Chapter 27
Rotation operator and angular momentum

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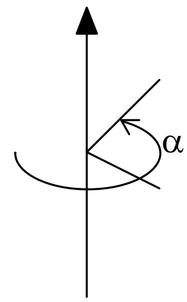
Eugene Paul "E. P." Wigner (Hungarian **Wigner Jenő Pál**; November 17, 1902 – January 1, 1995) was a Hungarian American physicist and mathematician. He received a share of the Nobel Prize in Physics in 1963 "for his contributions to the theory of the atomic nucleus and the elementary particles, particularly 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. Some contemporaries referred to Wigner as *the Silent Genius* and some even considered him the intellectual equal to Albert Einstein, though without his prominence. Wigner is important 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, and for his several mathematical theorems. It was Eugene Wigner who first identified Xe-135 "poisoning" in nuclear reactors, and for this reason it is sometimes referred to as *Wigner poisoning*.

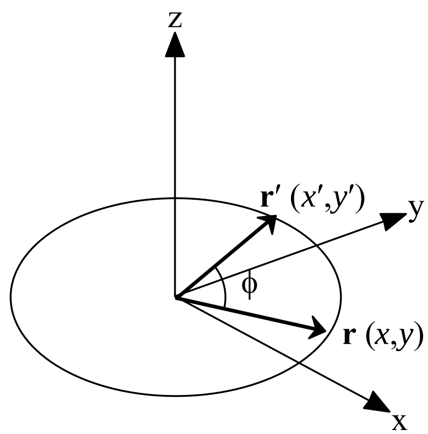
http://en.wikipedia.org/wiki/Eugene_Wigner

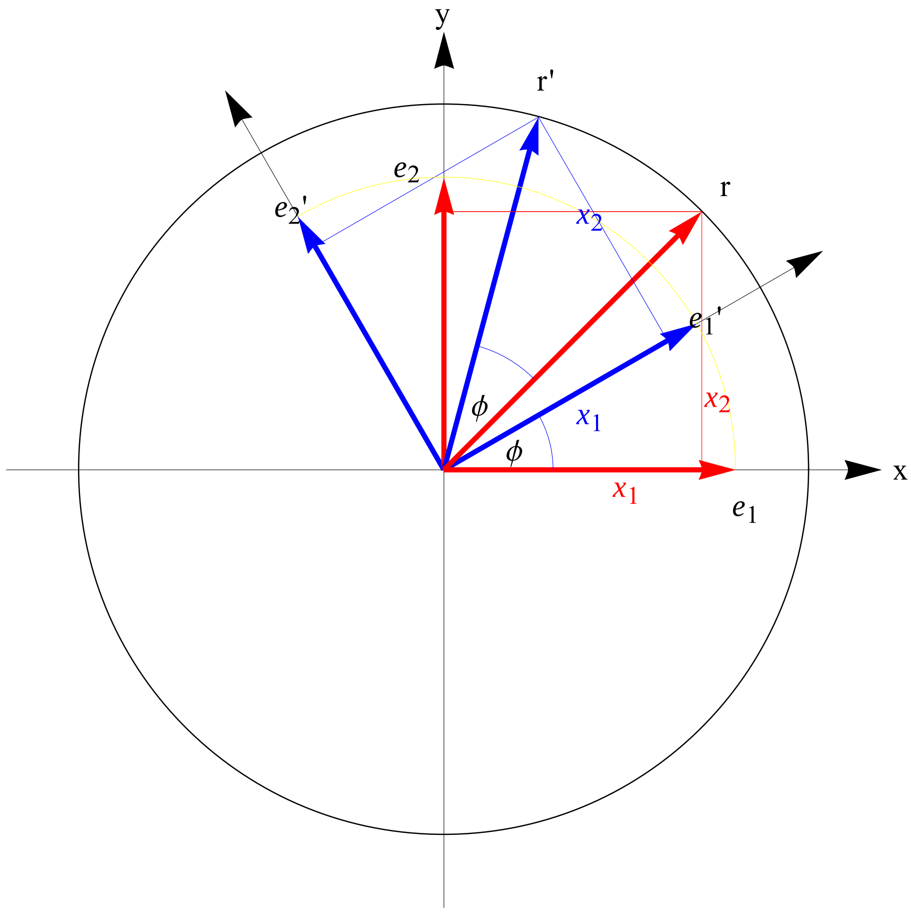
27.1 Overview of 2D rotation around a fixed axis

((Classical mechanics)) See Chapter 1S for the discussion of the rotation.



$\Re_{\mathbf{u}}(\alpha)$ is geometrical rotation characterized by the axis of rotation (***u***) and the angle of rotation (α).





$$\mathbf{e}_1 \cdot \mathbf{e}_1' = \cos\phi \qquad \mathbf{e}_2 \cdot \mathbf{e}_1' = \sin\phi$$
$$\mathbf{e}_1 \cdot \mathbf{e}_2' = -\sin\phi, \qquad \mathbf{e}_2 \cdot \mathbf{e}_2' = \cos\phi$$

We define ***r*** and ***r***' as

$$\mathbf{r}' = (x_1', x_2') = x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2 = x_1\mathbf{e}_1' + x_2\mathbf{e}_2'$$

and

$$\mathbf{r} = (x_1, x_2) = x_1\mathbf{e}_1 + x_2\mathbf{e}_2$$

$$\mathbf{e}_1 \cdot (x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2) = \mathbf{e}_1 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2')$$
$$\mathbf{e}_2 \cdot (x_1'\mathbf{e}_1 + x_2'\mathbf{e}_2) = \mathbf{e}_2 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2')$$

or

$$x_1' = \mathbf{e}_1 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\cos\phi - x_2\sin\phi$$
$$x_2' = \mathbf{e}_2 \cdot (x_1\mathbf{e}_1' + x_2\mathbf{e}_2') = x_1\sin\phi + x_2\cos\phi$$

or

$$\begin{pmatrix} x_1' \\ x_2' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

((**Note**))

Rotation around the *z* axis in the complex plane

$$x'+iy' = e^{i\phi}(x+iy) = (\cos\phi + i\sin\phi)(x+iy) = x\cos\phi - y\sin\phi + i(x\sin\phi + y\cos\phi)$$

