Matrix representation of rotation operator: general case

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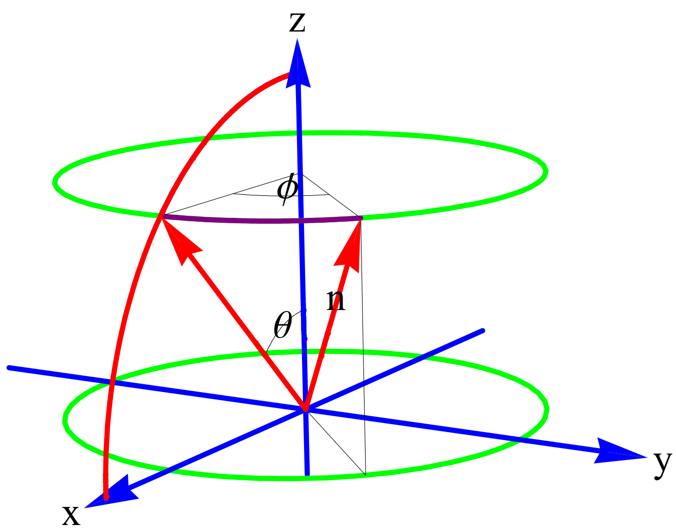
Eugene Paul "E. P." Wigner (November 17, 1902 – January 1, 1995), was a Hungarian American theoretical physicist and mathematician. He received a share of the Nobel Prize in Physics in 1963 "for his contributions to the theory of the atomic nucleus and the elementary particles, particularly through the discovery and application of fundamental symmetry principles"; the other half of the award was shared between Maria Goeppert-Mayer and J. Hans D. Jensen. Wigner is notable for having laid the foundation for the theory of symmetries in quantum mechanics as well as for his research into the structure of the atomic nucleus. Wigner is also important for his work in pure mathematics, having authored a number of theorems. In particular, Wigner's theorem is a cornerstone in the mathematical formulation of quantum mechanics.

http://en.wikipedia.org/wiki/Eugene_Wigner

1. Representation of rotations

Let the polar and the azimuthal angles that characterize $\boldsymbol{n}$ be θ and ϕ, respectively. We first rotate about the y axis by angle θ. We subsequently rotate by ϕ about the z axis.



The rotation operator is defined as

$$\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta) = \exp(-\frac{i}{\hbar}\phi\hat{J}_z)\exp(-\frac{i}{\hbar}\phi\hat{J}_y).$$

The matrix element is given by

$$\begin{aligned}\langle j,m'|\hat{R}|j,m\rangle &= \langle j,m'|\hat{R}_z(\phi)\hat{R}_y(\theta)|j,m\rangle \\ &= \langle j,m'|\hat{R}_y(\theta)|j,m\rangle(-im'\phi) \\ &= d^{(j)}_{m'm}(\theta)e^{-im'\phi} = D^{(j)}_{m'm}(\theta,\phi)\end{aligned}$$

These matrix elements are sometimes called Wigner functions after E.P. Wigner, who made pioneering contributions to the group-theoretical properties of rotations in quantum mechanics.

The problem of finding the representative matrices of the full rotation group has been reduced to that of finding $d^{(j)}_{m'm}(\theta)$.

2. Rotation operator with *j* = 1/2

The rotation operator with $j = 1/2$ is given by

$$\hat{R} = D^{(1/2)}(\theta,\phi) = \begin{pmatrix} e^{-i\frac{\phi}{2}} & 0 \\ 0 & e^{i\frac{\phi}{2}} \end{pmatrix} \begin{pmatrix} \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) & -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) & e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix}.$$

The eigenkets $|+\rangle_n$ and $|-\rangle_n$ are obtained as

$$|+\rangle_n = \hat{R}|+\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix},$$

and

$$|-\rangle_n = \hat{R}|-\rangle = \begin{pmatrix} -e^{-i\frac{\phi}{2}}\sin(\frac{\theta}{2}) \\ e^{i\frac{\phi}{2}}\cos(\frac{\theta}{2}) \end{pmatrix},$$

where $\boldsymbol{n}$ is the unit vector given by

$$\boldsymbol{n} = (\boldsymbol{n}_x, \boldsymbol{n}_y, \boldsymbol{n}_z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

