Uhin Funtzio Totala (erradiala eta angeluarra)

$$\Psi_{n,l,m}= R_{n,l}(r)\, Y_l^m(\theta,\, \phi) \qquad (1)$$

Funtzio erradiala:

$$R_{n,l}(r)= \left(\frac{2\,Z}{\text{na}}\right)^{3/2} \Phi_{n,l}(\rho) \qquad (2)$$

non

$$\Phi_{n,l}(r) = \sqrt{\frac{(n-l-1)!}{2\,n(n+l)!}}\ \left(\frac{2\,Z\,\rho}{n}\right)^l\ \text{Exp}\left[-\frac{2\,Z\,\rho}{n}\,/2\right] L_{n-l-1}^{2\,l+1}\left(\frac{2\,Z\,\rho}{n}\right) \qquad (3)$$

eta

$$\rho=\frac{r}{a} \qquad (4)$$

$$\text{a}=\frac{\hbar^2(4\,\pi\,\epsilon_0)}{\mu\, e^2} \qquad (5)$$

Egin beharra :

1. Definitu funtzio erradiala $R_{n,l}$
2. Definitu uhin funtzio totala $\Psi_{n,l,m}$ a
3. Definitu 1s, 2s, 3s, 2 p_x, 2 p_y, 2 p_z, funtzioak

Uhin Funtzioak

In[13]:=
```
Unprotect[Φ];
Clear[Φ]; Unprotect[a, Z]; Clear[a, Z]; Protect[a, Z];
Φ[n_Integer, l_Integer][ρ_] := Module[{const},
const = Sqrt[(n - l - 1)! / ((n + l)! 2 n)];
  const (2 Z ρ / n)^l LaguerreL[n - l - 1, 2 l + 1, 2 Z ρ / n] Exp[- Z ρ / n]]
Protect[Φ];

Unprotect[R];
Clear[R];
R[n_, l_][r_] := (2 Z / (n a))^(3 / 2) Φ[n, l][r / a]
Unprotect[a, Z];

(*   np_x(r, θ,ϕ) = 1/Sqrt[2] {Y_1^-1(θ,ϕ)-Y_1^1(θ,ϕ)} R_n,1(r)   *)
(* np_x zatia berdina da n guztientzat: *)

Clear[pxAng]
a = .5292;
Z = 1;

pxAng[θ, ϕ] :=
 (SphericalHarmonicY[1, -1, θ, ϕ] - SphericalHarmonicY[1, 1, θ, ϕ]) / Sqrt[2] // ComplexExpand
```

Harmoniko-Esferiko eta Kartessiarren arteko erlazioa:

$$\cos(\theta) = \frac{z}{r}$$

$$\sin(\theta) = \frac{\sqrt{x^2+y^2}}{r}$$

$$\sin(\phi) = \frac{y}{\sqrt{x^2+y^2}}$$

$$\cos(\phi) = \frac{x}{\sqrt{x^2+y^2}}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

In[25]:=
```
convCarts = { r → Sqrt[x ^ 2 + y ^ 2 + z ^ 2]};
convCartp = {Cos[θ] → z / r, Sin[θ] → Sqrt[x ^ 2 + y ^ 2] / r,
   Cos[ϕ] → x / Sqrt[x ^ 2 + y ^ 2], Sin[ϕ] → y / Sqrt[x ^ 2 + y ^ 2]};
```

In[27]:=
```
pxAng[θ, ϕ] /. convCartp;
```

Definitu:

px[r, θ, ϕ][n]

non n$p_x(r, \theta, \phi)$ (2 $p_x(r, \theta, \phi)$, 3 $p_x(r, \theta, \phi)$, lortu ditzakegun.)

