Mathematica for the Hydrogen wave function

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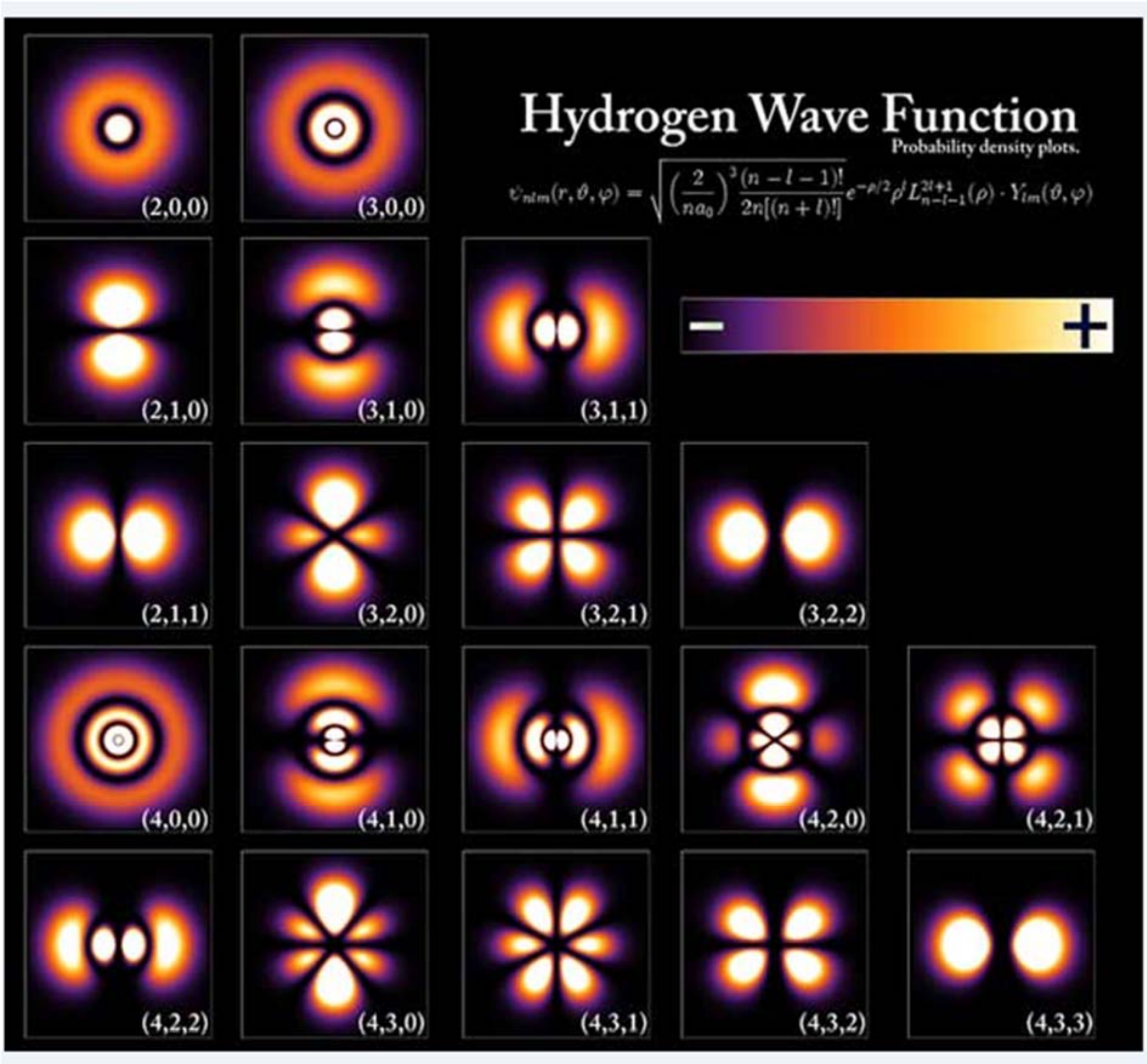

1. Plot of the wave function using Mathematica

Here we show how to make a plot of the wave function using the Mathematica. The wave function of the hydrogen is given by the form

$$\psi_{nlm}(\boldsymbol{r}) = R_{nl}(r)Y_l^m(\theta,\phi),$$

where

$$R_{nl}(r)=\sqrt{\frac{4Z^3(n-l-1)!}{a^3n^4(n+l)!}}e^{-\frac{Zr}{na}}(\frac{2Zr}{na})^l L_{n-l-1}^{2l+1}(\frac{2Zr}{na}),$$

and $Y_l^m(\theta,\phi)$ is the spherical harmonics.

We want to make a contour plot of the square of the amplitude of wave function,

$$|\psi_{nlm}(\boldsymbol{r})|^2=|R_{nl}(r)|^2|Y_l^m(\theta,\phi)|^2=\alpha=\text{constant}$$

where

$$r=\sqrt{x^2+y^2+z^2}\,,\qquad \theta=acr\cos[\frac{z}{\sqrt{x^2+y^2+z^2}}],\qquad \phi=\arctan(\frac{y}{x})\,.$$

α is changed as a parameter. For simplicity, we examine the contour plot when $x = 0$. In this case we get the ContourPlot of the probability in the (y, z) plane. In this plot, we change the value of α as a parameter.

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2. Example: ContourPlot of $|\psi_{nlm}(\boldsymbol{r})|^2$ with x = 0 in the (y, z) plane.

ContourPlot of prbability density $|\psi_{nlm}|^2$ for various states of hydrogen in the (y,z) plane with x = 0.

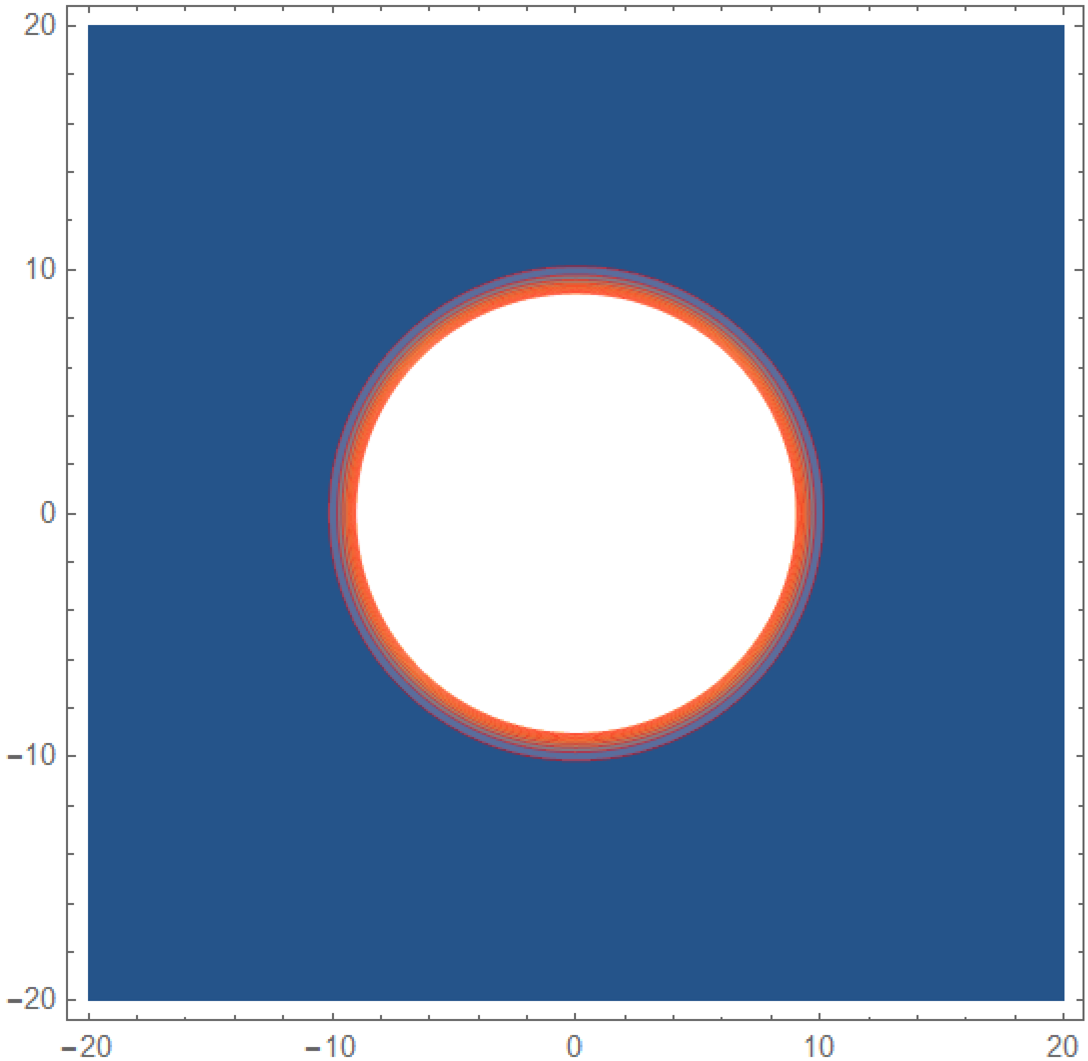
$n = 1$ $l = 0$, $m = 0$

$n = 2$ $l = 0$ $m = 0$
$n = 2$ $l = 1$ $m = 1$, $m = 0$

$n = 3$ $l = 2$ $m = 2$, $m =1$, $m = 0$
$n = 3$ $l = 1$ $m = 1$, $m = 0$
$n = 3$ $l = 0$ $m = 0$

$n = 4$ $l = 3$ $m = 3$, $m = 2$, $m =1$, $m = 0$
$n = 4$ $l = 2$ $m = 2$, $m = 1$, $m = 0$
$n = 4$ $l = 1$ $m = 1$, $m = 0$
$n = 4$ $l = 0$ $m = 0$

K1[1, 0, 0]



