HW #7

1. Free Particle

Because all momentum operators commute, trivially $[\vec{p}, H] = 0$. In order to show that the orbital angular momentum operators commute with the Hamiltonian, we first calculate $[L_i, p_j] = [\epsilon_{ikl}\, x_k\, p_l, p_j] = \epsilon_{ikl}\, i\hbar\, \delta_{kj}\, p_l = i\hbar\, \epsilon_{ijl}\, p_l$. Therefore, $[L_i, H] = [L_i, \frac{1}{2m} p_j\, p_j] = \frac{1}{2m}(p_j[L_i, p_j] + [L_i, p_j]\, p_j) = \frac{1}{2m}(p_j\, i\hbar\, \epsilon_{ijl}\, p_l + i\hbar\, \epsilon_{ijl}\, p_l\, p_j) = 0$ because of the anti-symmetry of the Levi-Civita symbol and the commutativity of two momentum operators. The conservation of three momentum operators is due to the spatial translational invariance along three independen directions, while the conservation of three angular momentum operators is due to the rotational invariance around three different axes.

2. Axially symmetric system

The Hamiltonian $H = \frac{\vec{p}^2}{2m} + V(z)$ has an axial symmetry around the z-axis as well as the translational invariance along the x- and y-axis. Therefore, we expect the conservation of L_z, p_x, and p_y. They are all shown to commute with the kinetic energy term in the previous problem, and hence the only commutators we need to calculate are those with the potential energy term. $[p_x, H] = [p_x, V(z)] = \frac{\hbar}{i} \nabla_x V(z) = 0$, and similarly $[p_y, H] = [p_y, V(z)] = \frac{\hbar}{i} \nabla_y V(z) = 0$. Finally, $[L_z, H] = [x\, p_y - y\, p_x, V(z)] = x \frac{\hbar}{i} \nabla_y V(z) - y \frac{\hbar}{i} \nabla_x V(z) = 0$. Therefore, L_z, p_x, and p_y are conserved as expected from the symmetry considerations.

3. Representation matrices

We use $J_z \mid j, m\rangle = m\hbar \mid j, m\rangle$, $J_+ \mid j, m\rangle = \sqrt{j(j+1) - m(m+1)} \mid j, m+1\rangle$, $J_- \mid j, m\rangle = \sqrt{j(j+1) - m(m-1)} \mid j, m-1\rangle$.

■ $j = 1$

■ $j = 5/2$

■ $j = 4$

■ $j = 9/2$

4. Spherical Harmonics

```
j = 2
```

2

```
J₊ = Table[If[k == l + 1, √(j (j + 1) - l (l + 1)), 0], {k, j, -j, -1}, {l, j, -j, -1}] ℏ
```

$\{\{0, 2\hbar, 0, 0, 0\}, \{0, 0, \sqrt{6}\,\hbar, 0, 0\}, \{0, 0, 0, \sqrt{6}\,\hbar, 0\}, \{0, 0, 0, 0, 2\hbar\}, \{0, 0, 0, 0, 0\}\}$

```
J₋ = Transpose[J₊]
```

$\{\{0, 0, 0, 0, 0\}, \{2\hbar, 0, 0, 0, 0\}, \{0, \sqrt{6}\,\hbar, 0, 0, 0\}, \{0, 0, \sqrt{6}\,\hbar, 0, 0\}, \{0, 0, 0, 2\hbar, 0\}\}$

■ $L_+ \, Y_2{}^2 = 0$

```
SphericalHarmonicY[2, 2, θ, ϕ]
```

$\frac{1}{4} e^{2 i \phi} \sqrt{\frac{15}{2\pi}} \, \text{Sin}[\theta]^2$

$\frac{\hbar}{I} E^{I\phi}$ (I D[%, θ] - Cot[θ] D[%, ϕ])

