Atomske orbite vodoniku slicnih atoma

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```
> restart : with(plots) : fonte :=
  titlefont=[TIMES,ROMAN,11] :
  read `R.txt` : # parties radiales.
  read `Y.txt` : # parties angulaires en
  sphériques.
  read `Yc.txt`: # parties angulaires en
  cartésiennes (x,y,z,r).
```

Uglovne komponente

Razvijanje normiranih funkcija

Verifikacija koeficijenata nomalizacije R[n,L]:

```
> assume(Z>0) :
  dP := (r*R[n,L])^2 ;
  #seq(seq(lprint([n,L],int(dP,r =
  0..infinity)), L=0..n-1), n=1..7) ;
  unassign('n','L') :
```

$$dP := r^2 {R_{n,L}}^2$$

Dodatak - koeficijent srazmernosti

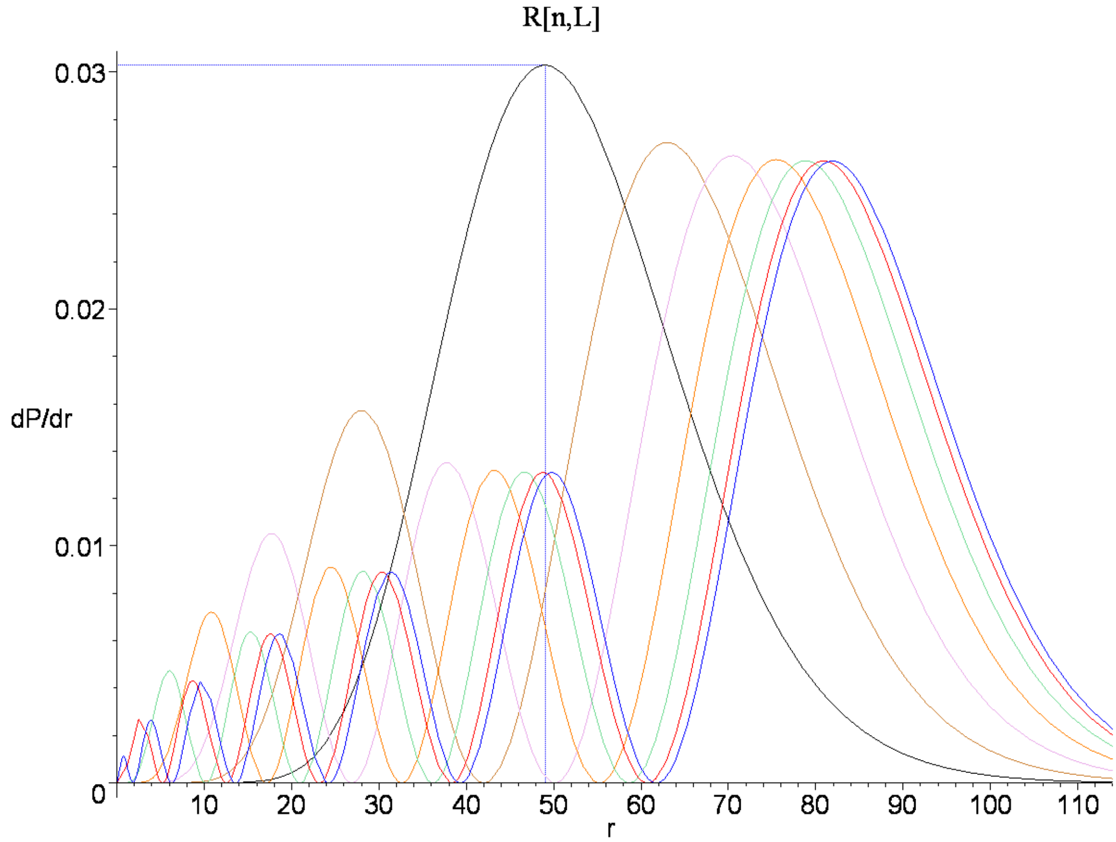
```
> r^2*R[n,L]^2/(r^2*R[n,L]^2/(r+h+me));
```

$$r + h + me$$

Representacija dP/dr = r.R.[n,L]:

```
> Z := 1 : n := 7 :
  couleurs :=
  [blue,red,aquamarine,coral,plum,gold,black]
  :
  top :=
  simplify(subs(r=n^2,eval(subs(L=n-1,dP)))):
  maxi :=
  plot([[n^2,0],[n^2,top],[0,top]],color=blue,
  linestyle=2) :
  sq := seq(plot(dP, r = 0..n*(n+10)-5,
```

```
color=couleurs[L+1]),L=0..n-1) :
display([sq,maxi],title=`R[n,L]`,fonte,
labels=[`r `,`dP/dr`],tickmarks=[10,3]);
unassign('n','L','Z') :
```

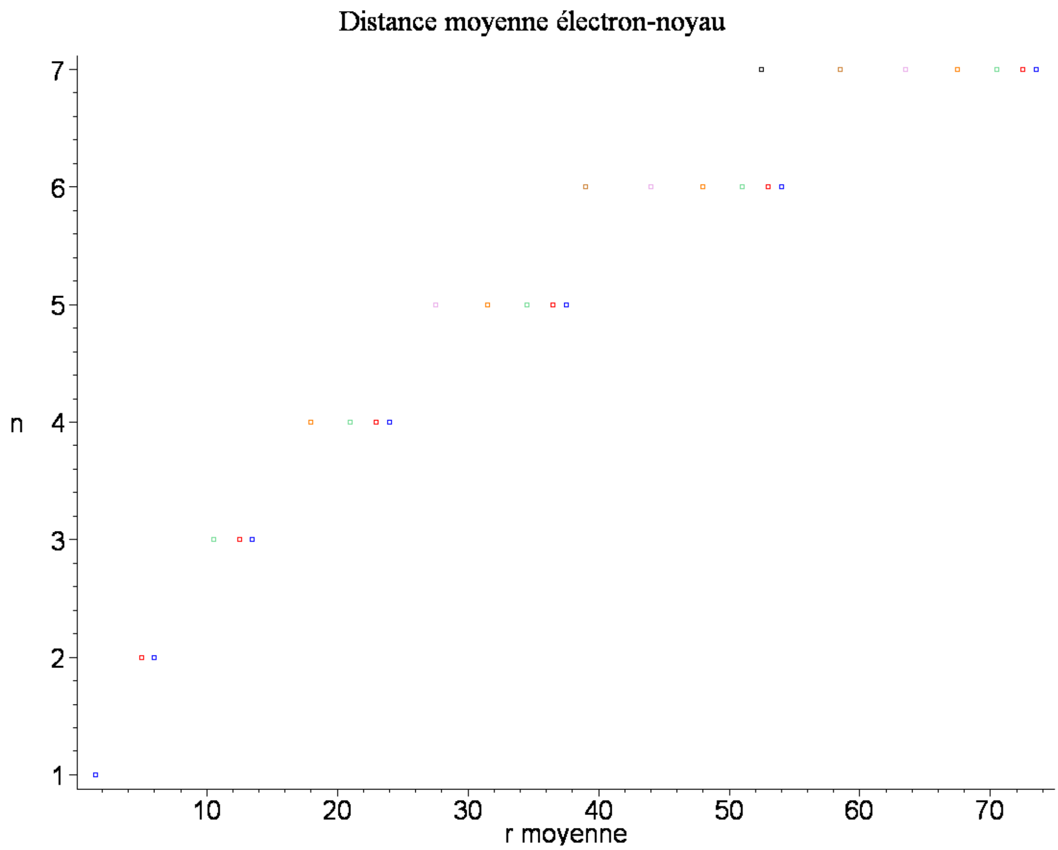


Srednje rastojanje elektron-jezgro

```
> assume(Z,posint):
  rm := Int(r*dP, r=0..infinity);
```

$$rm := \int_0^{\infty} r^3 R_{n,L}^2 \, dr$$

```
> #seq(lprint(`------`$2,seq(lprint([n,L],
  value(rm)), L=0..n-1)), n=1..7);
> ### WARNING: the definition of the type
  `symbol` has changed'; see help page for
  details
  gr:=seq(seq(plot([[eval(subs(Z=1,value(rm)))
  ,n]],color=couleurs[L+1],style=point,symbol=
  box),L=0..n-1),n=1..7):
  display([gr],title=`Distance moyenne
  électron-noyau`,fonte,labels=[`r moyenne`,`n
  `],tickmarks=[5,7]);
```



Uglovne komponente

Razvijanje ne normiranih funkcija Y[L,m]

Koeficijenti uglovnih komponenata