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Morer generally, since $x_3' = x_3$, we have

$$\mathbf{r}' = \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \Re_z(\phi)\mathbf{r}$$

where

$$\Re_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} =$$

27.2 Rotation matrix

$$\mathbf{r} = \sum_{j=1}^{3} x_j \mathbf{e}_j, \qquad \mathbf{r}' = \sum_{j=1}^{3} x_j' \mathbf{e}_j = \sum_{j=1}^{3} x_j \mathbf{e}_j'$$

$$\mathbf{r}' = \Re_z(\phi)\mathbf{r} = \Re_z(\phi)(\sum_{j=1}^{3} x_j \mathbf{e}_j) = \sum_{j=1}^{3} x_j \Re_z(\phi)\mathbf{e}_j = \sum_{j=1}^{3} x_j \mathbf{e}_j'$$

where

$$\Re_z(\phi)\mathbf{e}_j = \mathbf{e}_j'$$

Thus we have

$$(\sum_{j=1}^{3} x_j \mathbf{e}_j') \cdot \mathbf{e}_i = (\sum_{j=1}^{3} x_j' \mathbf{e}_j) \cdot \mathbf{e}_i$$

or

$$\sum_{j=1}^{3} x_j' \delta_{j,i} = x_i' = \sum_{j=1}^{3} (\mathbf{e}_i \cdot \mathbf{e}_j') x_j = \sum_{j=1}^{3} \Re_{ij} x_j$$

where

$$\Re_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j'$$

and

$$\begin{aligned}
&\Re_{11} = \mathbf{e}_1 \cdot \mathbf{e}_1' = \cos\phi, \quad &&\Re_{12} = \mathbf{e}_1 \cdot \mathbf{e}_2' = -\sin\phi, \quad &&\Re_{13} = \mathbf{e}_1 \cdot \mathbf{e}_3' = 0 \\
&\Re_{21} = \mathbf{e}_2 \cdot \mathbf{e}_1' = \sin\phi, \quad &&\Re_{22} = \mathbf{e}_2 \cdot \mathbf{e}_2' = \cos\phi, \quad &&\Re_{23} = \mathbf{e}_2 \cdot \mathbf{e}_3' = 0 \\
&\Re_{31} = \mathbf{e}_3 \cdot \mathbf{e}_1' = 0, \quad &&\Re_{32} = \mathbf{e}_3 \cdot \mathbf{e}_2' = 0, \quad &&\Re_{33} = \mathbf{e}_3 \cdot \mathbf{e}_3' = 1
\end{aligned}$$

$$\mathbf{r}' = \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} \Re_{11} & \Re_{12} & \Re_{13} \\ \Re_{21} & \Re_{22} & \Re_{23} \\ \Re_{31} & \Re_{32} & \Re_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

where

$$\Re_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(1) Rotation around the *z* axis, where ϕ (= ε) is infinitesimally small.

$$\Re_z(\phi) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 - \frac{\varepsilon^2}{2} & -\varepsilon & 0 \\ \varepsilon & 1 - \frac{\varepsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(2) Rotation around the *x* axis

$$\begin{pmatrix} y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix}$$

or

$$\Re_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\dfrac{\varepsilon^2}{2} & -\varepsilon \\ 0 & \varepsilon & 1-\dfrac{\varepsilon^2}{2} \end{pmatrix}$$

(2) Rotation around the *y* axis

$$\begin{pmatrix} z' \\ x' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} z \\ x \end{pmatrix}$$

or

$$\Re_y(\phi) = \begin{pmatrix} \cos\phi & 0 & \sin\phi \\ 0 & 1 & 0 \\ -\sin\phi & 0 & \cos\phi \end{pmatrix} = \begin{pmatrix} 1-\dfrac{\varepsilon^2}{2} & 0 & \varepsilon \\ 0 & 1 & 0 \\ -\varepsilon & 0 & 1-\dfrac{\varepsilon^2}{2} \end{pmatrix}$$

We have the relation to the order of ε^2

$$\Re_x(\varepsilon)\Re_y(\varepsilon) - \Re_y(\varepsilon)\Re_x(\varepsilon) = \begin{pmatrix} 0 & -\varepsilon^2 & 0 \\ \varepsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \Re_z(\varepsilon^2) - I$$

$$\Re_y(\varepsilon)\Re_z(\varepsilon) - \Re_z(\varepsilon)\Re_y(\varepsilon) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\varepsilon^2 \\ 0 & \varepsilon^2 & 0 \end{pmatrix} = \Re_x(\varepsilon^2) - I$$

$$\Re_z(\varepsilon)\Re_x(\varepsilon) - \Re_x(\varepsilon)\Re_z(\varepsilon) = \begin{pmatrix} 0 & 0 & \varepsilon^2 \\ 0 & 0 & 0 \\ -\varepsilon^2 & 0 & 0 \end{pmatrix} = \Re_y(\varepsilon^2) - I$$

where *I* is the unit matrix of 3 x 3.

27.3 Mathematica

((**Mathematica**))

```
Rz = {{1 - ϵ^2/2, -ϵ, 0}, {ϵ, 1 - ϵ^2/2, 0}, {0, 0, 1}};

Rx = {{1, 0, 0}, {0, 1 - ϵ^2/2, -ϵ}, {0, ϵ, 1 - ϵ^2/2}};

Ry = {{1 - ϵ^2/2, 0, ϵ}, {0, 1, 0}, {-ϵ, 0, 1 - ϵ^2/2}};

Rx.Ry - Ry.Rx // Expand // MatrixForm
```

$$\begin{pmatrix} 0 & -\epsilon^2 & \frac{\epsilon^3}{2} \\ \epsilon^2 & 0 & \frac{\epsilon^3}{2} \\ \frac{\epsilon^3}{2} & \frac{\epsilon^3}{2} & 0 \end{pmatrix}$$

```
Ry.Rz - Rz.Ry // Expand // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\epsilon^3}{2} & \frac{\epsilon^3}{2} \\ \frac{\epsilon^3}{2} & 0 & -\epsilon^2 \\ \frac{\epsilon^3}{2} & \epsilon^2 & 0 \end{pmatrix}$$

```
Rz.Rx - Rx.Rz // Expand // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\epsilon^3}{2} & \epsilon^2 \\ \frac{\epsilon^3}{2} & 0 & \frac{\epsilon^3}{2} \\ -\epsilon^2 & \frac{\epsilon^3}{2} & 0 \end{pmatrix}$$

27.4 Rotation operator in Quantum mechanics

After the geometrical rotation;

$$\mathbf{r} \to \Re\mathbf{r} = \mathbf{r}' \text{ (geometrical rotation)}$$

we assume that the state vector changes from the old state $|\psi\rangle$ to the new state $|\psi'\rangle$.

$$|\psi'\rangle = \hat{R}|\psi\rangle,$$

or

$$\langle\psi'| = \langle\psi|\hat{R}^{+},$$

where $\hat{R}$ is a rotation operator in the quantum mechanics. It is natural to assume that

$$\langle\psi'|\hat{\mathbf{r}}|\psi'\rangle = \langle\psi|\hat{\mathbf{r}}'|\psi\rangle = \langle\psi|\Re\hat{\mathbf{r}}|\psi\rangle,$$

or

$$\langle\psi|\hat{R}^{+}\hat{\mathbf{r}}\hat{R}|\psi\rangle = \langle\psi|\Re\hat{\mathbf{r}}|\psi\rangle,$$

or

$$\hat{R}^{+}\hat{\mathbf{r}}\hat{R} = \Re\hat{\mathbf{r}}. \qquad (1)$$

The rotation operator is a unitary operator.