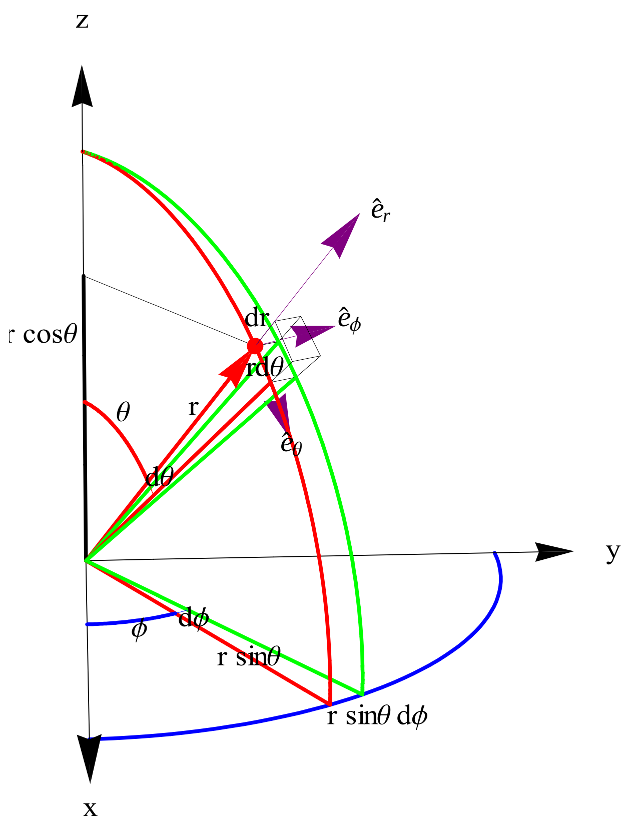
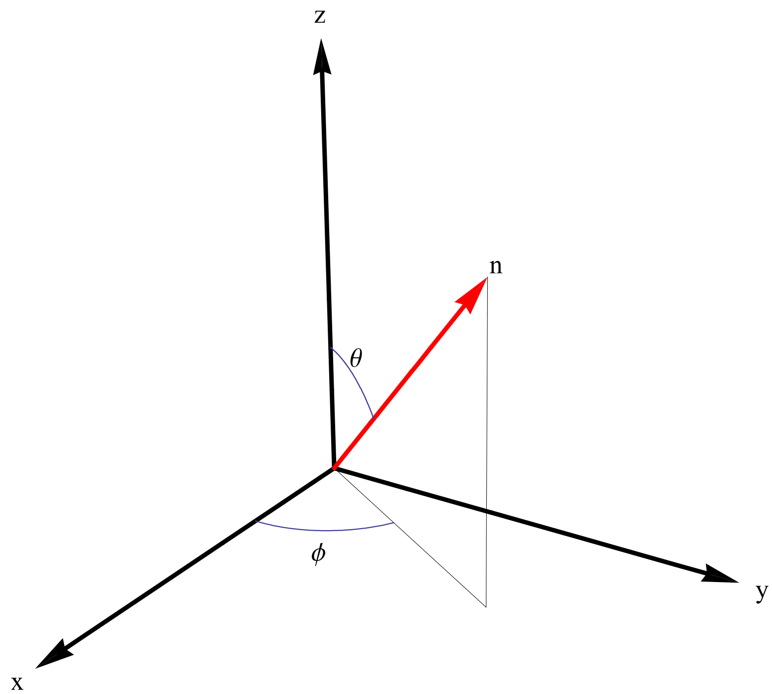


Fig. Spherical co-ordinates. $r = 1$. $\hat{n} = \mathbf{e}_r$.