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K1[2, 0, 0]
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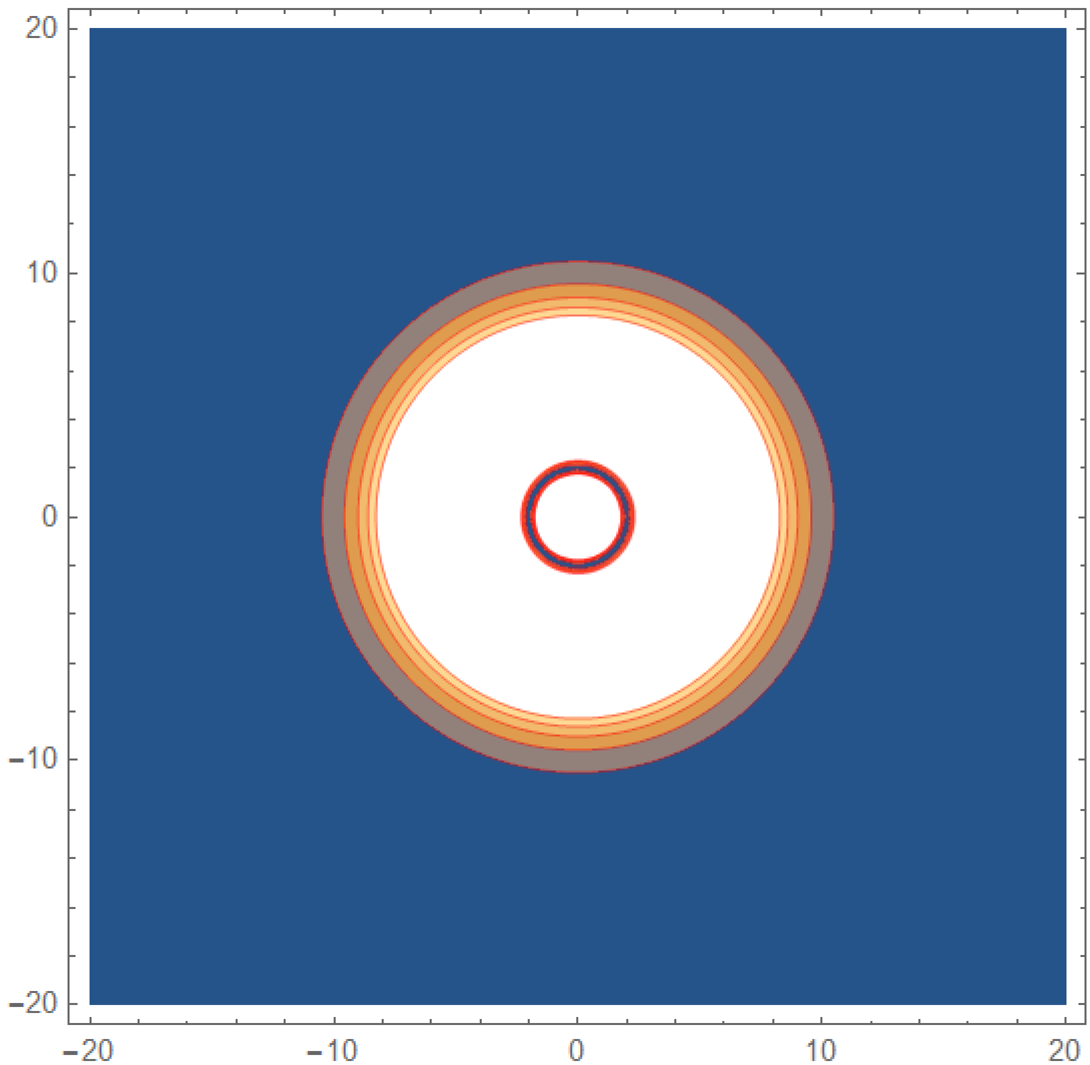
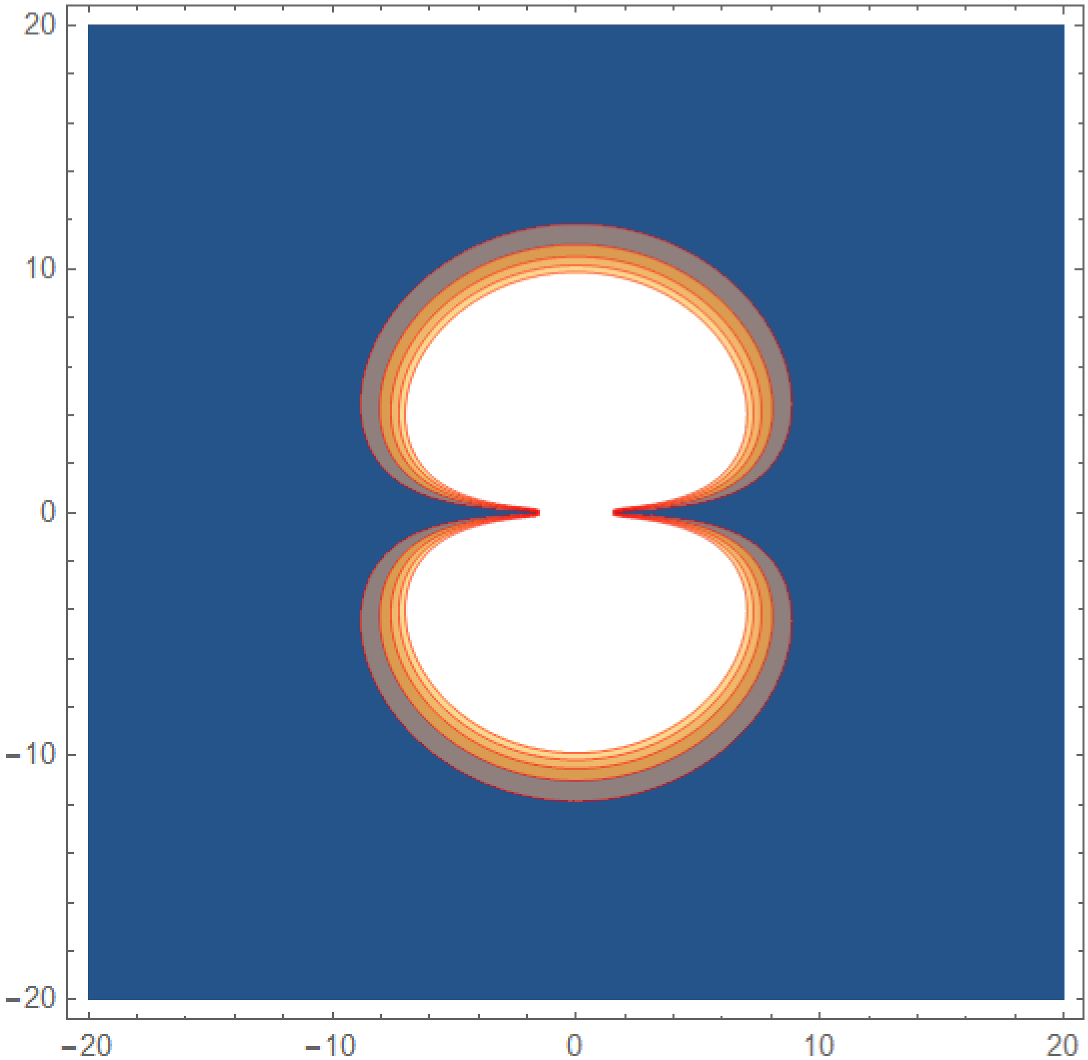
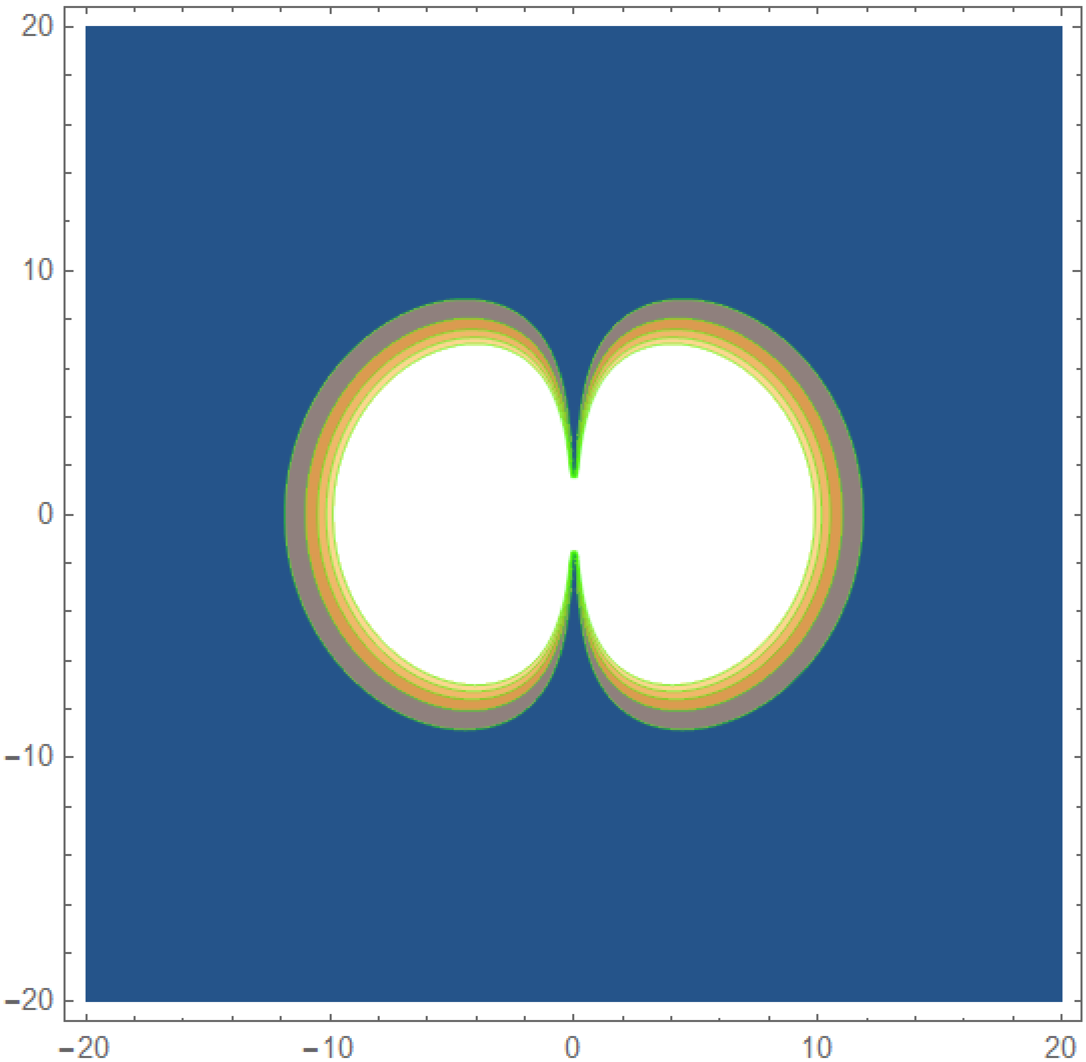


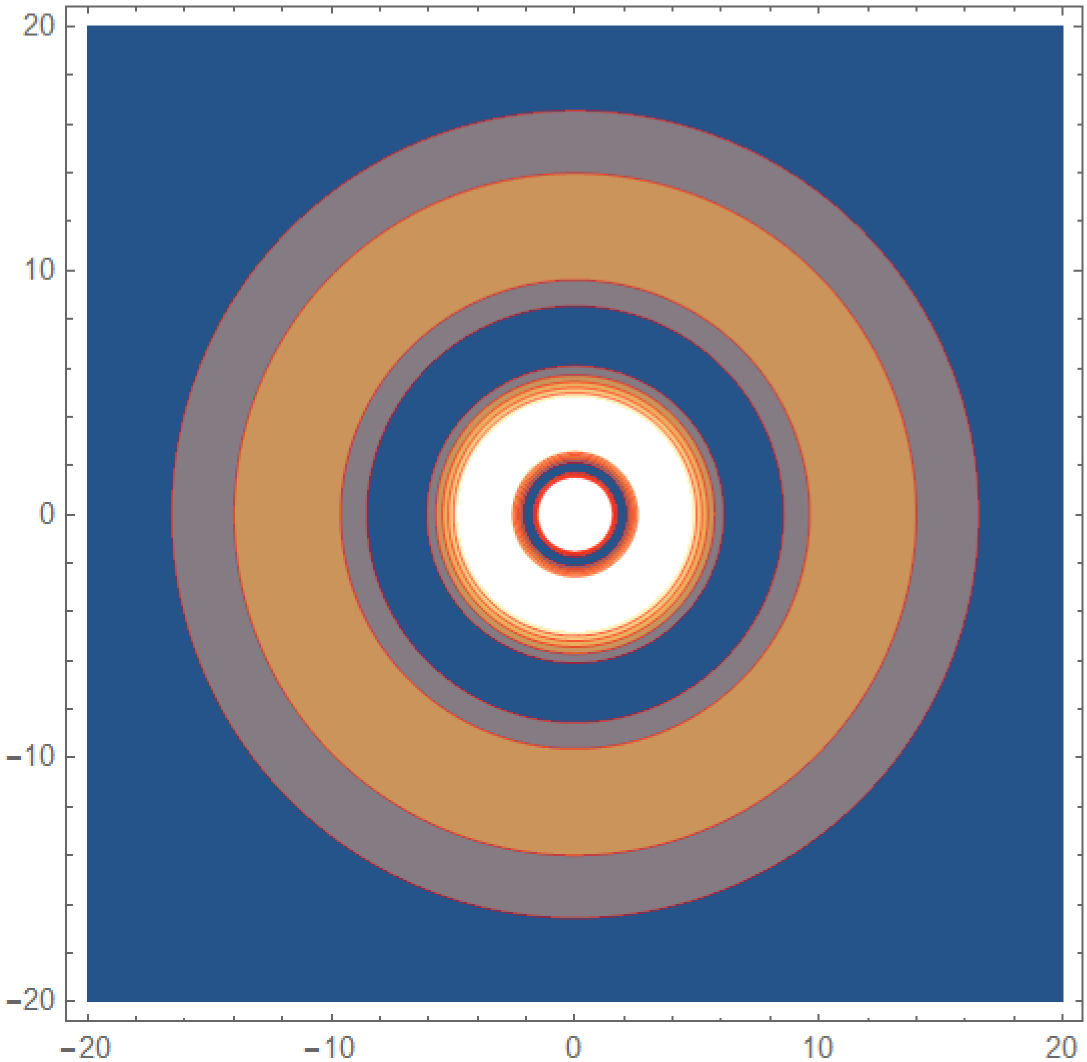
K1[2, 1, 0]



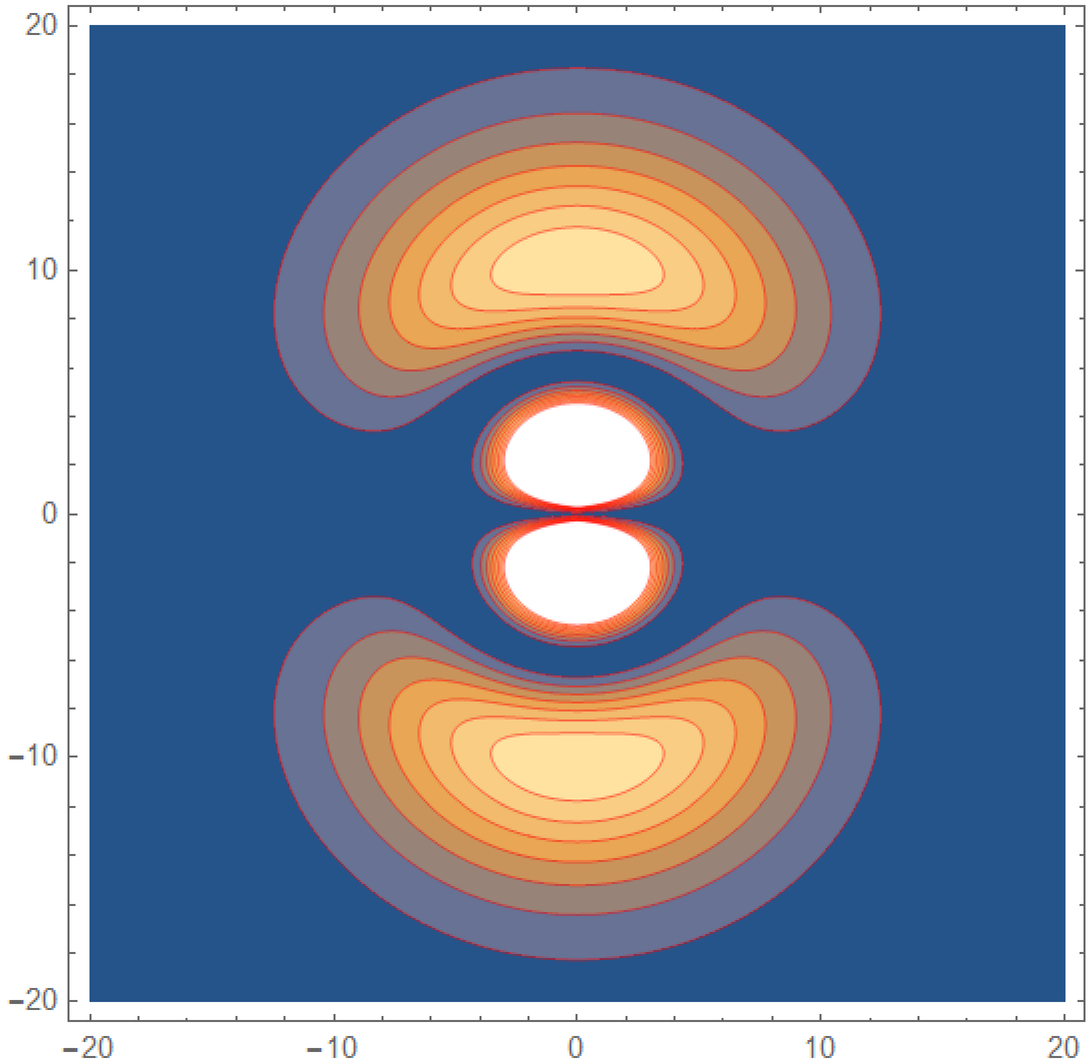
K1[2, 1, 1]



