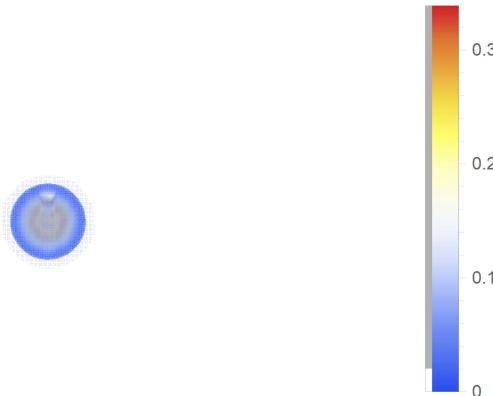


# Atomic Orbitals :

```
In[°]:= a0 = Quantity["BohrRadius"] / Quantity["Meters"];  
  
ψ[{n_, l_, m_}, {r_, θ_, φ_}] := With[{ρ = 2 r / n a0}, Sqrt[(2 r / n a0)^3 (n - l - 1)! / (2 n ((n + l) !))]  
e^(ρ^2/2) ρ^l LaguerreL[n + 1, 2 l + 1, ρ] SphericalHarmonicY[l, m, θ, φ]]  
  
s1 = DensityPlot3D[Abs@ψ[{1, 0, 0}], {Sqrt[x^2 + y^2 + z^2],  
ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}]^2, {x, -35 a0, 35 a0},  
{y, -35 a0, 35 a0}, {z, -35 a0, 35 a0}, PlotLegends → Automatic,  
PlotLabel → "1s", AxesLabel → Automatic,  
PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

1s

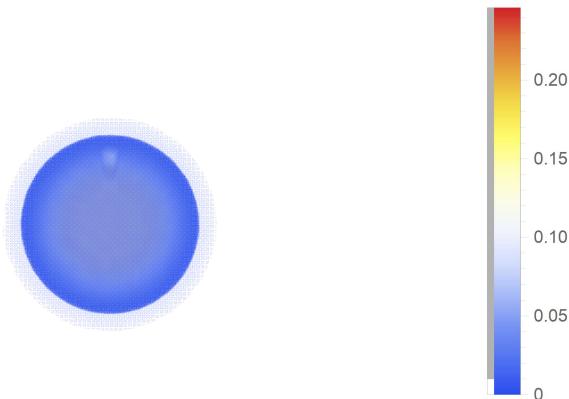
Out[°]=



```
In[6]:= s2 = DensityPlot3D[
  (Abs@ψ[{2, 0, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -40 a0, 40 a0}, {y, -40 a0, 40 a0}, {z, -40 a0, 40 a0},
  PlotLegends → Automatic, PlotLabel → "2s", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

2s

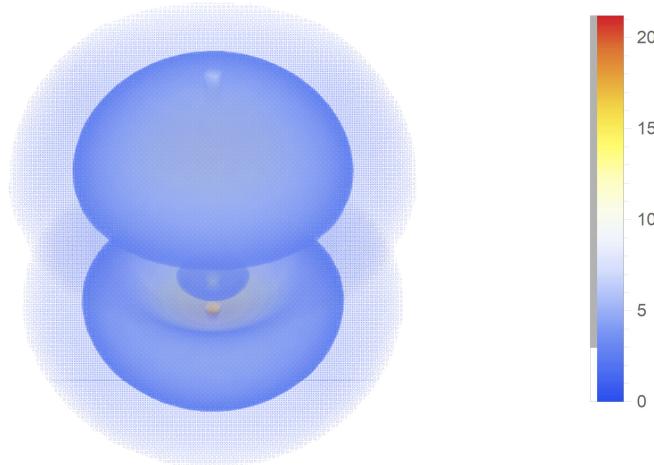
Out[6]=



```
In[6]:= p1 = DensityPlot3D[
  (Abs@ψ[{2, 1, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -25 a0, 25 a0}, {y, -25 a0, 25 a0}, {z, -25 a0, 25 a0},
  PlotLegends → Automatic, PlotLabel → "2pz", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

2pz

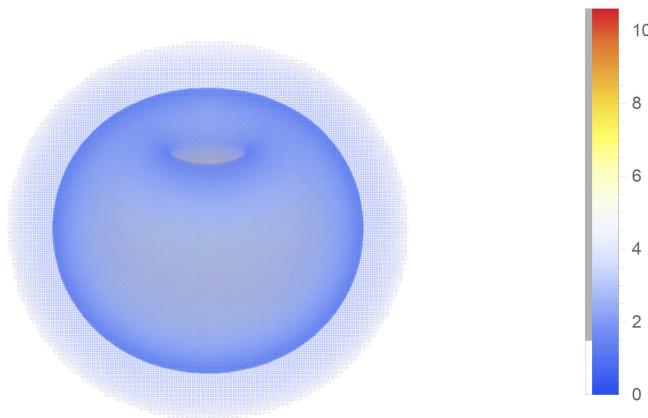
Out[6]=



