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 $J_z\,|\,j, m\rangle = m\hbar\,|\,j, m\rangle$, $J_+\,|\,j, m\rangle = \sqrt{j(j+1) - m(m+1)}\,\left|\,j, m+1\right\rangle$, $J_-\,|\,j, m\rangle = \sqrt{j(j+1) - m(m-1)}\,\left|\,j, m-1\right\rangle$.

■ $j = 1$

```
Jz = DiagonalMatrix[{1, 0, -1}] ħ
```

{{ħ, 0, 0}, {0, 0, 0}, {0, 0, -ħ}}

```
J+ = {{0, √2, 0}, {0, 0, √2}, {0, 0, 0}} ħ
```

{{0, $\sqrt{2}$ ħ, 0}, {0, 0, $\sqrt{2}$ ħ}, {0, 0, 0}}

```
J- = Transpose[J+]
```

{{0, 0, 0}, {$\sqrt{2}$ ħ, 0, 0}, {0, $\sqrt{2}$ ħ, 0}}

```
Jz.J+ - J+.Jz
```

{{0, $\sqrt{2}\,ħ^2$, 0}, {0, 0, $\sqrt{2}\,ħ^2$}, {0, 0, 0}}

```
% - ℏ J+
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

```
Jz.J- - J-.Jz
```

$\{\{0, 0, 0\}, \{-\sqrt{2}\, \hbar^2, 0, 0\}, \{0, -\sqrt{2}\, \hbar^2, 0\}\}$

```
% + ℏ J-
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

```
J+.J- - J-.J+
```

$\{\{2\hbar^2, 0, 0\}, \{0, 0, 0\}, \{0, 0, -2\hbar^2\}\}$

```
% - 2 ℏ Jz
```

{{0, 0, 0}, {0, 0, 0}, {0, 0, 0}}

■ $j = 5/2$

$j = \frac{5}{2}$

$\frac{5}{2}$

```
Jz = DiagonalMatrix[Table[k, {k, j, -j, -1}]] ℏ
```

$\{\{\frac{5\hbar}{2}, 0, 0, 0, 0, 0\}, \{0, \frac{3\hbar}{2}, 0, 0, 0, 0\}, \{0, 0, \frac{\hbar}{2}, 0, 0, 0\}, \{0, 0, 0, -\frac{\hbar}{2}, 0, 0\}, \{0, 0, 0, 0, -\frac{3\hbar}{2}, 0\}, \{0, 0, 0, 0, 0, -\frac{5\hbar}{2}\}\}$

$J_+ = \text{Table}[\text{If}[k == l + 1, \sqrt{j (j + 1) - l (l + 1)}, 0], \{k, j, -j, -1\}, \{l, j, -j, -1\}]\, \hbar$

$\{\{0, \sqrt{5}\, \hbar, 0, 0, 0, 0\}, \{0, 0, 2\sqrt{2}\, \hbar, 0, 0, 0\}, \{0, 0, 0, 3\hbar, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{2}\, \hbar, 0\}, \{0, 0, 0, 0, 0, \sqrt{5}\, \hbar\}, \{0, 0, 0, 0, 0, 0\}\}$

```
J- = Transpose[J+]
```

$\{\{0, 0, 0, 0, 0, 0\}, \{\sqrt{5}\, \hbar, 0, 0, 0, 0, 0\}, \{0, 2\sqrt{2}\, \hbar, 0, 0, 0, 0\}, \{0, 0, 3\hbar, 0, 0, 0\}, \{0, 0, 0, 2\sqrt{2}\, \hbar, 0, 0\}, \{0, 0, 0, 0, \sqrt{5}\, \hbar, 0\}\}$

```
Jz.J+ - J+.Jz
```

$\{\{0, \sqrt{5}\, \hbar^2, 0, 0, 0, 0\}, \{0, 0, 2\sqrt{2}\, \hbar^2, 0, 0, 0\}, \{0, 0, 0, 3\hbar^2, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{2}\, \hbar^2, 0\}, \{0, 0, 0, 0, 0, \sqrt{5}\, \hbar^2\}, \{0, 0, 0, 0, 0, 0\}\}$

```
% - ℏ J+
```