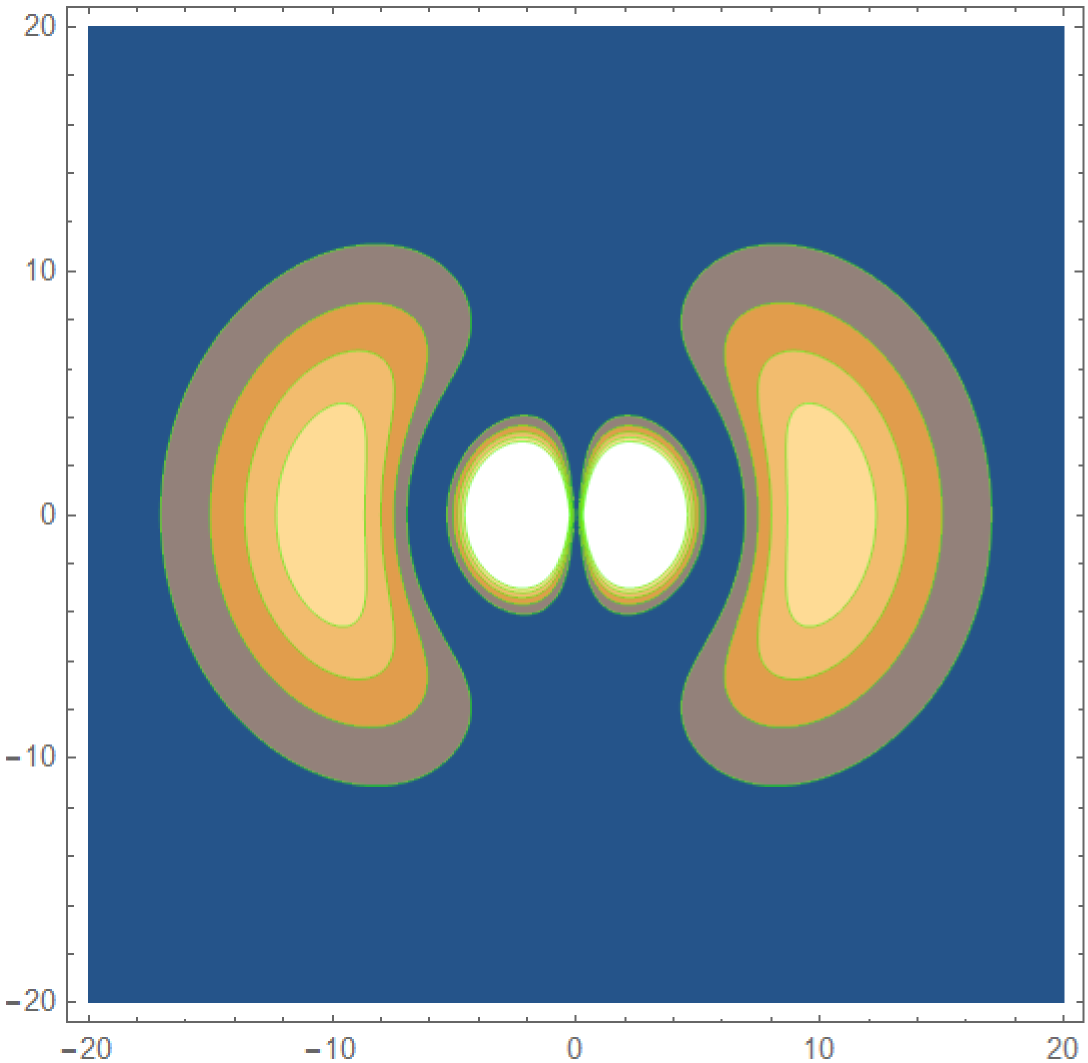
K1[3, 0, 0]



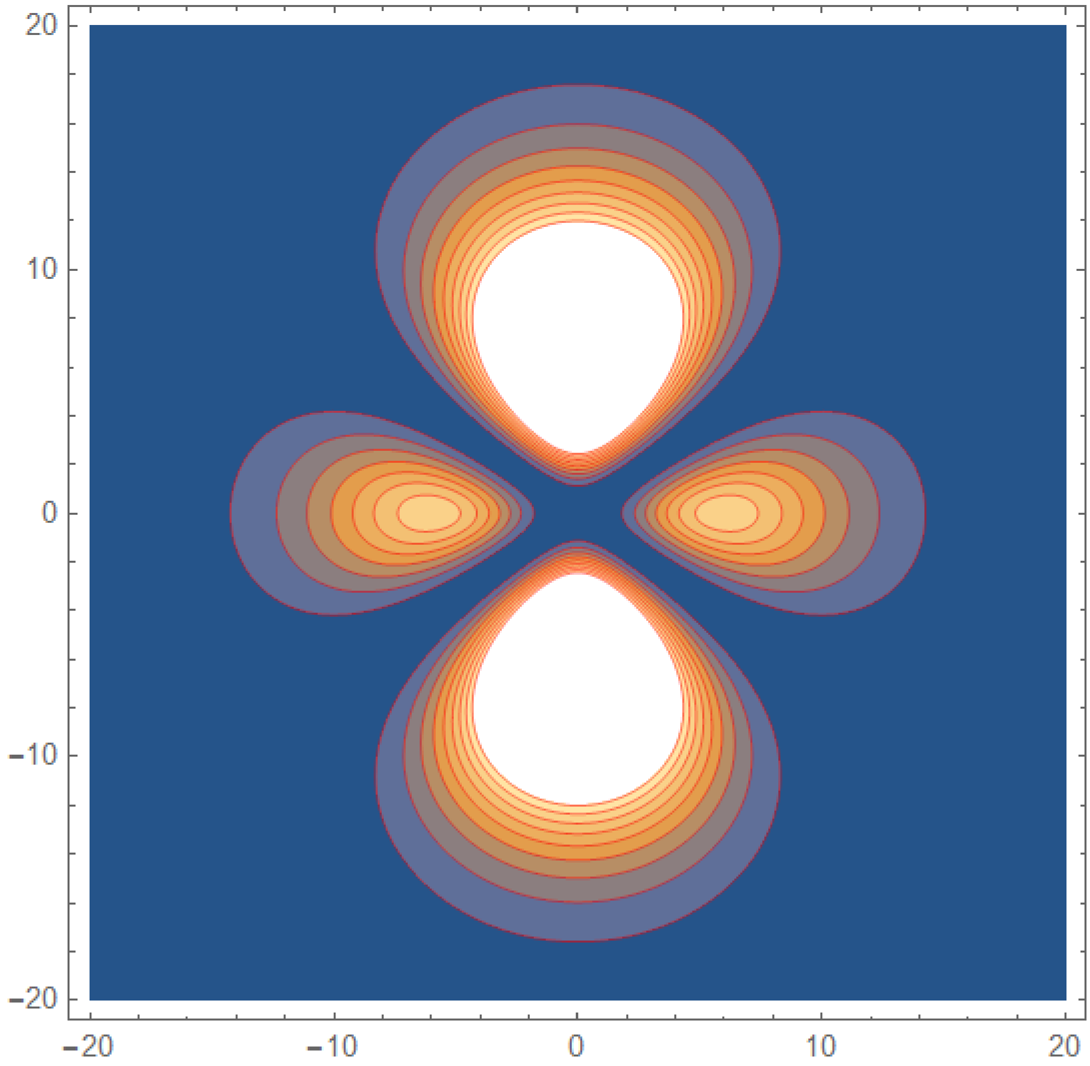
K1[3, 1, 0]

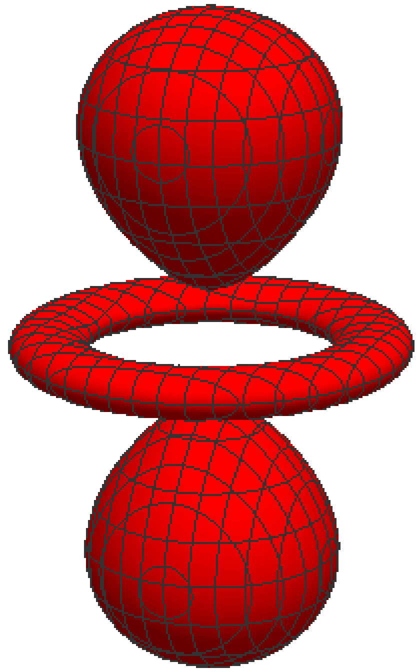


K1[3, 1, 1]



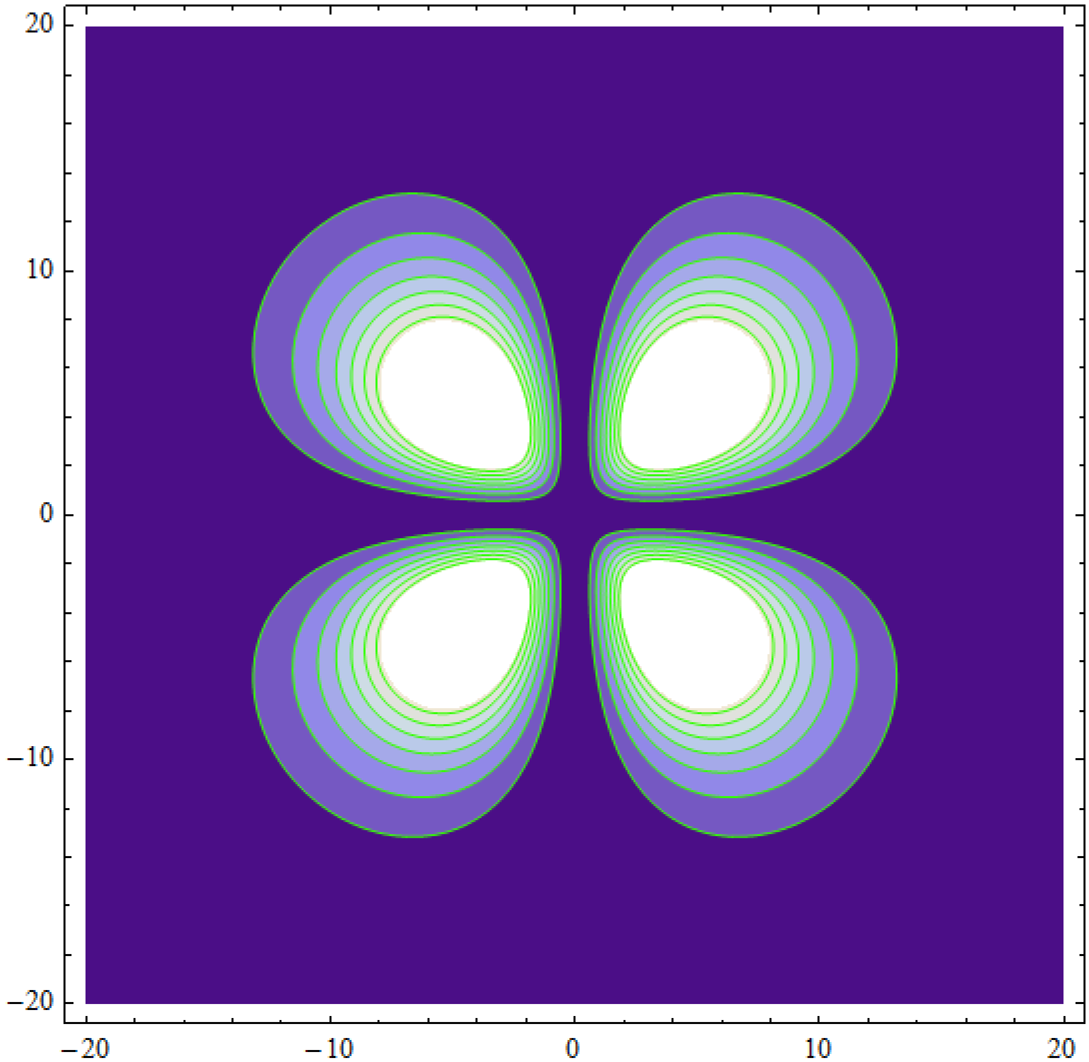
K1[3, 2, 0]

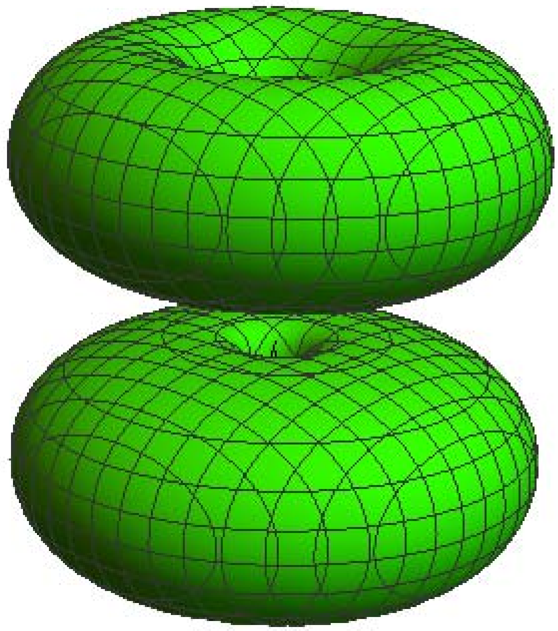




ContourPlot3D of $|\psi_{3,2,0}(\boldsymbol{r})|^2$ in the (x, y, z) plane.