```
In[®]:= P1 = DensityPlot3D[
  (Abs@ψ[{2, 1, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -30 a0, 30 a0}, {y, -30 a0, 30 a0}, {z, -30 a0, 30 a0},
  PlotLegends → Automatic, PlotLabel → "2py & 2px", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

2py & 2px

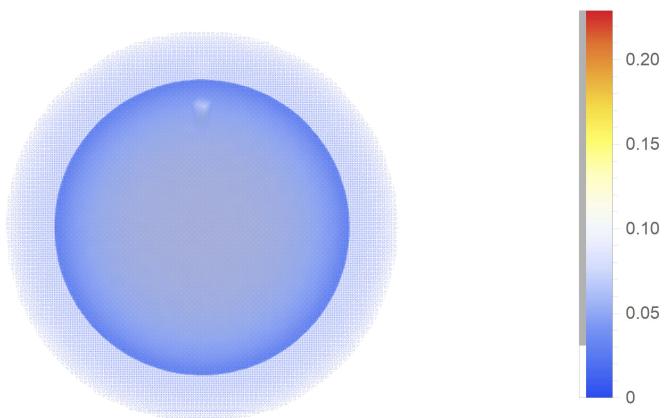
Out[<sup>®</sup>]=



```
In[6]:= s3 = DensityPlot3D[
  (Abs@ψ[{3, 0, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -40 a0, 40 a0}, {y, -40 a0, 40 a0}, {z, -40 a0, 40 a0},
  PlotLegends → Automatic, PlotLabel → "3s", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

3s

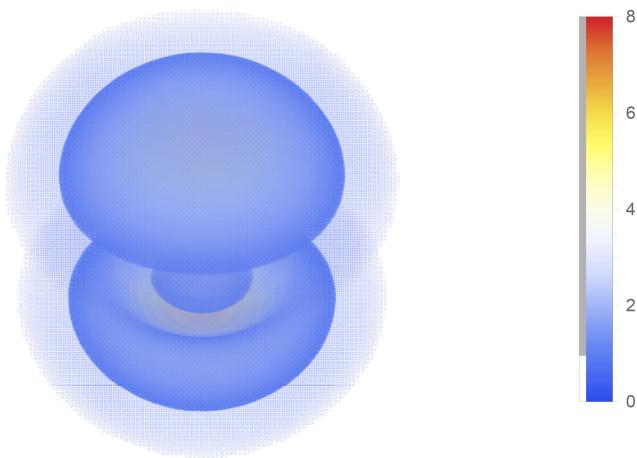
Out[6]=



```
In[6]:= p2 = DensityPlot3D[
  (Abs@ψ[{3, 1, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -45 a0, 45 a0}, {y, -45 a0, 45 a0}, {z, -45 a0, 45 a0},
  PlotLegends → Automatic, PlotLabel → "3pz", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

3pz

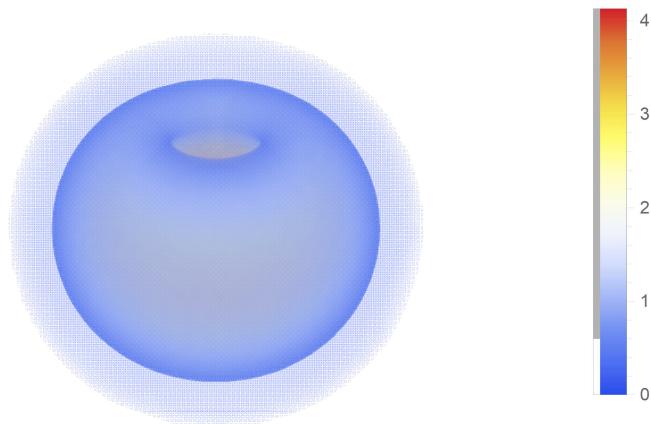
Out[6]=



```
In[6]:= P2 = DensityPlot3D[
  (Abs@ψ[{3, 1, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -50 a0, 50 a0}, {y, -50 a0, 50 a0}, {z, -50 a0, 50 a0},
  PlotLegends → Automatic, PlotLabel → "3py and 3px", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]

3py and 3px
```