{{0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}}

$J_z.J_- - J_-.J_z$

$\{\{0, 0, 0, 0, 0, 0\}, \{-\sqrt{5}\,\hbar^2, 0, 0, 0, 0, 0\}, \{0, -2\sqrt{2}\,\hbar^2, 0, 0, 0, 0\}, \{0, 0, -3\hbar^2, 0, 0, 0\}, \{0, 0, 0, -2\sqrt{2}\,\hbar^2, 0, 0\}, \{0, 0, 0, 0, -\sqrt{5}\,\hbar^2, 0\}\}$

$\% + \hbar\, J_-$

$\{\{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}\}$

$J_+.J_- - J_-.J_+$

$\{\{5\hbar^2, 0, 0, 0, 0, 0\}, \{0, 3\hbar^2, 0, 0, 0, 0\}, \{0, 0, \hbar^2, 0, 0, 0\}, \{0, 0, 0, -\hbar^2, 0, 0\}, \{0, 0, 0, 0, -3\hbar^2, 0\}, \{0, 0, 0, 0, 0, -5\hbar^2\}\}$

$\% - 2\hbar\, J_z$

$\{\{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0\}\}$

■ *j* = 4

j = 4

4

J_z = DiagonalMatrix[Table[k, {k, j, -j, -1}]] $\hbar$

$\{\{4\hbar, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 3\hbar, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 2\hbar, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, \hbar, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, -\hbar, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, -2\hbar, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, -3\hbar, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, -4\hbar\}\}$

J_+ = Table[If[k == l + 1, $\sqrt{j\,(j+1) - l\,(l+1)}$, 0], {k, j, -j, -1}, {l, j, -j, -1}] $\hbar$

$\{\{0, 2\sqrt{2}\,\hbar, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, \sqrt{14}\,\hbar, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 3\sqrt{2}\,\hbar, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{5}\,\hbar, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 2\sqrt{5}\,\hbar, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 3\sqrt{2}\,\hbar, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, \sqrt{14}\,\hbar, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 2\sqrt{2}\,\hbar\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0\}\}$

J_- = Transpose[J_+]

$\{\{0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{2\sqrt{2}\,\hbar, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, \sqrt{14}\,\hbar, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 3\sqrt{2}\,\hbar, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 2\sqrt{5}\,\hbar, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{5}\,\hbar, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 3\sqrt{2}\,\hbar, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, \sqrt{14}\,\hbar, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 2\sqrt{2}\,\hbar, 0\}\}$

$J_z.J_+ - J_+.J_z$

$\{\{0, 2\sqrt{2}\,\hbar^2, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, \sqrt{14}\,\hbar^2, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 3\sqrt{2}\,\hbar^2, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{5}\,\hbar^2, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 2\sqrt{5}\,\hbar^2, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 3\sqrt{2}\,\hbar^2, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, \sqrt{14}\,\hbar^2, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 2\sqrt{2}\,\hbar^2\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0\}\}$

```
% - ℏ J+
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}}

```
Jz.J- - J-.Jz
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0}, {$-2\sqrt{2}\,\hbar^2$, 0, 0, 0, 0, 0, 0, 0, 0}, {0, $-\sqrt{14}\,\hbar^2$, 0, 0, 0, 0, 0, 0, 0}, {0, 0, $-3\sqrt{2}\,\hbar^2$, 0, 0, 0, 0, 0, 0}, {0, 0, 0, $-2\sqrt{5}\,\hbar^2$, 0, 0, 0, 0, 0}, {0, 0, 0, 0, $-2\sqrt{5}\,\hbar^2$, 0, 0, 0, 0}, {0, 0, 0, 0, 0, $-3\sqrt{2}\,\hbar^2$, 0, 0, 0}, {0, 0, 0, 0, 0, 0, $-\sqrt{14}\,\hbar^2$, 0, 0}, {0, 0, 0, 0, 0, 0, 0, $-2\sqrt{2}\,\hbar^2$, 0}}

```
% + ℏ J-
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}}