$$\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle,$$

or

$$\hat{R}^{+}\hat{R} = \hat{R}\hat{R}^{+} = \hat{1} \text{ (Unitary operator)}$$

From Eq. (1),

$$\hat{\mathbf{r}}\hat{R} = \hat{R}\Re\hat{\mathbf{r}}.$$

Here we calculate

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

$\hat{R}|\mathbf{r}\rangle$ is the eigenket of $\hat{\mathbf{r}}$ with the eigenvalue $\Re\mathbf{r}$. So that we can write

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

When

$$\Re\mathbf{r} = \mathbf{r}_0$$

or

$$\mathbf{r} = \Re^{-1}\mathbf{r}_0$$

$$\hat{R}|\Re^{-1}\mathbf{r}_0\rangle = |\mathbf{r}_0\rangle$$

or

$$|\Re^{-1}\mathbf{r}_0\rangle = \hat{R}^{+}|\mathbf{r}_0\rangle .$$

For any $\mathbf{r}$,

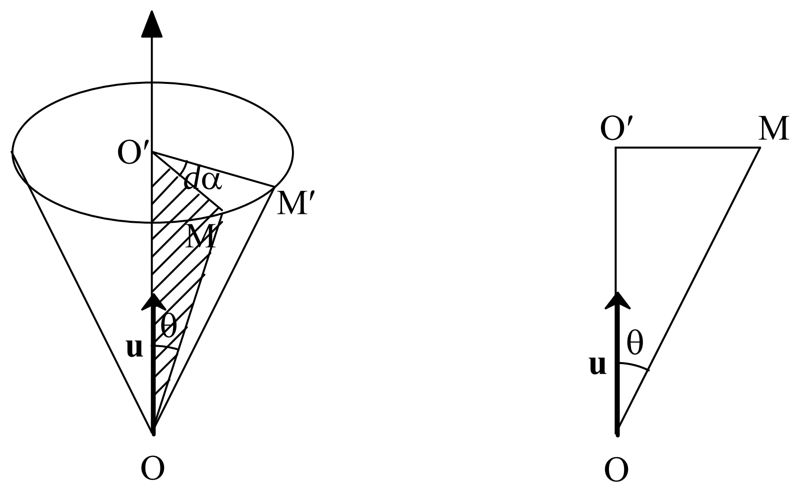
$$|\Re^{-1}\mathbf{r}\rangle = \hat{R}^{+}|\mathbf{r}\rangle$$

$$\hat{R}\hat{R}^{+}|\mathbf{r}\rangle = \hat{R}|\Re^{-1}\mathbf{r}\rangle = |\Re\Re^{-1}\mathbf{r}\rangle = |\mathbf{r}\rangle$$

In summary

1. $\hat{R}^{+}\hat{R} = \hat{R}\hat{R}^{+} = \hat{1}$
2. $\hat{R}|\mathbf{r}\rangle = |\Re\mathbf{r}\rangle$
3. $\langle\mathbf{r}|\hat{R}^{+} = \langle\Re\mathbf{r}|$
4. $\hat{R}^{+}|\mathbf{r}\rangle = |\Re^{-1}\mathbf{r}\rangle$
5. $\langle\mathbf{r}|\hat{R} = \langle\Re^{-1}\mathbf{r}|$

27.5 Theorem



$\Re_{\mathbf{u}}(d\alpha)$: infinitesimal rotation around the ***u*** axis.

$$\overrightarrow{OM'} = \Re_u(\alpha)\overrightarrow{OM} = \overrightarrow{OM} + d\alpha(\mathbf{u}\times\overrightarrow{OM})$$

$$|\,\mathbf{u}\times\overrightarrow{OM}\,| = \overline{OM}\sin\theta = \overline{O'M}$$

$$\overline{MM'} = \overline{O'M}d\alpha = \overline{OM}\sin\theta d\alpha$$

The direction of $\overrightarrow{MM'}$ coincides with that of $\mathbf{u}\times\overrightarrow{OM}$.

$$\Re_{\mathbf{u}}(d\alpha)\overrightarrow{OM} = \overrightarrow{OM'} = \overrightarrow{OM} + \overrightarrow{MM'} = \overrightarrow{OM} + d\alpha(\mathbf{u}\times\overrightarrow{OM})$$

((Theorem))

Every finite rotation can be decomposed into an infinite number of infinitesimal rotations.

$$\Re_{\mathbf{u}}(\alpha + d\alpha) = \Re_{\mathbf{u}}(\alpha)\Re_{\mathbf{u}}(d\alpha) = \Re_{\mathbf{u}}(d\alpha)\Re_{\mathbf{u}}(\alpha) \qquad (1)$$

Note the following relation which will be useful.

$$\Re_y(-d\alpha')\Re_x(d\alpha)\Re_y(d\alpha')\Re_x(-d\alpha) = \Re_z(d\alpha d\alpha') \qquad (2)$$

$$\Re_{\mathbf{u}}^{-1}(d\alpha) = \Re_{-\mathbf{u}}(d\alpha) \qquad (3)$$

The proof of Eqs. (1) and (2) can be given using Mathematica.

27.6 Proof by Mathematica

((**Mathematica**))
How can we define the rotation operator in the Mathematica?
(1) We need a package called "Calculus`VectorAnalysis`"

```
Needs["Calculus`VectorAnalysis`"]
```

(2) We use the Cartesian coordinate.

```
SetCoordinates[Cartesian[x,y,z]]
```

(3) Definition of the vectors, $\boldsymbol{e}_x$, $\boldsymbol{e}_y$, $\boldsymbol{e}_z$, and $\boldsymbol{r}$

(4) Definition of the geometrical rotation operator $R_u(\alpha)$

```
R[u_,α_]:=#+α CrossProduct[u,#]&
```

(5) Rotation:

```
R[u,α][r]
```

((**Mathematica**))

Geometrical rotation

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

Needs["VectorAnalysis`"];

SetCoordinates[Cartesian[x, y, z]];

ex = {1, 0, 0}; ey = {0, 1, 0}; ez = {0, 0, 1}; r = {x, y, z};
```

Definition of geometrical rotation

```
R[u_, δ_] := # + δ CrossProduct[u, #] &;

R[ez, dα][r]

{x - dα y, dα x + y, z}
```

Theorem 1

$\mathbb{R}[ez,d\alpha 1]\mathbb{R}[ez,d\alpha 2]=\mathbb{R}[ez,d\alpha 2]\mathbb{R}[ez,d\alpha 1]=\mathbb{R}[ez,d\alpha 1+d\alpha 2]$

where $\mathbb{R}$ is a geometrical rotation

$d\alpha 1$ and $d\alpha 2$ are infinitesimal rotation angles

```
r1 = R[ez, dα1][R[ez, dα2][r]] // Simplify

{x - dα1 dα2 x - (dα1 + dα2) y, dα2 x + y + dα1 (x - dα2 y), z}
```

```
r2 = R[ez, dα2][R[ez, dα1][r]] // Simplify
```
{x − dα1 dα2 x − (dα1 + dα2) y, dα2 x + y + dα1 (x − dα2 y), z}