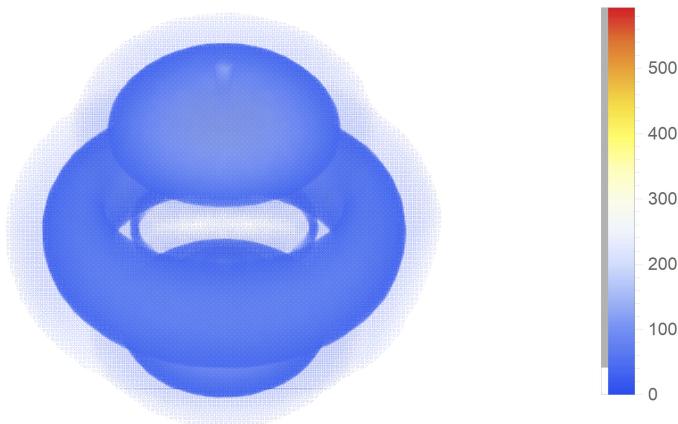
Out[6]=



```
In[6]:= d1 = DensityPlot3D[
  (Abs@ψ[{3, 2, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -55 a0, 55 a0}, {y, -55 a0, 55 a0}, {z, -60 a0, 60 a0},
  PlotLegends → Automatic, PlotLabel → "3d_z^2", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

3d\_z^2

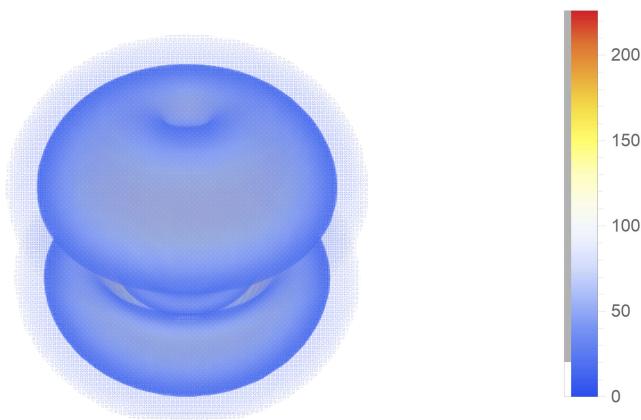
Out[6]=



```
In[6]:= D1 = DensityPlot3D[
  (Abs@ψ[{3, 2, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -65 a0, 65 a0}, {y, -65 a0, 65 a0}, {z, -65 a0, 65 a0},
  PlotLegends → Automatic, PlotLabel → "3d_xz and 3d_yz", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

3d\_xz and 3d\_yz

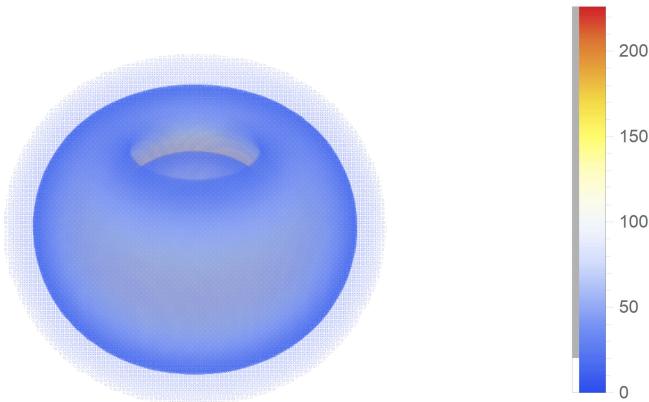
Out[<sup>6</sup>]=



```
In[6]:= Dd1 = DensityPlot3D[(Abs@ψ[{3, 2, -2},  
 {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^2,  
 {x, -67 a0, 67 a0}, {y, -67 a0, 67 a0}, {z, -67 a0, 67 a0}, PlotLegends → Automatic,  
 PlotLabel → "3d_xy and 3d_x2-y2", AxesLabel → Automatic,  
 PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

3d\_xy and 3d\_x2-y2

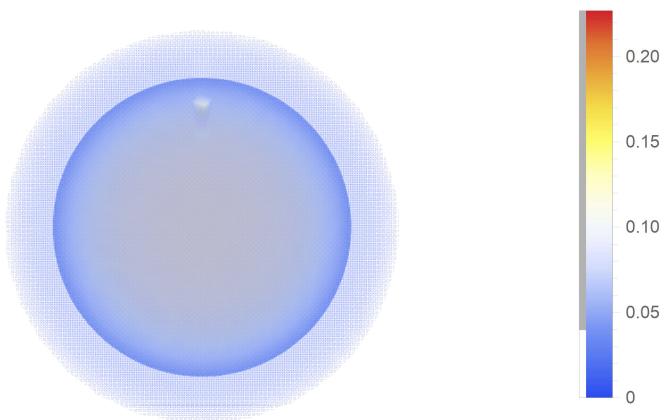
Out[<sup>6</sup>]=



