Hydrogen Radial and Angular Wave Func

```
(%i62) kill(all);
(%o0) done
```

1 Define operators

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

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

$$(\%o2)\quad N(f):=\int_0^{\infty} \text{conjugate}(f)\, f\, r^2 \,dr$$

```
(%i3) /* Norm of spherical function */
      NY(f) := integrate(integrate(conjugate(f)*f*sin(theta), theta, 0, %
```

$$(\%o3)\quad NY(f):=\int_0^{2\pi}\int_0^{\pi} \text{conjugate}(f)\, f\, \sin(\theta)\, d\theta\, d\phi$$

```
(%i4) /* Norm of 3d function */
      N3(f) := integrate(integrate(integrate(conjugate(f)*f*sin(theta),
      phi, 0, 2*%pi)*r^2, r, 0, inf);
```

$$(\%o4)\quad N3(f):=\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \text{conjugate}(f)\, f\, \sin(\theta)\, d\theta\, d\phi\, r^2\, dr$$

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

$$(\%o5)\quad Ex(f,op):=\int_0^{\infty} \text{conjugate}(f)\, op\, f\, r^2 \,dr$$

```
(%i6) /* Expectation value of 3D wave function */
      Ex3(f,op) := integrate(integrate(integrate(conjugate(f)*op*f*sin(t
      phi, 0, 2*%pi)*r^2, r, 0, inf);
```

$$(\%o6)\quad Ex3(f,op):=\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \text{conjugate}(f)\, op\, f\, \sin(\theta)\, d\theta\, d\phi\, r^2\, dr$$

```
(%i7) /* Integral of two 3D wave functions */
      Ex32(f1,op,f2) := integrate(integrate(integrate(conjugate(f1)*op*f
      phi, 0, 2*%pi)*r^2, r, 0, inf);
```

$$(\%o7)\quad Ex32(f1,op,f2):=\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \text{conjugate}(f1)\, op\, f2\, \sin(\theta)\, d\theta\, d\phi\, r^2\, dr$$

Define energy levels of Hydrogen

2 Define Radial Eigenfunctions

(%i8) rhon: 2*Z*r/(n*a);

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

1s radial function

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

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

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

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

2s radial function

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

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

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

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

2p radial function

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

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

3s radial function

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

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

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

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

3p radial function

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

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

3d radial function

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

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

Derivatives of Eigenfunctions

(%i18)
```
for i: 0 thru 5 do (
dR[i]: ratsimp(diff(R[i],r)),
print (i, ":   ", dR[i])
);
```

$$0: \quad -\frac{2\,Z^{5/2}\,\%e^{-\frac{r\,Z}{a}}}{a^{5/2}}$$

$$1: \quad \frac{\sqrt{Z}\,(\sqrt{2}\,r\,Z^3-2^{5/2}\,a\,Z^2)\,\%e^{-\frac{r\,Z}{2\,a}}}{8\,a^{7/2}}$$

$$2: \quad -\frac{\sqrt{Z}\,(\sqrt{6}\,r\,Z^3-2\,\sqrt{6}\,a\,Z^2)\,\%e^{-\frac{r\,Z}{2\,a}}}{24\,a^{7/2}}$$

$$3: \quad -\frac{\sqrt{Z}\,(4\,\sqrt{3}\,r^2\,Z^4-20\,3^{3/2}\,a\,r\,Z^3+2\,3^{9/2}\,a^2\,Z^2)\,\%e^{-\frac{r\,Z}{3\,a}}}{729\,a^{9/2}}$$

$$4: \quad \frac{\sqrt{Z}\,(4\,r^2\,Z^4-48\,a\,r\,Z^3+72\,a^2\,Z^2)\,\%e^{-\frac{r\,Z}{3\,a}}}{243\,\sqrt{6}\,a^{9/2}}$$

$$5: \quad -\frac{\sqrt{Z}\,(2\,\sqrt{30}\,r^2\,Z^4-12\,\sqrt{30}\,a\,r\,Z^3)\,\%e^{-\frac{r\,Z}{3\,a}}}{3645\,a^{9/2}}$$

(%o18) *done*

Normalization check

```
(%i19) for i: 0 thru 5 do (
       print (i, "  N(R): ", N(R[i]), "    N(dR): ", N(dR[i]))
       );
```