```
r3 = R[ez, dα1 + dα2][r] // Simplify
```
{x − (dα1 + dα2) y, (dα1 + dα2) x + y, z}

```
r3 - r1 // Simplify
```
{dα1 dα2 x, dα1 dα2 y, 0}

```
r3 - r2 // Simplify
```
{dα1 dα2 x, dα1 dα2 y, 0}

Theorem 2
ℝ[ey,-dα2]ℝ[ex,dα1]ℝ[ey,dα2]ℝ[ex,-dα1]=ℝ[ez,dα1 dα2]

```
s1 = R[ex, -dα1][r];
```
{x, y + dα1 z, −dα1 y + z}

```
s2 = R[ey, dα2][s1] // Simplify;
```
{x + dα2 (−dα1 y + z), y + dα1 z, −dα2 x − dα1 y + z}

```
s3 = R[ex, dα1][s2] // Simplify;
{x + dα2 (-dα1 y + z), dα1 dα2 x + y + dα1^2 y, -dα2 x + z + dα1^2 z}

s4 = R[ey, -dα2][s3] // Simplify;
{(1 + dα2^2) x - dα1 dα2 (y + dα1 z), dα1 dα2 x + y + dα1^2 y, -dα1 dα2^2 y + z + dα1^2 z + dα2^2 z}

s5 = R[ez, dα1 dα2][r] // Simplify
{x - dα1 dα2 y, dα1 dα2 x + y, z}

s5 - s4 // Simplify
{dα2 (-dα2 x + dα1^2 z), -dα1^2 y, dα1 dα2^2 y - dα1^2 z - dα2^2 z}
```

Theorem 3
ℝ[-ez,dα]ℝ[ez,dα]=1