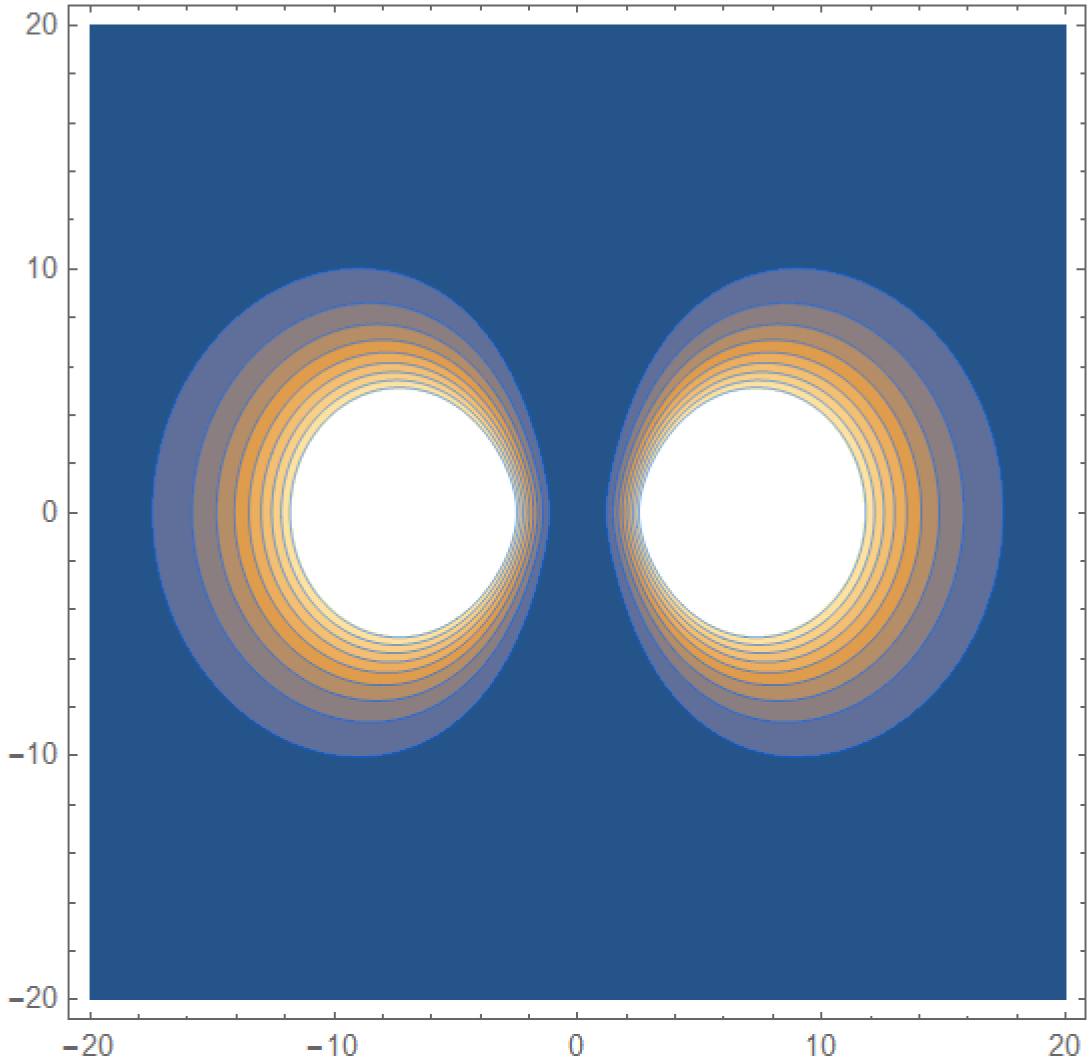
K1[3, 2, 1]

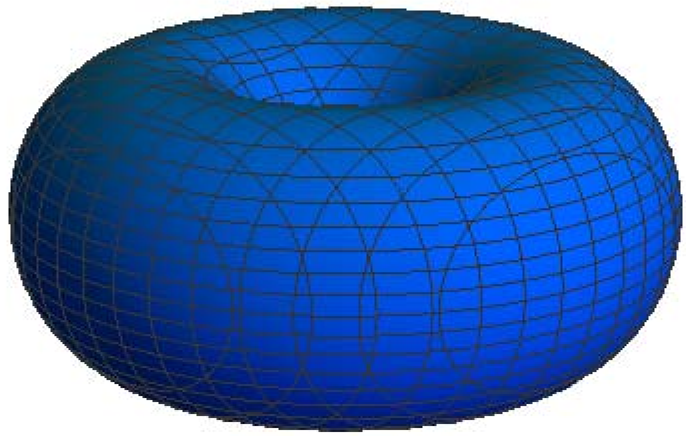




ContourPlot3D of $|\psi_{3,2,1}(\boldsymbol{r})|^2$ in the (x, y, z) plane.

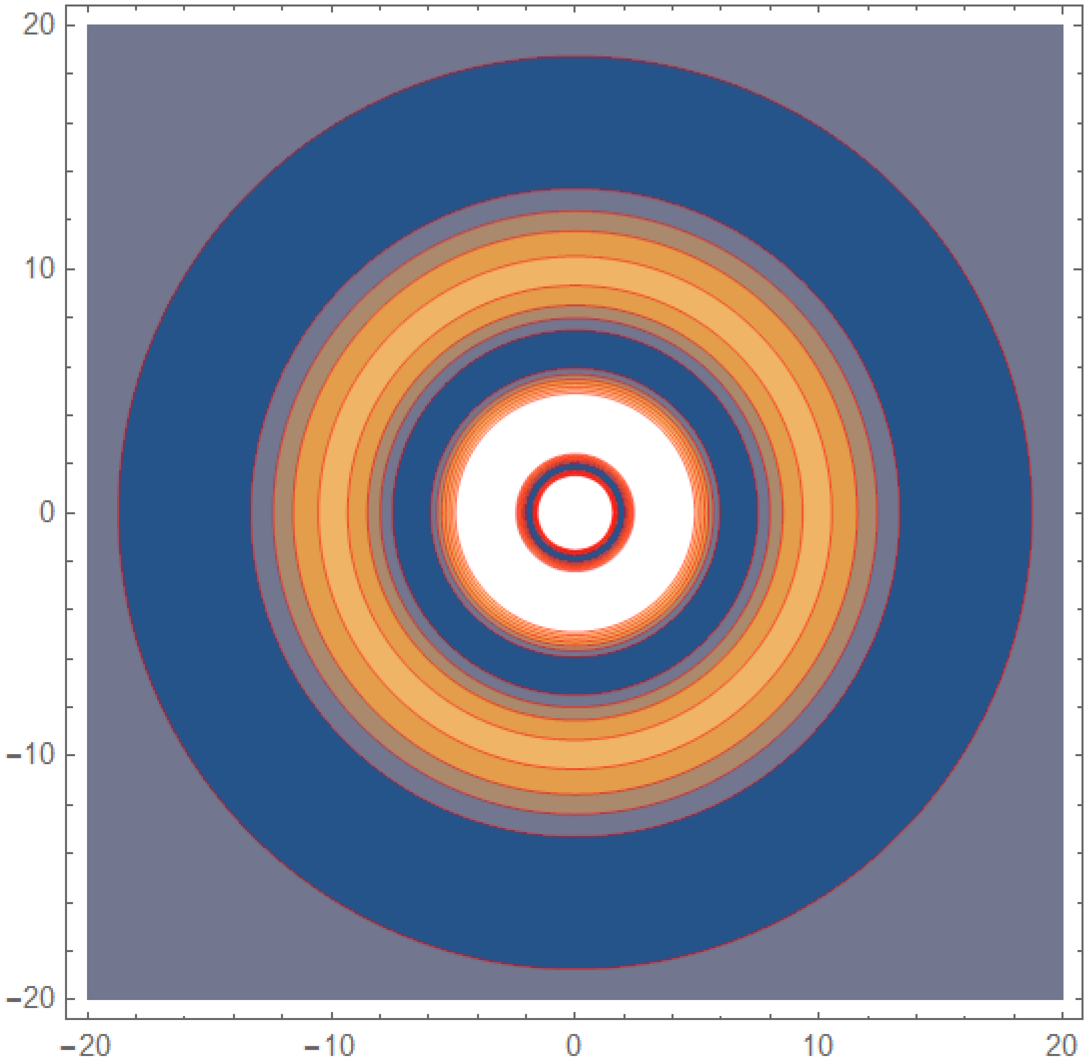
```
K1[3, 2, 2]
```





ContourPlot3D of $\left|\psi_{3,2,2}(\boldsymbol{r})\right|^2$ in the (x, y, z) plane.

K1[4, 0, 0]