```
> unassign('n','L','Z','m') :
C := sqrt(1/Int(Int(Y[L,m]^2*sin(theta),
theta = 0..Pi), phi = 0..2*Pi)) ;
seq(seq(print([L,m],simplify(value(C))),
m=-L..L), L=0..5) ;
```

$$C := \sqrt{\frac{1}{\int_0^{2\pi}\int_0^{\pi} {Y_{L,m}}^2 \sin(\theta)\, d\theta\, d\phi}}$$

$$[0, 0], \frac{1}{2}\frac{1}{\sqrt{\pi}}$$

$$[1, -1], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[1, 0], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[1, 1], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[2, -2], \frac{1}{4}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, -1], \frac{1}{2}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, 0], \frac{1}{4}\frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[2, 1], \frac{1}{2}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, 2], \frac{1}{4}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[3, -3], \frac{1}{8}\frac{\sqrt{35}\sqrt{2}}{\sqrt{\pi}}$$

$$[3, -2], \frac{1}{4}\frac{\sqrt{105}}{\sqrt{\pi}}$$

$$[3, -1], \frac{1}{8}\frac{\sqrt{21}\sqrt{2}}{\sqrt{\pi}}$$

$$[3, 0], \frac{1}{4}\frac{\sqrt{7}}{\sqrt{\pi}}$$

$$[3, 1], \frac{1}{8}\frac{\sqrt{21}\sqrt{2}}{\sqrt{\pi}}$$

$$[3, 2], \frac{1}{4} \frac{\sqrt{105}}{\sqrt{\pi}}$$

$$[3, 3], \frac{1}{8} \frac{\sqrt{35}\sqrt{2}}{\sqrt{\pi}}$$

$$[4, -4], \frac{3}{16} \frac{\sqrt{35}}{\sqrt{\pi}}$$

$$[4, -3], \frac{3}{8} \frac{\sqrt{35}\sqrt{2}}{\sqrt{\pi}}$$

$$[4, -2], \frac{3}{8} \frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[4, -1], \frac{3}{8} \frac{\sqrt{5}\sqrt{2}}{\sqrt{\pi}}$$

$$[4, 0], \frac{3}{16} \frac{1}{\sqrt{\pi}}$$

$$[4, 1], \frac{3}{8} \frac{\sqrt{5}\sqrt{2}}{\sqrt{\pi}}$$

$$[4, 2], \frac{3}{8} \frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[4, 3], \frac{3}{8} \frac{\sqrt{35}\sqrt{2}}{\sqrt{\pi}}$$

$$[4, 4], \frac{3}{16} \frac{\sqrt{35}}{\sqrt{\pi}}$$

$$[5, -5], \frac{3}{32} \frac{\sqrt{77}\sqrt{2}}{\sqrt{\pi}}$$

$$[5, -4], \frac{3}{16} \frac{\sqrt{385}}{\sqrt{\pi}}$$

$$[5, -3], \frac{1}{32} \frac{\sqrt{385}\sqrt{2}}{\sqrt{\pi}}$$

$$[5, -2], \frac{1}{8} \frac{\sqrt{1155}}{\sqrt{\pi}}$$

$$[5, -1], \frac{1}{16} \frac{\sqrt{165}}{\sqrt{\pi}}$$

$$[5, 0], \frac{1}{16} \frac{\sqrt{11}}{\sqrt{\pi}}$$

$$[5, 1], \frac{1}{16} \frac{\sqrt{165}}{\sqrt{\pi}}$$

$$[5, 2], \frac{1}{8} \frac{\sqrt{1155}}{\sqrt{\pi}}$$

$$[5, 3], \frac{1}{32} \frac{\sqrt{385}\sqrt{2}}{\sqrt{\pi}}$$

$$[5, 4], \frac{3}{16} \frac{\sqrt{385}}{\sqrt{\pi}}$$

$$[5, 5], \frac{3}{32} \frac{\sqrt{77}\sqrt{2}}{\sqrt{\pi}}$$

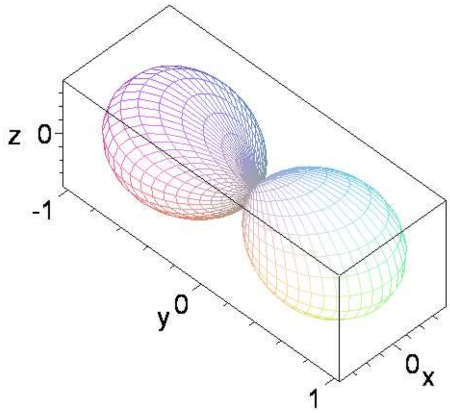
Reprezentacija ne normiranih Y[L,m]

```
> setoptions3d (grid=[50, 50],
  scaling=constrained, style=hidden,
  tickmarks=[3, 3, 3],fonte, axes=box):
  domaine := phi = 0..Pi, theta = 0..2*Pi :
  #pour les anglo-saxons theta et phi sont
  permutés ...
```

Orbitale p: L = 1 ; m = -1 (py) ; m = 0 (pz) ; m = 1 (px)

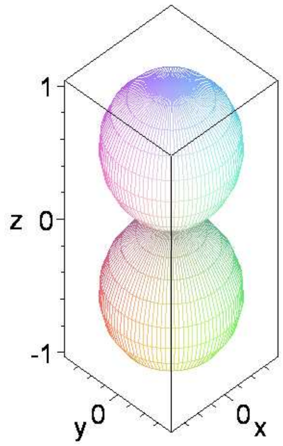
```
> py := sphereplot( Y[1,-1]^2, domaine,
  title = `m = - 1  py`) : py ;
```

m = - 1 py

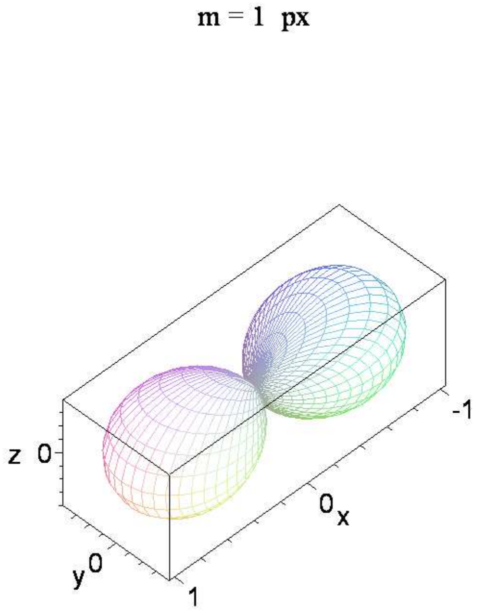



```
> pz := sphereplot( Y[1,0]^2 , domaine,
  title = `m = 0  pz`) : pz ;
```

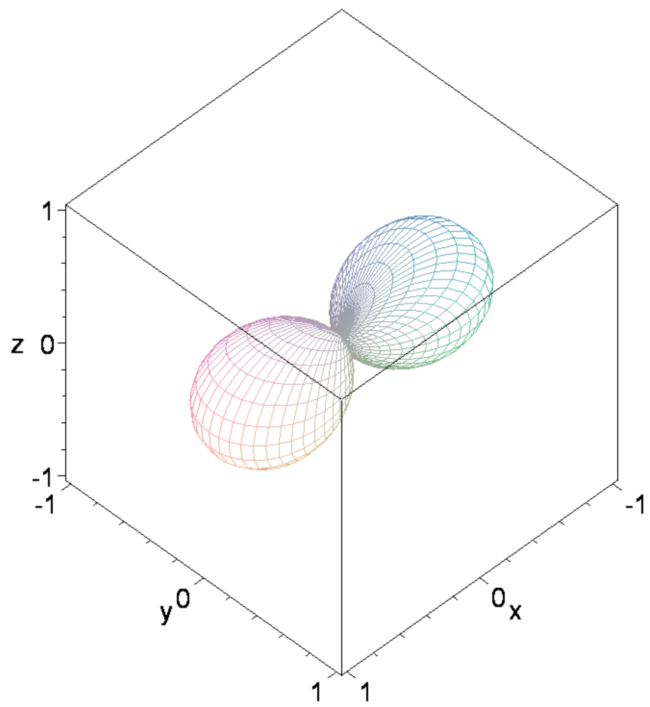
m = 0 pz



```
> px := sphereplot( Y[1,1]^2 , domaine,
  title = `m = 1  px`) : px ;
```




```
> display ([px, py, pz],insequence=true ) ;
```

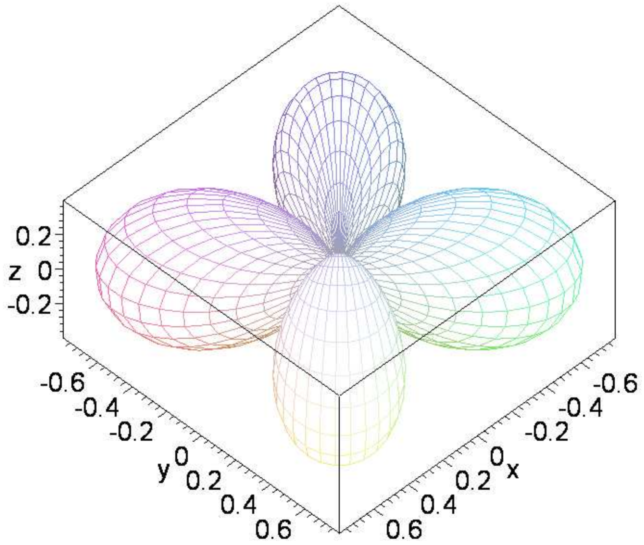


<u>Orbitales d</u>: L = 2 ; m = -2 (dxy) ; m = -1 (dyz) ; m = 0 (dz^2) ; m =1 (dxz) ; m = 2 (dx^2-y^2)

```
> sphereplot( abs(Y[2,-2]), domaine, title
```

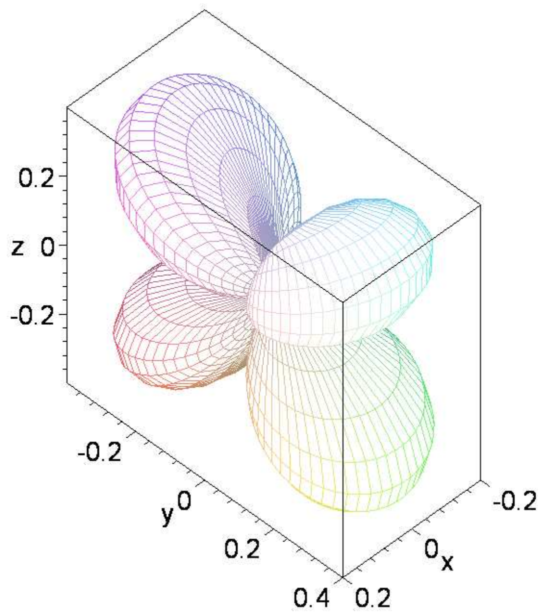
```
  =`m = -2  dxy`) ;
```

m = -2 dxy



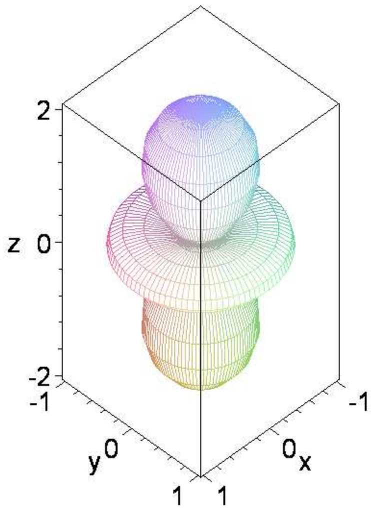