```
In[6]:= s4 = DensityPlot3D[
  (Abs@ψ[{4, 0, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -62 a0, 62 a0}, {y, -62 a0, 62 a0}, {z, -62 a0, 62 a0},
  PlotLegends → Automatic, PlotLabel → "4s", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

4s

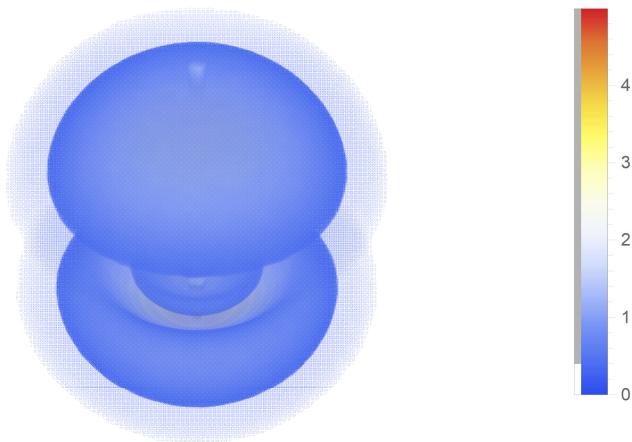
Out[6]=



```
In[6]:= p3 = DensityPlot3D[
  (Abs@ψ[{4, 1, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -70 a0, 70 a0}, {y, -70 a0, 70 a0}, {z, -70 a0, 70 a0},
  PlotLegends → Automatic, PlotLabel → "4pz", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

4pz

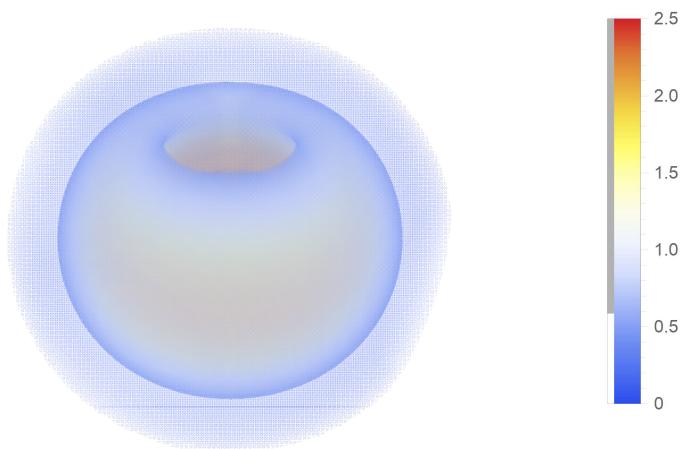
Out[6]=



```
In[6]:= P3 = DensityPlot3D[
  (Abs@ψ[{4, 1, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -70 a0, 70 a0}, {y, -70 a0, 70 a0}, {z, -70 a0, 70 a0},
  PlotLegends → Automatic, PlotLabel → "4px & 4py", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]

