

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) := \int_0^{\infty} conjugate(f) f r^2 dr
```

```
(%i3) /* Norm of spherical function */
NY(f) := integrate(integrate(conjugate(f)*f*sin(theta), theta, 0, %pi), phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o3) NY(f) := \int_0^{2\pi} \int_0^{\pi} conjugate(f) f sin(\theta) d\theta d\phi
```

```
(%i4) /* Norm of 3d function */
N3(f) := integrate(integrate(integrate(conjugate(f)*f*sin(theta), theta, 0, %pi), phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o4) N3(f) := \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} conjugate(f) f sin(\theta) d\theta d\phi 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) := \int_0^{\infty} 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(theta)*sin(phi), theta, 0, %pi), phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o6) Ex3(f,op) := \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} conjugate(f) op f sin(\theta) d\theta d\phi r^2 dr
```

```
(%i7) /* Integral of two 3D wave functions */
Ex32(f1,op,f2) := integrate(integrate(integrate(conjugate(f1)*op*f2*sin(theta)*sin(phi), theta, 0, %pi), phi, 0, 2*%pi)*r^2, r, 0, inf);
(%o7) Ex32(f1,op,f2) := \int_0^{\infty} \int_0^{2\pi} \int_0^{\pi} conjugate(f1) op f2 sin(\theta) d\theta d\phi 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 Spherical 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);

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

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);

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

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 $d\psi = dR[n] * Y[l, m]$**

```
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:  $\frac{Z^{3/2} e^{-\frac{rZ}{a_0}}}{\sqrt{\pi} a_0^{3/2}}$ 
n=2, l=0, ml=0, psi:  $\frac{Z^{3/2} \left(2 - \frac{rZ}{a_0}\right) e^{-\frac{rZ}{2a_0}}}{2^{5/2} \sqrt{\pi} a_0^{3/2}}$ 
n=2, l=1, ml=0, psi:  $\frac{\sqrt{3} r \cos(\theta) Z^{5/2} e^{-\frac{rZ}{2a_0}}}{4 \sqrt{6} \sqrt{\pi} a_0^{5/2}}$ 
n=2, l=1, ml=1, psi:  $-\frac{\sqrt{3} e^{i\phi} r \sin(\theta) Z^{5/2} e^{-\frac{rZ}{2a_0}}}{2^{5/2} \sqrt{6} \sqrt{\pi} a_0^{5/2}}$ 
n=3, l=0, ml=0, psi:  $\frac{Z^{3/2} \left(\frac{4r^2 Z^2}{9a_0^2} - \frac{4rZ}{a_0} + 6\right) e^{-\frac{rZ}{3a_0}}}{2 \cdot 3^{5/2} \sqrt{\pi} a_0^{3/2}}$ 
n=3, l=1, ml=0, psi:  $\frac{r \cos(\theta) Z^{5/2} \left(4 - \frac{2rZ}{3a_0}\right) e^{-\frac{rZ}{3a_0}}}{3^{5/2} \sqrt{6} \sqrt{\pi} a_0^{5/2}}$ 
n=3, l=1, ml=1, psi:  $-\frac{e^{i\phi} r \sin(\theta) Z^{5/2} \left(4 - \frac{2rZ}{3a_0}\right) e^{-\frac{rZ}{3a_0}}}{\sqrt{2} \cdot 3^{5/2} \sqrt{6} \sqrt{\pi} a_0^{5/2}}$ 
n=3, l=2, ml=0, psi:  $\frac{\sqrt{5} r^2 (3 \cos(\theta)^2 - 1) Z^{7/2} e^{-\frac{rZ}{3a_0}}}{81 \sqrt{30} \sqrt{\pi} a_0^{7/2}}$ 
n=3, l=2, ml=1, psi:  $-\frac{\sqrt{2} \sqrt{15} e^{i\phi} r^2 \cos(\theta) \sin(\theta) Z^{7/2} e^{-\frac{rZ}{3a_0}}}{81 \sqrt{30} \sqrt{\pi} a_0^{7/2}}$ 
n=3, l=2, ml=2, psi:  $\frac{\sqrt{15} e^{2i\phi} r^2 \sin(\theta)^2 Z^{7/2} e^{-\frac{rZ}{3a_0}}}{81 \sqrt{2} \sqrt{30} \sqrt{\pi} a_0^{7/2}}$ 
(%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 of orbital velocities

```

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

(%i52) op: a[0]/(1+epsilon*cos(theta));
(%o52) 
$$\frac{a_0}{\epsilon \cos(\theta)+1}$$


```

□ 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)
);
```

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

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

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

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

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

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

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

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

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

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

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

$$\frac{\sqrt{3} \sin(\theta) Z^{5/2} e^{i\phi} e^{-\frac{rZ}{2a_0}}}{2^{3/2} \sqrt{6} \sqrt{\pi} a_0^{5/2}}$$

$$\frac{\sqrt{3} \sin(\theta) Z^{5/2} e^{i\phi} e^{-\frac{rZ}{2a_0}}}{2^{3/2} \sqrt{6} \sqrt{\pi} a_0^{5/2}}$$

5.2 Compacted 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)
);
```

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

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

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

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

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

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

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

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

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

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

(%o54) done

6 Expectation values of orbital radii in theta pl (see notation of Atkins)