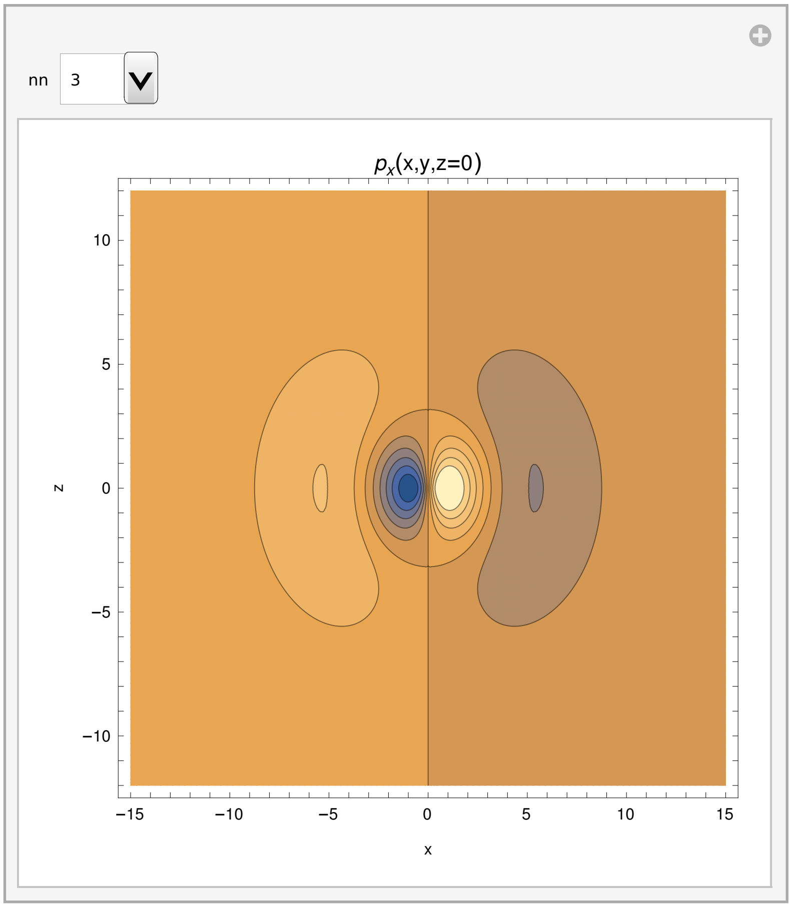
In[28]:=
```
Unprotect[px];
Clear[px]
px[r_, θ_, ϕ_][n_] := Module[{ },
  int = (SphericalHarmonicY[1, -1, θ, ϕ] - SphericalHarmonicY[1, 1, θ, ϕ]) / Sqrt[2] //
    ComplexExpand ;
  R[n, 1][r] * int ]
Protect[px];
```

These functions are all proportional to x and decay exponentially with r. These two elements controls their shape.

Make a contour plot of 2 $p_x(x, y, z = 0)$

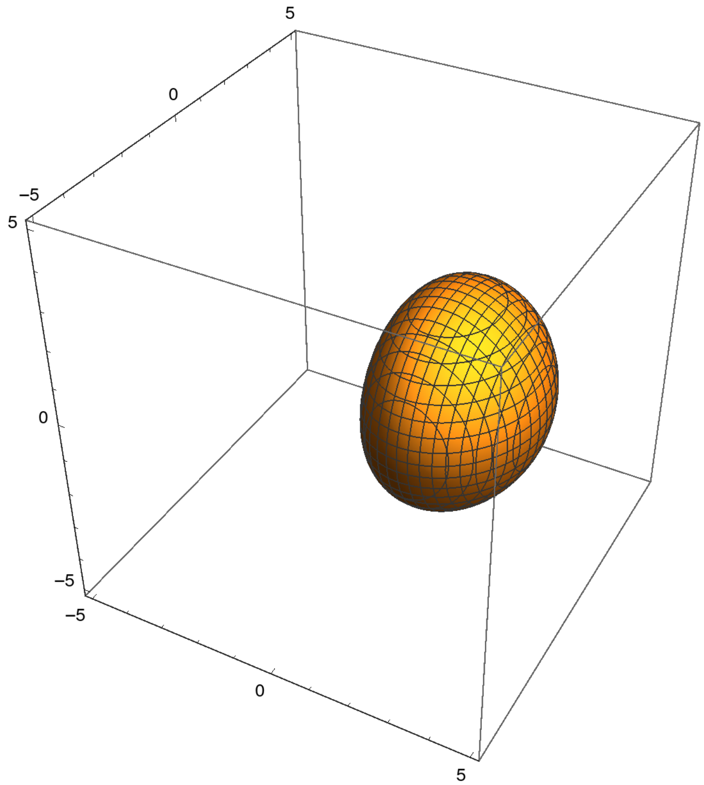
In[ ]:=
```
Manipulate[ContourPlot[
  Evaluate[px[r, θ, ϕ][nn] /. convCartp /. convCarts /. z → 0], {x, -15, 15}, {y, -12, 12},
  PlotPoints → 100, Contours → 10, PlotRange → All, FrameLabel → {"x", "z"},
  PlotLabel → "px(x,y,z=0)"], {nn, 1, 5, 1}, ControlType → PopupMenu]
```

Out[ ]=



In[32]:=
```
p1 = ContourPlot3D[Evaluate[px[r, θ, ϕ][2] == 0.04 /. convCartp /. convCarts],
  {x, -5, 5}, {y, -5, 5}, {z, -5, 5}]
```