3. Rotation operator with *j* = 1

The rotation operator with $J = 1$ is given by

$$\hat{R} = D^{(1)}(\theta,\phi) = \begin{pmatrix} e^{-i\phi}(\frac{1+\cos\theta}{2}) & -e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{-i\phi}(\frac{1-\cos\theta}{2}) \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ e^{i\phi}(\frac{1-\cos\theta}{2}) & e^{i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{i\phi}(\frac{1+\cos\theta}{2}) \end{pmatrix}.$$

The eigenkets $|1\rangle_n$, $|0\rangle_n$, and $|-1\rangle_n$ are obtained as

$$|1\rangle_n = \hat{R}|1\rangle = \begin{pmatrix} \frac{1+\cos\theta}{2}e^{-i\phi} \\ \frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2}e^{i\phi} \end{pmatrix},$$

$$|0\rangle_n = \hat{R}|0\rangle = \begin{pmatrix} -\frac{\sin\theta}{\sqrt{2}}e^{-i\phi} \\ \cos\theta \\ \frac{\sin\theta}{\sqrt{2}}e^{i\phi} \end{pmatrix},$$

$$|-1\rangle_n = \hat{R}|-1\rangle = \begin{pmatrix} \frac{1-\cos\theta}{2}e^{-i\phi} \\ -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1+\cos\theta}{2}e^{i\phi} \end{pmatrix}.$$

For $\phi = 0$, the rotation operator is given by

$$\hat{R} = D^{(1)}(\theta,\phi) = \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix},$$

and

$$|1\rangle_n = \hat{R}|1\rangle = \begin{pmatrix} \frac{1+\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} \end{pmatrix},$$

$$|0\rangle_n = \hat{R}|0\rangle = \begin{pmatrix} -\frac{\sin\theta}{\sqrt{2}} \\ \cos\theta \\ \frac{\sin\theta}{\sqrt{2}} \end{pmatrix},$$

$$\left|-1\right\rangle_n = \hat{R}\left|-1\right\rangle = \begin{pmatrix} \dfrac{1-\cos\theta}{2} \\ -\dfrac{\sin\theta}{\sqrt{2}} \\ \dfrac{1+\cos\theta}{2} \end{pmatrix}.$$

((**Mathematica**))

Matrices j = 1

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

Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m]


Jx = Table[Jx[1, n, m], {n, 1, -1, -1}, {m, 1, -1, -1}];

Jy = Table[Jy[1, n, m], {n, 1, -1, -1}, {m, 1, -1, -1}];

Jz = Table[Jz[1, n, m], {n, 1, -1, -1}, {m, 1, -1, -1}];

Ry[θ_] := MatrixExp[-ⅈ Jy θ] // Simplify

Rz[ϕ_] := MatrixExp[-ⅈ Jz ϕ] // Simplify

Rz[ϕ].Ry[θ] // MatrixForm
```

$$\begin{pmatrix} e^{-i\phi}\,\mathrm{Cos}\left[\frac{\theta}{2}\right]^2 & -\frac{e^{-i\phi}\,\mathrm{Sin}[\theta]}{\sqrt{2}} & e^{-i\phi}\,\mathrm{Sin}\left[\frac{\theta}{2}\right]^2 \\ \frac{\mathrm{Sin}[\theta]}{\sqrt{2}} & \mathrm{Cos}[\theta] & -\frac{\mathrm{Sin}[\theta]}{\sqrt{2}} \\ e^{i\phi}\,\mathrm{Sin}\left[\frac{\theta}{2}\right]^2 & \frac{e^{i\phi}\,\mathrm{Sin}[\theta]}{\sqrt{2}} & e^{i\phi}\,\mathrm{Cos}\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

```
u1 = Rz[ϕ].Ry[θ].{1, 0, 0} // Simplify
```

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

```
u2 = Rz[ϕ].Ry[θ].{0, 1, 0} // Simplify
```

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