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K1[4, 1, 0]
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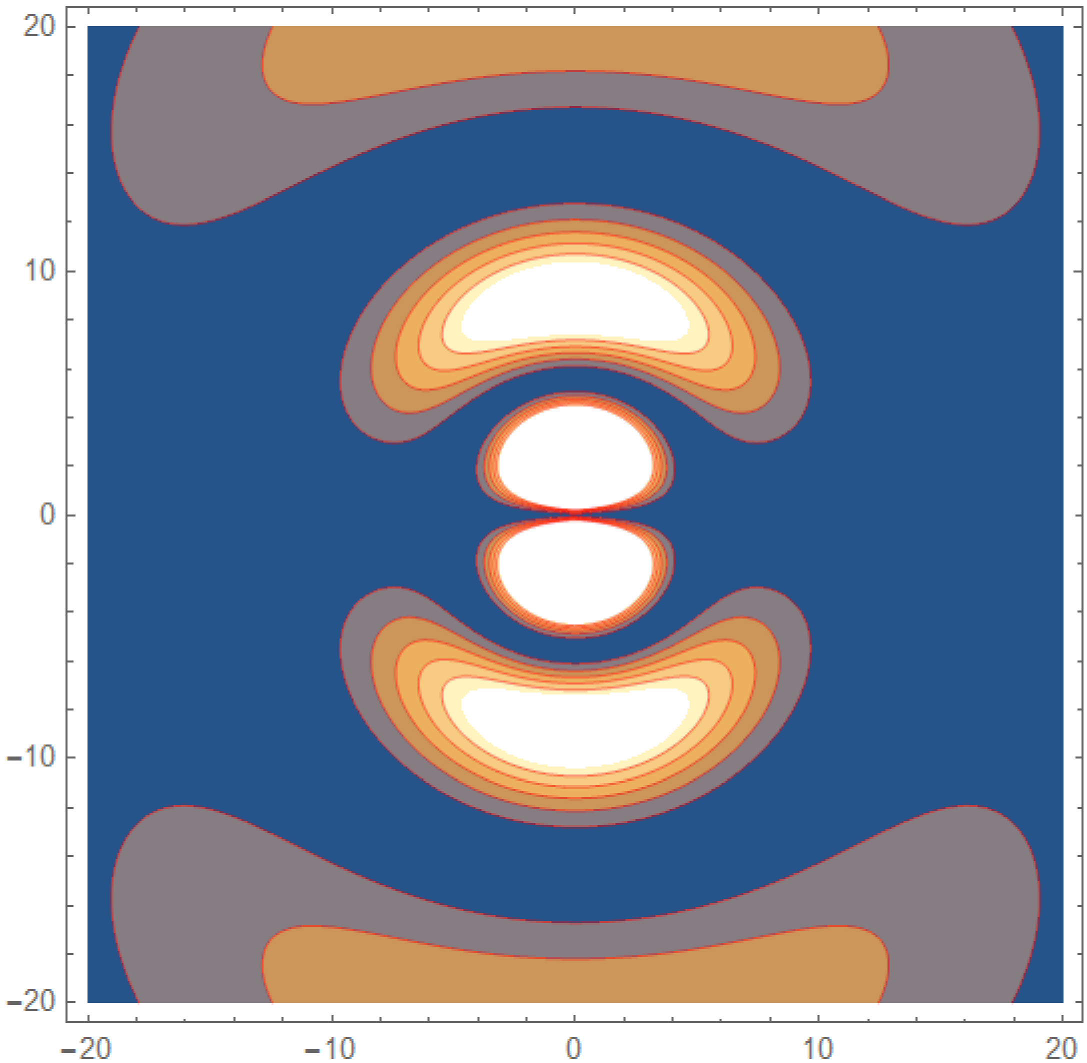
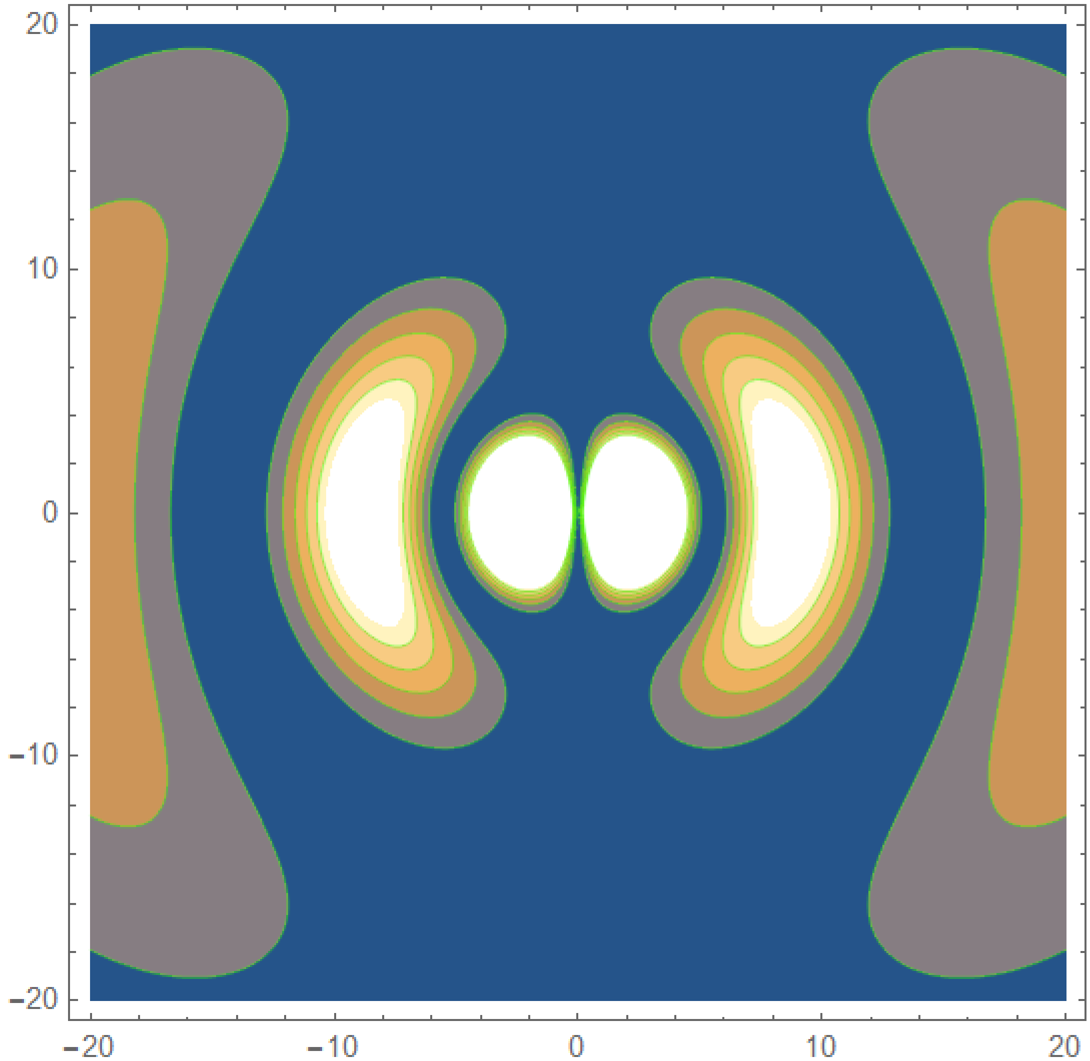
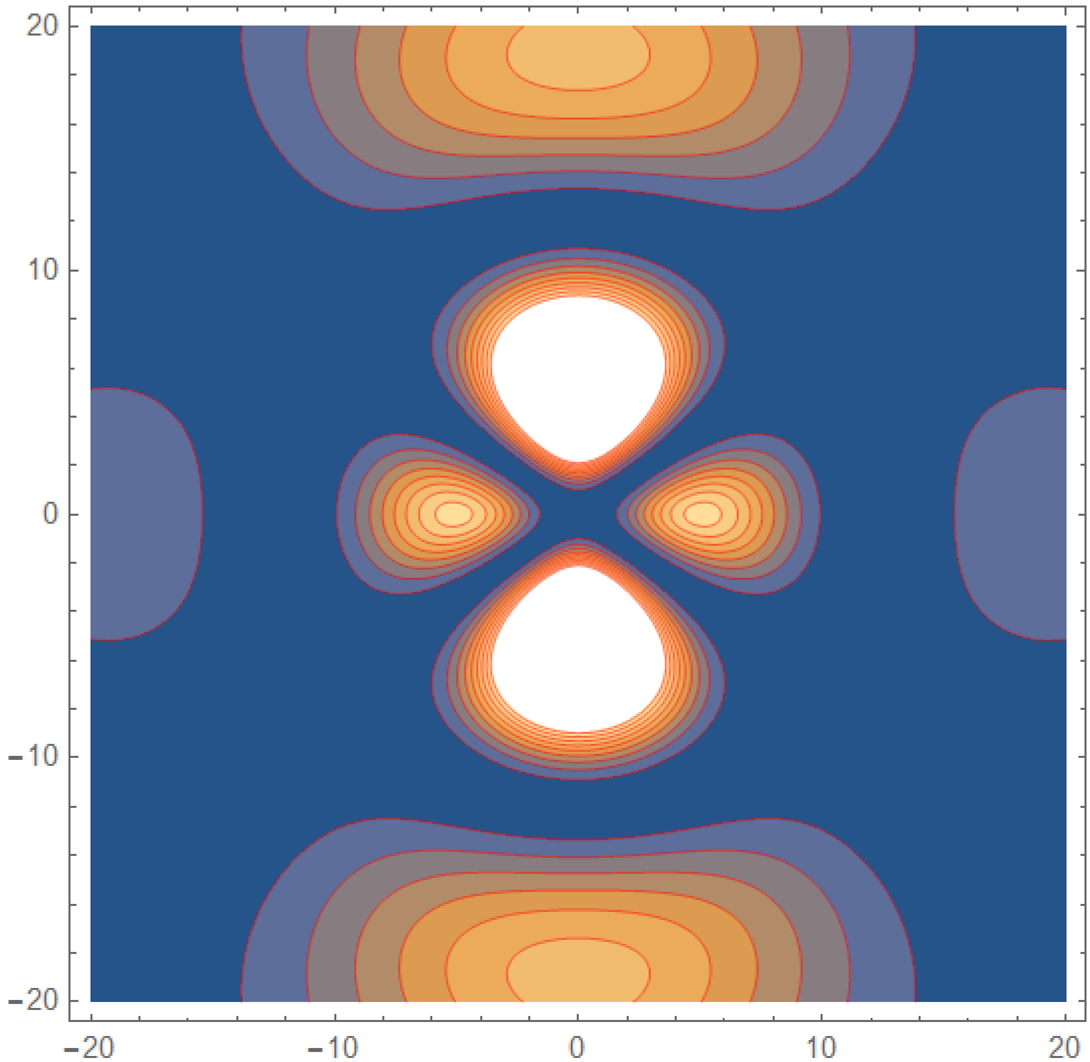
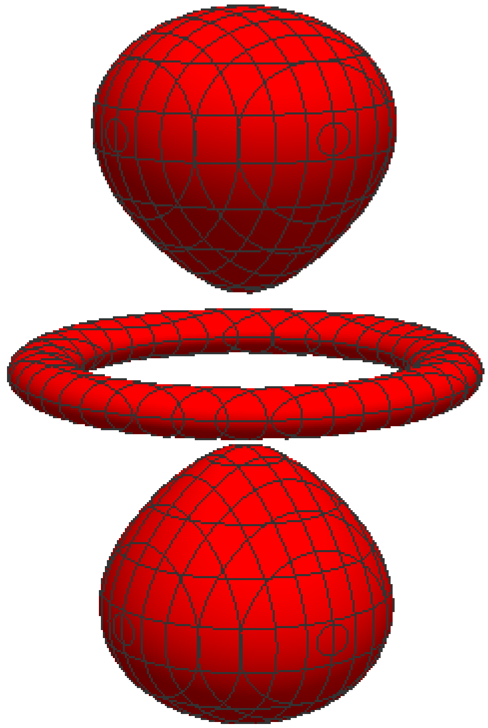


K1[4, 1, 1]



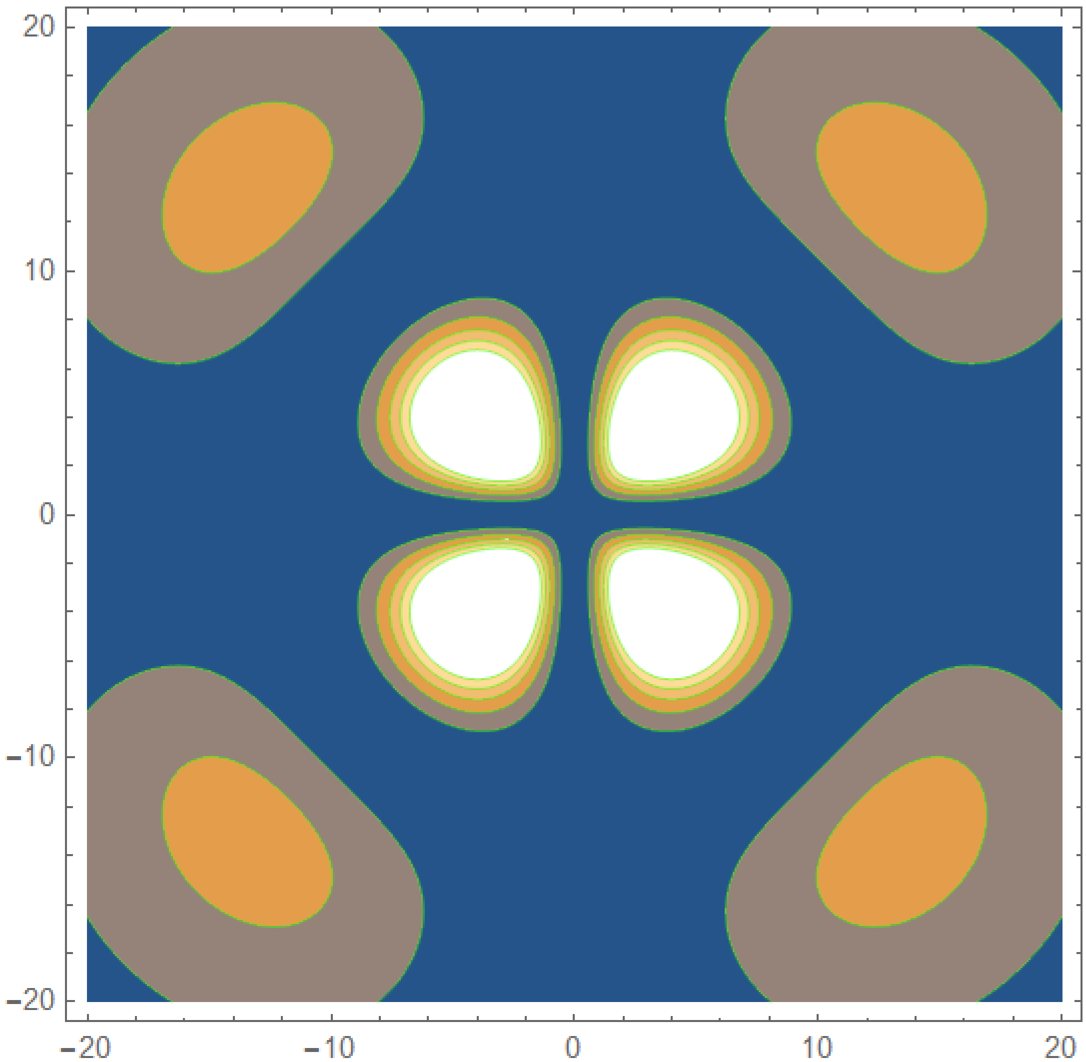
K1[4, 2, 0]

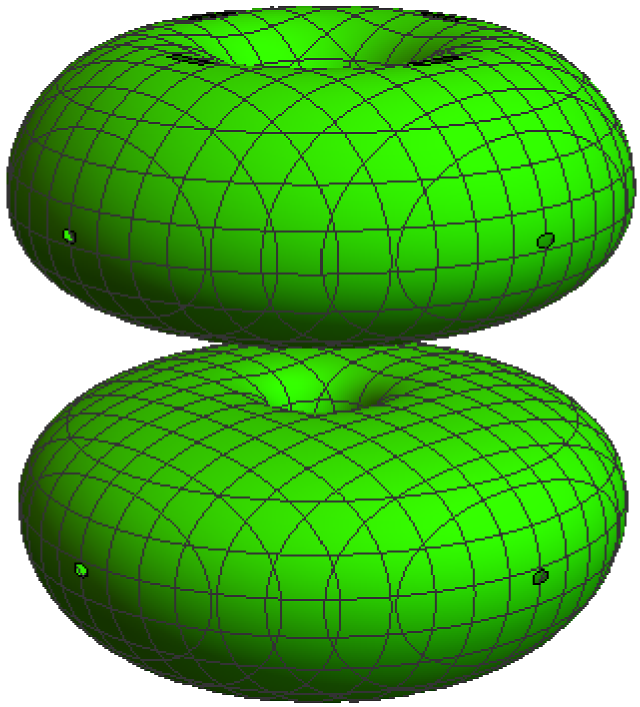




ContourPlot3D of $|\psi_{4,2,0}(\boldsymbol{r})|^2$ in the (x, y, z) plane.