4px & 4py
```

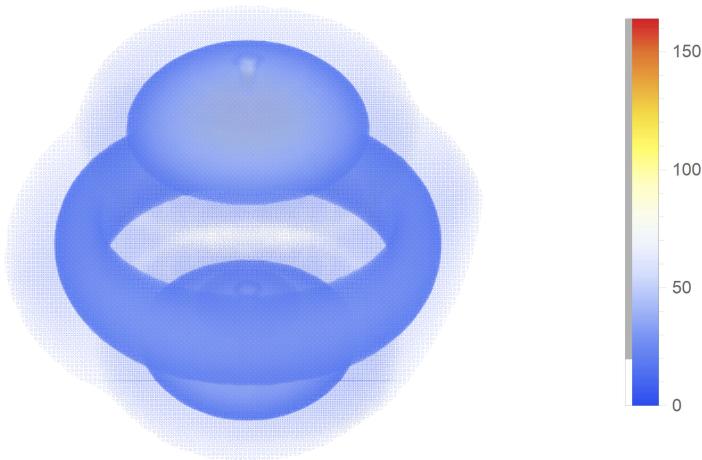
Out[6]=



```
In[6]:= d2 = DensityPlot3D[
  (Abs@ψ[{4, 2, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -73 a0, 73 a0}, {y, -73 a0, 73 a0}, {z, -80 a0, 80 a0},
  PlotLegends → Automatic, PlotLabel → "4d_z^2", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

4d\_z^2

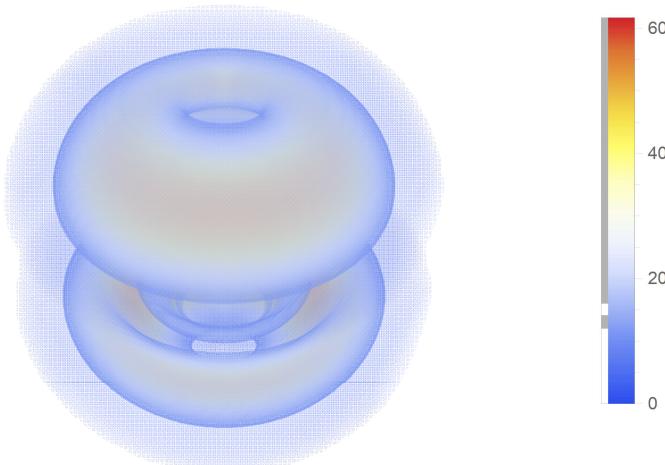
Out[6]=



```
In[6]:= D2 = DensityPlot3D[
  (Abs@ψ[{4, 2, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -80 a0, 80 a0}, {y, -80 a0, 80 a0}, {z, -80 a0, 80 a0},
  PlotLegends → Automatic, PlotLabel → "4d_xz & 4d_yz", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
```

4d\_xz & 4d\_yz

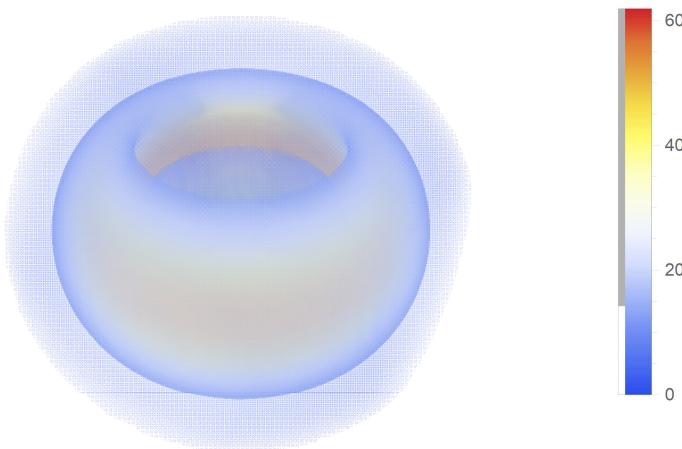
Out[<sup>6</sup>]=



```
In[6]:= Dd2 = DensityPlot3D[
  (Abs@ψ[{4, 2, 2}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -80 a0, 80 a0}, {y, -80 a0, 80 a0}, {z, -80 a0, 80 a0},
  PlotLegends → Automatic, PlotLabel → "4d_xy & 4d_x2-y2", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]

4d_xy & 4d_x2-y2
```