```
u3 = Rz[ϕ].Ry[θ].{0, 0, 1} // Simplify
```

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

4. Mathematica for the rotation operator with *J*=3/2

The rotation operator with $J = 3/2$ is given by

$$\hat{R} = D^{(3/2)}(\theta,\phi)$$

$$= \begin{pmatrix} {}^{\frac{-3i\phi}{2}}\cos^3(\frac{\theta}{2}) & -\frac{\sqrt{3}}{4}e^{\frac{-3i\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta & \frac{\sqrt{3}}{2}e^{\frac{-3i\phi}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta & -e^{\frac{-3i\phi}{2}}\sin^3(\frac{\theta}{2}) \\ \frac{\sqrt{3}}{4}e^{\frac{-i\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta & \frac{1}{4}e^{\frac{-i\phi}{2}}[\cos\left(\frac{\theta}{2}\right)+3\cos\left(\frac{3\theta}{2}\right)] & \frac{1}{4}e^{\frac{-i\phi}{2}}[\sin\left(\frac{\theta}{2}\right)-3\sin\left(\frac{3\theta}{2}\right)] & \frac{\sqrt{3}}{2}e^{\frac{-i\phi}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta \\ \frac{\sqrt{3}}{2}e^{\frac{i\phi}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta & \frac{1}{4}e^{\frac{i\phi}{2}}[-\sin\left(\frac{\theta}{2}\right)+3\sin\left(\frac{3\theta}{2}\right)] & \frac{1}{4}e^{\frac{i\phi}{2}}[\cos\left(\frac{\theta}{2}\right)+3\cos\left(\frac{3\theta}{2}\right)] & -\frac{\sqrt{3}}{4}e^{\frac{i\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta \\ e^{\frac{i3\phi}{2}}\sin^3(\frac{\theta}{2}) & \frac{\sqrt{3}}{2}e^{\frac{i3\phi}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta & \frac{\sqrt{3}}{4}e^{\frac{i3\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta & e^{\frac{i3\phi}{2}}\cos^3(\frac{\theta}{2}) \end{pmatrix}$$

$$\left|\frac{3}{2}\right\rangle_n = \hat{R}\left|\frac{3}{2}\right\rangle = \begin{pmatrix} {}^{\frac{-3i\phi}{2}}\cos^3(\frac{\theta}{2}) \\ \frac{\sqrt{3}}{4}e^{\frac{-i\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta \\ \frac{\sqrt{3}}{2}e^{\frac{i\iota}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta \\ e^{\frac{i3\phi}{2}}\sin^3(\frac{\theta}{2}) \end{pmatrix},$$

$$\left|\frac{1}{2}\right\rangle_n = \hat{R}\left|\frac{1}{2}\right\rangle = \begin{pmatrix} -\frac{\sqrt{3}}{4}e^{\frac{-3i\phi}{2}}\csc(\frac{\theta}{2})\sin^2\theta \\ \frac{1}{4}e^{\frac{-i\phi}{2}}[\cos\left(\frac{\theta}{2}\right)+3\cos\left(\frac{3\theta}{2}\right)] \\ \frac{1}{4}e^{\frac{i\phi}{2}}[-\sin\left(\frac{\theta}{2}\right)+3\sin\left(\frac{3\theta}{2}\right)] \\ \frac{\sqrt{3}}{2}e^{\frac{i3\phi}{2}}\sin\left(\frac{\theta}{2}\right)\sin\theta \end{pmatrix},$$

$$\left|-\frac{1}{2}\right\rangle_n = \hat{R}\left|-\frac{1}{2}\right\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2} e^{\frac{-3i\phi}{2}} \sin\left(\frac{\theta}{2}\right)\sin\theta \\ \frac{1}{4} e^{\frac{-i\phi}{2}} [\sin\left(\frac{\theta}{2}\right) - 3\sin\left(\frac{3\theta}{2}\right)] \\ \frac{1}{4} e^{\frac{i\phi}{2}} [\cos\left(\frac{\theta}{2}\right) + 3\cos\left(\frac{3\theta}{2}\right)] \\ \frac{\sqrt{3}}{4} e^{\frac{i3\phi}{2}} \csc(\frac{\theta}{2})\sin^2\theta \end{pmatrix},$$

$$\left|-\frac{3}{2}\right\rangle_n = \hat{R}\left|-\frac{3}{2}\right\rangle = \begin{pmatrix} -e^{\frac{-3i\phi}{2}} \sin^3(\frac{\theta}{2}) \\ \frac{\sqrt{3}}{2} e^{\frac{-i\phi}{2}} \sin\left(\frac{\theta}{2}\right)\sin\theta \\ -\frac{\sqrt{3}}{4} e^{\frac{i\phi}{2}} \csc(\frac{\theta}{2})\sin^2\theta \\ e^{\frac{i3\phi}{2}} \cos^3(\frac{\theta}{2}) \end{pmatrix}.$$

Matrices with j = 3/2

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

Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m]


Jx = Table[Jx[3/2, n, m], {n, 3/2, -3/2, -1}, {m, 3/2, -3/2, -1}];

Jy = Table[Jy[3/2, n, m], {n, 3/2, -3/2, -1}, {m, 3/2, -3/2, -1}];

Jz = Table[Jz[3/2, n, m], {n, 3/2, -3/2, -1}, {m, 3/2, -3/2, -1}];

Ry[θ_] := MatrixExp[-ⅈ Jy θ] // Simplify;

Rz[ϕ_] := MatrixExp[-ⅈ Jz ϕ] // Simplify;

u1 = Rz[ϕ].Ry[θ].{1, 0, 0, 0} // Simplify
```