```
s6 = R[-ez, dα][r]
{x + dα y, -dα x + y, z}

s7 = R[ez, dα][s6] // Simplify
{(1 + dα^2) x, (1 + dα^2) y, z}
```

27.7 Expression of rotation operator

$$\Re_z^{-1}(d\alpha)\mathbf{r} = \Re_{-z}(d\alpha)\mathbf{r} = \mathbf{r} + d\alpha(-\mathbf{e}_z \times \mathbf{r}) = \mathbf{r} - d\alpha(\mathbf{e}_z \times \mathbf{r})$$

Using

$$\mathbf{e}_z \times \mathbf{r} = \begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ 0 & 0 & 1 \\ x & y & z \end{vmatrix} = (-y, x, 0)$$

$$\Re_z^{-1}(d\alpha)\mathbf{r} = (x + y d\alpha, y - x d\alpha, z)$$

((Note)) Another simple way to get the above result is as follows.

$$(x' + iy') = e^{-i\alpha}(x + iy) = (1 - i\alpha)(x + iy) = x + \alpha y + i(y - \alpha x)$$

or

$$x' = x + y d\alpha$$
$$y' = y - x d\alpha$$

Therefore we have

$$\begin{aligned}\langle \mathbf{r}|\psi'\rangle &= \langle \mathbf{r}|\hat{R}_z(d\alpha)|\psi\rangle = \langle \Re_z^{-1}(d\alpha)\mathbf{r}|\psi\rangle \\ &= \psi(x+yd\alpha, y-xd\alpha, z) \\ &= \psi + d\alpha(y\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial y}) \\ &= \psi(x,y,z) - d\alpha(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})\psi(x,y,z) \\ &= \langle \mathbf{r}|1 - \frac{i}{\hbar}d\alpha\hat{L}_z|\psi\rangle\end{aligned}$$

where

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

or

$$\hat{R}_z(d\alpha) = \hat{1} - \frac{i}{\hbar}d\alpha\hat{L}_z$$

((Note))

$$\langle \mathbf{r}|(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)|\psi\rangle = \langle r|\hat{L}_z|\psi\rangle = \frac{\hbar}{i}(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})\langle \mathbf{r}|\psi\rangle$$

We have the relation

$$\hat{R}_z^{+}(d\alpha)\hat{\mathbf{r}}\hat{R}_z(d\alpha) = \Re\hat{\mathbf{r}}$$

$$\Re_z(d\alpha)\mathbf{r} = \mathbf{r} + d\alpha(\mathbf{e}_z \times \mathbf{r}) = (x - yd\alpha, y + xd\alpha, z)$$

and

$$\Re_z(d\alpha)\hat{\mathbf{r}} = (\hat{x} - \hat{y}d\alpha, \hat{y} + \hat{x}d\alpha, \hat{z})$$

Then

$$\hat{R}_z^{+}(d\alpha)\hat{\mathbf{r}}\hat{R}_z(d\alpha) = \Re_z(d\alpha)\hat{\mathbf{r}}$$

or

$$\hat{R}_z^{+}(d\alpha)\hat{x}\hat{R}_z(d\alpha) = \hat{x} - \hat{y}d\alpha$$

$$\hat{R}_z^{+}(d\alpha)\hat{y}\hat{R}_z(d\alpha) = \hat{y} + \hat{x}d\alpha$$

$$\hat{R}_z^{+}(d\alpha)\hat{z}\hat{R}_z(d\alpha) = \hat{z}$$

((Finite rotation))

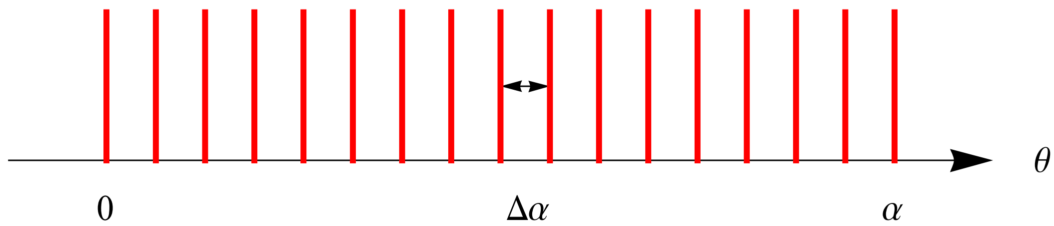


Fig. $\alpha = N\Delta\alpha$.

$$\hat{R}_z(\alpha = 0) = \hat{1}$$

$$\hat{R}_z(\alpha) = \lim_{N\to\infty}[\hat{R}_z(\Delta\alpha)]^N = \lim_{N\to\infty}(\hat{1} - \frac{i}{\hbar}\Delta\alpha\hat{L}_z)^N = \lim_{N\to\infty}(\hat{1} - \frac{i}{\hbar}\frac{\alpha}{N}\hat{L}_z)^N$$
$$= \exp(-\frac{i}{\hbar}\alpha\hat{L}_z)$$

((**Note**))

$$\lim_{N\to\infty}(\hat{1} - \frac{i}{\hbar}\frac{\alpha}{N}\hat{L}_z)^N = \lim_{N\to\infty}[(\hat{1} + \frac{\mu}{N})^{\frac{N}{\mu}}]^{\mu} = e^{\mu}$$

where

$$\mu = -\frac{i}{\hbar}\alpha\hat{L}_z$$

In general,

$$\hat{R}_u(\alpha) = \exp(-\frac{i}{\hbar}\alpha\hat{\mathbf{L}}\cdot\mathbf{u})$$

In the case of an arbitrary quantum mechanical system, using the general angular momentum $\hat{\mathbf{J}}$ instead of $\hat{\mathbf{L}}$:

$$\hat{R}_u(\alpha) = \exp(-\frac{i}{\hbar}\alpha\hat{\mathbf{J}}\cdot\mathbf{u})$$

27.8 Commutation relations of the components of the angular momentum

$$\Re_y(-d\alpha')\Re_x(d\alpha)\Re_y(d\alpha')\Re_x(-d\alpha) = \Re_z(d\alpha d\alpha') \quad (2)$$

Note

$$\left|\Re_1\Re_2\mathbf{r}\right\rangle = \hat{R}_1\left|\Re_2\mathbf{r}\right\rangle = \hat{R}_1\hat{R}_2\left|\mathbf{r}\right\rangle$$

Similarly

$$\left|\Re_1\Re_2\Re_3\mathbf{r}\right\rangle = \hat{R}_1\left|\Re_2\Re_3\mathbf{r}\right\rangle = \hat{R}_1\hat{R}_2\left|\Re_3\mathbf{r}\right\rangle = \hat{R}_1\hat{R}_2\hat{R}_3\left|\mathbf{r}\right\rangle$$

Thus from the relation

$$\left|\Re_y(-d\alpha')\Re_x(d\alpha)\Re_y(d\alpha')\Re_x(-d\alpha)\mathbf{r}\right\rangle = \left|\Re_z(d\alpha d\alpha')\mathbf{r}\right\rangle$$

we get

$$\hat{R}_y(-d\alpha')\hat{R}_x(d\alpha)\hat{R}_y(d\alpha')\hat{R}_x(-d\alpha)\left|\mathbf{r}\right\rangle = \hat{R}_z(d\alpha d\alpha')\left|\mathbf{r}\right\rangle$$

or

$$[(\hat{1}+\frac{i}{\hbar}d\alpha'\hat{J}_y - \frac{(d\alpha')^2}{2\hbar^2}\hat{J}_y{}^2][\hat{1}-\frac{i}{\hbar}d\alpha\hat{J}_x - \frac{(d\alpha)^2}{2\hbar^2}\hat{J}_x{}^2][\hat{1}-\frac{i}{\hbar}d\alpha'\hat{J}_y - \frac{(d\alpha')^2}{2\hbar^2}\hat{J}_y{}^2](\hat{1}+\frac{i}{\hbar}d\alpha\hat{J}_x - \frac{(d\alpha)^2}{2\hbar^2}\hat{J}_x{}^2]$$

$$= \hat{1} - \frac{i}{\hbar}d\alpha d\alpha'\hat{J}_z$$

The left-hand side $= \hat{1} - \frac{d\alpha d\alpha'}{\hbar^2}(\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x) + ...$ Expanding the left-hand side and setting the coefficients of dαdα' equal, we find

$$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$$

In general

$$[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k$$

(i) $\hat{J}_i$ is the generator of rotation about the *i*-th axis.
(ii) Rotations about different axes fail to commute.

$$\hat{R}^{+}(d\alpha)\hat{R}(d\alpha) = \hat{1} \text{ (unitary operator)}$$

$$(\hat{1} + \frac{i}{\hbar} d\alpha \hat{J}_z^{+})(\hat{1} - \frac{i}{\hbar} d\alpha \hat{J}_z) = \hat{1}$$

or

$$\hat{J}_z^{+} = \hat{J}_z \text{ (Hermitian)}$$

((Note)) Here we consider the discussion by Sakurai.

$$\Re_x(\varepsilon)\Re_y(\varepsilon) - \Re_y(\varepsilon)\Re_x(\varepsilon) = \Re_z(\varepsilon^2) - I$$

The rotation analogue would read

$$\hat{R}_x(\varepsilon)\hat{R}_y(\varepsilon) - \hat{R}_y(\varepsilon)\hat{R}_x(\varepsilon) = \hat{R}_z(\varepsilon^2) - \hat{I}$$