```
J+.J- - J-.J+
```

{{$8\hbar^2$, 0, 0, 0, 0, 0, 0, 0, 0}, {0, $6\hbar^2$, 0, 0, 0, 0, 0, 0, 0}, {0, 0, $4\hbar^2$, 0, 0, 0, 0, 0, 0}, {0, 0, 0, $2\hbar^2$, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, $-2\hbar^2$, 0, 0, 0}, {0, 0, 0, 0, 0, 0, $-4\hbar^2$, 0, 0}, {0, 0, 0, 0, 0, 0, 0, $-6\hbar^2$, 0}, {0, 0, 0, 0, 0, 0, 0, 0, $-8\hbar^2$}}

```
% - 2 ℏ Jz
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0}}

■ $j = 9/2$

```
j = 9/2
```

$\frac{9}{2}$

```
Jz = DiagonalMatrix[Table[k, {k, j, -j, -1}]] ℏ
```

{{$\frac{9\hbar}{2}$, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, $\frac{7\hbar}{2}$, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, $\frac{5\hbar}{2}$, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, $\frac{3\hbar}{2}$, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, $\frac{\hbar}{2}$, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, $-\frac{\hbar}{2}$, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, $-\frac{3\hbar}{2}$, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, $-\frac{5\hbar}{2}$, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, $-\frac{7\hbar}{2}$, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, $-\frac{9\hbar}{2}$}}

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

$\{\{0, 3\hbar, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 4\hbar, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, \sqrt{21}\hbar, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{6}\hbar, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 5\hbar, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 2\sqrt{6}\hbar, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, \sqrt{21}\hbar, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 4\hbar, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0, 3\hbar\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}\}$

```
J- = Transpose[J+]
```

$\{\{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{3\hbar, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 4\hbar, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, \sqrt{21}\hbar, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 2\sqrt{6}\hbar, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 5\hbar, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 2\sqrt{6}\hbar, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, \sqrt{21}\hbar, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 4\hbar, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 3\hbar, 0\}\}$

```
Jz.J+ - J+.Jz
```

$\{\{0, 3\hbar^2, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 4\hbar^2, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, \sqrt{21}\hbar^2, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 2\sqrt{6}\hbar^2, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 5\hbar^2, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 2\sqrt{6}\hbar^2, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, \sqrt{21}\hbar^2, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 4\hbar^2, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0, 3\hbar^2\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}\}$

```
% - ħ J+
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}}

```
Jz.J- - J-.Jz
```

$\{\{0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{-3\hbar^2, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, -4\hbar^2, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, -\sqrt{21}\hbar^2, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, -2\sqrt{6}\hbar^2, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, -5\hbar^2, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, -2\sqrt{6}\hbar^2, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, -\sqrt{21}\hbar^2, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, -4\hbar^2, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, -3\hbar^2, 0\}\}$

```
% + ħ J-
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}}

```
J+.J- - J-.J+
```

$\{\{9\hbar^2, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 7\hbar^2, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 5\hbar^2, 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 3\hbar^2, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, \hbar^2, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, -\hbar^2, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, -3\hbar^2, 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, -5\hbar^2, 0, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, -7\hbar^2, 0\}, \{0, 0, 0, 0, 0, 0, 0, 0, 0, -9\hbar^2\}\}$

```
% - 2 ℏ J_z
```

{{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0},
{0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0, 0, 0}}

4. Spherical Harmonics

```
j = 2
```

2

$J_+ = \text{Table}\left[\text{If}\left[k == l + 1, \sqrt{j\,(j+1) - l\,(l+1)}, 0\right], \{k, j, -j, -1\}, \{l, j, -j, -1\}\right] \hbar$

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

$J_- = \text{Transpose}[J_+]$

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

■ $L_+ \, Y_2{}^2 = 0$

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

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

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

0

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

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

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

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

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

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

0

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

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

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

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

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

$$\operatorname{Simplify}\left[\% - \sqrt{6}\,\hbar\, \operatorname{SphericalHarmonicY}[2, 0, \theta, \phi]\right]$$

0

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

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

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

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

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

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

0

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

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

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

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

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

```
Simplify[% - 2 ℏ SphericalHarmonicY[2, -2, θ, ϕ]]
```