```
> sphereplot( abs(Y[2,-1]), domaine, title
  =`m = -1  dyz`) ;
```

m = -1 dyz



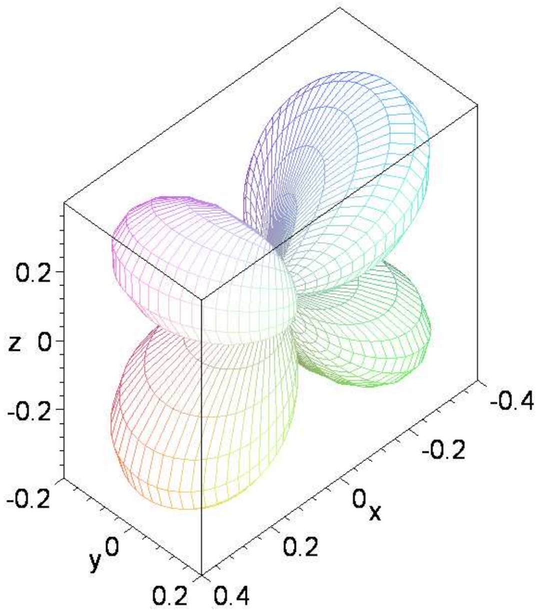

```
> sphereplot(      Y[2,0] , domaine, title
  =`m = 0  dz¸`) ;
```

m = 0 dz¿



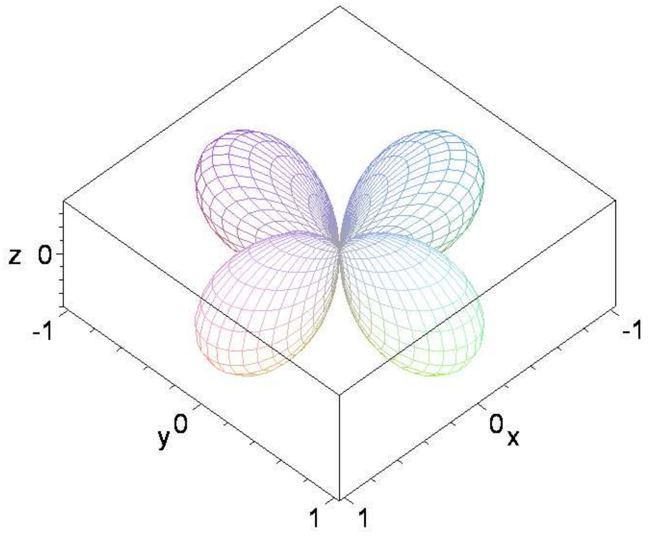

```
> sphereplot( abs(Y[2,1]) , domaine, title
  =`m = 1  dxz`) ;
```

m = 1 dxz




```
> sphereplot( abs(Y[2,2]) , domaine, title
  =`m = 2  d(x¿-y¿)`) ;
```

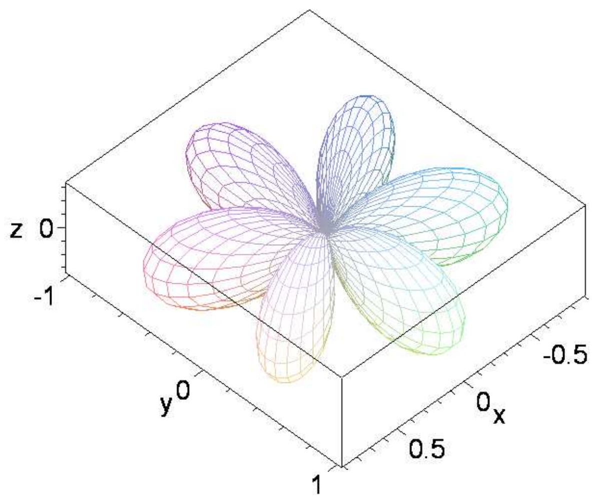
m = 2 d(x_-y_)



Orbitale f: L = 3 ;

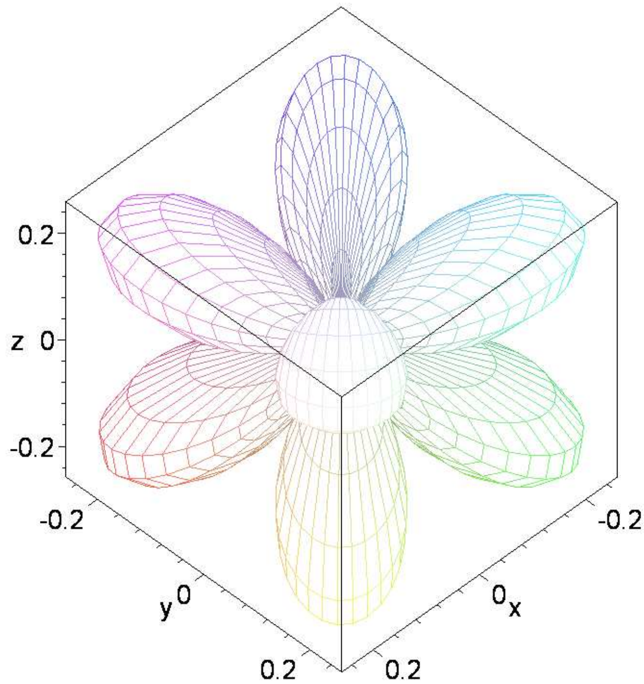
```
> sphereplot( abs(Y[3,-3]), domaine, title
  =`m = - 3`) ;
```

m = - 3



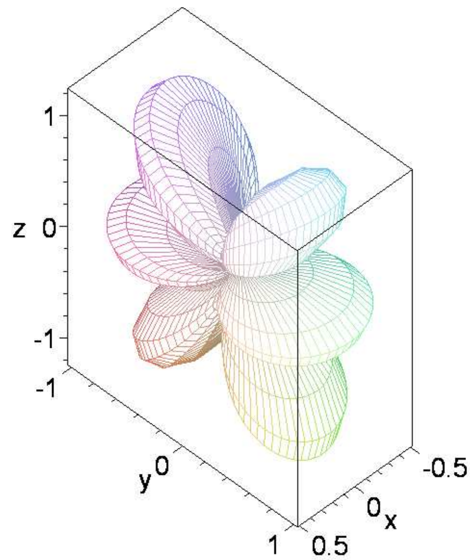

```
> sphereplot( abs(Y[3,-2]), domaine, title
  =`m = - 2`) ;
```

m = - 2



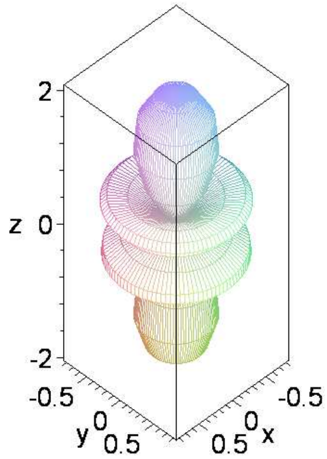

```
> sphereplot( abs(Y[3,-1]), domaine, title
  =`m = - 1`) ;
```

m = - 1



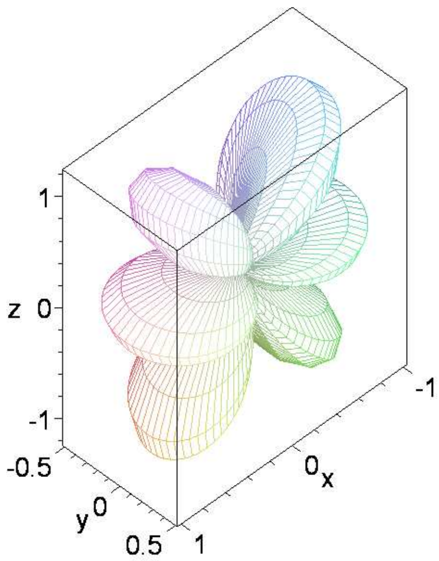

```
> sphereplot( abs(Y[3,0]) , domaine, title
  =`m = 0`) ; # idem  y -> z
```

m = 0

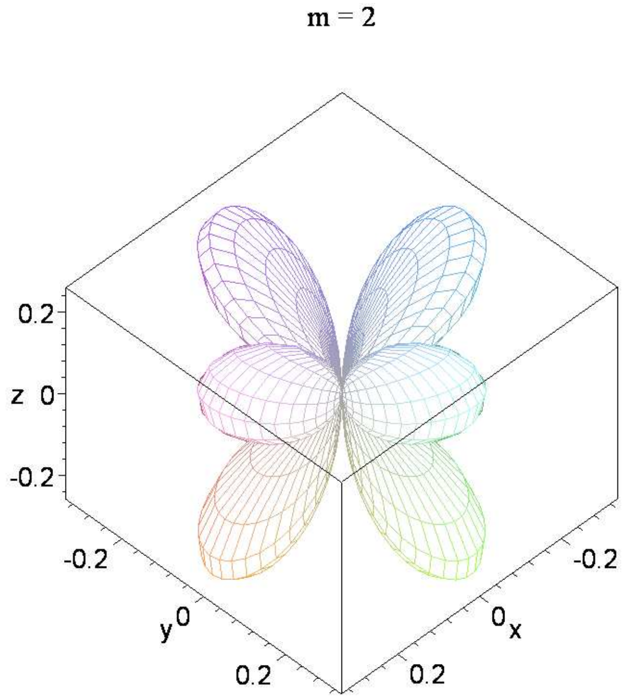



```
> sphereplot( abs(Y[3,1]) , domaine, title
  =`m = 1`) ; # idem  z -> x
```

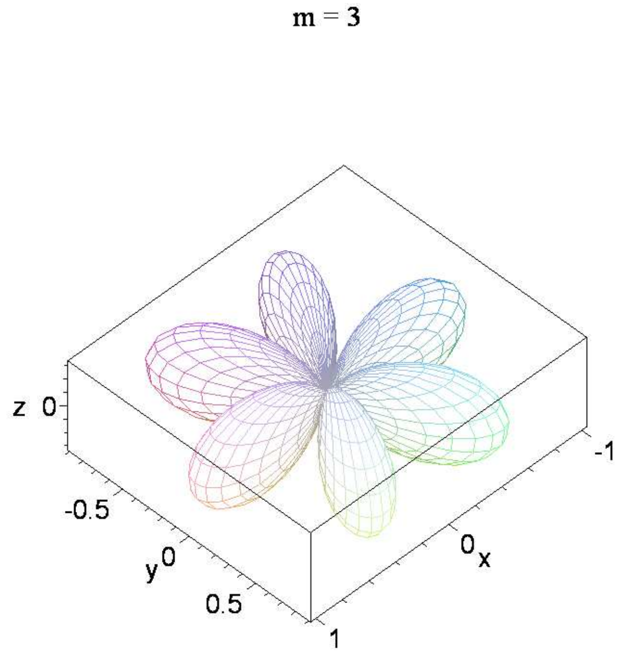
m = 1