$$[\hat{1} - \frac{i}{\hbar}\varepsilon\hat{J}_x - \frac{\varepsilon^2}{2\hbar^2}\hat{J}_x{}^2][\hat{1} - \frac{i}{\hbar}\varepsilon\hat{J}_y - \frac{\varepsilon^2}{2\hbar^2}\hat{J}_y{}^2] - [\hat{1} - \frac{i}{\hbar}\varepsilon\hat{J}_y - \frac{\varepsilon^2}{2\hbar^2}\hat{J}_y{}^2][\hat{1} - \frac{i}{\hbar}\varepsilon\hat{J}_x - \frac{\varepsilon^2}{2\hbar^2}\hat{J}_x{}^2]$$

$$= [\hat{1} - \frac{i}{\hbar}\varepsilon^2\hat{J}_z - \frac{\varepsilon 4}{2\hbar^2}\hat{J}_x{}^2] - \hat{1}$$

27.9 Invariance of $\hat{H}$ is invariant under the rotation

Suppose that the Hamiltonian $\hat{H}$ is invariant under the rotation (spherically symmetric).

$$\langle\psi'|\hat{H}|\psi'\rangle = \langle\psi|\hat{H}|\psi\rangle$$

with

$$|\psi'\rangle = \hat{R}|\psi\rangle$$

or

$$\langle\psi'| = \langle\psi|\hat{R}^{+}$$

Then we have

$$\langle\psi|\hat{R}^{+}\hat{H}\hat{R}|\psi\rangle=\langle\psi|\hat{H}|\psi\rangle$$

or

$$\hat{R}^{+}\hat{H}\hat{R}=\hat{H}$$

or

$$[\hat{H},\hat{R}]=\hat{0}$$

Since

$$\hat{R}=\exp[-\frac{i}{\hbar}\hat{J}.\mathbf{n}\theta]$$

or

$$\hat{R}=\hat{1}-\frac{i}{\hbar}\hat{J}.\mathbf{n}\delta\theta \text{ (infinitesimal rotation).}$$

or

$$[\hat{H},\hat{J}.\mathbf{n}]=\hat{0}$$

or

$$[\hat{H},\hat{J}_x]=\hat{0},\qquad [\hat{H},\hat{J}_y]=\hat{0},\qquad [\hat{H},\hat{J}_z]=\hat{0}$$

Using these relations, we also have the commutation relation

$$[\hat{H},\hat{J}_x{}^2+\hat{J}_y{}^2+\hat{J}_z{}^2]=\hat{0}.$$

((**Proof**))

$$[\hat{H},\hat{J}_x{}^2]=\hat{H}\hat{J}_x\hat{J}_x-\hat{J}_x\hat{J}_x\hat{H}=\hat{H}\hat{J}_x\hat{J}_x-\hat{J}_x\hat{H}\hat{J}_x=[\hat{H},\hat{J}_x]\hat{J}_x=\hat{0}$$

Thus we have the two commutation relations.

$$[\hat{H},\hat{J}_z]=\hat{0},\qquad [\hat{H},\hat{J}^2]=\hat{0}$$

Simultaneous eigenket

$$\hat{H}|n, j, m\rangle = E_n |n, j, m\rangle$$

$$\hat{J}_z |n, j, m\rangle = \hbar m |n, j, m\rangle$$

$$\hat{J}^2 |n, j, m\rangle = \hbar^2 j(j+1) |n, j, m\rangle$$

27.10 Commutation relations

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z, \qquad [\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x, \qquad [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$$

Generalization: definition of an angular momentum.
The origin of the above relations lies in the geometric properties of rotations in three-dimensional space.

Now we define an angular momentum $\hat{J}_i$ (i = x, y, z) as any set of three observables satisfying

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z, \qquad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x, \qquad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

$$\hat{J}^2 = \hat{J}_x^{\ 2} + \hat{J}_y^{\ 2} + \hat{J}_z^{\ 2}$$

$$[\hat{J}^2, \hat{J}_x] = \hat{0}, \quad [\hat{J}^2, \hat{J}_y] = \hat{0}, \quad [\hat{J}^2, \hat{J}_z] = \hat{0}$$

27.11 General theory of angular momentum

(a) $\hat{J}_+$ and $\hat{J}_-$

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$$

where

$$\hat{J}_+^{\ +} = \hat{J}_-, \qquad \hat{J}_-^{\ +} = \hat{J}_+$$

$$[\hat{J}_z, \hat{J}_+] = \hbar \hat{J}_+, \qquad [\hat{J}_z, \hat{J}_-] = -\hbar \hat{J}_-, \qquad [\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_z$$

$$[\hat{J}^2, \hat{J}_+] = [\hat{J}^2, \hat{J}_-] = [\hat{J}^2, \hat{J}_z] = \hat{0}$$

$$\hat{J}_+ \hat{J}_- = \hat{J}^2 - \hat{J}_z^{\ 2} + \hbar \hat{J}_z$$

$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_z{}^2 - \hbar\hat{J}_z$$

Thus we have

$$\hat{J}^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z{}^2$$

Formula:

$$[\mathbf{a}\cdot\hat{\mathbf{J}}, \mathbf{b}\cdot\hat{\mathbf{J}}] = i\hbar(\mathbf{a}\times\mathbf{b})\cdot\hat{\mathbf{J}}$$

((Proof))

$$I = [\mathbf{a}\cdot\hat{\mathbf{J}}, \mathbf{b}\cdot\hat{\mathbf{J}}] = \sum_{i,j} a_i b_j [\hat{J}_i, \hat{J}_j]$$

Since

$$[\hat{J}_i, \hat{J}_j] = i\hbar\varepsilon_{ijk}\hat{J}_k$$

then

$$I = \sum_{i,j} a_i b_j i\hbar\varepsilon_{ijk}\hat{J}_k = i\hbar(\mathbf{a}\times\mathbf{b})\cdot\hat{J}$$

(b) Notation for the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$

For any ket $|\psi\rangle$

$$\langle\psi|\hat{J}^2|\psi\rangle = \langle\psi|\hat{J}_x{}^2|\psi\rangle + \langle\psi|\hat{J}_y{}^2|\psi\rangle + \langle\psi|\hat{J}_z{}^2|\psi\rangle$$
$$= \langle\psi|\hat{J}_x{}^+\hat{J}_x|\psi\rangle + \langle\psi|\hat{J}_y{}^+\hat{J}_y|\psi\rangle + \langle\psi|\hat{J}_z{}^+\hat{J}_z|\psi\rangle \geq 0$$

For an eigenket $|\psi_\alpha\rangle$

$$\hat{J}^2|\psi_\alpha\rangle = \alpha|\psi_\alpha\rangle$$

$$\langle\psi_\alpha|\hat{J}^2|\psi_\alpha\rangle = \alpha\langle\psi_\alpha|\psi_\alpha\rangle = \alpha \geq 0$$

We shall write

$$\hat{J}^2|\psi_\alpha\rangle = \hbar^2 j(j+1)|\psi_\alpha\rangle = \lambda\hbar^2|\psi_\alpha\rangle$$

where

$$\lambda = j(j+1) \geq 0$$

27.12 Eigenvalue equations for $\hat{J}^2$ and $\hat{J}_z$

$$|\psi_\alpha\rangle = |j,m\rangle$$

$|j.m\rangle$ is the simultaneous eigenket of $\hat{J}^2$ and $\hat{J}_z$, since $[\hat{J}^2, \hat{J}_z] = \hat{0}$

$$\hat{J}^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle$$

$$\hat{J}_z |j,m\rangle = \hbar m |j,m\rangle$$

Eigenvalues of $\hat{J}^2$ and $\hat{J}_z$

Lemma 1 (Properties of eigenvalues of $\hat{J}^2$ and $\hat{J}_z$)

j and *m* satisfy the inequality

$-j \leq m \leq j$

((**Proof**))

$$\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle \geq 0$$

$$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle \geq 0$$

We find

$$\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle = \langle j,m|\hat{J}^2 - \hat{J}_z^2 - \hbar\hat{J}_z|j,m\rangle = \hbar^2[j(j+1) - m(m+1)] \geq 0$$

and

$$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = \langle j,m|\hat{J}^2 - \hat{J}_z^2 + \hbar\hat{J}_z|j,m\rangle = \hbar^2[j(j+1) - m(m-1)] \geq 0$$

