

## Uhin Funtzio Totala (erradiala eta angeluarra)

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In[69]:= 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 = .5292;
Z = 1;
```

```
In[83]:= 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]};
```

$$nd_{z^2}(\theta, \phi) = R_{n,2}(r) Y_2^0(\theta, \phi)$$

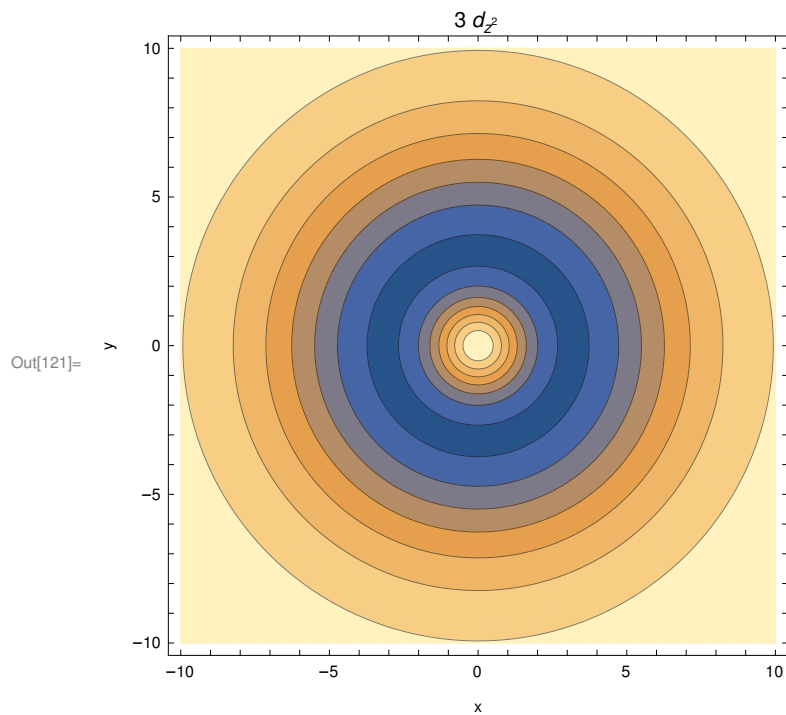
```

In[113]:= Unprotect[dz2Ang];
Clear[dz2Ang]
dz2Ang[ $\theta$ _,  $\phi$ _] := SphericalHarmonicY[2, 0,  $\theta$ ,  $\phi$ ]
Protect[dz2Ang];

Unprotect[dz2];
Clear[dz2]
dz2[r_,  $\theta$ _,  $\phi$ ][n_] :=
  SphericalHarmonicY[2, 0,  $\theta$ ,  $\phi$ ] * R[n, 2][r]
Protect[dz2];

ContourPlot[Evaluate[dz2[r,  $\theta$ ,  $\phi$ ][3] /. convCartp /. convCarts /. z  $\rightarrow$  0],
  {x, -10, 10}, {y, -10, 10},
  PlotPoints  $\rightarrow$  50, PlotRange  $\rightarrow$  All, FrameLabel  $\rightarrow$  {"x", "y"}, PlotLabel  $\rightarrow$  3 " $d_z^2$ " ]

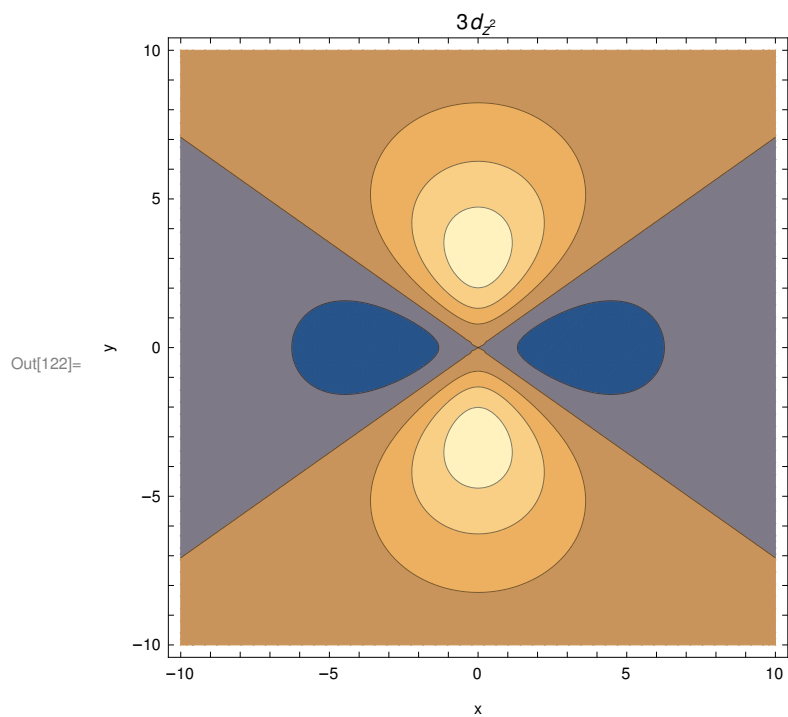
```



```

In[122]:= ContourPlot[
  Evaluate[dz2[r,  $\theta$ ,  $\phi$ ][3] /. convCartp /. convCarts /. y  $\rightarrow$  0, {x, -10, 10}, {z, -10, 10},
  PlotPoints  $\rightarrow$  50, PlotRange  $\rightarrow$  All, FrameLabel  $\rightarrow$  {"x", "y"}, PlotLabel  $\rightarrow$  "3dz2"}]

```



```

In[123]:= Manipulate[ContourPlot3D[{Evaluate[dz2[r,  $\theta$ ,  $\phi$ ][nn] == 0.08 / nn /. convCartp /. convCarts],
  Evaluate[dz2[r,  $\theta$ ,  $\phi$ ][nn] == -0.08 / nn /. convCartp /. convCarts]},
  {x, -50, 50}, {y, -50, 50}, {z, -50, 50}, Contours  $\rightarrow$  10,
  PlotPoints  $\rightarrow$  20, PlotRange  $\rightarrow$  All, PlotLabel  $\rightarrow$  nn " $d_z^2$ ",
  {nn, 3, 7, 1}, ControlType  $\rightarrow$  PopupMenu]

```

Out[123]=