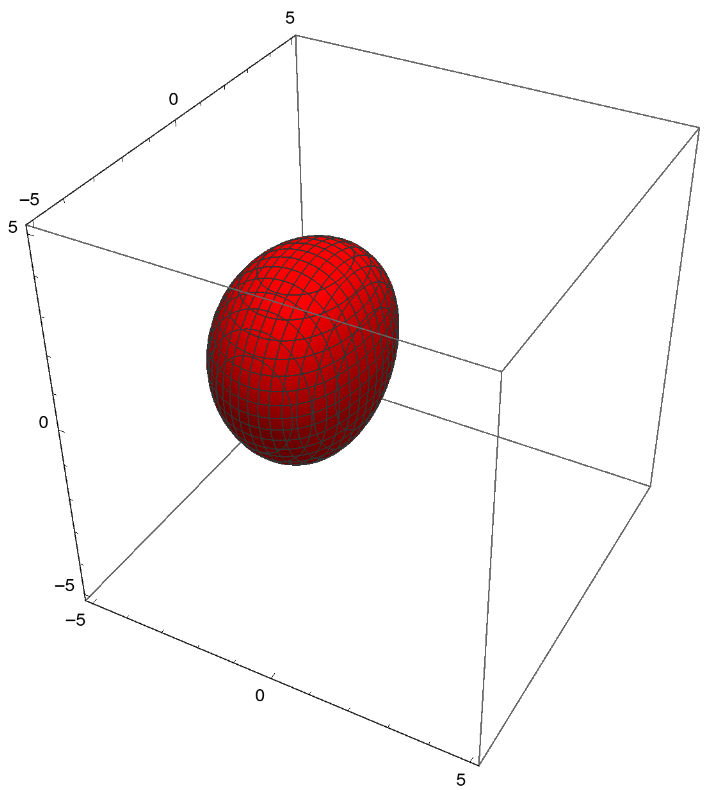
Out[32]=



In[33]:=

```
p2 = ContourPlot3D[Evaluate[px[r, θ, ϕ][2] == -0.04 /. convCartp /. convCarts],
  {x, -5, 5}, {y, -5, 5}, {z, -5, 5}, ContourStyle → Directive[Red]]
```

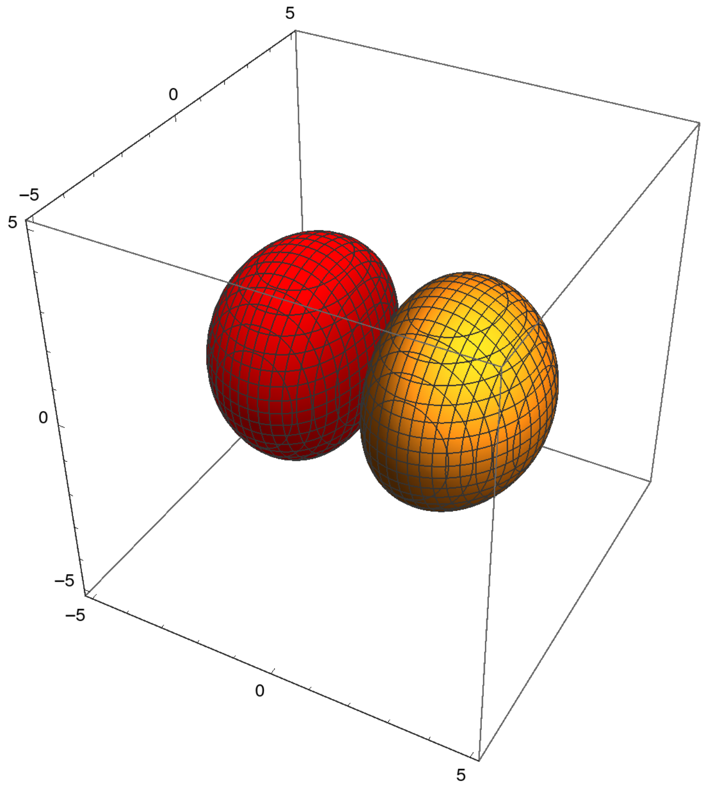
Out[33]=



In[34]:=

```
Show[p1, p2]
```

Out[34]=



In[ ]:=

```
Manipulate[ContourPlot3D[{Evaluate[px[r, θ, ϕ][nn] == 0.04 /. convCartp /. convCarts],
   Evaluate[px[r, θ, ϕ][nn] == -0.04 /. convCartp /. convCarts]}, {x, -5, 5},
  {y, -5, 5}, {z, -5, 5}, PlotRange → All], {nn, 1, 5, 1}, ControlType → PopupMenu]
```

Out[ ]=