```
(%i55) op: a[0]/(1+epsilon*cos(theta));
```

```
(%o55) 
$$\frac{a_0}{\epsilon \cos(\theta) + 1}$$

```

```
(%i56) for i: 0 thru 9 do (
  re: Ex3(psi[i], op),
  print ("*****"),
  print (qn[i], ", <r>:", re)
);
```

$$n=1, l=0, ml=0, \langle r \rangle: \frac{a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{\log(1-\epsilon)}{\epsilon} \right)}{2}$$

$$n=2, l=0, ml=0, \langle r \rangle: \frac{a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{\log(1-\epsilon)}{\epsilon} \right)}{2}$$

$$n=2, l=1, ml=0, \langle r \rangle: \frac{3 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon^3} - \frac{\epsilon+2}{2 \epsilon^2} + \frac{\epsilon-2}{2 \epsilon^2} - \frac{\log(1-\epsilon)}{\epsilon^3} \right)}{2}$$

$$n=2, l=1, ml=1, \langle r \rangle: \frac{3 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{\log(\epsilon+1)}{\epsilon^3} + \frac{\epsilon+2}{2 \epsilon^2} - \frac{\log(1-\epsilon)}{\epsilon} - \frac{\epsilon-2}{2 \epsilon^2} + \frac{\log(1-\epsilon)}{\epsilon^3} \right)}{4}$$

$$n=3, l=0, ml=0, \langle r \rangle: \frac{a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{\log(1-\epsilon)}{\epsilon} \right)}{2}$$

$$n=3, l=1, ml=0, \langle r \rangle: \frac{3 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon^3} - \frac{\epsilon+2}{2 \epsilon^2} + \frac{\epsilon-2}{2 \epsilon^2} - \frac{\log(1-\epsilon)}{\epsilon^3} \right)}{2}$$

$$n=3, l=1, ml=1, \langle r \rangle: \frac{3 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{\log(\epsilon+1)}{\epsilon^3} + \frac{\epsilon+2}{2 \epsilon^2} - \frac{\log(1-\epsilon)}{\epsilon} - \frac{\epsilon-2}{2 \epsilon^2} + \frac{\log(1-\epsilon)}{\epsilon^3} \right)}{4}$$

$$n=3, l=2, ml=0, \langle r \rangle: \left(5 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{6 \log(\epsilon+1)}{\epsilon^3} + \frac{9 \log(\epsilon+1)}{\epsilon^5} + \frac{3 \epsilon^3 + 12 \epsilon^2 - 18 \epsilon - 36}{4 \epsilon^4} - \frac{3 \epsilon^3 - 12 \epsilon^2 - 18 \epsilon + 36}{4 \epsilon^4} - \frac{\log(1-\epsilon)}{\epsilon} + \frac{6 \log(1-\epsilon)}{\epsilon^3} - \frac{9 \log(1-\epsilon)}{\epsilon^5} \right) \right) / 8$$

$$n=3, l=2, ml=1, \langle r \rangle: \frac{15 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon^3} - \frac{\log(\epsilon+1)}{\epsilon^5} - \frac{3 \epsilon^3 + 8 \epsilon^2 - 6 \epsilon - 12}{12 \epsilon^4} + \frac{3 \epsilon^3 - 8 \epsilon^2 - 6 \epsilon + 12}{12 \epsilon^4} - \frac{\log(1-\epsilon)}{\epsilon^3} + \frac{\log(1-\epsilon)}{\epsilon^5} \right)}{4}$$

$$n=3, l=2, ml=2, \langle r \rangle: \left(15 a_0 \left(\frac{\log(\epsilon+1)}{\epsilon} - \frac{2 \log(\epsilon+1)}{\epsilon^3} + \frac{\log(\epsilon+1)}{\epsilon^5} + \frac{9 \epsilon^3 + 20 \epsilon^2 - 6 \epsilon - 12}{12 \epsilon^4} - \frac{9 \epsilon^3 - 20 \epsilon^2 - 6 \epsilon + 12}{12 \epsilon^4} - \frac{\log(1-\epsilon)}{\epsilon} + \frac{2 \log(1-\epsilon)}{\epsilon^3} - \frac{\log(1-\epsilon)}{\epsilon^5} \right) \right) / 16$$

□ **7 Expectation values of orbital radii in phi plane
(see notation of Atkins)**

⌈ (%i57) op: a[0]/(1+epsilon*cos(phi));

⌋ (%o57)
$$\frac{a_0}{\epsilon \cos(\phi) + 1}$$

```

(%i58) for i: 0 thru 9 do (
      re: Ex3(psi[i], op),
      print ("*****"),
      print (qn[i], ", <r>: ", re)
    );
Is  $\sqrt{1-\epsilon^2}-\epsilon+1$  positive, negative, or zero? p;
Is  $|\sqrt{1-\epsilon^2}-1|-\epsilon$  positive, negative, or zero? n;
*****
n=1, l=0, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=2, l=0, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=2, l=1, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=2, l=1, ml=1, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=0, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=1, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=1, ml=1, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=2, ml=0, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=2, ml=1, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
*****
n=3, l=2, ml=2, <r>:  $\frac{a_0}{\sqrt{1-\epsilon^2}}$ 
(%o58) done

```