0 N(R): 1 N(dR): $\frac{Z^2}{a^2}$

1 N(R): 1 N(dR): $\frac{Z^2}{4\,a^2}$

2 N(R): 1 N(dR): $\frac{Z^2}{12\,a^2}$

3 N(R): 1 N(dR): $\frac{Z^2}{9\,a^2}$

4 N(R): 1 N(dR): $\frac{5\,Z^2}{81\,a^2}$

5 N(R): 1 N(dR): $\frac{Z^2}{45\,a^2}$

(%o19) *done*

3 Spherial Harmonics

Define Eigenfunctions

Y(0,0)

```
(%i20) Y[0]: 1/(2*sqrt(%pi));
```

(%o20) $\frac{1}{2\sqrt{\pi}}$

Y(1,0)

```
(%i21) Y[1]: 1/2*sqrt(3/%pi)*cos(theta);
```

(%o21) $\frac{\sqrt{3}\cos(\theta)}{2\sqrt{\pi}}$

Y(1,1)

```
(%i22) Y[2]: -1/2*sqrt(3/(2*%pi))*sin(theta)*exp(%i*phi);
```

(%o22) $-\frac{\sqrt{3}\,\%e^{\%i\,\phi}\sin(\theta)}{2^{3/2}\sqrt{\pi}}$

Y(2,0)

```
(%i23) Y[3]: 1/4*sqrt(5/%pi)*(3*cos(theta)^2-1);
```

(%o23) $\frac{\sqrt{5}\,(3\cos(\theta)^2-1)}{4\sqrt{\pi}}$

Y(2,1)

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

(%o24) $$-\frac{\sqrt{15}\,\%e^{\%i\,\phi}\cos(\theta)\sin(\theta)}{2^{3/2}\sqrt{\pi}}$$

Y(2,2)

(%i25) `Y[5]: 1/4*sqrt(15/(2*%pi))*sin(theta)^2*exp(2*%i*phi);`

(%o25) $$\frac{\sqrt{15}\,\%e^{2\,\%i\,\phi}\sin(\theta)^2}{2^{5/2}\sqrt{\pi}}$$

Y(3,0)

(%i26) `Y[6]: 1/4*sqrt(7/%pi)*(5*cos(theta)^3-3*cos(theta));`

(%o26) $$\frac{\sqrt{7}\,(5\cos(\theta)^3-3\cos(\theta))}{4\sqrt{\pi}}$$

Y(3,1)

(%i27) `Y[7]: -1/8*sqrt(21/(%pi))*sin(theta)*(5*cos(theta)^2-1)*exp(%i*phi`

(%o27) $$-\frac{\sqrt{21}\,\%e^{\%i\,\phi}\,(5\cos(\theta)^2-1)\sin(\theta)}{8\sqrt{\pi}}$$

Y(3,2)

(%i28) `Y[8]: 1/4*sqrt(105/(2*%pi))*sin(theta)^2*cos(theta)*exp(2*%i*phi);`

(%o28) $$\frac{\sqrt{105}\,\%e^{2\,\%i\,\phi}\cos(\theta)\sin(\theta)^2}{2^{5/2}\sqrt{\pi}}$$

Y(3,3)

(%i29) `Y[9]: -1/8*sqrt(35/(%pi))*sin(theta)^3*exp(3*%i*phi);`

(%o29) $$-\frac{\sqrt{35}\,\%e^{3\,\%i\,\phi}\sin(\theta)^3}{8\sqrt{\pi}}$$

theta-derivative of Y

```
(%i30) for i: 0 thru 9 do (
       dYt[i]: ratsimp(diff(Y[i],theta)),
       print (i, ":   ", dYt[i])
       );
```

0 : 0

1 : $-\frac{\sqrt{3}\sin(\theta)}{2\sqrt{\pi}}$

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

3 : $-\frac{3\sqrt{5}\cos(\theta)\sin(\theta)}{2\sqrt{\pi}}$

4 : $\frac{\sqrt{2}\sqrt{15}\,\%e^{\%i\,\phi}\sin(\theta)^2-\sqrt{2}\sqrt{15}\,\%e^{\%i\,\phi}\cos(\theta)^2}{4\sqrt{\pi}}$

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

6 : $-\frac{(15\sqrt{7}\cos(\theta)^2-3\sqrt{7})\sin(\theta)}{4\sqrt{\pi}}$

7 : $\frac{10\sqrt{21}\,\%e^{\%i\,\phi}\cos(\theta)\sin(\theta)^2-5\sqrt{21}\,\%e^{\%i\,\phi}\cos(\theta)^3+\sqrt{21}\,\%e^{\%i\,\phi}\cos(\theta)}{8\sqrt{\pi}}$