0

■ $L_- \, Y_2{}^2 = 2\hbar \, Y_2{}^1$

```
SphericalHarmonicY[2, 2, θ, ϕ]
```

$\frac{1}{4} e^{2 i \phi} \sqrt{\frac{15}{2\pi}} \, \text{Sin}[\theta]^2$

$\frac{\hbar}{I} E^{-I\phi}$ (-I D[%, θ] - Cot[θ] D[%, ϕ])

$-e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \hbar \, \text{Cos}[\theta] \, \text{Sin}[\theta]$

% - 2 ℏ SphericalHarmonicY[2, 1, θ, ϕ]

0

■ $L_- \, Y_2{}^1 = \sqrt{6} \, \hbar \, Y_2{}^0$

```
SphericalHarmonicY[2, 1, θ, ϕ]
```

$-\frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \text{Cos}[\theta] \, \text{Sin}[\theta]$

$\frac{\hbar}{I} E^{-I\phi}$ (-I D[%, θ] - Cot[θ] D[%, ϕ])

$-i \, e^{-i\phi} \hbar \left(\frac{1}{2} i \, e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \text{Cos}[\theta]^2 - i \left(-\frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \text{Cos}[\theta]^2 + \frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \, \text{Sin}[\theta]^2 \right) \right)$

Simplify[% - $\sqrt{6}$ ℏ SphericalHarmonicY[2, 0, θ, ϕ]]

0

■ $L_- Y_2^0 = \sqrt{6}\,\hbar\, Y_2^{-1}$

```
SphericalHarmonicY[2, 0, θ, ϕ]
```

$$\frac{1}{4}\sqrt{\frac{5}{\pi}}\left(-1+3\,\text{Cos}[\theta]^2\right)$$

$$\frac{\hbar}{\text{I}}\,\text{E}^{-\text{I}\,\phi}\,(-\text{I}\,\text{D}[\%,\theta]-\text{Cot}[\theta]\,\text{D}[\%,\phi])$$

$$\frac{3}{2}\,e^{-i\phi}\sqrt{\frac{5}{\pi}}\,\hbar\,\text{Cos}[\theta]\,\text{Sin}[\theta]$$

$$\% - \sqrt{6}\,\hbar\,\text{SphericalHarmonicY}[2,-1,\theta,\phi]$$

0

■ $L_- Y_2^{-1} = 2\,\hbar\, Y_2^{-2}$

```
SphericalHarmonicY[2, -1, θ, ϕ]
```

$$\frac{1}{2}\,e^{-i\phi}\sqrt{\frac{15}{2\pi}}\,\text{Cos}[\theta]\,\text{Sin}[\theta]$$

$$\frac{\hbar}{\text{I}}\,\text{E}^{-\text{I}\,\phi}\,(-\text{I}\,\text{D}[\%,\theta]-\text{Cot}[\theta]\,\text{D}[\%,\phi])$$

$$-i\,e^{-i\phi}\,\hbar\left(\frac{1}{2}\,i\,e^{-i\phi}\sqrt{\frac{15}{2\pi}}\,\text{Cos}[\theta]^2-i\left(\frac{1}{2}\,e^{-i\phi}\sqrt{\frac{15}{2\pi}}\,\text{Cos}[\theta]^2-\frac{1}{2}\,e^{-i\phi}\sqrt{\frac{15}{2\pi}}\,\text{Sin}[\theta]^2\right)\right)$$

$$\text{Simplify}[\% - 2\,\hbar\,\text{SphericalHarmonicY}[2,-2,\theta,\phi]]$$

0

■ $L_- Y_2^{-2} = 0$

```
SphericalHarmonicY[2, -2, θ, ϕ]
```

$$\frac{1}{4}\,e^{-2i\phi}\sqrt{\frac{15}{2\pi}}\,\text{Sin}[\theta]^2$$

$$\frac{\hbar}{\text{I}}\,\text{E}^{-\text{I}\,\phi}\,(-\text{I}\,\text{D}[\%,\theta]-\text{Cot}[\theta]\,\text{D}[\%,\phi])$$