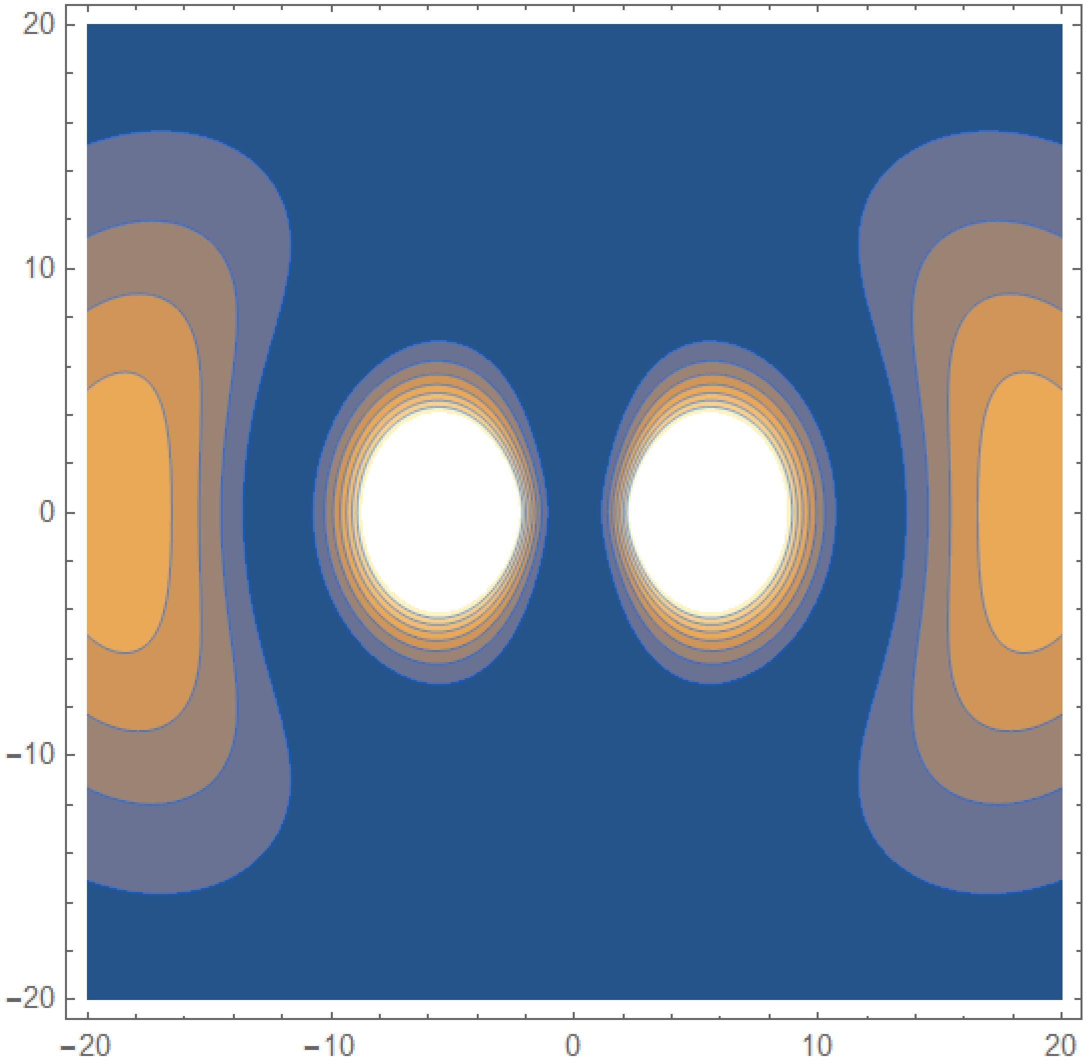
K1[4, 2, 1]



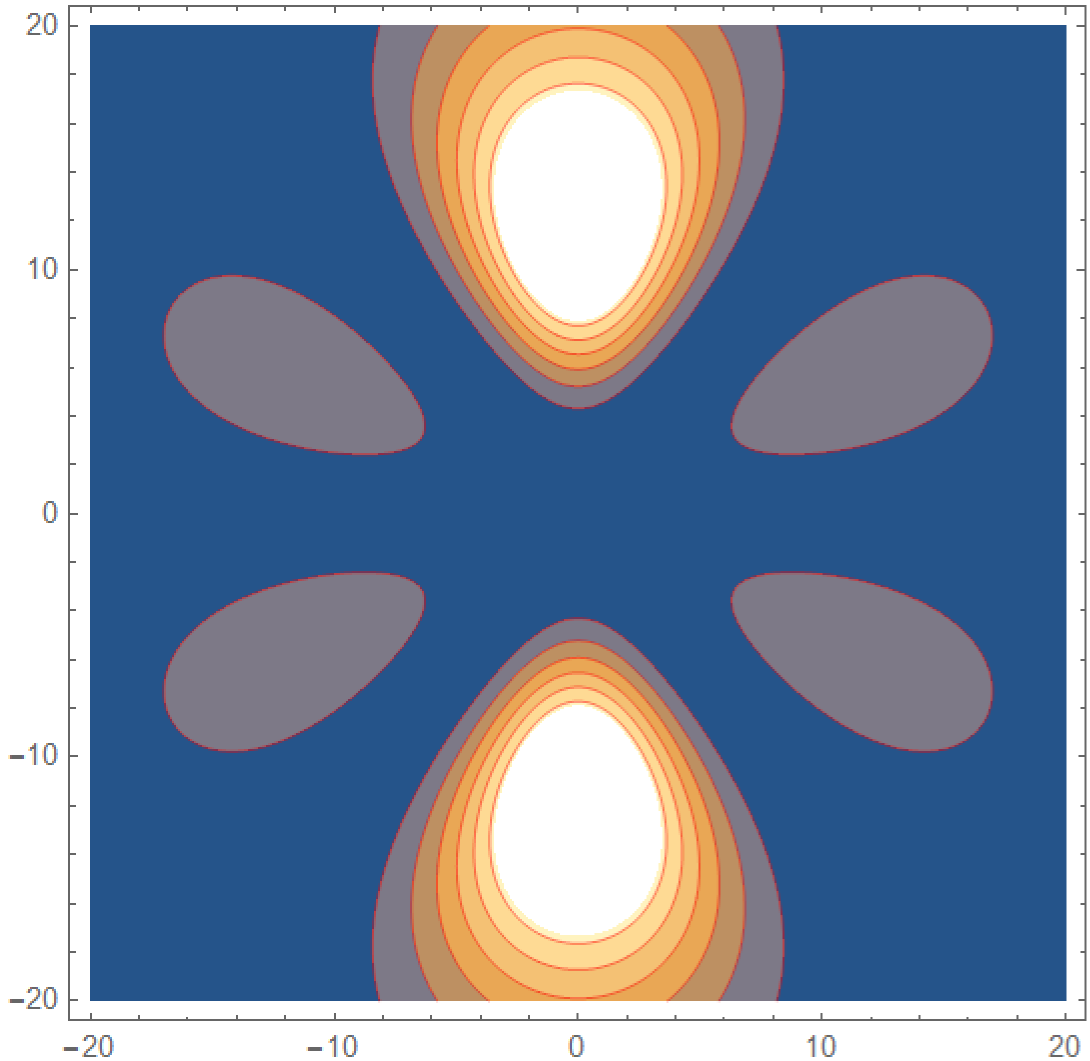


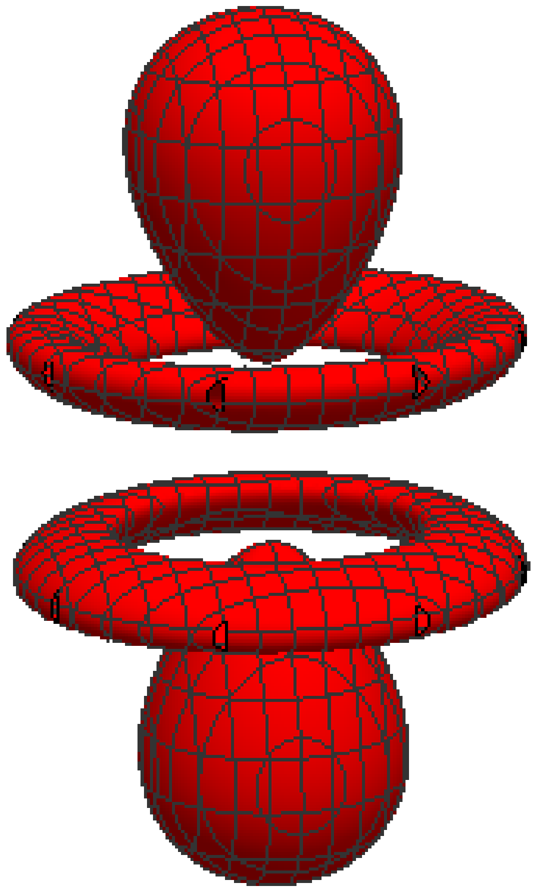
ContourPlot3D of $\left|\psi_{4,2,1}(\boldsymbol{r})\right|^2$ in the (x, y, z) plane.

```
K1[4, 2, 2]
```



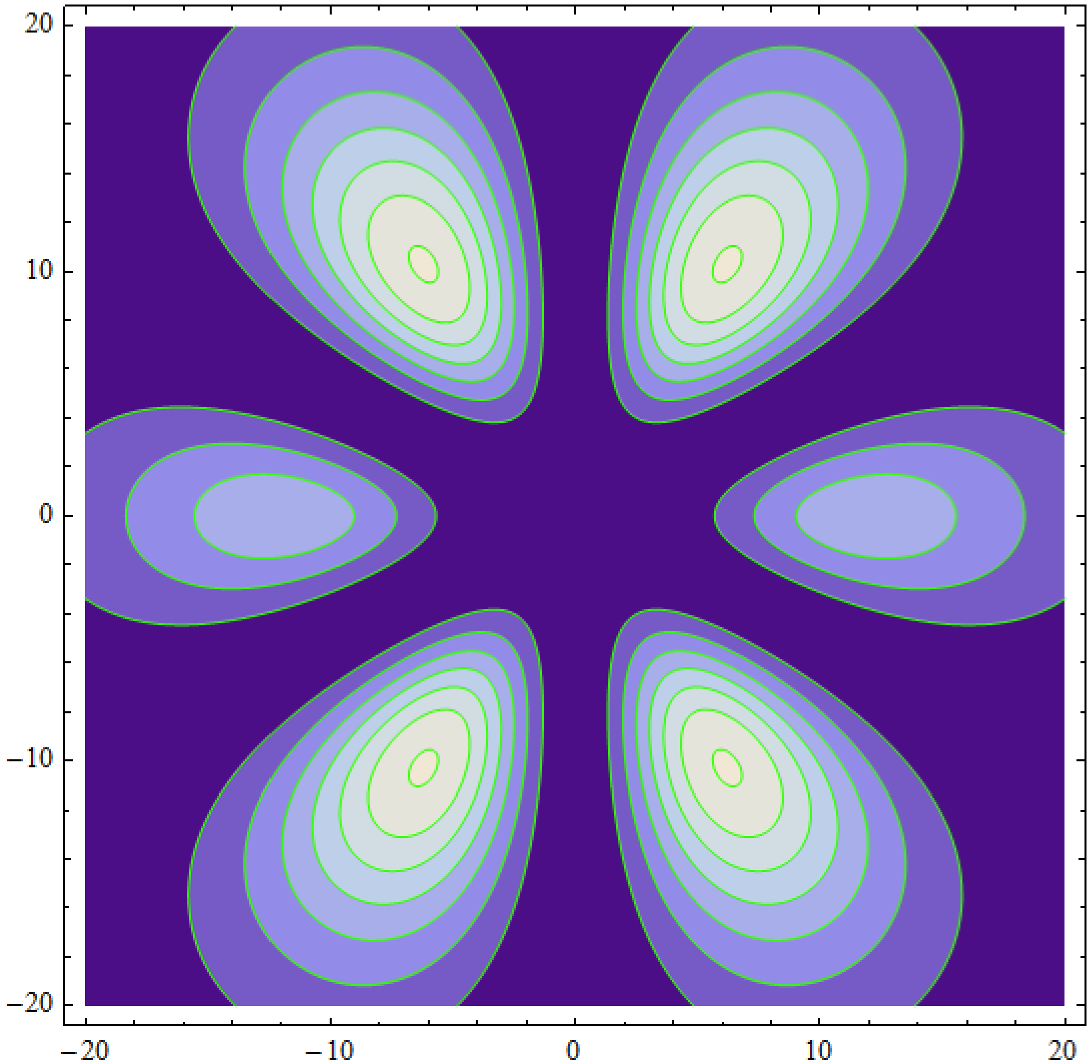
K1[4, 3, 0]