```
> sphereplot( abs(Y[3,2]) , domaine, title
  =`m = 2`) ;
```



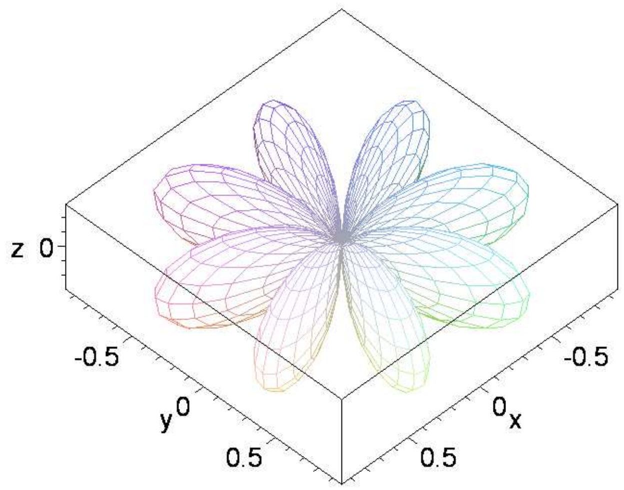

```
> sphereplot( abs(Y[3,3]) , domaine, title
  =`m = 3`) ;
```



Orbitale g: L = 4 ;

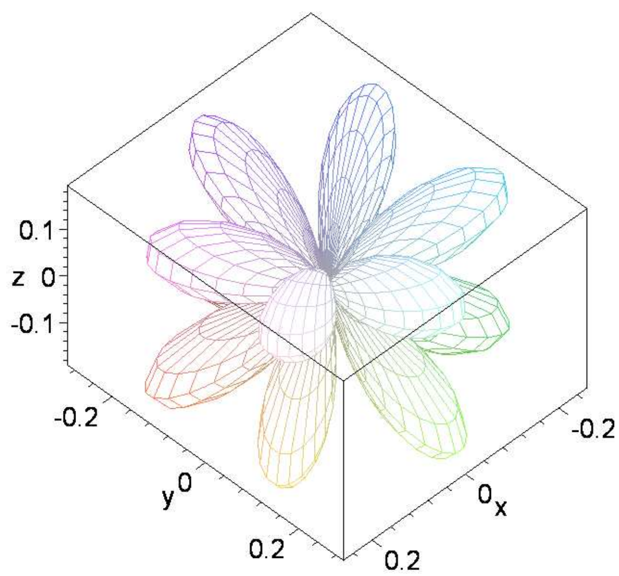
```
> sphereplot( abs(Y[4,-4]), domaine, title
  =`m = - 4`) ;
```

m = - 4



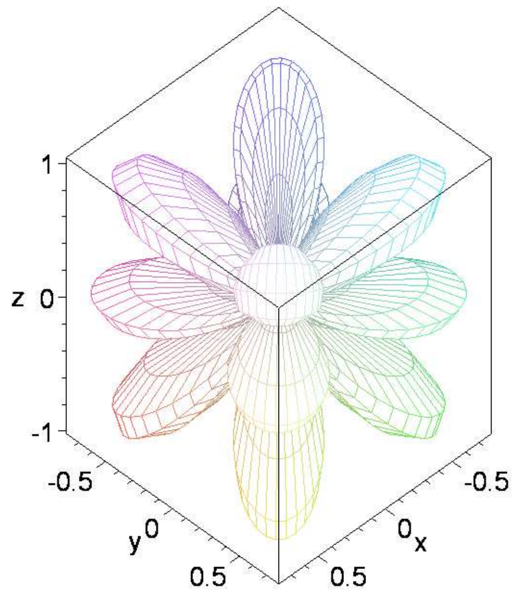

```
> sphereplot( abs(Y[4,-3]), domaine, title
  =`m = - 3`) ;
```

m = - 3



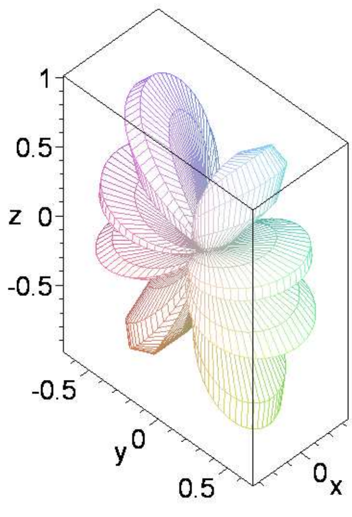

```
> sphereplot( abs(Y[4,-2]), domaine, title
  =`m = - 2`) ;
```

m = - 2



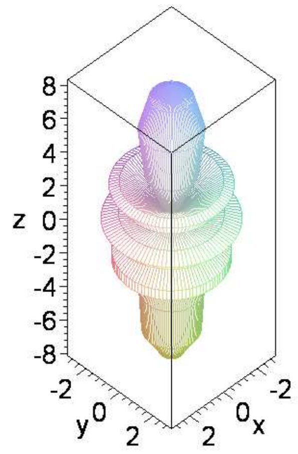

```
> sphereplot( abs(Y[4,-1]), domaine, title
  =`m = - 1`) ;
```

m = - 1



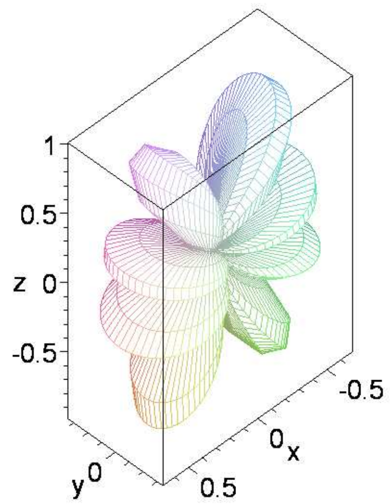

```
> sphereplot( abs(Y[4,0]) , domaine, title
  =`m = 0`) ;
```

m = 0



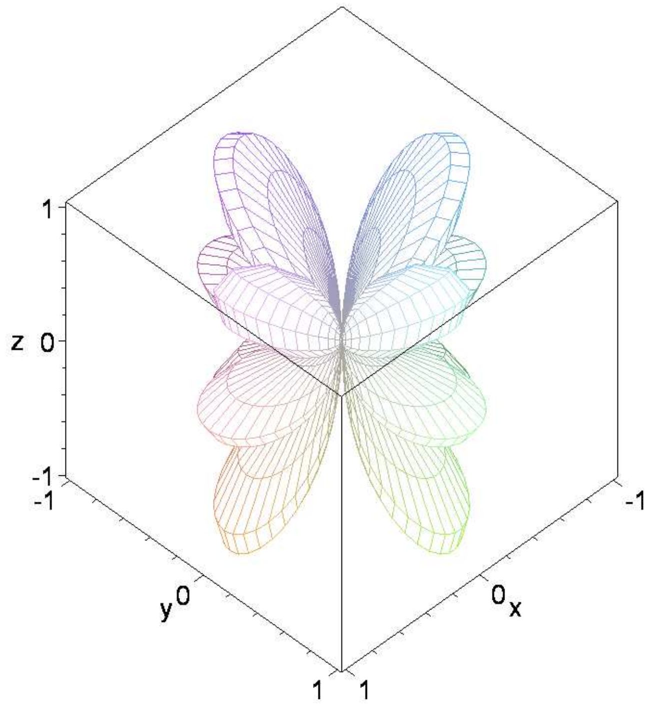

```
> sphereplot( abs(Y[4,1]) , domaine, title
  =`m = 1`) ;
```

m = 1



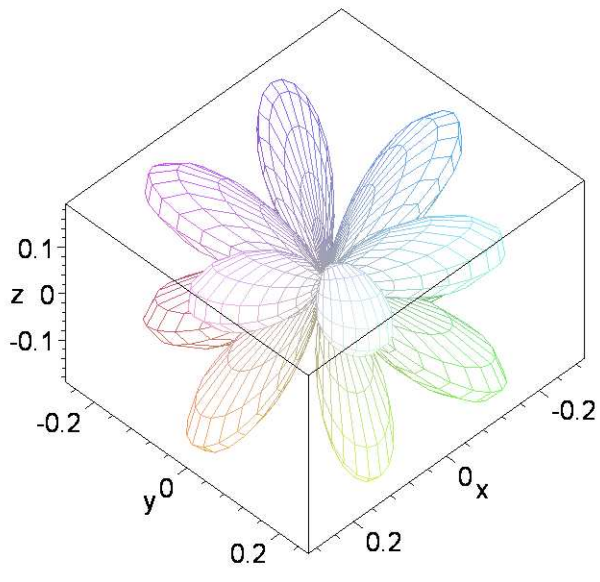

```
> sphereplot( abs(Y[4,2]) , domaine, title
  =`m = 2`) ;
```

m = 2



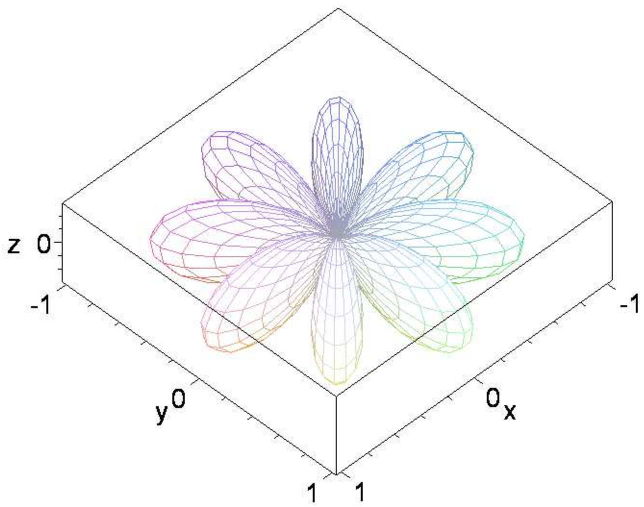

```
> sphereplot( abs(Y[4,3]) , domaine, title
  =`m = 3`) ;
```

m = 3




```
> sphereplot( abs(Y[4,4]) , domaine, title
  =`m = 4`) ;
```

m = 4



Krive izogustine

Talasne funkcije Psi[n,n-1,0], nezavisne od de phi:

```
> Z := 1 :
  n := 2 :
> Rr := R[n,n-1] ;
  Psi2 := (Rr*Y[n-1,0])^2 ;
```

$$Rr := \frac{1}{12}\sqrt{6}\, r\, \mathbf{e}^{(-1/2\, r)}$$

$$\Psi 2 := \frac{1}{24} r^2 \left(\mathbf{e}^{(-1/2\, r)}\right)^2 \cos(\theta)^2$$

```
> rmax := max(solve(diff(Rr^2,r),r)) ;
  Psi2max:=simplify(subs(r=rmax,theta=0,Psi
  2));
  domaine3d := x=-3*rmax..3*rmax,
  y=-3*rmax..3*rmax,view=0..Psi2max :
```

$$rmax := 2$$

$$Psi2max := \frac{1}{6}\mathbf{e}^{(-2)}$$

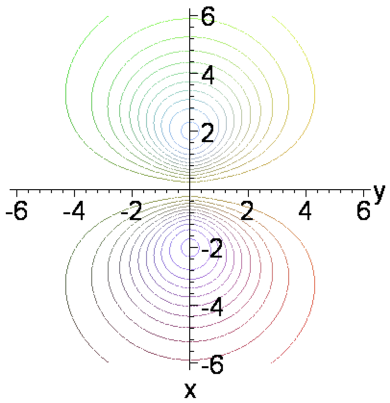
Reprezentacija na kupi u ravni koja prolazi kroz

Oz.

