\ ml=0,\ psi:\ \frac{\sqrt{5}\,r^2(3\cos(\theta)^2-1)Z^{7/2}\,\%e^{-\frac{r\,Z}{3\,a_0}}}{81\sqrt{30}\sqrt{\pi}\,a_0^{7/2}}$$

$$n=3,\ l=2,\ ml=1,\ psi:\ -\frac{\sqrt{2}\sqrt{15}\,\%e^{\%i\,\phi}\,r^2\cos(\theta)\sin(\theta)Z^{7/2}\,\%e^{-\frac{r\,Z}{3\,a_0}}}{81\sqrt{30}\sqrt{\pi}\,a_0^{7/2}}$$

$$n=3,\ l=2,\ ml=2,\ psi:\ \frac{\sqrt{15}\,\%e^{2\,\%i\,\phi}\,r^2\sin(\theta)^2\,Z^{7/2}\,\%e^{-\frac{r\,Z}{3\,a_0}}}{81\sqrt{2}\sqrt{30}\sqrt{\pi}\,a_0^{7/2}}$$

(%o49) *done*

Normalization check

```
(%i50) for i: 0 thru 9 do
       print (i, "  N3(psi): ", N3(psi[i]));
0   N3(psi):  1
1   N3(psi):  1
2   N3(psi):  1
3   N3(psi):  1
4   N3(psi):  1
5   N3(psi):  1
6   N3(psi):  1
7   N3(psi):  1
8   N3(psi):  1
9   N3(psi):  1
(%o50) done
```

5 Expectation values orbital velocities

```
(%i51) assume(epsilon>0, epsilon<1);
(%o51) [ε>0,ε<1]
```

```
(%i52) op: a[0]/(1+epsilon*cos(theta));
(%o52)        a_0
       ε cos(θ)+1
```

5.1 Detailed results

```
(%i53) for i: 0 thru 9 do (
           P: r*psi[i],
           d2P: diff(P, r, 2),
           v2: expand(ratsimp(-h[bar]^2/P * d2P)),
           v: Ex3(psi[i], op),
           print ("*****************************************************"),
           print (qn[i], ", psi: ", psi[i]),
           print ("***** d2P: ", d2P),
           print ("***** v2: ", v2)
       );
```

*****

$$n=1,\ l=0,\ ml=0,\ psi:\ \frac{Z^{3/2}\,\%e^{-\frac{r\,Z}{a_0}}}{\sqrt{\pi}\,a_0^{3/2}}$$

$$***** d2P:\ \frac{r\,Z^{7/2}\,\%e^{-\frac{r\,Z}{a_0}}}{\sqrt{\pi}\,a_0^{7/2}}-\frac{2\,Z^{5/2}\,\%e^{-\frac{r\,Z}{a_0}}}{\sqrt{\pi}\,a_0^{5/2}}$$

$$***** v2:\ \frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{h_{bar}^2\,Z^2}{a_0^2}$$

*****

$$n=2,\ l=0,\ ml=0,\ psi:\ \frac{Z^{3/2}\left(2-\frac{r\,Z}{a_0}\right)\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{\pi}\,a_0^{3/2}}$$

$$***** d2P:\ \frac{r\,Z^{7/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{\pi}\,a_0^{7/2}}-\frac{Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{3/2}\sqrt{\pi}\,a_0^{5/2}}+\frac{r\,Z^{7/2}\left(2-\frac{r\,Z}{a_0}\right)\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{9/2}\sqrt{\pi}\,a_0^{7/2}}-\frac{Z^{5/2}\left(2-\frac{r\,Z}{a_0}\right)\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{\pi}\,a_0^{5/2}}$$

$$***** v2:\ \frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{h_{bar}^2\,Z^2}{4\,a_0^2}$$

*****

$$n=2,\ l=1,\ ml=0,\ psi:\ \frac{\sqrt{3}\,r\cos(\theta)\,Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{4\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$***** d2P:\ \frac{\sqrt{3}\,r^2\cos(\theta)\,Z^{9/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{16\sqrt{6}\sqrt{\pi}\,a_0^{9/2}}-\frac{\sqrt{3}\,r\cos(\theta)\,Z^{7/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2\sqrt{6}\sqrt{\pi}\,a_0^{7/2}}+\frac{\sqrt{3}\cos(\theta)\,Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$***** v2:\ -\frac{h_{bar}^2\,Z^2}{4\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{2\,h_{bar}^2}{r^2}$$

*****

$$n=2,\ l=1,\ ml=1,\ psi:\ -\frac{\sqrt{3}\,\%e^{\%i\,\phi}\,r\sin(\theta)\,Z^{5/2}\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{5/2}\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

$$***** d2P:\ -\frac{\sqrt{3}\,r^2\sin(\theta)\,Z^{9/2}\,\%e^{\%i\,\phi-\frac{r\,Z}{2\,a_0}}}{2^{9/2}\sqrt{6}\sqrt{\pi}\,a_0^{9/2}}+\frac{\sqrt{3}\,r\sin(\theta)\,Z^{7/2}\,\%e^{\%i\,\phi-\frac{r\,Z}{2\,a_0}}}{2^{3/2}\sqrt{6}\sqrt{\pi}\,a_0^{7/2}}-\frac{\sqrt{3}\sin(\theta)\,Z^{5/2}\,\%e^{\%i\,\phi-\frac{r\,Z}{2\,a_0}}}{2^{3/2}\sqrt{6}\sqrt{\pi}\,a_0^{5/2}}$$

5.2 compact results

```
(%i54) for i: 0 thru 9 do (
           P: r*psi[i],
           d2P: diff(P, r, 2),
           v2: expand(ratsimp(-h[bar]^2/P * d2P)),
           v: Ex3(psi[i], op),
           print ("*****************************************************"),
           print (qn[i], ", v2: ", v2)
       );
```

****

$$n=1,\ l=0,\ ml=0,\ v2:\ \frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{h_{bar}^2\,Z^2}{a_0^2}$$

****

$$n=2,\ l=0,\ ml=0,\ v2:\ \frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{h_{bar}^2\,Z^2}{4\,a_0^2}$$

****

$$n=2,\ l=1,\ ml=0,\ v2:\ -\frac{h_{bar}^2\,Z^2}{4\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{2\,h_{bar}^2}{r^2}$$

****

$$n=2,\ l=1,\ ml=1,\ v2:\ -\frac{h_{bar}^2\,Z^2}{4\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{2\,h_{bar}^2}{r^2}$$

****

$$n=3,\ l=0,\ ml=0,\ v2:\ \frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{h_{bar}^2\,Z^2}{9\,a_0^2}$$

****

$$n=3,\ l=1,\ ml=0,\ v2:\ -\frac{h_{bar}^2\,Z^2}{9\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{2\,h_{bar}^2}{r^2}$$

****

$$n=3,\ l=1,\ ml=1,\ v2:\ -\frac{h_{bar}^2\,Z^2}{9\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{2\,h_{bar}^2}{r^2}$$

****

$$n=3,\ l=2,\ ml=0,\ v2:\ -\frac{h_{bar}^2\,Z^2}{9\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{6\,h_{bar}^2}{r^2}$$

****

$$n=3,\ l=2,\ ml=1,\ v2:\ -\frac{h_{bar}^2\,Z^2}{9\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{6\,h_{bar}^2}{r^2}$$

****

$$n=3,\ l=2,\ ml=2,\ v2:\ -\frac{h_{bar}^2\,Z^2}{9\,a_0^2}+\frac{2\,h_{bar}^2\,Z}{a_0\,r}-\frac{6\,h_{bar}^2}{r^2}$$

(%o54) done