```
(%i3) kill(all);
(%o0) done
```

(%i1) batchload("D:/Doc/Artikel-Eck/ECE-Theorie/Paper253/RY-Hydrogen.wxm

0 : $$-\frac{2\,Z^{5/2}\,\%e^{-\frac{r\,Z}{a_0}}}{a_0^{5/2}}$$

1 : $$\frac{\sqrt{Z}\,(\sqrt{2}\,r\,Z^3-2^{5/2}\,a_0\,Z^2)\,\%e^{-\frac{r\,Z}{2\,a_0}}}{8\,a_0^{7/2}}$$

2 : $$-\frac{\sqrt{Z}\,(\sqrt{6}\,r\,Z^3-2\,\sqrt{6}\,a_0\,Z^2)\,\%e^{-\frac{r\,Z}{2\,a_0}}}{24\,a_0^{7/2}}$$

3 : $$-\frac{\sqrt{Z}\,(4\,\sqrt{3}\,r^2\,Z^4-20\,3^{3/2}\,a_0\,r\,Z^3+2\,3^{9/2}\,a_0^2\,Z^2)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{729\,a_0^{9/2}}$$

4 : $$\frac{\sqrt{Z}\,(4\,r^2\,Z^4-48\,a_0\,r\,Z^3+72\,a_0^2\,Z^2)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{243\,\sqrt{6}\,a_0^{9/2}}$$

5 : $$-\frac{\sqrt{Z}\,(2\,\sqrt{30}\,r^2\,Z^4-12\,\sqrt{30}\,a_0\,r\,Z^3)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{3645\,a_0^{9/2}}$$

0 : $$\frac{2\,Z^{7/2}\,\%e^{-\frac{r\,Z}{a_0}}}{a_0^{7/2}}$$

1 : $$-\frac{\sqrt{Z}\,(r\,Z^4-6\,a_0\,Z^3)\,\%e^{-\frac{r\,Z}{2\,a_0}}}{2^{7/2}\,a_0^{9/2}}$$

2 : $$\frac{\sqrt{Z}\,(r\,Z^4-4\,a_0\,Z^3)\,\%e^{-\frac{r\,Z}{2\,a_0}}}{8\,\sqrt{6}\,a_0^{9/2}}$$

3 : $$\frac{\sqrt{Z}\,(4\,\sqrt{3}\,r^2\,Z^5-28\,3^{3/2}\,a_0\,r\,Z^4+38\,3^{5/2}\,a_0^2\,Z^3)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{2187\,a_0^{11/2}}$$

4 : $$-\frac{\sqrt{Z}\,(2\,\sqrt{6}\,r^2\,Z^5-6^{5/2}\,a_0\,r\,Z^4+3\,6^{5/2}\,a_0^2\,Z^3)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{2187\,a_0^{11/2}}$$

5 : $$\frac{\sqrt{Z}\,(2\,\sqrt{30}\,r^2\,Z^5-24\,\sqrt{30}\,a_0\,r\,Z^4+36\,\sqrt{30}\,a_0^2\,Z^3)\,\%e^{-\frac{r\,Z}{3\,a_0}}}{10935\,a_0^{11/2}}$$

0 N(R): 1 N(dR): $\frac{Z^2}{a_0^2}$ N(d2R): $\frac{Z^4}{a_0^4}$

1 N(R): 1 N(dR): $\frac{Z^2}{4\,a_0^2}$ N(d2R): $\frac{3\,Z^4}{16\,a_0^4}$

2 N(R): 1 N(dR): $\frac{Z^2}{12\,a_0^2}$ N(d2R): $\frac{Z^4}{48\,a_0^4}$

3 N(R): 1 N(dR): $\frac{Z^2}{9\,a_0^2}$ N(d2R): $\frac{49\,Z^4}{729\,a_0^4}$

4 N(R): 1 N(dR): $\frac{5\,Z^2}{36\,a_0^2}$ N(d2R): $\frac{Z^4}{}$

1 Operators

```
(%i2) /* radial part of delta operator */
      D2r(f) := (expand(1/r^2*diff(r^2*diff(f,r),r)));
```

$$(\%o2)\quad D2r(f):=\mathrm{expand}\left(\frac{1}{r^2}\,\mathrm{diff}(r^2\,\mathrm{diff}(f,r),r)\right)$$

```
(%i3) /* full delta operator */
      Delta_s(psi) := 1/r^2*diff(r^2*diff(psi,r),r)
      + 1/(r^2*sin(theta))*diff(sin(theta)*diff(psi,theta),theta)
      + 1/(r^2*sin(theta)^2)*diff(psi,phi,2);
```