$$\left\{e^{-\frac{3 i \phi}{2}} \mathrm{Cos}\left[\frac{\theta}{2}\right]^3, \frac{1}{4}\sqrt{3}\, e^{-\frac{i \phi}{2}} \mathrm{Csc}\left[\frac{\theta}{2}\right] \mathrm{Sin}[\theta]^2, \frac{1}{2}\sqrt{3}\, e^{\frac{i \phi}{2}} \mathrm{Sin}\left[\frac{\theta}{2}\right] \mathrm{Sin}[\theta], e^{\frac{3 i \phi}{2}} \mathrm{Sin}\left[\frac{\theta}{2}\right]^3\right\}$$

```
u2 = Rz[ϕ].Ry[θ].{0, 1, 0, 0} // Simplify
```

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

```
u3 = Rz[ϕ].Ry[θ].{0, 0, 1, 0} // Simplify
```

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

```
u4 = Rz[ϕ].Ry[θ].{0, 0, 0, 1} // Simplify
```

$$\left\{-e^{-\frac{3 i \phi}{2}} \mathrm{Sin}\left[\frac{\theta}{2}\right]^3, \frac{1}{2}\sqrt{3}\, e^{-\frac{i \phi}{2}} \mathrm{Sin}\left[\frac{\theta}{2}\right] \mathrm{Sin}[\theta], -\frac{1}{4}\sqrt{3}\, e^{\frac{i \phi}{2}} \mathrm{Csc}\left[\frac{\theta}{2}\right] \mathrm{Sin}[\theta]^2, e^{\frac{3 i \phi}{2}} \mathrm{Cos}\left[\frac{\theta}{2}\right]^3\right\}$$

5. Mathematica for the rotation operator with *J*=2

Matrices j = 2

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

Jx[ℓ_, n_, m_] := 1/2 Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jy[ℓ_, n_, m_] := -1/2 ⅈ Sqrt[(ℓ - m) (ℓ + m + 1)] KroneckerDelta[n, m + 1] +
  1/2 ⅈ Sqrt[(ℓ + m) (ℓ - m + 1)] KroneckerDelta[n, m - 1]

Jz[ℓ_, n_, m_] := m KroneckerDelta[n, m]


Jx = Table[Jx[2, n, m], {n, 2, -2, -1}, {m, 2, -2, -1}];

Jy = Table[Jy[2, n, m], {n, 2, -2, -1}, {m, 2, -2, -1}];

Jz = Table[Jz[2, n, m], {n, 2, -2, -1}, {m, 2, -2, -1}];

Ry[θ_] := MatrixExp[-ⅈ Jy θ] // Simplify

Rz[ϕ_] := MatrixExp[-ⅈ Jz ϕ] // Simplify

u1 = Rz[ϕ].Ry[θ].{1, 0, 0, 0, 0} // Simplify
```

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