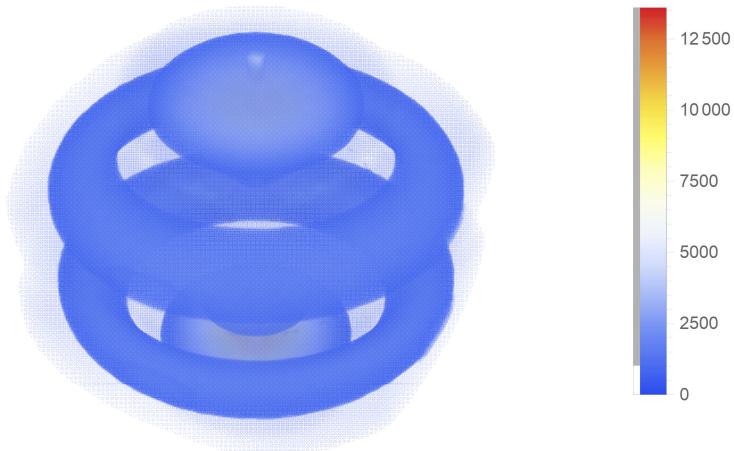
Out[<sup>6</sup>]=



```
In[6]:= f1 = DensityPlot3D[
  (Abs@ψ[{4, 3, 0}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -80 a0, 80 a0}, {y, -80 a0, 80 a0}, {z, -100 a0, 100 a0},
  PlotLegends → Automatic, PlotLabel → "4f_z^3", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]

4f_z^3
```

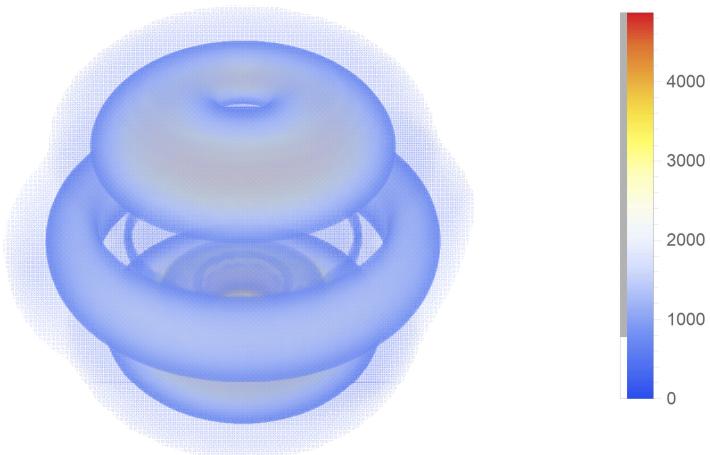
Out[6]=



```
In[6]:= f2 = DensityPlot3D[
  (Abs@ψ[{4, 3, 1}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -90 a0, 90 a0}, {y, -90 a0, 90 a0}, {z, -100 a0, 100 a0},
  PlotLegends → Automatic, PlotLabel → "4f_xz2 & 4f_yz2", AxesLabel → Automatic,
  PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]

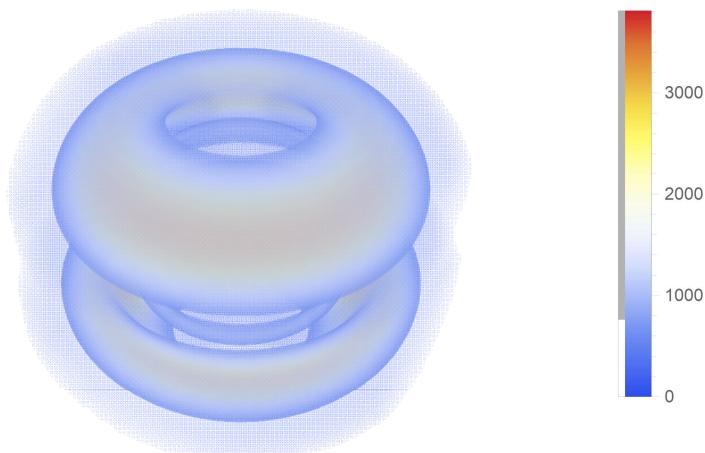
4f_xz2 & 4f_yz2
```

Out[<sup>6</sup>]=



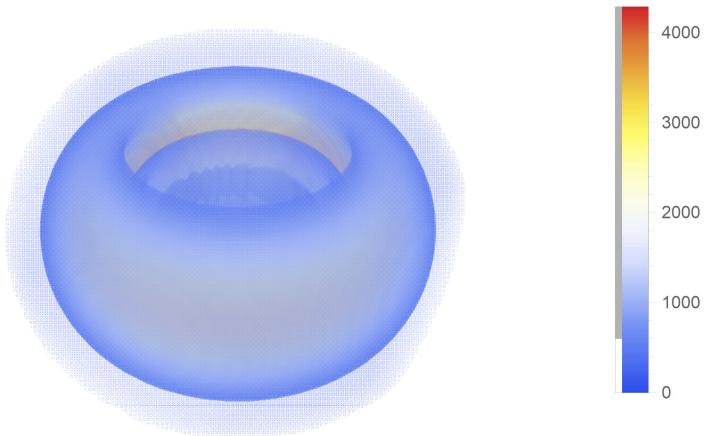
```
In[6]:= f3 = DensityPlot3D[
  (Abs@ψ[{4, 3, 2}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -90 a0, 90 a0}, {y, -90 a0, 90 a0}, {z, -100 a0, 100 a0},
  PlotLegends → Automatic, PlotLabel → "4_fxyz & 4_fz(x2-y2)",
  AxesLabel → Automatic, PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
4_fxyz & 4_fz(x2-y2)
```