0

■ $L_{-}\ Y_2^{-2} = 0$

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

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

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

0

5. Shape of orbitals

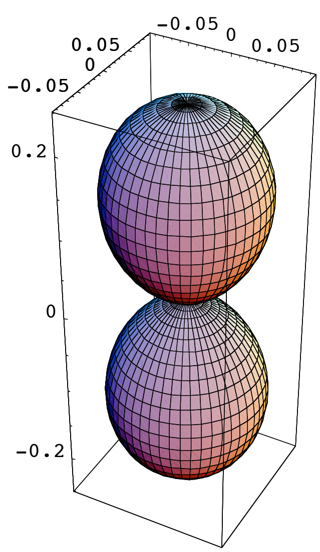
The power of polynomials corresponds to *l* of spherical harmonics.

```
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, 2 π}, PlotPoints → 50]
```



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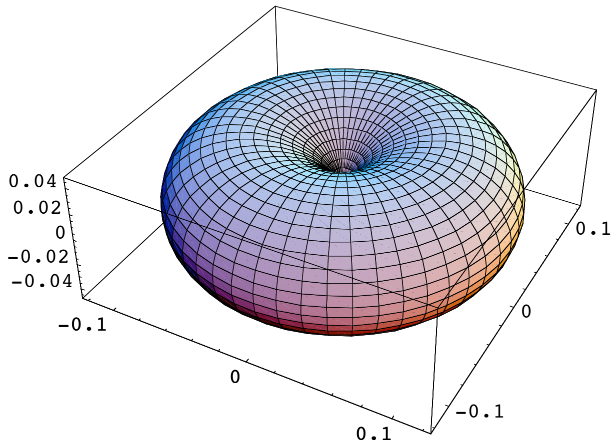
```
ParametricPlot3D[Abs[(SphericalHarmonicY[1, 1, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π}, PlotPoints → 50]
```



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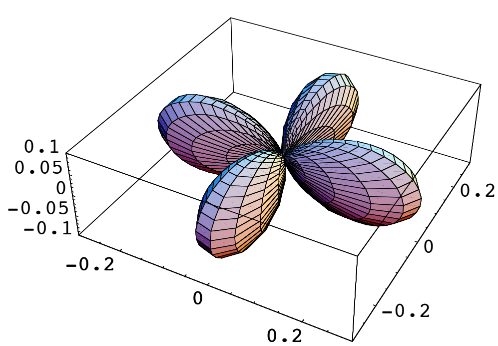
```
Table[SphericalHarmonicY[2, m, θ, ϕ], {m, 2, -2, -1}]
```