```
> g1 :=
  polarplot([rmax,t,t=0..2*Pi],color=blu
  e,linestyle=2,scaling=constrained):
  g2
  :=seq(implicitplot(subs(theta=Pi/2-the
  ta,Psi2)=i/10*Psi2max,r=0..5*rmax,thet
  a=0..2*Pi,coords=polar,color=red,
  scaling=constrained,
  numpoints=2000,color=COLOR(HUE,i/10)),
  i=[1,3,5,7,9]) :
  display([g1,g2]);
Error, (in display) cannot display 2D
and 3D plots together
```

Reprezentacija u 3D za z = Psi¸ = f(x,y):

```
> z :=simplify(subs(cos(theta) = y/r, r=
  sqrt(x^2+y^2), Psi2)) :
  plot3d(z, domaine3d,
  numpoints=10000,style=contour,
  contours
  =10,orientation=[-90,0],tickmarks=[3,3
  ,3],axes=normal) ;
```



O radijalnim funkcijama

Ove funkcije imaju oblik: $R_{n,L} := A_{n,L}\, \rho^L\, \mathrm{Lg}(\rho)\, \mathbf{e}^{\left(-\frac{1}{2}\rho\right)}$

gde Lg je polinom stepena n-L-1 i $\rho := \frac{2\,Z\,r}{n\,a}$

Koeficijenti Lg dati su relacijom rekurentnosti: $c_0 := 1$; `c[p] := ((p-n+L)/(2*p*(L+1)+p*(p-1))*c[p-1])`

```
missing operator or `;`
```

Racun koeficijenata:

```
> for n to 7 do
    for L from 0 to n-1 do
      c[0,n,L] := 1 :
      for p to n-L-1 do
        c[p,n,L] :=
  (p-n+L)/(2*p*(L+1)+p*(p-1))*c[p-1,n,L]:
        #lprint(n,L,p,c[p,n,L]);
      od;
    od;
  od;
  unassign('p') :
```

Konstrukcija polinoma Lg:

```
> for n to 7 do
    for L from 0 to n-1 do
      Lg[n,L] := sum(c[p,n,L]*rho^p, p =
  0..n-L-1):
      #lprint(n,L,Lg[n,L]) :
    od;
  od;
```

Odakle proisticu ne normirane radijalne funkcije:

```
> for n to 7 do
    for L from 0 to n-1 do
      R[n,L] := rho^L*Lg[n,L]*exp(-rho/2) :
      R[n,L] := subs(rho = 2*Z*r/n,R[n,L]):
      lprint(n,L,R[n,L]):
    od;
  od;
1    0    exp(-r)
2    0    (1-1/2*r)*exp(-1/2*r)
2    1    r*exp(-1/2*r)
```

```
3    0    (1-2/3*r+2/27*r^2)*exp(-1/3*r)
3    1    2/3*r*(1-1/6*r)*exp(-1/3*r)
3    2    4/9*r^2*exp(-1/3*r)
4    0    (1-3/4*r+1/8*r^2-1/192*r^3)*exp(-1/4*r)
4    1    1/2*r*(1-1/4*r+1/80*r^2)*exp(-1/4*r)
4    2    1/4*r^2*(1-1/12*r)*exp(-1/4*r)
4    3    1/8*r^3*exp(-1/4*r)
5    0    (1-4/5*r+4/25*r^2-4/375*r^3+2/9375*r^4)*e
xp(-1/5*r)
5    1    2/5*r*(1-3/10*r+3/125*r^2-1/1875*r^3)*exp
(-1/5*r)
5    2    4/25*r^2*(1-2/15*r+2/525*r^2)*exp(-1/5*r)
5    3    8/125*r^3*(1-1/20*r)*exp(-1/5*r)
5    4    16/625*r^4*exp(-1/5*r)
6    0    (1-5/6*r+5/27*r^2-5/324*r^3+1/1944*r^4-1/
174960*r^5)*exp(-1/6*r)
6    1    1/3*r*(1-1/3*r+1/30*r^2-1/810*r^3+1/68040
*r^4)*exp(-1/6*r)
6    2    1/9*r^2*(1-1/6*r+1/126*r^2-1/9072*r^3)*ex
p(-1/6*r)
6    3    1/27*r^3*(1-1/12*r+1/648*r^2)*exp(-1/6*r)
6    4    1/81*r^4*(1-1/30*r)*exp(-1/6*r)
6    5    1/243*r^5*exp(-1/6*r)
7    0    (1-6/7*r+10/49*r^2-20/1029*r^3+2/2401*r^4
-4/252105*r^5+4/37059435*r^6)*exp(-1/7*r)
7    1    2/7*r*(1-5/14*r+2/49*r^2-2/1029*r^3+2/504
21*r^4-1/3529470*r^5)*exp(-1/7*r)
7    2    4/49*r^2*(1-4/21*r+4/343*r^2-2/7203*r^3+1
/453789*r^4)*exp(-1/7*r)
7    3    8/343*r^3*(1-3/28*r+1/294*r^2-1/30870*r^3
)*exp(-1/7*r)
7    4    16/2401*r^4*(1-2/35*r+2/2695*r^2)*exp(-1/
7*r)
7    5    32/16807*r^5*(1-1/42*r)*exp(-1/7*r)
7    6    64/117649*r^6*exp(-1/7*r)
```

Racun koeficijenata normiranja :

```
> for n to 7 do
    for L from 0 to n-1 do
      assume(Z>0):
      A[n,L] := 1/sqrt(int((r*R[n,L])^2, r =
```

```
0..infinity));
      Z := 'Z' :
      R[n,L] := simplify(A[n,L]*R[n,L],symbolic)
:
      lprint([n,L],R[n,L]) :
    od;
od;
Error, (in assume) cannot assume on a constant
object
```

Ukratko,radi se o dobro poznatim Lagerovim polinomima:

```
> L := 'L' :
  with(orthopoly,L):
  seq(seq(print([n,l],L(n-l-1,2*l+1,x)),l=0..n-1)
  ,n=1..7);
```

$$[1, 0], 1$$

$$[2, 0], 2 - x$$

$$[2, 1], 1$$

$$[3, 0], 3 - 3\,x + \frac{1}{2}x^2$$

$$[3, 1], 4 - x$$

$$[3, 2], 1$$

$$[4, 0], 4 - 6\,x + 2\,x^2 - \frac{1}{6}x^3$$

$$[4, 1], 10 - 5\,x + \frac{1}{2}x^2$$

$$[4, 2], 6 - x$$

$$[4, 3], 1$$

$$[5, 0], 5 - 10\,x + 5\,x^2 - \frac{5}{6}x^3 + \frac{1}{24}x^4$$

$$[5, 1], 20 - 15\,x + 3\,x^2 - \frac{1}{6}x^3$$

$$[5, 2], 21 - 7x + \frac{1}{2}x^2$$

$$[5, 3], 8 - x$$

$$[5, 4], 1$$

$$[6, 0], 6 - 15x + 10x^2 - \frac{5}{2}x^3 + \frac{1}{4}x^4 - \frac{1}{120}x^5$$

$$[6, 1], 35 - 35x + \frac{21}{2}x^2 - \frac{7}{6}x^3 + \frac{1}{24}x^4$$

$$[6, 2], 56 - 28x + 4x^2 - \frac{1}{6}x^3$$

$$[6, 3], 36 - 9x + \frac{1}{2}x^2$$

$$[6, 4], 10 - x$$

$$[6, 5], 1$$

$$[7, 0], 7 - 21x + \frac{35}{2}x^2 - \frac{35}{6}x^3 + \frac{7}{8}x^4 - \frac{7}{120}x^5 + \frac{1}{720}x^6$$

$$[7, 1], 56 - 70x + 28x^2 - \frac{14}{3}x^3 + \frac{1}{3}x^4 - \frac{1}{120}x^5$$

$$[7, 2], 126 - 84x + 18x^2 - \frac{3}{2}x^3 + \frac{1}{24}x^4$$

$$[7, 3], 120 - 45x + 5x^2 - \frac{1}{6}x^3$$

$$[7, 4], 55 - 11x + \frac{1}{2}x^2$$

$$[7, 5], 12 - x$$

$$[7, 6], 1$$

O uglovnim talasnim funkcijama

Ove funkcije imaju oblik: $Y_{L,m} := \sin(\theta)^{|m|} Le_{L,m}\, f(|m|\phi)$
odakle Le[L,m] je izvod reda |m| Lezandrovog polinoma stepena L varijable z = cos(theta)

$$Legendre_L := \frac{(-1)^L\,(D^{(L)})((1-z^2)^L)}{2^L\,L!};$$

$$Le_{L,m} := (D^{|m|})(Legendre_L) = \frac{(-1)^L\,(D^{(L+|m|)})((1-z^2)^L)}{2^L\,L!}$$