8 : $-\frac{\sqrt{2}\sqrt{105}\,\%e^{2\,\%i\,\phi}\sin(\theta)^3-2^{3/2}\sqrt{105}\,\%e^{2\,\%i\,\phi}\cos(\theta)^2\sin(\theta)}{8\sqrt{\pi}}$

9 : $-\frac{3\sqrt{35}\,\%e^{3\,\%i\,\phi}\cos(\theta)\sin(\theta)^2}{8\sqrt{\pi}}$

(%o30) *done*

phi-derivative of Y

```
(%i31) for i: 0 thru 9 do (
       dYp[i]: ratsimp(diff(Y[i],phi)),
       print (i, ":   ", dYp[i])
       );
```

$$0: \quad 0$$

$$1: \quad 0$$

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

$$3: \quad 0$$

$$4: \quad -\frac{\sqrt{15}\ \%i\ \%e^{\%i\ \phi}\ \cos(\theta)\sin(\theta)}{2^{3/2}\sqrt{\pi}}$$

$$5: \quad \frac{\sqrt{15}\ \%i\ \%e^{2\ \%i\ \phi}\ \sin(\theta)^2}{2^{3/2}\sqrt{\pi}}$$

$$6: \quad 0$$

$$7: \quad -\frac{(5\sqrt{21}\ \%i\ \%e^{\%i\ \phi}\ \cos(\theta)^2 - \sqrt{21}\ \%i\ \%e^{\%i\ \phi})\sin(\theta)}{8\sqrt{\pi}}$$

$$8: \quad \frac{\sqrt{105}\ \%i\ \%e^{2\ \%i\ \phi}\ \cos(\theta)\sin(\theta)^2}{2^{3/2}\sqrt{\pi}}$$

$$9: \quad -\frac{3\sqrt{35}\ \%i\ \%e^{3\ \%i\ \phi}\ \sin(\theta)^3}{8\sqrt{\pi}}$$

(%o31) *done*

Normalization check

```
(%i32) for i: 0 thru 9 do (
       print (i, "  NY(Y): ", NY(Y[i]), "    NY(dY/dtheta): ", NY(dYt[i]),
       );
```

0	*NY(Y):*	1	*NY(dY/dtheta):*	0	*NY(dY/dphi):* 0
1	*NY(Y):*	1	*NY(dY/dtheta):*	2	*NY(dY/dphi):* 0
2	*NY(Y):*	1	*NY(dY/dtheta):*	$\frac{1}{2}$	*NY(dY/dphi):* 1
3	*NY(Y):*	1	*NY(dY/dtheta):*	6	*NY(dY/dphi):* 0
4	*NY(Y):*	1	*NY(dY/dtheta):*	$\frac{7}{2}$	*NY(dY/dphi):* 1
5	*NY(Y):*	1	*NY(dY/dtheta):*	1	*NY(dY/dphi):* 4
6	*NY(Y):*	1	*NY(dY/dtheta):*	12	*NY(dY/dphi):* 0
7	*NY(Y):*	1	*NY(dY/dtheta):*	$\frac{17}{2}$	*NY(dY/dphi):* 1
8	*NY(Y):*	1	*NY(dY/dtheta):*	5	*NY(dY/dphi):* 4
9	*NY(Y):*	1	*NY(dY/dtheta):*	$\frac{3}{2}$	*NY(dY/dphi):* 9

(%o32) *done*

*4 Wave functions psi(r,theta,phi)=R[n]*Y[l,m]*

```
psi[n=1, l=0, ml=0]
(%i33) qn[0]: "n=1, l=0, ml=0"$
(%i34) psi[0]:  R[0]*Y[0]$
psi[n=2, l=0, ml=0]
(%i35) qn[1]: "n=2, l=0, ml=0"$
(%i36) psi[1]:  R[1]*Y[0]$
psi[n=2, l=1, ml=0]
(%i37) qn[2]: "n=2, l=1, ml=0"$
(%i38) psi[2]:  R[2]*Y[1]$
psi[n=2, l=1, ml=1]
(%i39) qn[3]: "n=2, l=1, ml=1"$
(%i40) psi[3]:  R[2]*Y[2]$
psi[n=3, l=0, ml=0]
(%i41) qn[4]: "n=3, l=0, ml=0"$
(%i42) psi[4]:  R[3]*Y[0]$
psi[n=3, l=1, ml=0]
(%i43) qn[5]: "n=3, l=1, ml=0"$
(%i44) psi[5]:  R[4]*Y[1]$
psi[n=3, l=1, ml=1]
(%i45) qn[6]: "n=3, l=1, ml=1"$
(%i46) psi[6]:  R[4]*Y[2]$
psi[n=3, l=2, ml=0]
(%i47) qn[7]: "n=3, l=2, ml=0"$
(%i48) psi[7]:  R[5]*Y[3]$
```