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

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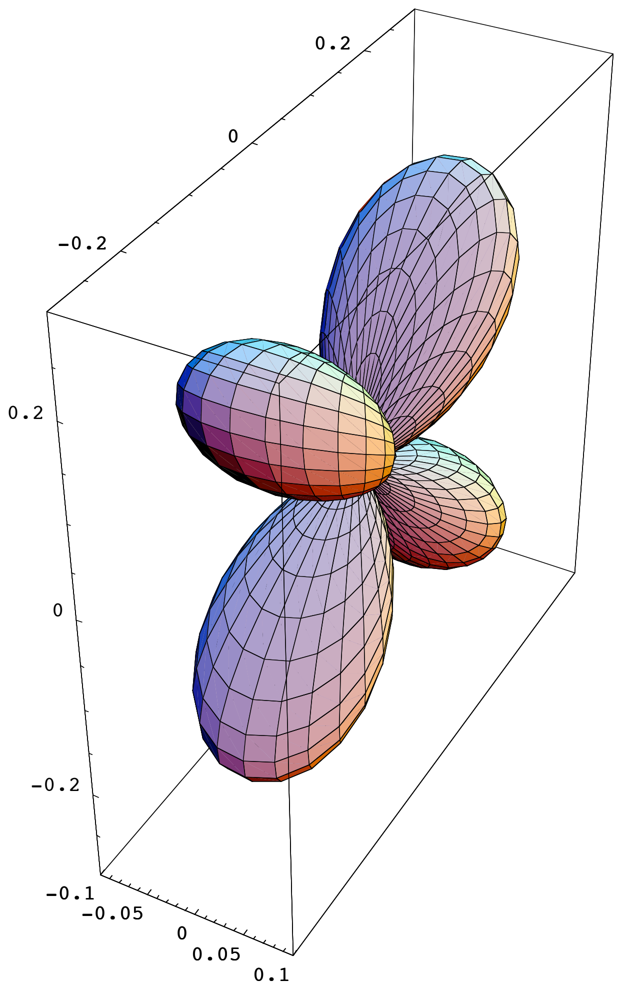
```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[2, 1, θ, ϕ] + SphericalHarmonicY[2, -1, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.1, 0.1}, {-0.3, 0.3}, {-0.3, 0.3}}]
```

```
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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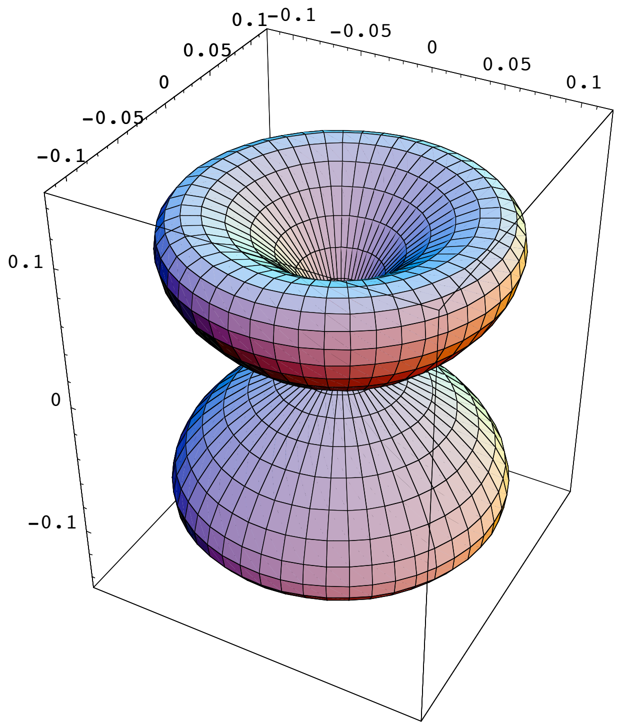
```
ParametricPlot3D[
 Abs[(SphericalHarmonicY[2, 1, θ, ϕ])^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π},
 {ϕ, 0, 2 π}, PlotPoints → 50, PlotRange → {{-0.12, 0.12}, {-0.12, 0.12}, {-0.15, 0.15}}]
```



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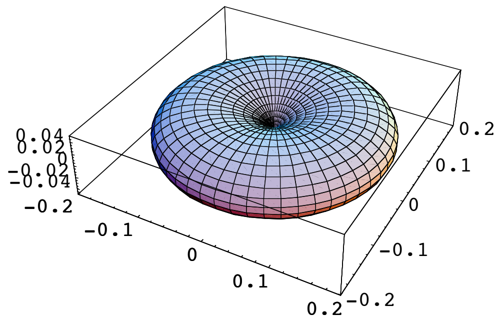
```
Table[SphericalHarmonicY[3, m, θ, ϕ], {m, 3, -3, -1}]
```