```
missing operator or `;`
```

Koeficijenti Le[L,m] dati su rekurentnom relacijom:

$$b_{L,m,p+2} := \frac{((p+|m|)\,(p+1+|m|) - L\,(L+1))\,b_{L,m,p}}{(p+1)\,(p+2)}$$

```
>
Warning, premature end of input
```

Racun koeficijenata:

```
> for L from 0 to 5 do
    for m from -L to L do
      mm := abs(m) : pmax := L-mm :
      b[L,m,pmax+1] := 0 : b[L,m,pmax] := 1 :
      for p from pmax-1 to 0 by -1 do
        b[L,m,p] :=
  b[L,m,p+2]*(p+1)*(p+2)/((p+mm)*(p+1+mm)-L*(L+1)
  );
      od;
    od;
  od;
```

Konstrukcija polinoma Le[L,m]:

```
> unassign('p') :
  for L from 0 to 5 do
    for m from -L to L do
      Le[L,m] := sum(b[L,m,p]*cos(theta)^p, p =
  0..L-abs(m)) :
      #lprint([L,m],Le[L,m]) :
    od;
  od;
```

Konstrukcija funkcija Y[L,m]:

```
> unassign('L','m','p'):
  for L from 0 to 5 do
    for m from -L to L do
      if m < 0 then Le[L,m] :=
  Le[L,m]*sin(theta)^abs(m)*sin(abs(m)*phi)
                  else Le[L,m] :=
  Le[L,m]*sin(theta)^abs(m)*cos(abs(m)*phi) :
      fi;
    od;
  od;
```

Razvijanje rezultata:

```
> seq(seq(lprint([L,m],Le[L,m]),m=-L..L),L=0..5);
[0, 0]   1
[1, -1]   sin(theta)*sin(phi)
[1, 0]   cos(theta)
[1, 1]   sin(theta)*cos(phi)
[2, -2]   sin(theta)^2*sin(2*phi)
[2, -1]   sin(theta)*cos(theta)*sin(phi)
[2, 0]   -1/3+cos(theta)^2
[2, 1]   sin(theta)*cos(theta)*cos(phi)
[2, 2]   sin(theta)^2*cos(2*phi)
[3, -3]   sin(theta)^3*sin(3*phi)
[3, -2]   sin(theta)^2*cos(theta)*sin(2*phi)
[3, -1]   (-1/5+cos(theta)^2)*sin(theta)*sin(phi)
[3, 0]   -3/5*cos(theta)+cos(theta)^3
[3, 1]   (-1/5+cos(theta)^2)*sin(theta)*cos(phi)
[3, 2]   sin(theta)^2*cos(theta)*cos(2*phi)
[3, 3]   sin(theta)^3*cos(3*phi)
[4, -4]   sin(theta)^4*sin(4*phi)
[4, -3]   sin(theta)^3*cos(theta)*sin(3*phi)
[4, -2]   (-1/7+cos(theta)^2)*sin(theta)^2*sin(2*
phi)
[4, -1]   (-3/7*cos(theta)+cos(theta)^3)*sin(thet
a)*sin(phi)
[4, 0]   3/35-6/7*cos(theta)^2+cos(theta)^4
[4, 1]   (-3/7*cos(theta)+cos(theta)^3)*sin(theta
)*cos(phi)
[4, 2]   (-1/7+cos(theta)^2)*sin(theta)^2*cos(2*p
hi)
```

```
[4, 3]    sin(theta)^3*cos(theta)*cos(3*phi)
[4, 4]    sin(theta)^4*cos(4*phi)
[5, -5]    sin(theta)^5*sin(5*phi)
[5, -4]    sin(theta)^4*cos(theta)*sin(4*phi)
[5, -3]    (-1/9+cos(theta)^2)*sin(theta)^3*sin(3*
phi)
[5, -2]    (-1/3*cos(theta)+cos(theta)^3)*sin(thet
a)^2*sin(2*phi)
[5, -1]    (1/21-2/3*cos(theta)^2+cos(theta)^4)*si
n(theta)*sin(phi)
[5, 0]    5/21*cos(theta)-10/9*cos(theta)^3+cos(th
eta)^5
[5, 1]    (1/21-2/3*cos(theta)^2+cos(theta)^4)*sin
(theta)*cos(phi)
[5, 2]    (-1/3*cos(theta)+cos(theta)^3)*sin(theta
)^2*cos(2*phi)
[5, 3]    (-1/9+cos(theta)^2)*sin(theta)^3*cos(3*p
hi)
[5, 4]    sin(theta)^4*cos(theta)*cos(4*phi)
[5, 5]    sin(theta)^5*cos(5*phi)
```

Koeficijenti normiranja:

```
> seq(seq(print([L,m],1/sqrt(int(int(Le[L,m]^2*si
  n(theta),theta=0..Pi),phi=0..2*Pi))),m=-L..L),L
  =0..5);
```

$$[0, 0], \frac{1}{2}\frac{1}{\sqrt{\pi}}$$

$$[1, -1], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[1, 0], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[1, 1], \frac{1}{2}\frac{\sqrt{3}}{\sqrt{\pi}}$$

$$[2, -2], \frac{1}{4}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, -1], \frac{1}{2}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, 0], \frac{3}{4}\frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[2, 1], \frac{1}{2}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[2, 2], \frac{1}{4}\frac{\sqrt{15}}{\sqrt{\pi}}$$

$$[3, -3], \frac{1}{8}\frac{\sqrt{70}}{\sqrt{\pi}}$$

$$[3, -2], \frac{1}{4}\frac{\sqrt{105}}{\sqrt{\pi}}$$

$$[3, -1], \frac{5}{8}\frac{\sqrt{42}}{\sqrt{\pi}}$$

$$[3, 0], \frac{5}{4}\frac{\sqrt{7}}{\sqrt{\pi}}$$

$$[3, 1], \frac{5}{8}\frac{\sqrt{42}}{\sqrt{\pi}}$$

$$[3, 2], \frac{1}{4}\frac{\sqrt{105}}{\sqrt{\pi}}$$

$$[3, 3], \frac{1}{8}\frac{\sqrt{70}}{\sqrt{\pi}}$$

$$[4, -4], \frac{3}{16}\frac{\sqrt{35}}{\sqrt{\pi}}$$

$$[4, -3], \frac{3}{8}\frac{\sqrt{70}}{\sqrt{\pi}}$$

$$[4, -2], \frac{21}{8}\frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[4, -1], \frac{21}{8}\frac{\sqrt{10}}{\sqrt{\pi}}$$

$$[4, 0], \frac{105}{16}\frac{1}{\sqrt{\pi}}$$

$$[4, 1], \frac{21}{8}\frac{\sqrt{10}}{\sqrt{\pi}}$$

$$[4, 2], \frac{21}{8}\frac{\sqrt{5}}{\sqrt{\pi}}$$

$$[4, 3], \frac{3}{8}\frac{\sqrt{70}}{\sqrt{\pi}}$$

$$[4, 4], \frac{3}{16}\frac{\sqrt{35}}{\sqrt{\pi}}$$

$$[5, -5], \frac{3}{32}\frac{\sqrt{154}}{\sqrt{\pi}}$$

$$[5, -4], \frac{3}{16}\frac{\sqrt{385}}{\sqrt{\pi}}$$

$$[5, -3], \frac{9}{32}\frac{\sqrt{770}}{\sqrt{\pi}}$$

$$[5, -2], \frac{3}{8}\frac{\sqrt{1155}}{\sqrt{\pi}}$$

$$[5, -1], \frac{21}{16}\frac{\sqrt{165}}{\sqrt{\pi}}$$

$$[5, 0], \frac{63}{16}\frac{\sqrt{11}}{\sqrt{\pi}}$$

$$[5, 1], \frac{21}{16}\frac{\sqrt{165}}{\sqrt{\pi}}$$

$$[5, 2], \frac{3}{8}\frac{\sqrt{1155}}{\sqrt{\pi}}$$

$$[5, 3], \frac{9}{32}\frac{\sqrt{770}}{\sqrt{\pi}}$$

$$[5, 4], \frac{3}{16}\frac{\sqrt{385}}{\sqrt{\pi}}$$

$$[5, 5], \frac{3}{32}\frac{\sqrt{154}}{\sqrt{\pi}}$$

Racun Le[L,m] pomocu Legandrovog polinoma:

```
> unassign('L','m') :
  f := z -> (1-z^2)^L :
  P := (-1)^L/2^L/L!*(D@@(L+abs(m)))(f):
  seq(seq(print([L,m],simplify(P(z))),m=0..L),
  L = 0..5) ;
```

$$[0, 0], 1$$

$$[1, 0], \frac{1}{24}\mathbf{e}^{(-\sqrt{x^2+y^2})}\, y^2$$

$$[1, 1], 1$$

$$[2, 0], \frac{1}{384}\mathbf{e}^{(-2\sqrt{x^2+y^2})}\, y^4 - \frac{1}{2}$$

$$[2, 1], \frac{1}{8}\mathbf{e}^{(-\sqrt{x^2+y^2})}\, y^2$$

$$[2, 2], 3$$

$$[3, 0], \frac{5}{27648} e^{(-3\sqrt{x^2+y^2})} y^6 - \frac{1}{16} e^{(-\sqrt{x^2+y^2})} y^2$$

$$[3, 1], \frac{5}{384} e^{(-2\sqrt{x^2+y^2})} y^4 - \frac{3}{2}$$

$$[3, 2], \frac{5}{8} e^{(-\sqrt{x^2+y^2})} y^2$$

$$[3, 3], 15$$

$$[4, 0], \frac{35}{2654208} e^{(-4\sqrt{x^2+y^2})} y^8 - \frac{5}{768} e^{(-2\sqrt{x^2+y^2})} y^4 + \frac{3}{8}$$

$$[4, 1], \frac{35}{27648} e^{(-3\sqrt{x^2+y^2})} y^6 - \frac{5}{16} e^{(-\sqrt{x^2+y^2})} y^2$$

$$[4, 2], \frac{35}{384} e^{(-2\sqrt{x^2+y^2})} y^4 - \frac{15}{2}$$

$$[4, 3], \frac{35}{8} e^{(-\sqrt{x^2+y^2})} y^2$$

$$[4, 4], 105$$

$$[5, 0], \frac{7}{7077888} e^{(-5\sqrt{x^2+y^2})} y^{10} - \frac{35}{55296} y^6 e^{(-3\sqrt{x^2+y^2})}$$
$$+ \frac{5}{64} e^{(-\sqrt{x^2+y^2})} y^2$$

$$[5, 1], -\frac{35}{768} e^{(-2\sqrt{x^2+y^2})} y^4 + \frac{35}{294912} e^{(-4\sqrt{x^2+y^2})} y^8 + \frac{15}{8}$$

$$[5, 2], -\frac{35}{16} e^{(-\sqrt{x^2+y^2})} y^2 + \frac{35}{3072} y^6 e^{(-3\sqrt{x^2+y^2})}$$

$$[5, 3], \frac{105}{128} e^{(-2\sqrt{x^2+y^2})} y^4 - \frac{105}{2}$$

$$[5,4],\ \frac{315}{8}\,\mathbf{e}^{(-\sqrt{x^2+y^2})}\,y^2$$

$$[5,5],\ 945$$

ili poseban slucaj Jakobijevih polinoma,
uzimajuci izvod reda d'ordre $|m|$