0

5. Shape of orbitals

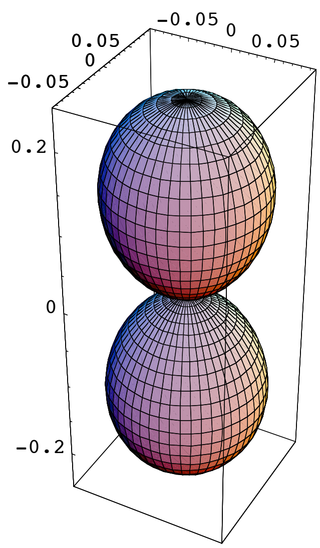
The power of polynomials corresponds to l of spherical harmonics.

```
Table[SphericalHarmonicY[1, m, θ, ϕ], {m, 1, -1, -1}]
```

$$\left\{-\frac{1}{2}\, e^{i\phi} \sqrt{\frac{3}{2\pi}}\, \mathrm{Sin}[\theta],\ \frac{1}{2}\sqrt{\frac{3}{\pi}}\, \mathrm{Cos}[\theta],\ \frac{1}{2}\, e^{-i\phi}\sqrt{\frac{3}{2\pi}}\, \mathrm{Sin}[\theta]\right\}$$

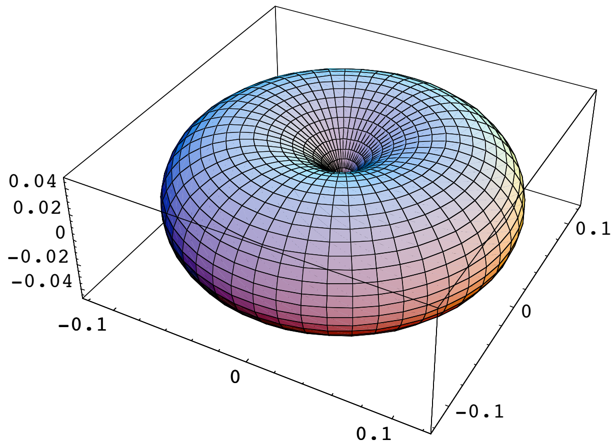
"z" is $Y_1{}^0$. "$x + i\,y$" is $Y_1{}^1$.

```
ParametricPlot3D[Abs[(SphericalHarmonicY[1, 0, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2π}, PlotPoints → 50]
```



- Graphics3D -

```
ParametricPlot3D[Abs[(SphericalHarmonicY[1, 1, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π}, PlotPoints → 50]
```



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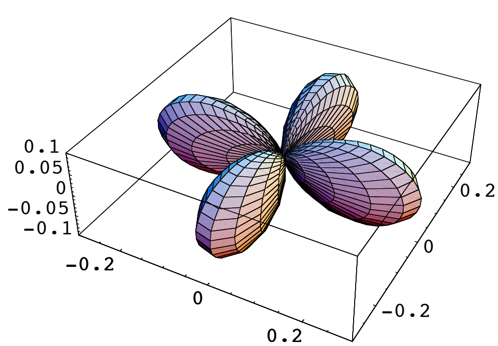
```
Table[SphericalHarmonicY[2, m, θ, ϕ], {m, 2, -2, -1}]
```

$$\left\{\frac{1}{4} e^{2 i \phi} \sqrt{\frac{15}{2\pi}} \text{Sin}[\theta]^2, -\frac{1}{2} e^{i\phi} \sqrt{\frac{15}{2\pi}} \text{Cos}[\theta] \text{Sin}[\theta], \frac{1}{4}\sqrt{\frac{5}{\pi}} (-1 + 3 \text{Cos}[\theta]^2), \frac{1}{2} e^{-i\phi} \sqrt{\frac{15}{2\pi}} \text{Cos}[\theta] \text{Sin}[\theta], \frac{1}{4} e^{-2 i \phi} \sqrt{\frac{15}{2\pi}} \text{Sin}[\theta]^2\right\}$$