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

```
(%i49) qn[8]: "n=3, l=2, ml=1"$
```

```
(%i50) psi[8]:  R[5]*Y[4]$
```

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

```
(%i51) qn[9]: "n=3, l=2, ml=2"$
```

```
(%i52) psi[9]:  R[5]*Y[5]$
```

```
(%i53) for i: 0 thru 9 do (
           print (qn[i], ", psi: ", psi[i])
       );
```

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

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

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

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

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

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

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

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

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

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

```
(%o53) done
```

Normalization check

```
(%i54) 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
(%o54) done
```

5 Expectation values for E1: -e hbar/(2m) sigmaZ BZ integral psi* sin^2(theta

```
(%i55) for i: 0 thru 9 do (
           op: -e*h[bar]/(2*m)*sigma[Z]*B[Z]*sin(theta)^2,
           print (qn[i], ",  Ex3(psi, op): ", Ex3(psi[i], op))
       );
```

n=1, l=0, ml=0 , Ex3(psi, op): $-\frac{h_{bar}\, e\, \sigma_Z\, B_Z}{3\, m}$

n=2, l=0, ml=0 , Ex3(psi, op): $-\frac{h_{bar}\, e\, \sigma_Z\, B_Z}{3\, m}$

n=2, l=1, ml=0 , Ex3(psi, op): $-\frac{h_{bar}\, e\, \sigma_Z\, B_Z}{5\, m}$

n=2, l=1, ml=1 , Ex3(psi, op): $-\frac{2\, h_{bar}\, e\, \sigma_Z\, B_Z}{5\, m}$

n=3, l=0, ml=0 , Ex3(psi, op): $-\frac{h_{bar}\, e\, \sigma_Z\, B_Z}{3\, m}$

n=3, l=1, ml=0 , Ex3(psi, op): $-\frac{h_{bar}\, e\, \sigma_Z\, B_Z}{5\, m}$

n=3, l=1, ml=1 , Ex3(psi, op): $-\frac{2\, h_{bar}\, e\, \sigma_Z\, B_Z}{5\, m}$

n=3, l=2, ml=0 , Ex3(psi, op): $-\frac{5\, h_{bar}\, e\, \sigma_Z\, B_Z}{21\, m}$

n=3, l=2, ml=1 , Ex3(psi, op): $-\frac{2\, h_{bar}\, e\, \sigma_Z\, B_Z}{7\, m}$

n=3, l=2, ml=2 , Ex3(psi, op): $-\frac{3\, h_{bar}\, e\, \sigma_Z\, B_Z}{7\, m}$

```
(%o55) done
```

6 Expectation values for E2: -e hbar/(2m) sigmaZ BZ integral psi* sin^2(theta

```
(%i56) for i: 0 thru 9 do (
           op: -e*h[bar]/(2*m)*sigma[Z]*B[Z]*sin(theta)^2,
           psi2: 1/r*diff(psi[i], r),
           print (qn[i], ",  Ex32(psi1, op, psi2): ", Ex32(psi[i], op, psi
       );
```

$$n=1,\ l=0,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{3\ a^2\ m}$$

$$n=2,\ l=0,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{24\ a^2\ m}$$

$$n=2,\ l=1,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{120\ a^2\ m}$$

$$n=2,\ l=1,\ ml=1,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{60\ a^2\ m}$$

$$n=3,\ l=0,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{81\ a^2\ m}$$

$$n=3,\ l=1,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{405\ a^2\ m}$$

$$n=3,\ l=1,\ ml=1,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{2\ h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{405\ a^2\ m}$$

$$n=3,\ l=2,\ ml=0,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{567\ a^2\ m}$$

$$n=3,\ l=2,\ ml=1,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{2\ h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{945\ a^2\ m}$$

$$n=3,\ l=2,\ ml=2,\ \ Ex32(psi1,\ op,\ psi2):\ \frac{h_{bar}\ e\ Z^2\ \sigma_Z\ B_Z}{315\ a^2\ m}$$

```
(%o56) done
```