```
> with(orthopoly,P):
  unassign('L','m') :
  seq(seq(print([L,m],simplify((D@@abs(m))(P(L
  ,z)))),m=0..L),L=0..5);
Error, (in with) extra arguments must be names
```

$$[0,0],\ 1$$

```
Error, (in unknown) division by zero
```

Sredingerova jednacina

Jednacina

```
> restart : with(linalg):
> eq:=
  laplacian(psi(r,theta,phi),[r,theta,phi],coo
  rds=spherical)
       + 2*m/hb^2*(E+k*e^2/r)*psi(r,theta,phi)
  ;

Warning, new definition for norm
Warning, new definition for trace
```

$$eq := \left(2\,r\sin(\theta)\left(\frac{\partial}{\partial r}\psi(r,\theta,\phi)\right) + r^2\sin(\theta)\left(\frac{\partial^2}{\partial r^2}\psi(r,\theta,\phi)\right) + \cos(\theta)\left(\frac{\partial}{\partial \theta}\psi(r,\theta,\phi)\right) + \sin(\theta)\left(\frac{\partial^2}{\partial \theta^2}\psi(r,\theta,\phi)\right) + \frac{\frac{\partial^2}{\partial \phi^2}\psi(r,\theta,\phi)}{\sin(\theta)}\right) \Big/ (r^2\sin(\theta))$$

$$+2\,\frac{m\left(E+\frac{k\,e^2}{r}\right)\psi(r,\theta,\phi)}{hb^2}$$

Mnozeci sa r¸*sin¸(theta)

```
> eq := expand(eq*r^2*sin(theta)^2);
```

$$eq := 2\,r\sin(\theta)^2\left(\frac{\partial}{\partial r}\psi(r,\theta,\phi)\right)$$
$$+r^2\sin(\theta)^2\left(\frac{\partial^2}{\partial r^2}\psi(r,\theta,\phi)\right)$$
$$+\sin(\theta)\cos(\theta)\left(\frac{\partial}{\partial \theta}\psi(r,\theta,\phi)\right)$$
$$+\sin(\theta)^2\left(\frac{\partial^2}{\partial \theta^2}\psi(r,\theta,\phi)\right)+\left(\frac{\partial^2}{\partial \phi^2}\psi(r,\theta,\phi)\right)$$
$$+2\,\frac{r^2\sin(\theta)^2\,m\,\psi(r,\theta,\phi)\,E}{hb^2}$$
$$+2\,\frac{r\sin(\theta)^2\,m\,\psi(r,\theta,\phi)\,k\,e^2}{hb^2}$$

Trazi se resenje $\psi(r,\theta,\phi)$ oblika $\mathrm{R}(r)\,\mathrm{f}(\theta)\,\mathrm{g}(\phi)$ i deli se sa psi

```
> eq :=
  expand(subs(psi(r,theta,phi)=R(r)*f(theta)*g
  (phi),eq/psi(r,theta,phi)));
```

$$eq := 2\,\frac{r\sin(\theta)^2\left(\frac{\partial}{\partial r}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+\frac{r^2\sin(\theta)^2\left(\frac{\partial^2}{\partial r^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)}$$
$$+\frac{\sin(\theta)\cos(\theta)\left(\frac{\partial}{\partial \theta}\mathrm{f}(\theta)\right)}{\mathrm{f}(\theta)}+\frac{\sin(\theta)^2\left(\frac{\partial^2}{\partial \theta^2}\mathrm{f}(\theta)\right)}{\mathrm{f}(\theta)}$$

$$+\frac{\frac{\partial^2}{\partial \phi^2}\mathrm{g}(\phi)}{\mathrm{g}(\phi)}+2\,\frac{r^2\sin(\theta)^2\,m\,E}{hb^2}+2\,\frac{r\sin(\theta)^2\,m\,k\,e^2}{hb^2}$$

Term koji zavici samo od phi je konstanta -m¸ jer g(phi) treba da ima period 2*Pi

Dakle g(phi) = exp(i*m*phi) gde je m relativno

```
> eq1 := eval(subs(g(phi) = exp(I*m*phi),eq))
  ;
```

$$eq1 := 2\,\frac{r\sin(\theta)^2\left(\frac{\partial}{\partial r}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+\frac{r^2\sin(\theta)^2\left(\frac{\partial^2}{\partial r^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)}$$
$$+\frac{\sin(\theta)\cos(\theta)\left(\frac{\partial}{\partial \theta}\mathrm{f}(\theta)\right)}{\mathrm{f}(\theta)}+\frac{\sin(\theta)^2\left(\frac{\partial^2}{\partial \theta^2}\mathrm{f}(\theta)\right)}{\mathrm{f}(\theta)}-m^2$$
$$+2\,\frac{r^2\sin(\theta)^2\,m\,E}{hb^2}+2\,\frac{r\sin(\theta)^2\,m\,k\,e^2}{hb^2}$$

Deleci sa sin¸(theta) dobijaju se 2 terma, jedan koji zavisi samo od r i drugi samo od theta .

Ova 2 terma su dakle konstantni i suprotni

```
> eq1 := expand(eq1/sin(theta)^2) ;
  eqr := select(has,eq1,r) - beta ;
  eqtheta := select(has,eq1,theta) + beta ;
```

$$eq1 := 2\,\frac{r\left(\frac{\partial}{\partial r}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+\frac{r^2\left(\frac{\partial^2}{\partial r^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+\frac{\cos(\theta)\left(\frac{\partial}{\partial \theta}\mathrm{f}(\theta)\right)}{\sin(\theta)\,\mathrm{f}(\theta)}$$
$$+\frac{\frac{\partial^2}{\partial \theta^2}\mathrm{f}(\theta)}{\mathrm{f}(\theta)}-\frac{m^2}{\sin(\theta)^2}+2\,\frac{r^2\,m\,E}{hb^2}+2\,\frac{r\,m\,k\,e^2}{hb^2}$$

$eqr :=$

$$2\,\frac{r\left(\frac{\partial}{\partial r}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+\frac{r^2\left(\frac{\partial^2}{\partial r^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)}+2\,\frac{r^2\,m\,E}{hb^2}+2\,\frac{r\,m\,k\,e^2}{hb^2}-\beta$$

$$eqtheta:=\frac{\cos(\theta)\left(\frac{\partial}{\partial\theta}\mathrm{f}(\theta)\right)}{\sin(\theta)\,\mathrm{f}(\theta)}+\frac{\frac{\partial^2}{\partial\theta^2}\mathrm{f}(\theta)}{\mathrm{f}(\theta)}-\frac{m^2}{\sin(\theta)^2}+\beta$$

Resenje jednacine po theta

Vrsi se promena varijabli z = cos(theta) d'oů f(theta) = P(z)

```
> with(DEtools,Dchangevar):
  eqz :=
  Dchangevar(f(theta)=P(z),theta=arccos(z),eqt
  heta,theta,z); # erreur !!!! manque un 2...
  eqz := collect(eqz,diff,factor) ;
  eqz := 'diff'((1-z^2)*diff(P(z),z),z) +
  (beta-m^2/(1-z^2))*P(z) ; # la bonne
  expression!
```

$$eqz:=-\frac{\cos(\arccos(z))\sqrt{1-z^2}\left(\frac{\partial}{\partial z}\mathrm{P}(z)\right)}{\sin(\arccos(z))\,\mathrm{P}(z)}$$

$$-\frac{\sqrt{1-z^2}\left(\frac{\left(\frac{\partial}{\partial z}\mathrm{P}(z)\right)z}{\sqrt{1-z^2}}-\sqrt{1-z^2}\left(\frac{\partial^2}{\partial z^2}\mathrm{P}(z)\right)\right)}{\mathrm{P}(z)}$$

$$-\frac{m^2}{\sin(\arccos(z))^2}+\beta$$

$$eqz:=-2\,\frac{z\left(\frac{\partial}{\partial z}\mathrm{P}(z)\right)}{\mathrm{P}(z)}-\frac{(z-1)\,(z+1)\left(\frac{\partial^2}{\partial z^2}\mathrm{P}(z)\right)}{\mathrm{P}(z)}$$

$$+\frac{-\beta+\beta z^2+m^2}{(z-1)(z+1)}$$

$$eqz := \left(\frac{\partial}{\partial z}(1-z^2)\left(\frac{\partial}{\partial z}\mathrm{P}(z)\right)\right)+\left(\beta-\frac{m^2}{1-z^2}\right)\mathrm{P}(z)$$

Resenja imaju oblik $\mathrm{P}(z) := (1-z^2)^{\left(\frac{|m|}{2}\right)}\mathrm{G}(z)$