$x^2 - y^2$ is $Y_2{}^2 + Y_2{}^{-2}$, $y z$ is $Y_2{}^1 + Y_2{}^{-1}$, $x^2 + y^2 - 2 z^2$ is $Y_2{}^0$

```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[2, 2, θ, ϕ] + SphericalHarmonicY[2, -2, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.3, 0.3}, {-0.3, 0.3}, {-0.1, 0.1}}]
```

```
ParametricPlot3D::ppcom : Function 1/2 Abs[(<<1>> + <<1>>)^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}
   cannot be compiled; plotting will proceed with the uncompiled function.
```



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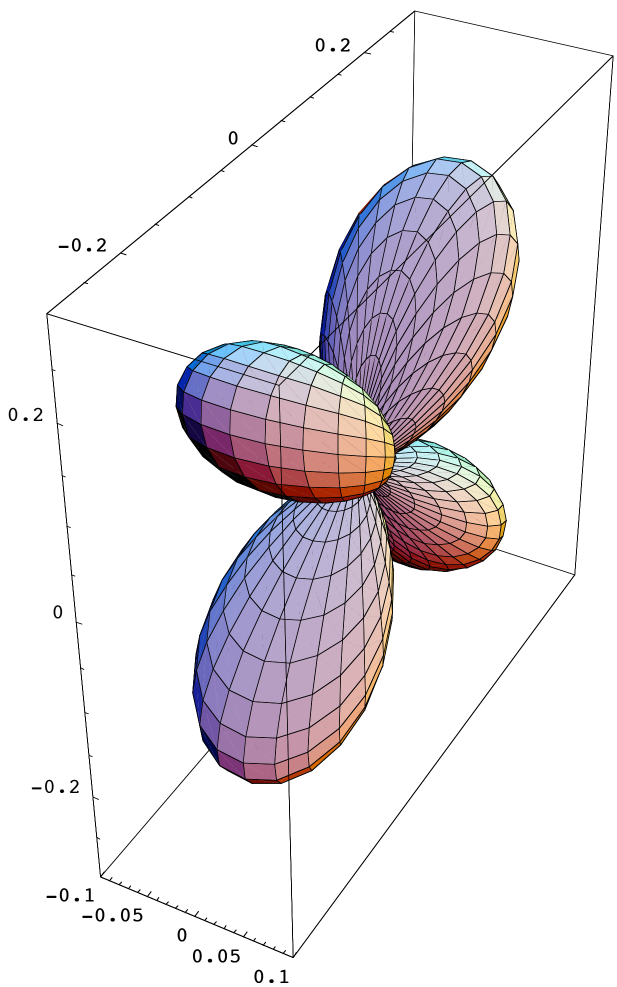
```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[2, 1, θ, ϕ] + SphericalHarmonicY[2, -1, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.1, 0.1}, {-0.3, 0.3}, {-0.3, 0.3}}]
```

```
ParametricPlot3D::ppcom : Function 1/2 Abs[(«1» + «1»)^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}
   cannot be compiled; plotting will proceed with the uncompiled function.
```