```
u2 = Rz[ϕ].Ry[θ].{0, 1, 0, 0, 0} // Simplify
```

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

```
u3 = Rz[ϕ].Ry[θ].{0, 0, 1, 0, 0} // Simplify
```

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

```
u4 = Rz[ϕ].Ry[θ].{0, 0, 0, 1, 0} // Simplify
```

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

```
u5 = Rz[ϕ].Ry[θ].{0, 0, 0, 0, 1} // Simplify
```

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

6. Spherical Harmonics as rotator matrices

Using the relation

$$\left|\Re\mathbf{r}\right\rangle = \hat{R}\left|\mathbf{r}\right\rangle .$$

we have

$$\begin{aligned}\left|\mathbf{n}\right\rangle &= \left|\Re\mathbf{e}_z\right\rangle = \hat{R}\left|\mathbf{e}_z\right\rangle = \hat{R}_z(\phi)\hat{R}_y(\theta)\left|\mathbf{e}_z\right\rangle \\ &= \sum_{m'}\hat{R}_z(\phi)\hat{R}_y(\theta)\left|\ell m'\right\rangle\left\langle lm'\right|\mathbf{e}_z\rangle\end{aligned}$$

Then

$$\left\langle lm\middle|\mathbf{n}\right\rangle = \sum_{m'}\left\langle lm\right|\hat{R}_z(\phi)\hat{R}_y(\theta)\left|lm'\right\rangle\left\langle lm'\middle|\mathbf{e}_z\right\rangle .$$

Here note that

$$\left\langle\mathbf{n}\middle|lm\right\rangle = Y_\ell^m(\mathbf{n}) = Y_\ell^m(\theta,\phi) ,$$

or

$$\left\langle lm\middle|\mathbf{n}\right\rangle = [Y_\ell^m(\theta,\phi)]^* .$$

We also note that

$$\left\langle lm\middle|\mathbf{e}_z\right\rangle = [Y_\ell^m(\theta,\phi)]^* ,$$

which is evaluated at $\theta = 0$ with ϕ undetermined. At $\theta = 0$, $Y_\ell^m(\theta,\phi)$ is known to vanish for $m\neq 0$;

$$\begin{aligned}\left\langle lm\middle|\mathbf{e}_z\right\rangle &= [Y_\ell^m(\theta=0,\phi)]^*\delta_{m,0} \\ &= \sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta=1)\delta_{m,0} \\ &= \sqrt{\frac{2\ell+1}{4\pi}}\delta_{m,0}\end{aligned}$$

$$[Y_\ell^m(\theta,\phi)]^* = \sum_{m'} \langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|lm'\rangle\langle lm'|\mathbf{e}_z\rangle$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\sum_{m'} \langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|lm'\rangle\delta_{m',0}$$
$$= \sqrt{\frac{2\ell+1}{4\pi}}\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle$$

or

$$\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle == \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^* .$$

Since

$$\hat{R}_z(\phi) = \exp[-\frac{i}{\hbar}\hat{J}_z\phi],$$

$$\langle lm|\hat{R}_z(\phi)\hat{R}_y(\theta)|l0\rangle = \langle lm|\exp[-\frac{i}{\hbar}\hat{J}_z\phi]\hat{R}_y(\theta)|l0\rangle$$
$$= e^{-im\phi}\langle lm|\hat{R}_y(\theta)|l0\rangle$$

or

$$e^{-im\phi}\langle lm|\hat{R}_y(\theta)|l0\rangle = \sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*,$$

or

$$\langle lm|\hat{R}_y(\theta)|l0\rangle = e^{-im\phi}\sqrt{\frac{4\pi}{2\ell+1}}[Y_\ell^m(\theta,\phi)]^*.$$

7. Calculation for the rotation operator for $j = 1$

