```
> restart:

> # ###################
  # Uebung 11, Aufgabe 2
  # ###################

> assume(e>0):
  assume(hbar>0):
  assume(m>0):

  # Bohrscher Radius.
  a := hbar^2/(m*e^2):

> # Radialanteile der Wellenfunktionen (dir R_nl sind urspruenglich
  bezueglich rho normiert).

  R_10 := 2 * exp(-rho):
  norm_ := int(subs(rho=r/a, R_10)^2 * r^2, r=0..infinity);
  R_10 := R_10 / sqrt(norm_);
  norm_ := int(subs(rho=r/a, R_10)^2 * r^2, r=0..infinity);

  R_20 := (1/sqrt(2)) * (1 - rho/2) * exp(-rho/2):
  norm_ := int(subs(rho=r/a, R_20)^2 * r^2, r=0..infinity);
  R_20 := R_20 / sqrt(norm_);
  norm_ := int(subs(rho=r/a, R_20)^2 * r^2, r=0..infinity);

  R_21 := (1/(2*sqrt(6))) * rho * exp(-rho/2):
  norm_ := int(subs(rho=r/a, R_21)^2 * r^2, r=0..infinity);
  R_21 := R_21 / sqrt(norm_);
  norm_ := int(subs(rho=r/a, R_21)^2 * r^2, r=0..infinity);

  R_31 := (8/(27*sqrt(6))) * rho * (1 - rho/6) * exp(-rho/3):
  norm_ := int(subs(rho=r/a, R_31)^2 * r^2, r=0..infinity);
  R_31 := R_31 / sqrt(norm_);
  norm_ := int(subs(rho=r/a, R_31)^2 * r^2, r=0..infinity);
```

$$norm\_ := \frac{hbar\sim^6}{m\sim^3 e\sim^6}$$

$$R\_10 := \frac{2\, e^{-\rho}\, m\sim^{3/2} e\sim^3}{hbar\sim^3}$$

$$norm\_ := 1$$

$$norm\_ := \frac{hbar\sim^6}{m\sim^3 e\sim^6}$$

$$R\_20 := \frac{1}{2}\,\frac{\sqrt{2}\left(1-\frac{1}{2}\rho\right) e^{-\frac{1}{2}\rho}\, m\sim^{3/2} e\sim^3}{hbar\sim^3}$$

$$norm\_ := 1$$

$$norm\_ := \frac{hbar\sim^6}{m\sim^3 e\sim^6}$$

$$R\_21 := \frac{1}{12}\,\frac{\sqrt{6}\,\rho\, e^{-\frac{1}{2}\rho}\, m\sim^{3/2} e\sim^3}{hbar\sim^3}$$

$$norm\_ := 1$$

$$norm\_ := \frac{hbar\sim^6}{m\sim^3 e\sim^6}$$

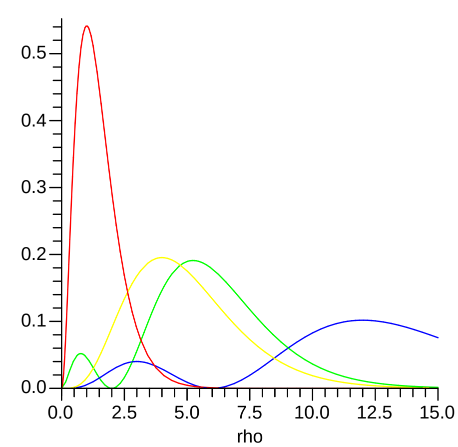
$$R\_31 := \frac{4}{81}\,\frac{\sqrt{6}\,\rho\left(1-\frac{1}{6}\rho\right) e^{-\frac{1}{3}\rho}\, m\sim^{3/2} e\sim^3}{hbar\sim^3}$$