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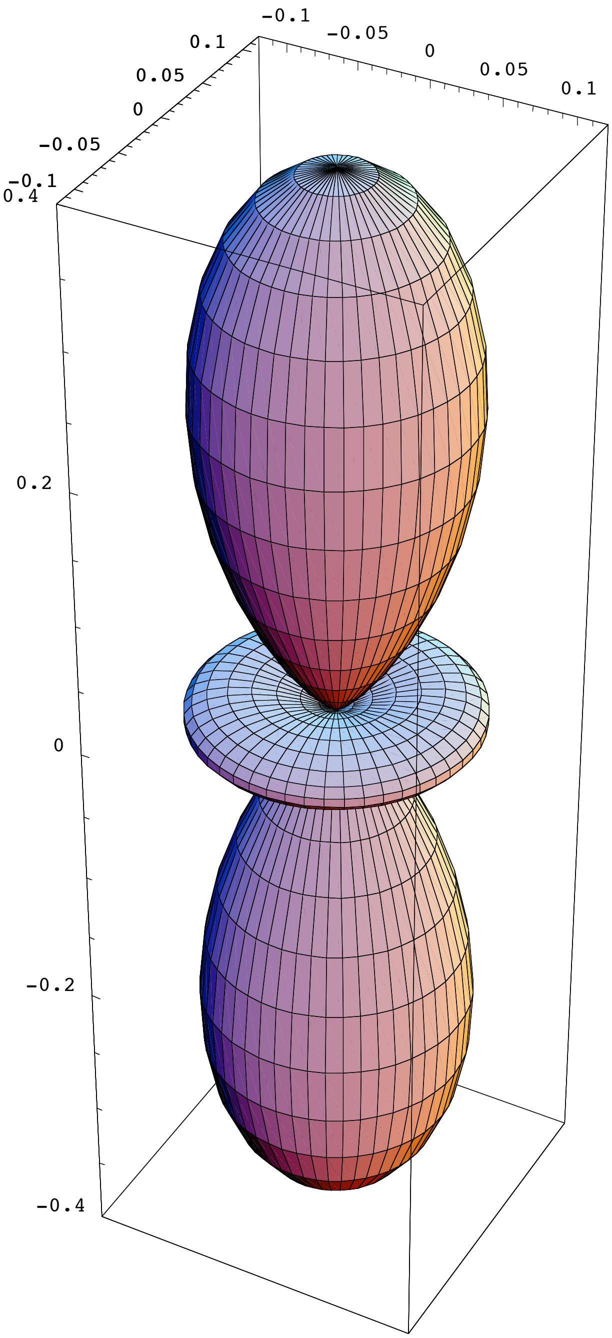
```
ParametricPlot3D[
 Abs[(SphericalHarmonicY[2, 0, θ, ϕ])^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π},
 {ϕ, 0, 2 π}, PlotPoints → 50, PlotRange → {{-0.12, 0.12}, {-0.12, 0.12}, {-0.4, 0.4}}]
```



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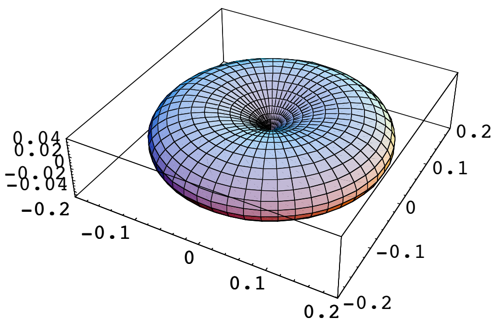
```
Table[SphericalHarmonicY[3, m, θ, ϕ], {m, 3, -3, -1}]
```

$$\left\{-\frac{1}{8} e^{3 i \phi} \sqrt{\frac{35}{\pi}} \operatorname{Sin}[\theta]^3, \frac{1}{4} e^{2 i \phi} \sqrt{\frac{105}{2 \pi}} \operatorname{Cos}[\theta] \operatorname{Sin}[\theta]^2, -\frac{1}{8} e^{i \phi} \sqrt{\frac{21}{\pi}} \left(-1+5 \operatorname{Cos}[\theta]^2\right) \operatorname{Sin}[\theta], \frac{1}{4} \sqrt{\frac{7}{\pi}} \left(-3 \operatorname{Cos}[\theta]+5 \operatorname{Cos}[\theta]^3\right), \frac{1}{8} e^{-i \phi} \sqrt{\frac{21}{\pi}} \left(-1+5 \operatorname{Cos}[\theta]^2\right) \operatorname{Sin}[\theta], \frac{1}{4} e^{-2 i \phi} \sqrt{\frac{105}{2 \pi}} \operatorname{Cos}[\theta] \operatorname{Sin}[\theta]^2, \frac{1}{8} e^{-3 i \phi} \sqrt{\frac{35}{\pi}} \operatorname{Sin}[\theta]^3\right\}$$