Then we have

$$[j(j+1) - m(m+1)] = (j-m)(j+m+1) \geq 0$$

$$[j(j+1)-m(m-1)]=(j-m+1)(j+m)\geq 0$$

Then

$$-(j+1)\leq m\leq j$$

and

$$-j\leq m\leq j+1$$

If $-j\leq m\leq j$, these two conditions are satisfied simultaneously.

Lemma II (Properties of the ket vector of $\hat{J}_{-}|j,m\rangle$)

(i) If m = -j, $\hat{J}_{-}|j,m\rangle=\hat{0}$

(ii) If m>-j, $\hat{J}_{-}|j,m\rangle$ is a non-null eigenket of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j(j+1)\hbar^2$ and $(m-1)\hbar$.

((**Proof of (i)**))

Since

$$\langle j,m|\hat{J}_{+}\hat{J}_{-}|j,m\rangle=\hbar^2[(j+m)(j-m+1)]=0$$

for m = -j, we get

$$\hat{J}_{-}|j,m\rangle=\hat{0}$$

for m=-j.

Conversely,
if

$$\hat{J}_{-}|j,m\rangle=\hat{0}$$

then

$$\langle j,m|\hat{J}_{+}\hat{J}_{-}|j,m\rangle=\hbar^2[(j+m)(j-m+1)]=0$$

Then we have j = -m.

((**Proof of (ii)**))

Since

$$[\hat{J}^2, \hat{J}_-] = \hat{0}$$

$$[\hat{J}^2, \hat{J}_-]|j,m\rangle = \hat{0}$$

or

$$\hat{J}^2\hat{J}_-|j,m\rangle = \hat{J}_-\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)\hat{J}_-|j,m\rangle$$

So $\hat{J}_-|j,m\rangle$ is an eigenket of $\hat{J}^2$ with the eigenvalue $\hbar^2 j(j+1)$.

Moreover,

$$[\hat{J}_z, \hat{J}_-]|j,m\rangle = -\hbar\hat{J}_-|j,m\rangle$$

or

$$\hat{J}_z\hat{J}_-|j,m\rangle = \hat{J}_-\hat{J}_z|j,m\rangle - \hbar\hat{J}_-|j,m\rangle = \hbar(m-1)\hat{J}_-|j,m\rangle$$

So $\hat{J}_-|j,m\rangle$ is an eigenket of $\hat{J}_z$ with the eigenvalue $\hbar(m-1)$.

Lemma III (Properties of the ket vector of $\hat{J}_+|j,m\rangle$)

(i) If $m = j$, $\hat{J}_+|j,m\rangle = \hat{0}$

(ii) If $m<j$, $\hat{J}_+|j,m\rangle$ is a non-null eigenket of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j(j+1)\hbar^2$ and $(m+1)\hbar$.

[Proof of (i)]

$$\langle j,m|\hat{J}_-\hat{J}_+|j,m\rangle = \hbar^2[(j-m)(j+m+1)] \geq 0$$

If $m = j$, then $\hat{J}_+|j,m\rangle = \hat{0}$.

[Proof of (ii)]

$$[\hat{J}^2, \hat{J}_+] = \hat{0}$$

or

$$[\hat{J}^2, \hat{J}_+]|j,m\rangle = \hat{0}$$

or

$$\langle j,m|\hat{J}^2\hat{J}_+|j,m\rangle = \hbar^2 j(j+1)\hat{J}_+|j,m\rangle$$

$\hat{J}_+|j,m\rangle$ is an eigenket of $\hat{J}^2$ with an eigenvalues $\hbar^2 j(j+1)$.

$$[\hat{J}_z,\hat{J}_+]|j,m\rangle = \hbar\hat{J}_+|j,m\rangle$$

or

$$\hat{J}_z\hat{J}_+|j,m\rangle = \hat{J}_+\hat{J}_z|j,m\rangle + \hbar\hat{J}_+|j,m\rangle = \hbar(m+1)|j,m\rangle$$

$\hat{J}_+|j,m\rangle$ is an eigenket of $\hat{J}_z$ with an eigenvalues $\hbar(m+1)$.

27.13 Determination of the spectrum of $\hat{J}^2$ and $\hat{J}_z$.

There exists a positive or zero integer p such that

$$m - p = -j \tag{1}$$

$|j,m\rangle$: [eigenvalues $\hbar m$, $\hbar^2 j(j+1)$]

$\hat{J}_-|j,m\rangle$: [$\hbar(m-1)$, $\hbar^2 j(j+1)$]

$(\hat{J}_-)^2|j,m\rangle$: [$\hbar(m-2)$, $\hbar^2 j(j+1)$]

....

$(\hat{J}_-)^p|j,m\rangle$: [$\hbar(m-\mathrm{p})$, $\hbar^2 j(j+1)$]

$$(\hat{J}_-)^{p+1}|j,m\rangle = \hat{0}$$

There exists a positive or zero integer such that

$$m + q = j, \tag{2}$$

$|j,m\rangle$: [eigenvalues $\hbar\mathrm{m}$, $\hbar^2 j(j+1)$]

$\hat{J}_+|j,m\rangle$: [$\hbar(m+1)$, $\hbar^2 j(j+1)$]

$$\left(\hat{J}_{+}\right)^2 |\, j,m\rangle : [\hbar(m+2),\ \hbar^2 j(j+1)]$$

....

$$\left(\hat{J}_{+}\right)^q |\, j,m\rangle : [\hbar(m+q),\ \hbar^2 j(j+1)]$$

$$\left(\hat{J}_{+}\right)^{q+1} |\, j,m\rangle = \hat{0}$$

Combining Eqs.(1) and (2),

$$p + q = 2j$$

Since p and q are integers, j is therefore an integer or a half-integer.

$$j = 0,\ 1/2,\ 1,\ 3/2,\ 2,\ ....$$

$$m = -j,\ -j+1, ..., j-1,\ j.$$

(i) If j is an integer, then m is an integer.
(ii) If j is a half-integer, then m is a half-integer.

27.14 $|\, j,m\rangle$ representation

$$\langle j,m|\hat{J}_{-}\hat{J}_{+}|\, j,m\rangle = \langle j,m|\hat{J}^2 - \hat{J}_z^{\,2} - \hbar\hat{J}_z|\, j,m\rangle = \hbar^2[(j-m)(j+m+1)]$$

Since

$$\hat{J}_{+}|\, j,m\rangle = \alpha|\, j,m+1\rangle$$

we have

$$\langle j,m|\hat{J}_{-}\hat{J}_{+}|\, j,m\rangle = |\alpha|^2 = \hbar^2[(j-m)(j+m+1)]$$

Thus

$$\hat{J}_{+}|\, j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}\,|\, j,m+1\rangle$$

Similarly

$$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = \langle j,m|\hat{J}^2 - \hat{J}_z{}^2 + \hbar\hat{J}_z|j,m\rangle = \hbar^2[(j+m)(j-m+1)]$$

Since

$$\hat{J}_-|j,m\rangle = \beta|j,m-1\rangle$$

we have

$$\langle j,m|\hat{J}_+\hat{J}_-|j,m\rangle = |\beta|^2 = \hbar^2[(j+m)(j-m+1)]$$

or

$$\hat{J}_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle$$

In summary:

$$\hat{J}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle$$

$$\hat{J}_z|j,m\rangle = \hbar m|j,m\rangle$$

$$\hat{J}_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle$$

$$\hat{J}_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle$$

27.15 Matrix element of the angular momentum

Using Mathematica, you determine the matrix elements of $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$

$$\hat{J}^2|j.m\rangle = \hbar^2 j(j+1)|j.m\rangle$$

$$\hat{J}_z|j,m\rangle = \hbar m|j,m\rangle$$

$$\hat{J}_+|j,m\rangle = \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle$$

$$\hat{J}_-|j,m\rangle = \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle$$

Since

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y$$

$$\hat{J}_- = \hat{J}_x - i\hat{J}_y$$

we get

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$$

$$\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) = -\frac{i}{2}(\hat{J}_+ - \hat{J}_-)$$

$$\begin{aligned}\hat{J}_x|j,m\rangle &= \frac{1}{2}(\hat{J}_+ + \hat{J}_-)|j,m\rangle \\ &= \frac{\hbar}{2}(\sqrt{(j-m)(j+m+1)}|j,m+1\rangle + \sqrt{(j+m)(j-m+1)}|j,m-1\rangle)\end{aligned}$$