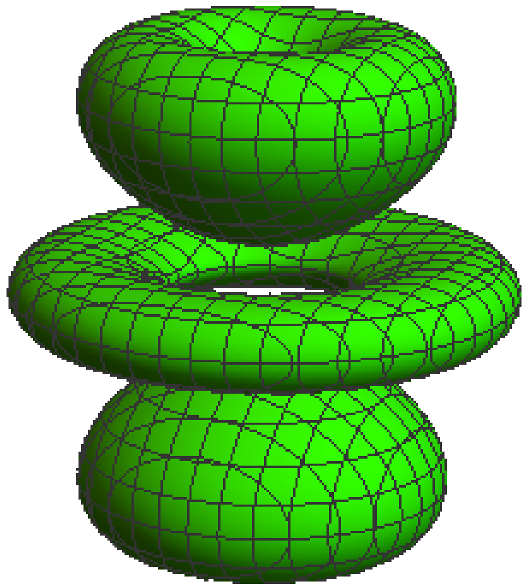




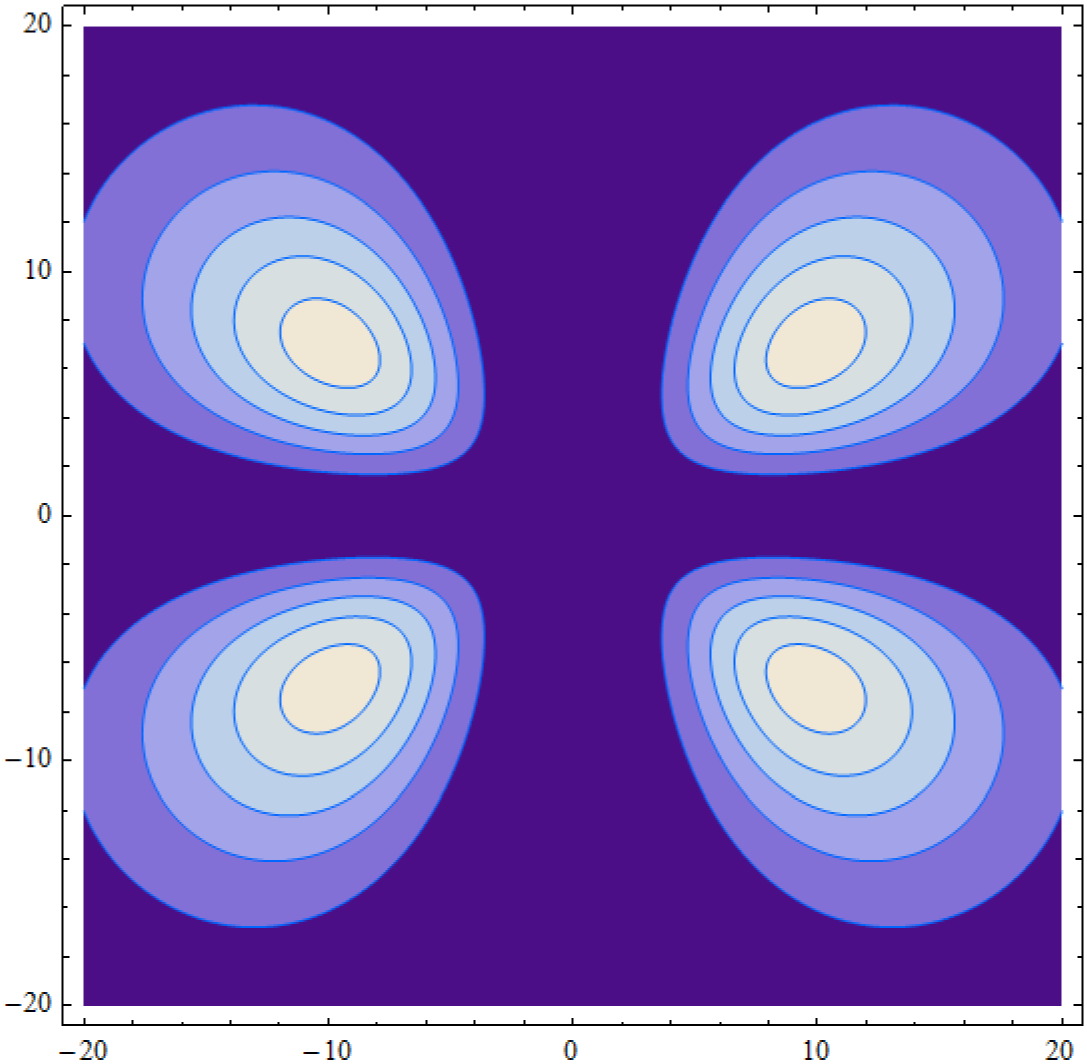
ContourPlot3D of $\left|\psi_{4,3,0}(\boldsymbol{r})\right|^2$ in the (x, y, z) plane.

```
K1[4, 3, 1]
```

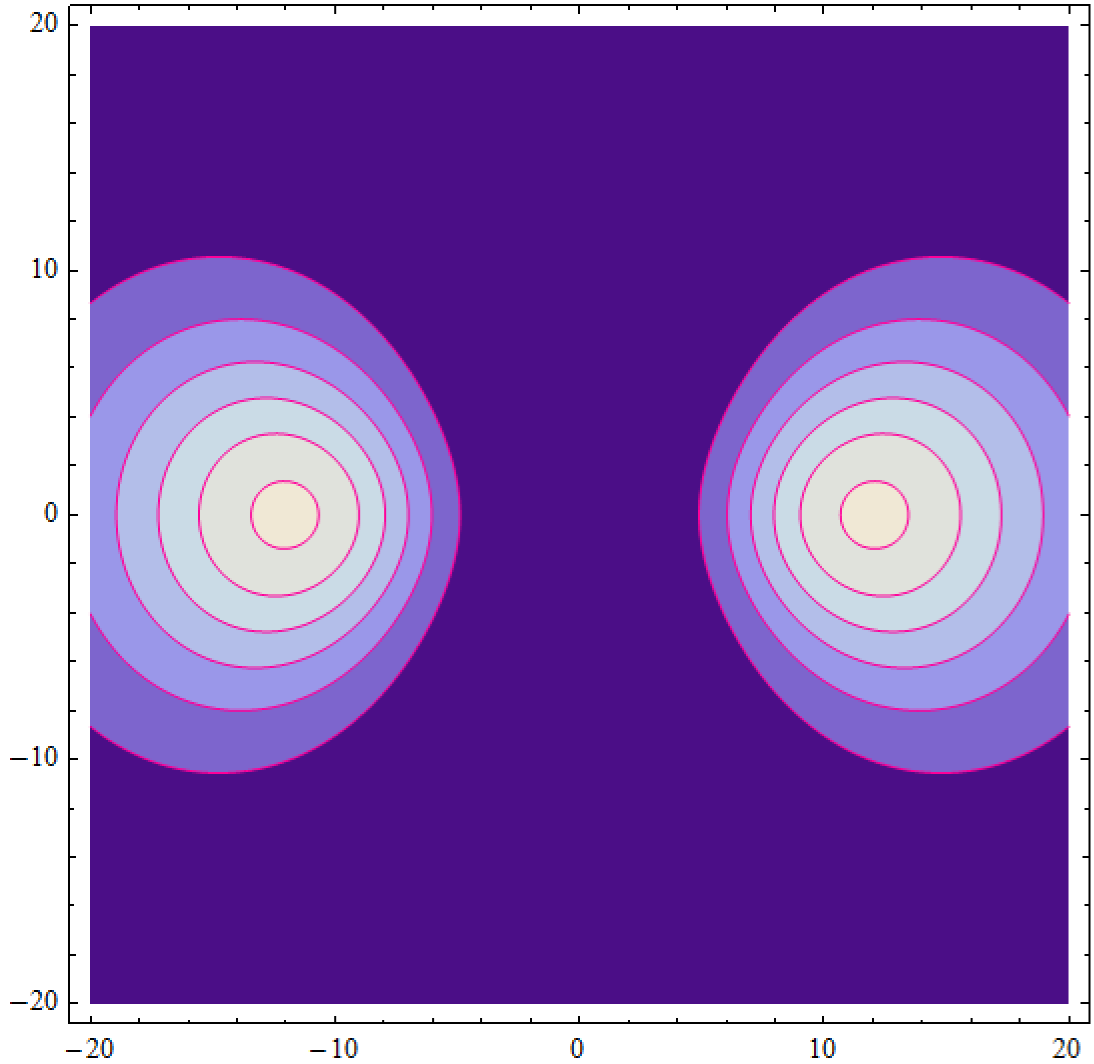




```
K1[4, 3, 2]
```



```
K1[4, 3, 3]
```



3. ((Mathematica-2) Plot3D

We also make a Plot3D of

$$|\psi_{nlm}(\boldsymbol{r})|^2 = |R_{nl}(r)|^2 |Y_l^m(\theta,\phi)|^2$$

as s function of (y, z), where

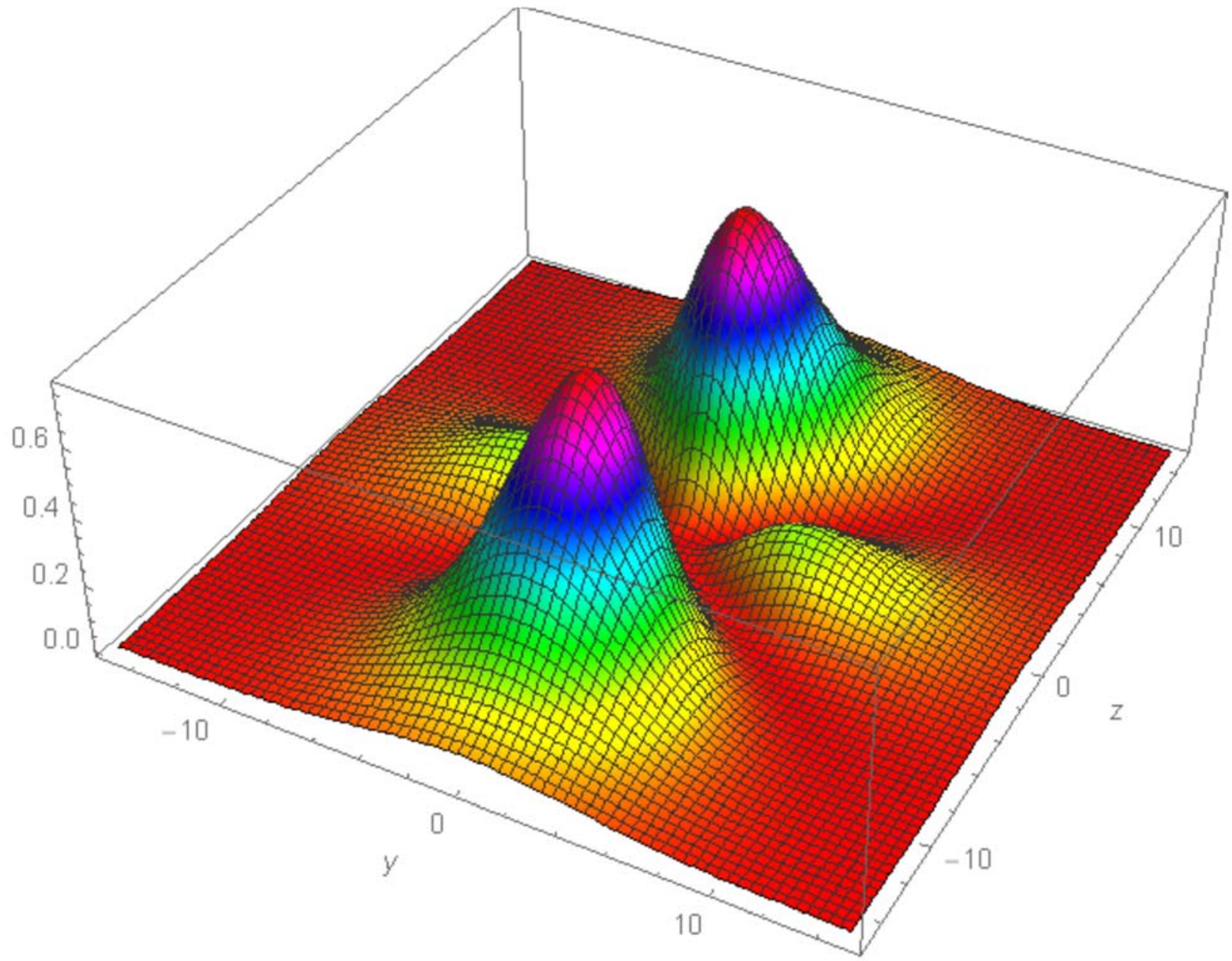
$$r = \sqrt{x^2 + y^2 + z^2}\,, \qquad \theta = acr\cos[\frac{z}{\sqrt{x^2 + y^2 + z^2}}], \qquad \phi = \arctan(\frac{y}{x})$$

The amplitude $|\psi_{nlm}(\boldsymbol{r})|^2 = |R_{nl}(r)|^2 |Y_l^m(\theta,\phi)|^2$ with $x = 0$, can be plotted in the (y, z) plane.

