

Uhin Funtzioak

```
In[55]:= Unprotect[R];
Clear[R];
R[n_, l_][r_] := (2 Z / (n a))^(3 / 2) Φ[n, l][r / a]
Unprotect[a, Z];

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

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

(* npx(r, θ, ϕ) = 
$$\frac{1}{\sqrt{2}} \{Y_1^{-1}(\theta, \phi) - Y_1^1(\theta, \phi)\} R_{n, 1}(r)$$
 *)
(* npx zatia berdina da n guztientzat: *)

a = .523;
Z = 1;
```

```
In[15]:= 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]};
```

$$nd_{xy}(r, \theta, \phi) = R_{n,2}(r) \frac{1}{i\sqrt{2}} \{Y_2^2(\theta, \phi) - Y_2^{-2}(\theta, \phi)\}$$

```
In[27]:= Clear[dxyAng]
dxyAng[θ_, ϕ_] := (1 / (I Sqrt[2])) *
  (SphericalHarmonicY[2, 2, θ, ϕ] - SphericalHarmonicY[2, -2, θ, ϕ]) // ComplexExpand

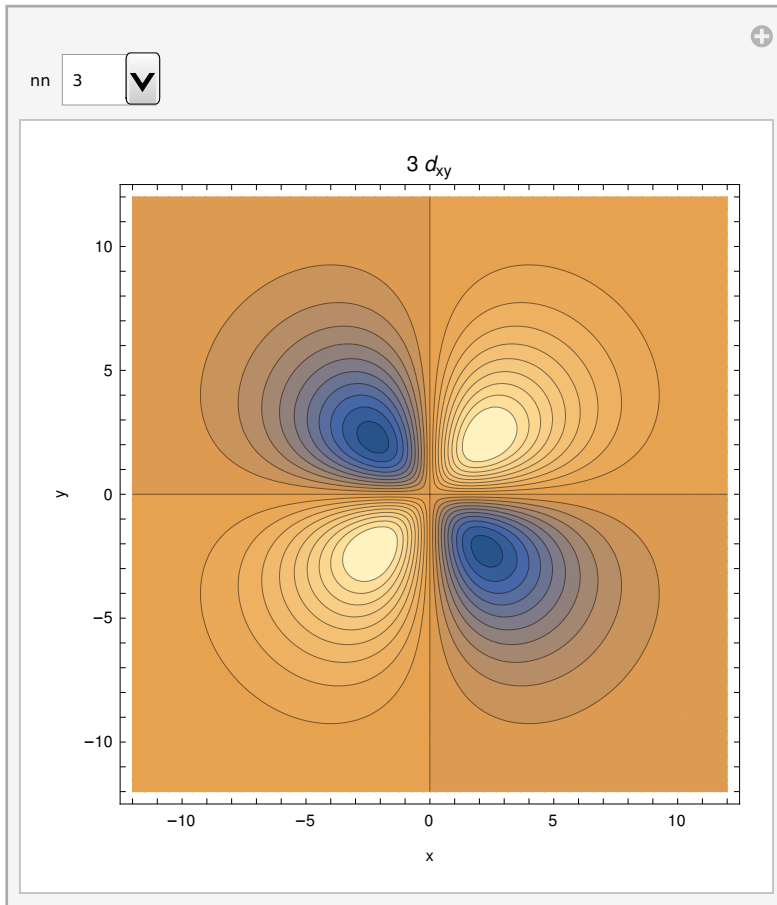
temp1 = (dxyAng[θ, ϕ] // TrigExpand) /. convCartp /. convCarts // FullSimplify;
dxyCart = ReplacePart[temp1, r^2, Position[temp1, x^2 + y^2 + z^2] // Flatten];

Clear[dxy]
dxy[r_, θ_, ϕ_][n_] := R[n, 2][r] * dxyAng[θ, ϕ];

dxyCartesian[n_] := dxyCart * R[n, 2][r]

Manipulate[ContourPlot[Evaluate[dxyCartesian[nn] /. convCarts /. z -> 0],
  {x, -20 * nn / 5, 20 * nn / 5}, {y, -20 * nn / 5, 20 * nn / 5}, Contours -> 20, PlotRange -> All,
  PlotPoints -> 50, FrameLabel -> {"x", "y"}, PlotLabel -> nn "dxy"],
{nn, 3, 6, 1}, ControlType -> PopupMenu]
```

Out[] =



In[35]:=

```
Manipulate[ContourPlot3D[Evaluate[
  {dxyCartesian[nn] == 0.02 / nn /. convCarts, dxyCartesian[nn] == -0.02 / nn /. convCarts}],
  {x, -20 * nn / 5, 20 * nn / 5}, {y, -20 * nn / 5, 20 * nn / 5}, {z, -20 * nn / 5, 20 * nn / 5},
  Contours -> 10, PlotPoints -> 20, PlotRange -> All, PlotLabel -> nn "dxy"],
  {nn, 3, 7, 1}, ControlType -> PopupMenu]
```

Out[35]=