$$(\%o3)\quad \mathrm{Delta\_s}(\Psi):=\frac{1}{r^2}\,\mathrm{diff}(r^2\,\mathrm{diff}(\Psi,r),r)+\frac{1}{r^2\sin(\theta)}\,\mathrm{diff}(\sin(\theta)\,\mathrm{diff}(\Psi,\theta),\theta)+\frac{1}{r^2\sin(\theta)^2}\,\mathrm{diff}(\Psi,\phi,2)$$

```
(%i4) grad_s(psi) := [diff(psi,r), 1/r*diff(psi,theta), 1/(r*sin(theta))
```

$$(\%o4)\quad \mathrm{grad\_s}(\Psi):=\left[\mathrm{diff}(\Psi,r),\frac{1}{r}\,\mathrm{diff}(\Psi,\theta),\frac{1}{r\sin(\theta)}\,\mathrm{diff}(\Psi,\phi)\right]$$

```
(%i5) f: h[bar]^3/(2*m);
      str: [a[0]=1, Z=1, c=c1];
```

$$(\%o5)\quad \frac{h_{bar}^3}{2\,m}$$

$$(\%o6)\quad [a_0=1,Z=1,c=c1]$$

2 Expectation values

2.1 Ekin, Lz, EkinLz, LzEkin

```
(%i9) i: 0$
      for n: 1 thru 3 do (
       for l: 0 thru n-1 do (
        for ml: 0 thru l do (
         EkinLz: f*          Ex32(psi[i], 1, Delta_s(diff(psi[i],phi))),
         LzEkin: f*          Ex32(psi[i], 1, diff(Delta_s(psi[i]),phi)),
         Lz:  h[bar]/%i*      Ex32(psi[i], 1, diff(psi[i],phi)),
         Ekin: h[bar]^2/(2*m)*Ex32(psi[i], 1, Delta_s(psi[i])),
         printf(true, "~s Ekin=~a Lz=~a EkinLz=~a LzEkin=~a~%", qn[i],
              Ekin, Lz, EkinLz, LzEkin),
         print(Ekin), print(Lz), print(EkinLz),print(LzEkin),
         print("------------"),
         i: i+1
      )));
```

"n=1, l=0, ml=0" Ekin=-h[bar]^2*Z^2/(2*a[0]^2*m) Lz=0 EkinLz=0 LzEkin=0

$$-\frac{h_{bar}^2 Z^2}{2 a_0^2 m}$$

0

0

0

"n=2, l=0, ml=0" Ekin=-h[bar]^2*Z^2/(8*a[0]^2*m) Lz=0 EkinLz=0 LzEkin=0

$$-\frac{h_{bar}^2 Z^2}{8 a_0^2 m}$$

0

0

0

"n=2, l=1, ml=0" Ekin=-h[bar]^2*Z^2/(8*a[0]^2*m) Lz=0 EkinLz=0 LzEkin=0

$$-\frac{h_{bar}^2 Z^2}{8 a_0^2 m}$$

0

0

0

"n=2, l=1, ml=1" Ekin=-h[bar]^2*Z^2/(8*a[0]^2*m) Lz=h[bar] EkinLz=-%i*h[ba

$$-\frac{h_{bar}^2 Z^2}{8 a_0^2 m}$$

$$h_{bar}$$

$$-\frac{\%i\, h_{bar}^3 Z^2}{8 a_0^2 m}$$

$$-\frac{\%i\, h_{bar}^3 Z^2}{8 a_0^2 m}$$

"n=3, l=0, ml=0" Ekin=-h[bar]^2*Z^2/(18*a[0]^2*m) Lz=0 EkinLz=0 LzEkin=0

$$-\frac{h_{bar}^2 Z^2}{18 a_0^2 m}$$

0

0

0