$$\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta) .$$

(a) Calculate the rotation operator $\hat{R}_y(\theta)$

$$\hat{R}_y(\phi) = \exp(-\frac{i}{\hbar}\hat{J}_y\theta)$$

$$= \hat{1} + \frac{1}{1!}(-\frac{i}{\hbar}\theta)\hat{J}_y + \frac{1}{2!}(-\frac{i}{\hbar}\theta)^2\hat{J}_y{}^2 + \frac{1}{3!}(-\frac{i}{\hbar}\theta)^3\hat{J}_y{}^3 + \frac{1}{4!}(-\frac{i}{\hbar}\theta)^4\hat{J}_y{}^4 + \frac{1}{5!}(-\frac{i}{\hbar}\theta)^5\hat{J}_y{}^5 + ...$$

$$= \hat{1} + \frac{1}{1!}(-\frac{i}{\hbar}\theta)\hat{J}_y + \frac{1}{2!}(-\frac{i}{\hbar}\theta)^2\hat{J}_y{}^2 + \frac{1}{3!}(-\frac{i}{\hbar}\theta)^3\hbar^2\hat{J}_y + \frac{1}{4!}(-\frac{i}{\hbar}\theta)^4\hbar^2\hat{J}_y{}^2 + \frac{1}{5!}(-\frac{i}{\hbar}\theta)^5\hbar^4\hat{J}_y + ...$$

$$= \hat{1} + \frac{\hat{J}_y}{\hbar}[(-i\theta) + \frac{1}{3!}(-i\theta)^3 + \frac{1}{5!}(-i\theta)^5 + ...] + \frac{\hat{J}_y{}^2}{\hbar^2}[\frac{1}{2!}(-i\theta)^2 + \frac{1}{4!}(-i\theta)^4 + \frac{1}{4!}(-i\theta)^6 + ...] +$$

$$= \hat{1} - \frac{\hat{J}_y}{\hbar}[(i\theta) + \frac{1}{3!}(i\theta)^3 + \frac{1}{5!}(i\theta)^5 + ...] + \frac{\hat{J}_y{}^2}{\hbar^2}[\frac{1}{2!}(i\theta)^2 + \frac{1}{4!}(i\theta)^4 + \frac{1}{4!}(i\theta)^6 + ...] +$$

where

$$\hat{J}_y = \frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \hat{J}_y{}^2 = \frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix},$$

$$\hat{J}_y{}^3 = \hbar^2\frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} = \hbar^2\hat{J}_y, \qquad \hat{J}_y{}^4 = \hat{J}_y{}^3\hat{J}_y = \hbar^2\hat{J}_y{}^2$$

$$\hat{J}_y{}^5 = \hat{J}_y{}^4\hat{J}_y = \hbar^2\hat{J}_y{}^3 = \hbar^4\hat{J}_y$$

Note that

$$\cos\theta - 1 = \frac{1}{2!}(i\theta)^2 + \frac{1}{4!}(i\theta)^4 + \frac{1}{6!}(i\theta)^6 + ...$$

$$i\sin\theta = (i\theta) + \frac{1}{3!}(i\theta)^3 + \frac{1}{5!}(i\theta)^5 + ...$$

$$\hat{R}_y(\phi) = \hat{1} - \frac{1}{\hbar}\hat{J}_y(i\sin\theta) + \frac{\hat{J}_y{}^2}{\hbar^2}(\cos\theta - 1)$$

$$= \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix}.$$

(b) Calculate the rotation operator $\hat{R}_y(\theta)$

$$\hat{R}_z(\phi) = \exp(-\frac{i}{\hbar}\hat{J}_z\phi) = \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\phi} \end{pmatrix}.$$

(c) Calculation of the rotation operator $\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta)$

The matrix of $\hat{R}$ is given by

$$\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta) = \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix},$$

or

$$\hat{R} = D^{(1)}(\theta,\phi) = \begin{pmatrix} e^{-i\phi}(\frac{1+\cos\theta}{2}) & -e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{-i\phi}(\frac{1-\cos\theta}{2}) \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ e^{i\phi}(\frac{1-\cos\theta}{2}) & e^{i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{i\phi}(\frac{1+\cos\theta}{2}) \end{pmatrix}.$$