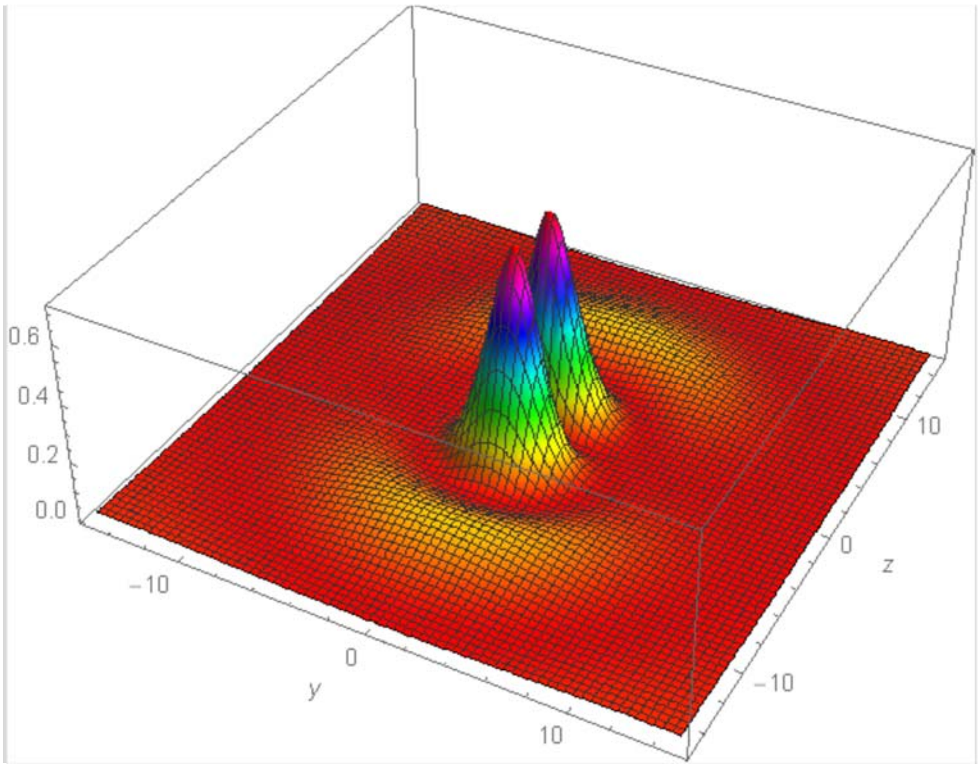
4. Example of Plot3D

We show some examples.

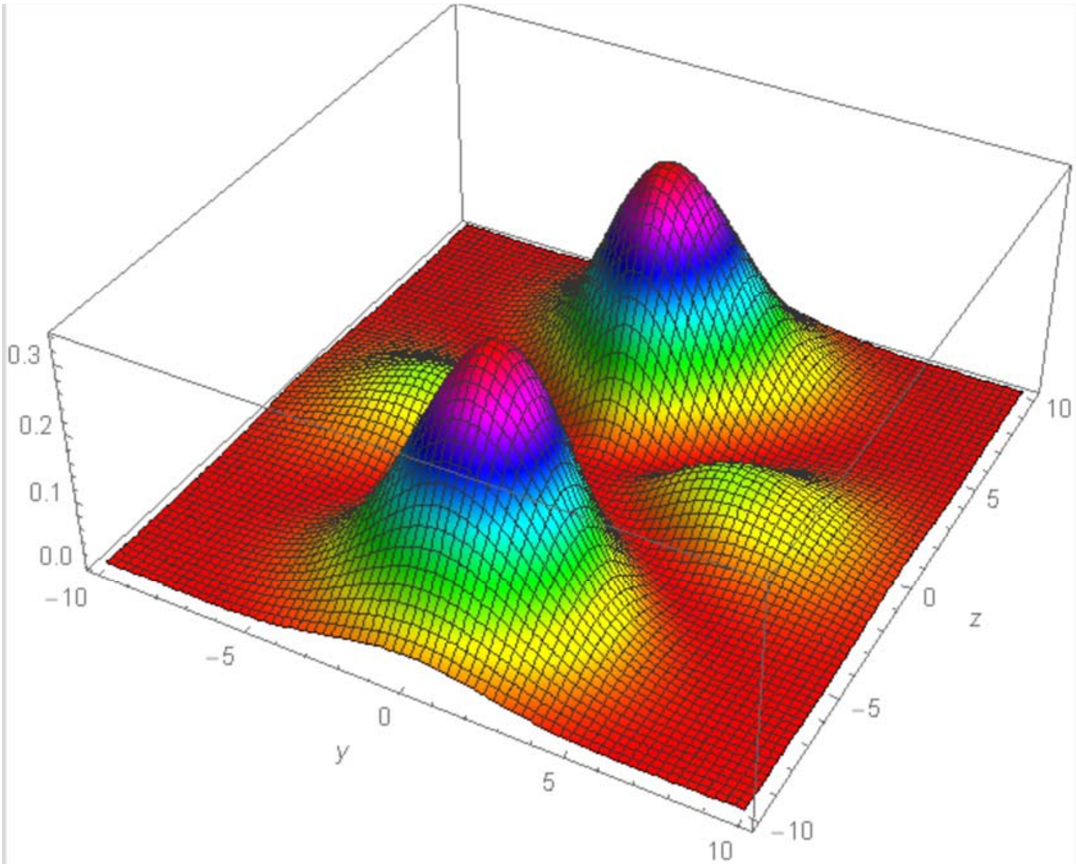
(a) $|n.l, m\rangle = |3,2,0\rangle$



(b) $|n.l, m\rangle = |4,1,0\rangle$



(c) $\left|n.l,m\right\rangle = \left|4,2,0\right\rangle$



APPENDIX
((**Mathematica-1**))
ContourPlot

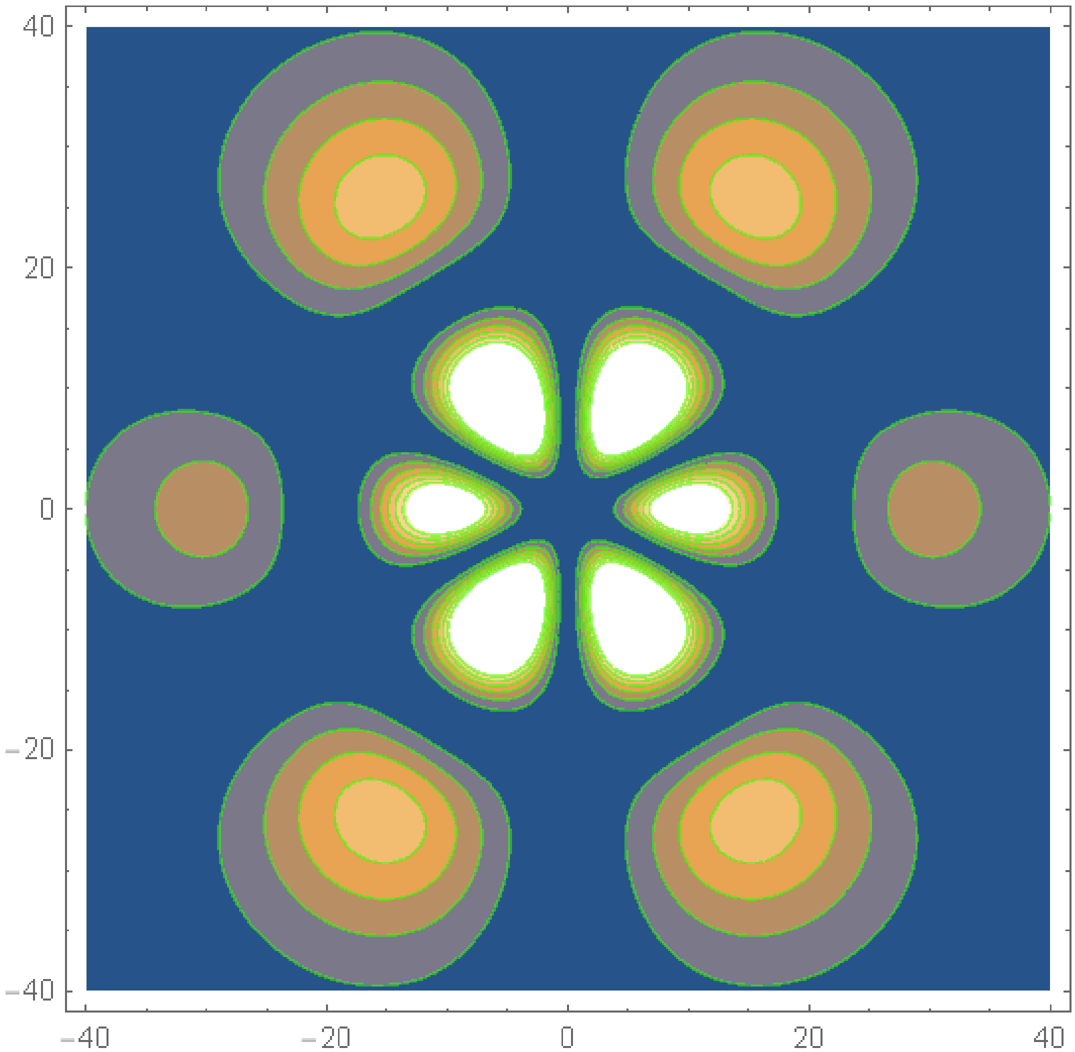
```
Clear["Global`*"];

r2xRule = {r → Sqrt[x^2 + y^2 + z^2], θ → ArcCos[z / Sqrt[x^2 + y^2 + z^2]],
    ϕ → ArcTan[x, y]};

rwave[n_, ℓ_, r_] :=
  1/Sqrt[(n + ℓ)!]
   (2^(1+ℓ) a0^(-ℓ-3/2) ⅇ^(-r/(a0 n)) n^(-ℓ-2) r^ℓ Sqrt[(n - ℓ - 1)!]
     LaguerreL[-1 + n - ℓ, 1 + 2 ℓ, (2 r)/(a0 n)]) /. a0 → 1;

Ψ[n_, l_, m_, r_, θ_, ϕ_] :=
 rwave[n, l, r]^2 Abs[SphericalHarmonicY[l, m, θ, ϕ]]^2;
```

$$r2xRule = \left\{r \to \sqrt{x^2+y^2+z^2},\ \theta \to \mathrm{ArcCos}\left[\frac{z}{\sqrt{x^2+y^2+z^2}}\right],\ \phi \to \mathrm{ArcTan}[x, y]\right\}$$

$$rwave[n\_, \ell\_, r\_] := \frac{1}{\sqrt{(n+\ell)!}}\left(2^{1+\ell}\, a0^{-\ell-\frac{3}{2}}\, e^{-\frac{r}{a0\, n}}\, n^{-\ell-2}\, r^{\ell} \sqrt{(n-\ell-1)!}\ \mathrm{LaguerreL}\left[-1+n-\ell,\ 1+2\ell,\ \frac{2r}{a0\, n}\right]\right) /.\ a0 \to 1$$

```
K1[n_, l_, m_] :=
 ContourPlot[Ψ[n, l, m, r, θ, ϕ] //. r2xRule //. {x → 0},
  {y, -40, 40}, {z, -40, 40}, PlotPoints → 100,
  ContourStyle → {Hue[0.3 m]}]
```

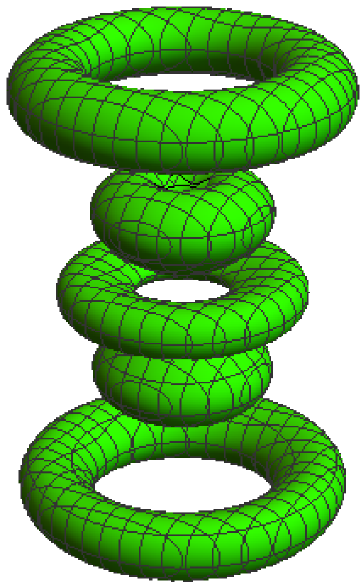
```
K1[5, 3, 1]
```



((**Mathematica-2**)) ContourPlot3D

```
Clear["Global`*"];

r2xRule = {r → Sqrt[x^2 + y^2 + z^2], θ → ArcCos[z / Sqrt[x^2 + y^2 + z^2]],
   ϕ → ArcTan[x, y]};
rwave[n_, ℓ_, r_] :=
  1/Sqrt[(n + ℓ)!]
    (2^(1+ℓ) a0^(-ℓ-3/2) E^(-r/(a0 n)) n^(-ℓ-2) r^ℓ Sqrt[(n - ℓ - 1)!]
      LaguerreL[-1 + n - ℓ, 1 + 2 ℓ, (2 r)/(a0 n)]) /. a0 → 1;

Ψ[n_, l_, m_, r_, θ_, ϕ_] :=
 rwave[n, l, r]^2 Abs[SphericalHarmonicY[l, m, θ, ϕ]]^2;
K1[n_, l_, m_] :=
 ContourPlot3D[Evaluate[Ψ[n, l, m, r, θ, ϕ] //. r2xRule],
  {x, -40, 40}, {y, -40, 40}, {z, -40, 40}, PlotPoints → 20,
  ContourStyle → {Hue[0.3 m]}, Boxed → False, Axes → False];
```

```
K1[5, 3, 1]
```



((**Mathematica-3**)) Plot3D

Probability Density

```
Clear["Global`*"];

<< "VectorAnalysis`"

r2xRule = {r, θ, ϕ} → CoordinatesFromCartesian[{x, y, z}, Spherical] // Thread;
```

$$\text{rwave}[n\_, \ell\_, r\_] := \frac{1}{\sqrt{(n+\ell)!}} \left(2^{1+\ell}\, a0^{-\ell-\frac{3}{2}}\, e^{-\frac{r}{a0\, n}}\, n^{-\ell-2}\, r^{\ell} \sqrt{(n-\ell-1)!}\ \text{LaguerreL}\left[-1+n-\ell,\, 1+2\,\ell,\, \frac{2\,r}{a0\,n}\right]\right) \text{/.}$$

```
  a0 → 1;
A1 = 1000;

Ψ[n_, l_, m_, r_, θ_, ϕ_] := A1 rwave[n, l, r]^2 Abs[SphericalHarmonicY[l, m, θ, ϕ]]^2;

K1[n_, l_, m_] := Plot3D[Ψ[n, l, m, r, θ, ϕ] //. r2xRule //. {x → 0}, {y, -50, 50}, {z, -50, 50},
  PlotPoints → 100, PlotRange → All, AxesLabel → {"y", "z"}, Mesh → 70,
  ColorFunction → Function[{x, y, z}, Hue[z]]]

K1[5, 3, 1]
```