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

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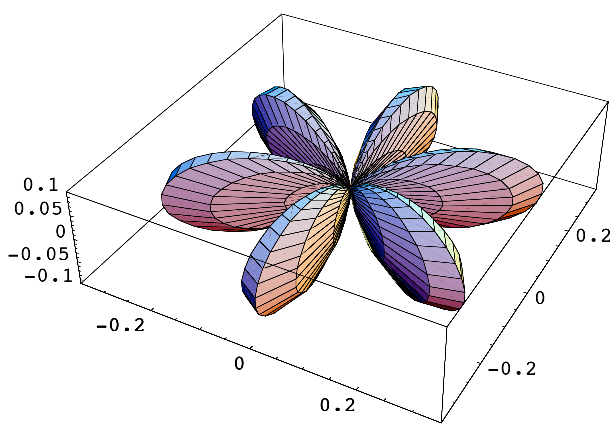
```
ParametricPlot3D[
 1/2 Abs[(SphericalHarmonicY[3, 3, θ, ϕ] + SphericalHarmonicY[3, -3, θ, ϕ])^2]
  {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π}, {ϕ, 0, 2 π},
 PlotPoints → 50, PlotRange → {{-0.35, 0.35}, {-0.35, 0.35}, {-0.1, 0.1}}]
```

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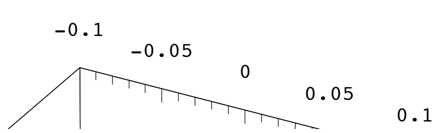
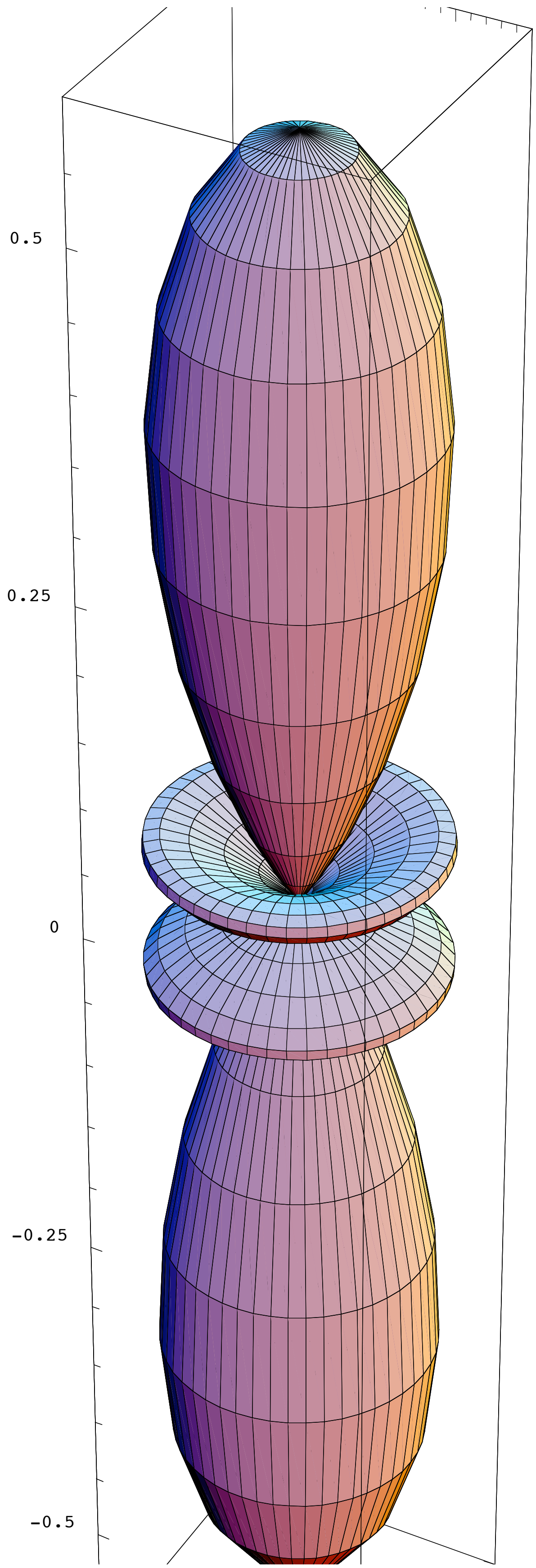
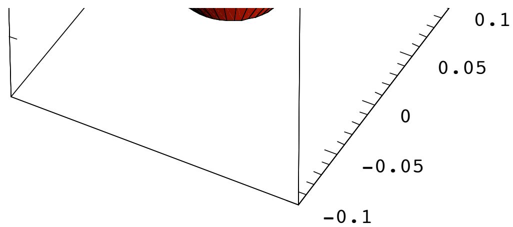
```
ParametricPlot3D[
 Abs[(SphericalHarmonicY[3, 0, θ, ϕ])^2] {Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]}, {θ, 0, π},
 {ϕ, 0, 2 π}, PlotPoints → 50, PlotRange → {{-0.1, 0.1}, {-0.1, 0.1}, {-0.6, 0.6}}]
```




0.5
0.25
0
-0.25
-0.5



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