```
> alias(alpha=(1-z^2)^(abs(m)/2)) :
> eqz1 := subs(P(z)= alpha*G(z),eqz);
  assume(m,integer) :
  eqz1 :=
  collect(simplify(eval(eqz1/alpha)),diff,fact
  or);
  eqz1 :=
  subs(G(z)=Sum(b[p]*z^p,p=0..nu),eqz1) ;
```

$$eqz1 := -2z\left(\frac{\partial}{\partial z}\alpha\,\mathrm{G}(z)\right)+(1-z^2)\left(\frac{\partial^2}{\partial z^2}\alpha\,\mathrm{G}(z)\right)$$

$$+\left(\beta-\frac{m^2}{1-z^2}\right)\alpha\,\mathrm{G}(z)$$

$$eqz1 := -2z(1+|m\sim|)\left(\frac{\partial}{\partial z}\mathrm{G}(z)\right)$$

$$-(z-1)(z+1)\left(\frac{\partial^2}{\partial z^2}\mathrm{G}(z)\right)-\mathrm{G}(z)(|m\sim|+m\sim^2-\beta)$$

$$eqz1 := -2z(1+|m\sim|)\left(\frac{\partial}{\partial z}\left(\sum_{p=0}^{\nu} b_p z^p\right)\right)$$

$$-(z-1)(z+1)\left(\frac{\partial^2}{\partial z^2}\left(\sum_{p=0}^{\nu} b_p z^p\right)\right)$$

$$-\left(\sum_{p=0}^{\nu} b_p z^p\right)(|m\sim|+m\sim^2-\beta)$$

```
> eqz1 := combine(eqz1) ;
```

$$eqz1 := \sum_{p=0}^{\nu} \left(-2\,(1+|m\sim|)\, b_p\, z^p\, p + (-z+1)\,(z+1)\left(\frac{b_p\, z^p\, p^2}{z^2} - \frac{b_p\, z^p\, p}{z^2}\right) + (-|m\sim| - m\sim^2 + \beta)\, b_p\, z^p \right)$$

Opsti term serije pise se:

```
> cp := expand(op(1,eqz1));
```

$$cp := -b_p\, z^p\, p - 2\, b_p\, z^p\, p\, |m\sim| + \frac{b_p\, z^p\, p^2}{z^2} - \frac{b_p\, z^p\, p}{z^2} - b_p\, z^p\, p^2 - b_p\, z^p\, |m\sim| - b_p\, z^p\, m\sim^2 + b_p\, z^p\, \beta$$

Da bi bio fizicki prihvatljiv treba da ovaj polinom ima konacni broj termova, p+2 na primer.
Koeficijen uz z^(p+2) treba da bude nula,sto daje rekurentnu relaciju izmedju koeficijenata:

```
> cp1 := subs(p=p+2,select(has,cp,z^(-2))) ;
  cp := remove(has,cp,z^(-2)) + cp1 ;
  b[p+2] :=simplify(solve(cp,b[p+2]));
```

$$cp1 := \frac{b_{p+2}\, z^{(p+2)}\, (p+2)^2}{z^2} - \frac{b_{p+2}\, z^{(p+2)}\, (p+2)}{z^2}$$

$$cp := -b_p\, z^p\, p - 2\, b_p\, z^p\, p\, |m\sim| - b_p\, z^p\, p^2 - b_p\, z^p\, |m\sim| - b_p\, z^p\, m\sim^2 + b_p\, z^p\, \beta + \frac{b_{p+2}\, z^{(p+2)}\, (p+2)^2}{z^2} - \frac{b_{p+2}\, z^{(p+2)}\, (p+2)}{z^2}$$

$$b_{p+2} := \frac{b_p\,(p + 2\,p\,|m\sim| + p^2 + |m\sim| + m\sim^2 - \beta)}{p^2 + 3\,p + 2}$$

Odakle je beta resavajuci b[p+2] = 0:

```
> beta := solve(b[p+2],beta) ;
```

$$\beta := p + 2\,p\,|m\sim| + p^2 + |m\sim| + m\sim^2$$

p i |m| su celi prirodni brojevi dakle p+|m| je to takodje. Stavlja se p+|m| = L:

```
> beta :=
  factor(simplify(subs(p=L-abs(m),beta)));
```

$$\beta := L\,(1 + L)$$

Resenje jednacine po r

```
> alias(alpha = 'alpha') :
  eqr ;
```

$$2\,\frac{r\left(\frac{\partial}{\partial r}\mathrm{R}(r)\right)}{\mathrm{R}(r)} + \frac{r^2\left(\frac{\partial^2}{\partial r^2}\mathrm{R}(r)\right)}{\mathrm{R}(r)} + 2\,\frac{r^2\,m\sim E}{hb^2} + 2\,\frac{r\,m\sim k\,e^2}{hb^2} - L\,(1 + L)$$

Notacija se uproscava stavljanjem: $E = -\frac{hb^2\,\alpha^2}{2\,m}$;

$k = \frac{hb^2\,\alpha\,n}{m\,e^2}$; $\rho := 2\,\alpha\,r$

```
> eqr1 := simplify(subs(E=-hb^2*alpha^2/2/m,
  k=hb^2*alpha*n/m/e^2, eqr)) :
  Dchangevar(r=rho/2/alpha, R(r) =
  R(rho),eqr1,r,rho) :
  eqrho := collect(%,diff,factor);
```

$eqrho :=$

$$\frac{\rho^2\left(\frac{\partial^2}{\partial \rho^2}\mathrm{R}(\rho)\right)}{\mathrm{R}(\rho)} + 2\,\frac{\rho\left(\frac{\partial}{\partial \rho}\mathrm{R}(\rho)\right)}{\mathrm{R}(\rho)} - L - L^2 - \frac{1}{4}\,\rho^2 + \rho\,n$$

Resenja imaju oblik $\mathbf{e}^{\left(-\frac{\rho}{2}\right)} \mathrm{F}(\rho)$:
Odakle diferencijalna jednacina dajuci F(rho), i zamenjujuci R(rho) i mnozeci sa $\mathbf{e}^{\left(\frac{\rho}{2}\right)}$:

```
> eqF :=
  collect(simplify(subs(R(rho)=exp(-rho/2)*F(rho),eqrho*F(rho))),diff,factor) ;
```

$$eqF := \rho^2 \left(\frac{\partial^2}{\partial \rho^2} \mathrm{F}(\rho)\right) - \rho\,(-2+\rho)\left(\frac{\partial}{\partial \rho} \mathrm{F}(\rho)\right) + \mathrm{F}(\rho)\,(-L - L^2 - \rho + \rho\, n)$$

Tacka rho=0 kao singularna trazi se F(rho) oblika
$\mathrm{F}(\rho) = \rho^s\,\mathrm{Lg}(\rho)$ avec s >= 0:

```
> eqL :=
  collect(simplify(subs(F(rho)=rho^s*Lg(rho),eqF*rho^(-s))),diff,factor);
```

$$eqL := \rho^2 \left(\frac{\partial^2}{\partial \rho^2} \mathrm{Lg}(\rho)\right) - \rho\,(-2\,s+\rho-2)\left(\frac{\partial}{\partial \rho} \mathrm{Lg}(\rho)\right) - \mathrm{Lg}(\rho)\,(-s^2 - s + L + \rho + \rho\, s + L^2 - \rho\, n)$$

Trazi se Lg(rho) u obliku polinoma.
Nezavisni terme od rho treba da bude nula odakle vrednosti za s:

```
> s :=
  solve(subs(rho=0,select(has,eqL,L)),s)[2];
  eqLg := collect(eqL/rho,diff,factor);
```

$$s := L$$

$$eqLg := \rho \left(\frac{\partial^2}{\partial \rho^2} \mathrm{Lg}(\rho)\right) + (2\,L - \rho + 2)\left(\frac{\partial}{\partial \rho} \mathrm{Lg}(\rho)\right) - \mathrm{Lg}(\rho)\,(1 + L - n)$$

```
> eqLg :=
  subs(Lg(rho)=Sum(c[p]*rho^p,p=0..nu),eqLg) ;
```

$$eqLg := \rho\left(\frac{\partial^2}{\partial\rho^2}\left(\sum_{p=0}^{\nu} c_p\,\rho^p\right)\right) + (2L-\rho+2)\left(\frac{\partial}{\partial\rho}\left(\sum_{p=0}^{\nu} c_p\,\rho^p\right)\right) - \left(\sum_{p=0}^{\nu} c_p\,\rho^p\right)(1+L-n)$$

```
> eqLg := combine(eqLg) ;
```

$$eqLg := \sum_{p=0}^{\nu}\left(\rho\left(\frac{c_p\,\rho^p\,p^2}{\rho^2} - \frac{c_p\,\rho^p\,p}{\rho^2}\right) + \frac{(2L-\rho+2)\,c_p\,\rho^p\,p}{\rho} + (-1-L+n)\,c_p\,\rho^p\right)$$

```
> cp := simplify(op(1,eqLg));
```

$$cp := \rho^{(p-1)}\,c_p\,p^2 + c_p\,\rho^{(p-1)}\,p + 2\,c_p\,\rho^{(p-1)}\,p\,L - c_p\,\rho^p\,p - c_p\,\rho^p - c_p\,\rho^p\,L + c_p\,\rho^p\,n$$

```
> cp1 := subs(p=p+1,select(has,cp,p-1));
```

$$cp1 := \rho^p\,c_{p+1}\,(p+1)^2 + c_{p+1}\,\rho^p\,(p+1) + 2\,c_{p+1}\,\rho^p\,(p+1)\,L$$

```
> cp := remove(has,cp,p-1) + cp1 ;
```

$$cp := -c_p\,\rho^p\,p - c_p\,\rho^p - c_p\,\rho^p\,L + c_p\,\rho^p\,n + \rho^p\,c_{p+1}\,(p+1)^2 + c_{p+1}\,\rho^p\,(p+1) + 2\,c_{p+1}\,\rho^p\,(p+1)\,L$$

```
> c[p+1] := solve(cp,c[p+1]);
```

$$c_{p+1} := \frac{c_p\,(p+1+L-n)}{p^2+3\,p+2+2\,L\,p+2\,L}$$

Lg posto ima samo konacni broj termova,na primer p+1, c[p+1] treba da bude nula, odakle n = p+1+L.
p i L kao celi prirodni brojevi, n je dakle ceo broj koji uzima vrednosti 1, 2, 3 ... (glavni kvantni broj).
Odakle L = n - 1 - p uzima vrednosti n - 1, n - 2, ... , 0 (sporedni kvantni broj).
Najzad |m| = L - p uzima vrednosti L, L - 1, ... , 0 (magnetni

kvantni broj).

```
> E := -(k*m*e^2/hb^2/n)^2*hb^2/2/m ;
```

$$E := -\frac{1}{2}\,\frac{k^2\,m\sim\,e^4}{hb^2\,n^2}$$

```
>
```