$(x+i\,y)^3$ is ${Y_3}^3$, $x^3-3\,x\,y^2$ is ${Y_3}^3-{Y_3}^{-3}$, $z(x^2-y^2)$ is ${Y_3}^2+{Y_3}^{-2}$, $(5\,z^2-3\,r^2)\,z$ is ${Y_3}^0$

```
ParametricPlot3D[
 Abs[(SphericalHarmonicY[3, 3, θ, ϕ])^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π},
 {ϕ, 0, 2 π}, PlotPoints → 50, PlotRange → {{-0.2, 0.2}, {-0.2, 0.2}, {-0.05, 0.05}}]
```



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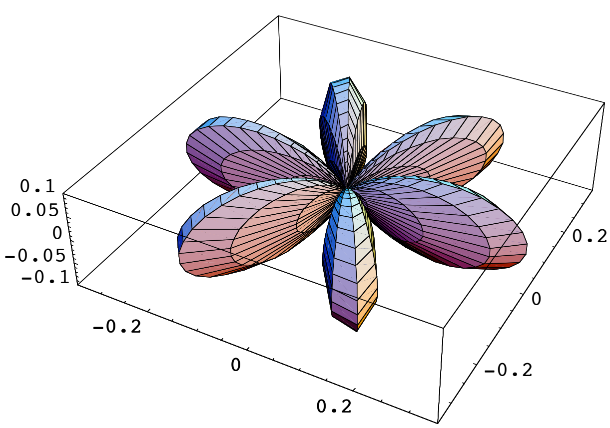
```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[3, 3, θ, ϕ] - SphericalHarmonicY[3, -3, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.35, 0.35}, {-0.35, 0.35}, {-0.1, 0.1}}]
```



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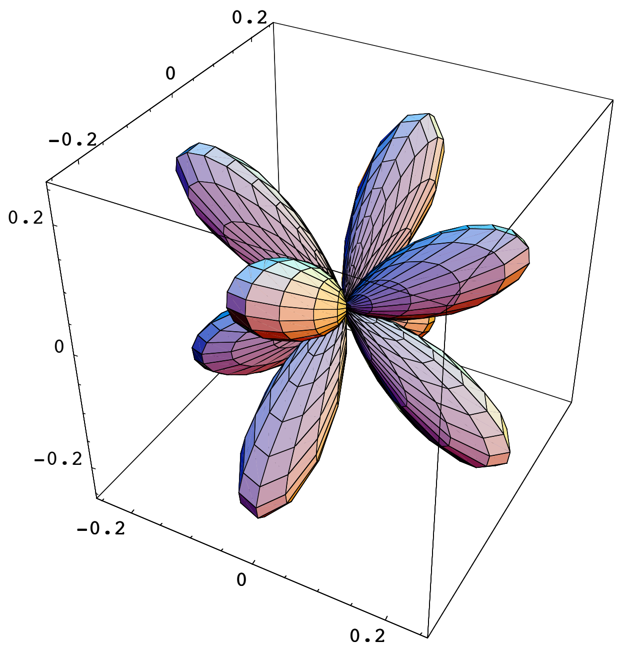
```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[3, 2, θ, ϕ] + SphericalHarmonicY[3, -2, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.26, 0.26}, {-0.26, 0.26}, {-0.26, 0.26}}]
```