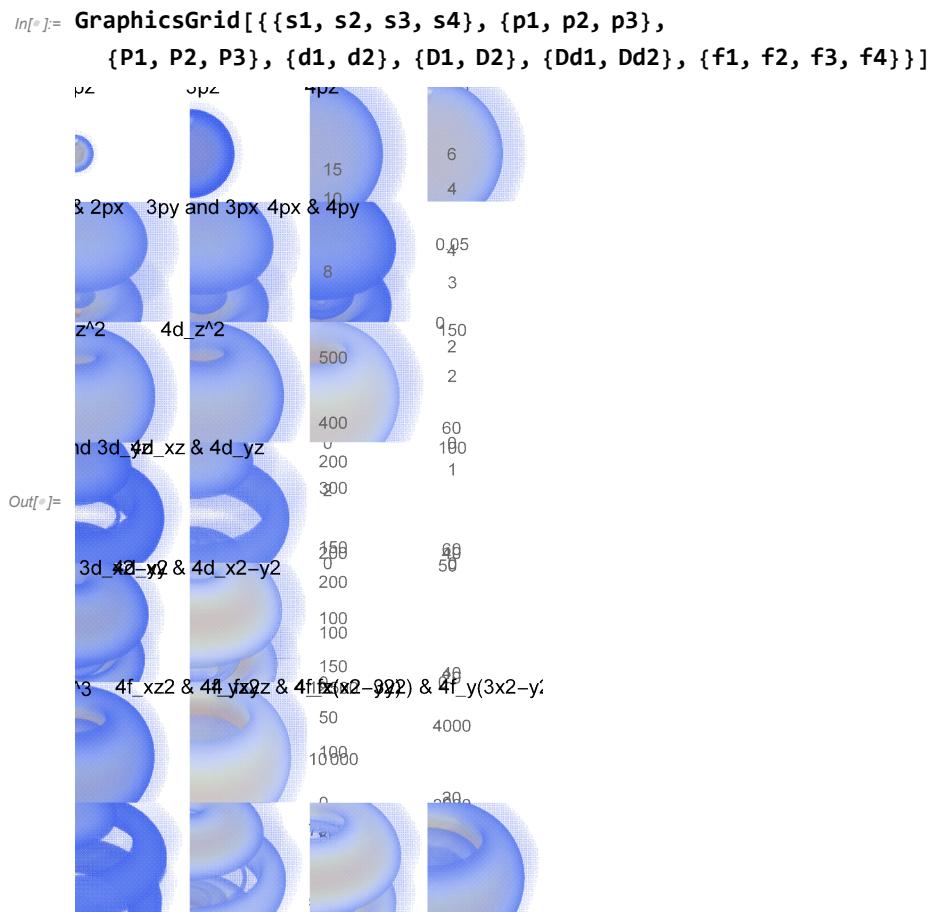
Out[<sup>6</sup>]=



```
In[®]:= f4 = DensityPlot3D[
  (Abs@ψ[{4, 3, 3}, {Sqrt[x^2 + y^2 + z^2], ArcTan[z, Sqrt[x^2 + y^2]], ArcTan[x, y]}])^
  2, {x, -95 a0, 95 a0}, {y, -95 a0, 95 a0}, {z, -100 a0, 100 a0},
  PlotLegends → Automatic, PlotLabel → "4f_x(x^2-3y^2) & 4f_y(3x^2-y^2)",
  AxesLabel → Automatic, PlotTheme → "NoAxes", ColorFunction → "TemperatureMap"]
4f_x(x^2-3y^2) & 4f_y(3x^2-y^2)
```

Out[<sup>®</sup>]=





In[<sup>24</sup>]:= **Show**[%24, **ImageSize** → **Full**]