$$norm\_ := 1 \qquad (1)$$

```
> # Test durch Einsetzen in die SG fuer radialsymmetrische Probleme.

  # Potential.
  V := -e^2/r:

  # Energieeigenwerte.
  E := (-m*e^4/(2*hbar^2)) * (1/n^2):

  # |1 0 0>

  simplify(
    subs(n=1, l=0,
      (-hbar^2/(2*m)) * diff(diff(subs(rho=r/a, R_10)*r, r), r) +
      (hbar^2/(2*m)) * (l*(l+1)/r^2) * subs(rho=r/a, R_10)*r +
      V * subs(rho=r/a, R_10)*r -
      E * subs(rho=r/a, R_10)*r
      )
  );

  # |2 0 0>

  simplify(
    subs(n=2, l=0,
      (-hbar^2/(2*m)) * diff(diff(subs(rho=r/a, R_20)*r, r), r) +
      (hbar^2/(2*m)) * (l*(l+1)/r^2) * subs(rho=r/a, R_20)*r +
      V * subs(rho=r/a, R_20)*r -
      E * subs(rho=r/a, R_20)*r
      )
  );

  # |2 1 0>

  simplify(
    subs(n=2, l=1,
      (-hbar^2/(2*m)) * diff(diff(subs(rho=r/a, R_21)*r, r), r) +
      (hbar^2/(2*m)) * (l*(l+1)/r^2) * subs(rho=r/a, R_21)*r +
      V * subs(rho=r/a, R_21)*r -
      E * subs(rho=r/a, R_21)*r
      )
  );

  # |3 1 0>

  simplify(
    subs(n=3, l=1,
      (-hbar^2/(2*m)) * diff(diff(subs(rho=r/a, R_31)*r, r), r) +
      (hbar^2/(2*m)) * (l*(l+1)/r^2) * subs(rho=r/a, R_31)*r +
      V * subs(rho=r/a, R_31)*r -
      E * subs(rho=r/a, R_31)*r
      )
  );
```

$$0$$
$$0$$
$$0$$
$$0 \qquad (2)$$

```
> # Radiale Aufenthaltswahrscheinlichkeit in Einheiten von a.
  plot(subs(r=rho*a, [a*R_10^2*r^2, a*R_20^2*r^2, a*R_21^2*r^2, a*
  R_31^2*r^2]), rho=0.0..15.0);
```




```
> # Grundzustandserwartungswerte.

  # Erwartungswert von 1 (ein Check).
  int(subs(rho=r/a, R_10)^2 * r^2, r=0..infinity);

  # Erwartungswert von r   -->   (3/2) * a.
  int(subs(rho=r/a, R_10)^2 * r^2 * r, r=0..infinity);

  # Erwartungswert von r^2   -->   3 * a^2.
  int(subs(rho=r/a, R_10)^2 * r^2 * r^2, r=0..infinity);

  # Erwartungswert von x   -->   0 (Rotationssymmetrie).

  # Erwartungswert von x^2   -->   a^2 (Symmetrie).
```

$$1$$

$$\frac{3}{2}\,\frac{hbar\sim^2}{m\sim e\sim^2}$$

$$\frac{3\, hbar\sim^4}{m\sim^2\, e\sim^4} \tag{3}$$

```
> 
  # |2 1 1>-Erwartungswerte.

  assume(phi, real):
  Y_11 := sqrt(3/(8*Pi)) * sin(theta) * exp(I*phi);

  # Erwartungswert von 1 (ein Check).
  int(subs(rho=r/a, R_21)^2 * r^2, r=0..infinity) *
    int(conjugate(Y_11)*Y_11 * sin(theta), theta=0..Pi) *
    int(1, phi=0..2*Pi);

  # Erwartungswert von x^2 = (r^2 * sin(theta)^2 * cos(phi)^2)   -->
    12 * a.
  int(subs(rho=r/a, R_21)^2 * r^2 * r^2, r=0..infinity) *
    int(conjugate(Y_11)*Y_11 * sin(theta) * sin(theta)^2, theta=0..
  Pi) *
    int(cos(phi)^2, phi=0..2*Pi);
```

$$Y\_11 := \frac{1}{4}\,\frac{\sqrt{6}\,\sin(\theta)\,e^{I\,\phi\sim}}{\sqrt{\pi}}$$

$$1$$

$$\frac{12\, hbar\sim^4}{m\sim^2\, e\sim^4} \tag{4}$$

>