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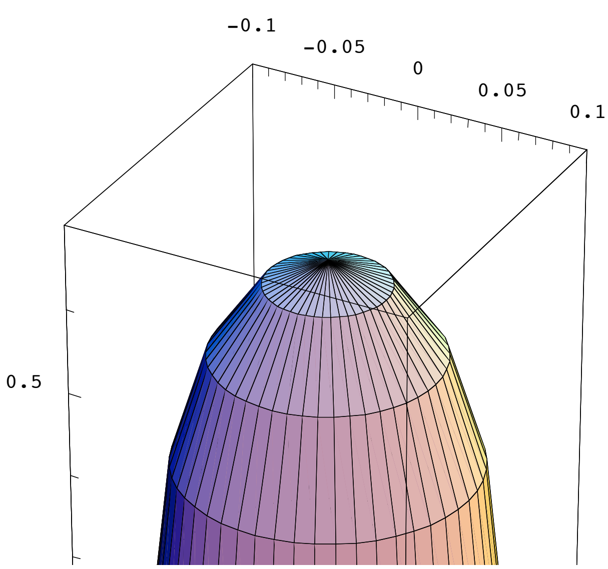
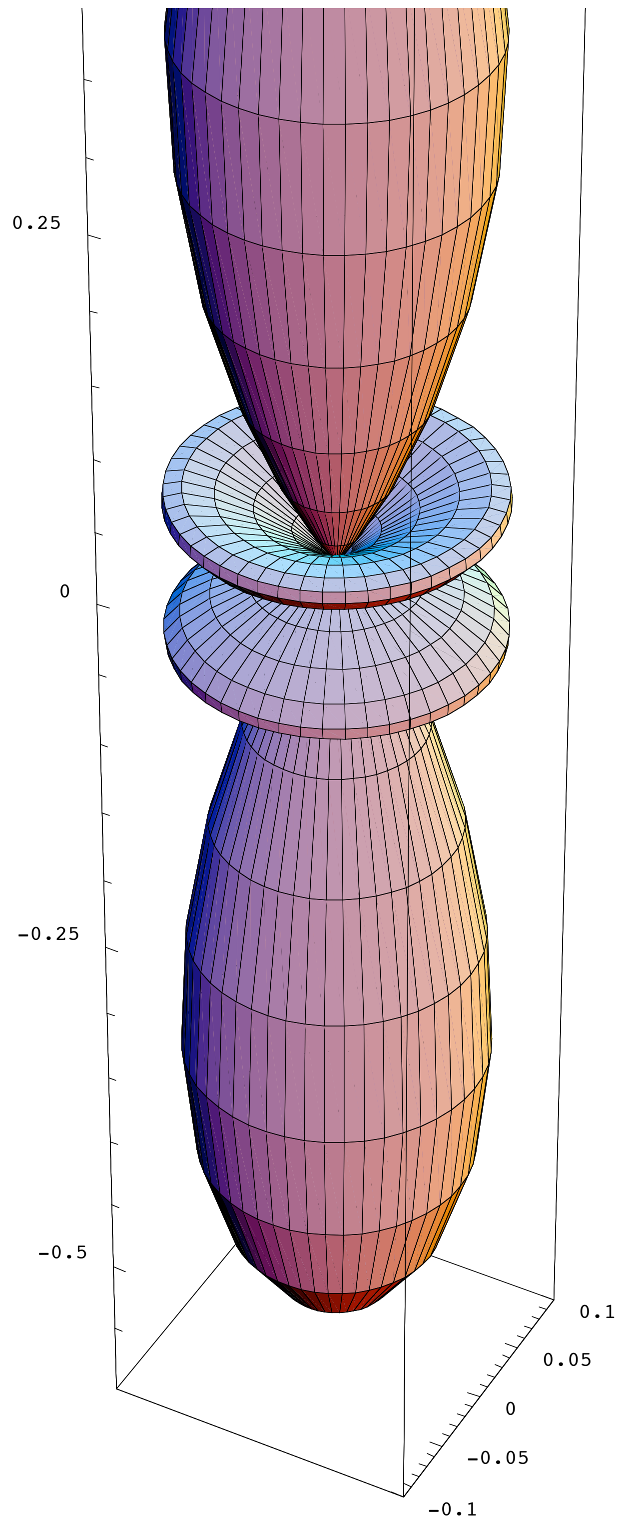
```
ParametricPlot3D[
 Abs[(SphericalHarmonicY[3, 0, θ, ϕ])^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π},
 {ϕ, 0, 2 π}, PlotPoints → 50, PlotRange → {{-0.1, 0.1}, {-0.1, 0.1}, {-0.6, 0.6}}]
```





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