7 Expectation values for E3: e/(2m) sigmaZ BZ integral psi* sin^2(theta) sigm

```
E3 = e hbar/(2m) ES3 sigmaZ BZ integral psi* sin^2(theta) sigma*L dtau
with
ES3 = j*(j+1)-l*(l-1)-s*(s+1)
```

```
(%i67) E3fun(l,s,j,ml,ms,mj,iR,iY) := (
           psi: R[iR]*Y[iY],
           EJ: j*(j+1)-l*(l-1)-s*(s+1),
           op: e*h[bar]/(2*m)*sigma[Z]*B[Z]*EJ*sin(theta)^2,
           E3: Ex3(psi, op)
       /*    print("l, s, j, ml, ms, mj, iR, iY = ", l,s,j,ml,ms,mj,iR,iY
             ", ES3 = ",ES3, ", E = ",E)
           print("ES3 = ",ES3, ", E = ",E)*/
       )$
```

```
(%i74) for l: 0 thru 3 do (
           for ml: -l thru l do (
               for ms1: 1 thru 2 do (
                   ms: ms1-3/2,
                   mj: ml + ms,
                   if ml=-l then s: 1/2 else s: ms,
                   j: abs(l + s),
                  /* if j>0 then (*/
                   iY: 0,
                   if l=1 and abs(ml)=1 then iY: 2,
                   if l=1 and abs(ml)=0 then iY: 1,
                   if l=2 and abs(ml)=2 then iY: 5,
                   if l=2 and abs(ml)=1 then iY: 4,
                   if l=2 and abs(ml)=0 then iY: 3,
                   if l=3 and abs(ml)=3 then iY: 9,
                   if l=3 and abs(ml)=2 then iY: 8,
                   if l=3 and abs(ml)=1 then iY: 7,
                   if l=3 and abs(ml)=0 then iY: 6,
                   EJ: 0, E3: 0,
                   E3fun(l, 1/2, j, ml, ms, mj, 0, iY),
                   printf(true, "l=~d,  ml=~d, j=~a,  s=~a,  ms=~a,  mj=~a
                   l, ml, j, s, ms, mj, EJ, E3),
                   print("                    EJ=", EJ, ", E3=", E3)
       )))$
l=0,  ml=0, j=1/2,  s=1/2,  ms=-1/2,  mj=-1/2
                    EJ= 0 , E3= 0
l=0,  ml=0, j=1/2,  s=1/2,  ms=1/2,  mj=1/2
                    EJ= 0 , E3= 0
l=1,  ml=-1, j=3/2,  s=1/2,  ms=-1/2,  mj=-3/2
                    EJ= 3 , E3= 6 h_bar e σ_Z B_Z / (5 m)
l=1,  ml=-1, j=3/2,  s=1/2,  ms=1/2,  mj=-1/2
                    EJ= 3 , E3= 6 h_bar e σ_Z B_Z / (5 m)
l=1,  ml=0, j=1/2,  s=-1/2,  ms=-1/2,  mj=-1/2
                    EJ= 0 , E3= 0
l=1,  ml=0, j=3/2,  s=1/2,  ms=1/2,  mj=1/2
                    EJ= 3 , E3= 3 h_bar e σ_Z B_Z / (5 m)
l=1,  ml=1, j=1/2,  s=-1/2,  ms=-1/2,  mj=1/2
                    EJ= 0 , E3= 0
l=1,  ml=1, j=3/2,  s=1/2,  ms=1/2,  mj=3/2
                    EJ= 3 , E3= 6 h_bar e σ_Z B_Z / (5 m)
l=2,  ml=-2, j=5/2,  s=1/2,  ms=-1/2,  mj=-5/2
                    EJ= 6 , E3= 18 h_bar e σ_Z B_Z / (7 m)
l=2,  ml=-2, j=5/2,  s=1/2,  ms=1/2,  mj=-3/2
                    EJ= 6 , E3= 18 h_bar e σ_Z B_Z / (7 m)
l=2,  ml=-1, j=3/2,  s=-1/2,  ms=-1/2,  mj=-3/2
                    EJ= 1 , E3= 2 h_bar e σ_Z B_Z
```