$$\begin{aligned}\hat{J}_y|j,m\rangle &= -\frac{i}{2}(\hat{J}_+ - \hat{J}_-)|j,m\rangle \\ &= -\frac{i\hbar}{2}(\sqrt{(j-m)(j+m+1)}|j,m+1\rangle - \sqrt{(j+m)(j-m+1)}|j,m-1\rangle)\end{aligned}$$

$$\hat{J}_z|j,m\rangle = \hbar m|j,m\rangle$$

Thus the matrix elements are expressed by

$$\begin{aligned}\langle j,m'|\hat{J}_x|j,m\rangle &= \frac{\hbar}{2}(\sqrt{(j-m)(j+m+1)}\langle j,m'|j,m+1\rangle + \sqrt{(j+m)(j-m+1)}\langle j,m'|j,m-1\rangle) \\ &= \frac{\hbar}{2}(\sqrt{(j-m)(j+m+1)}\delta_{m',m+1} + \sqrt{(j+m)(j-m+1)}\delta_{m',m-1})\end{aligned}$$

$$\begin{aligned}\langle j,m'|\hat{J}_y|j,m\rangle &= -\frac{i\hbar}{2}(\sqrt{(j-m)(j+m+1)}\langle j,m'|j,m+1\rangle - \sqrt{(j+m)(j-m+1)}\langle j,m'|j,m-1\rangle) \\ &= -\frac{i\hbar}{2}(\sqrt{(j-m)(j+m+1)}\delta_{m',m+1} - \sqrt{(j+m)(j-m+1)}\delta_{m',m-1})\end{aligned}$$

$$\langle j.m'|\hat{J}_z|j,m\rangle = m\hbar\langle j,m|j,m'\rangle = \hbar m\delta_{m,m'}$$

27.16 Matrix elements with *J*

$j = 1/2$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\hat{\sigma}_x,$$

$$\hat{J}_y = \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2}\hat{\sigma}_y,$$

$$\hat{J}_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\hat{\sigma}_z$$

where $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$ are the Pauli matrices.

$J = 1$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

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

$$\hat{J}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$J = 3/2$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}$$

$$\hat{J}_y = \begin{pmatrix} 0 & \frac{-i\sqrt{3}}{2} & 0 & 0 \\ \frac{i\sqrt{3}}{2} & 0 & -i & 0 \\ 0 & i & 0 & \frac{-i\sqrt{3}}{2} \\ 0 & 0 & \frac{i\sqrt{3}}{2} & 0 \end{pmatrix}$$

$$\hat{J}_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

$J = 2$

$$\hat{J}_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\hat{J}_y = \begin{pmatrix} 0 & -i & 0 & 0 & 0 \\ i & 0 & -i\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & i\sqrt{\frac{3}{2}} & 0 & -i\sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & i\sqrt{\frac{3}{2}} & 0 & -i \\ 0 & 0 & 0 & i & 0 \end{pmatrix}$$

$$\hat{J}_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

$J = 5/2$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{\sqrt{5}}{2} & 0 & 0 & 0 & 0 \\ \frac{\sqrt{5}}{2} & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & \frac{3}{2} & 0 & 0 \\ 0 & 0 & \frac{3}{2} & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & \frac{\sqrt{5}}{2} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{5}}{2} & 0 \end{pmatrix},$$

$$\hat{J}_y = \begin{pmatrix} 0 & \frac{-i\sqrt{5}}{2} & 0 & 0 & 0 & 0 \\ \frac{i\sqrt{5}}{2} & 0 & -i\sqrt{2} & 0 & 0 & 0 \\ 0 & i\sqrt{2} & 0 & -\frac{3i}{2} & 0 & 0 \\ 0 & 0 & \frac{3i}{2} & 0 & -i\sqrt{2} & 0 \\ 0 & 0 & 0 & i\sqrt{2} & 0 & \frac{-i\sqrt{5}}{2} \\ 0 & 0 & 0 & 0 & \frac{i\sqrt{5}}{2} & 0 \end{pmatrix}$$

$$\hat{J}_z = \begin{pmatrix} \frac{5}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{5}{2} \end{pmatrix}$$

$J = 3$

$$\hat{J}_x = \begin{pmatrix} 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{5}{2}} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{5}{2}} & 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & \sqrt{\frac{5}{2}} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{5}{2}} & 0 & \sqrt{\frac{3}{2}} \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} & 0 \end{pmatrix}$$

$$\hat{J}_y = \begin{pmatrix} 0 & -i\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ i\sqrt{\frac{3}{2}} & 0 & -i\sqrt{\frac{5}{2}} & 0 & 0 & 0 & 0 \\ 0 & i\sqrt{\frac{5}{2}} & 0 & -i\sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & i\sqrt{3} & 0 & -i\sqrt{\frac{5}{2}} & 0 \\ 0 & 0 & 0 & 0 & i\sqrt{\frac{5}{2}} & 0 & -i\sqrt{\frac{3}{2}} \\ 0 & 0 & 0 & 0 & 0 & i\sqrt{\frac{3}{2}} & 0 \end{pmatrix}$$

$$\hat{J}_z = \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}$$

$j = 7/2$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{\sqrt{7}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{\sqrt{7}}{2} & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & \frac{\sqrt{15}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{15}}{2} & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & \frac{\sqrt{15}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\sqrt{15}}{2} & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & \frac{\sqrt{7}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\sqrt{7}}{2} & 0 \end{pmatrix}$$

$$\hat{J}_x = \begin{pmatrix} 0 & \frac{-i\sqrt{7}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{i\sqrt{7}}{2} & 0 & -i\sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & i\sqrt{3} & 0 & \frac{-i\sqrt{15}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i\sqrt{15}}{2} & 0 & -2i & 0 & 0 & 0 \\ 0 & 0 & 0 & 2i & 0 & \frac{-i\sqrt{15}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{i\sqrt{15}}{2} & 0 & -i\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & i\sqrt{3} & 0 & \frac{-i\sqrt{7}}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{i\sqrt{7}}{2} & 0 \end{pmatrix}$$

$$\hat{J}_z = \begin{pmatrix} \frac{7}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{5}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{5}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{7}{2} \end{pmatrix}$$

27.17 Mathematica

We make a program for the matrix elements in Mathematica. For simplicity, we use the unit of $\hbar = 1$.

((Mathematica))

```
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];
```

Matices for J=3/2

```
Table[Jx[3 / 2, p, q], {p, 3 / 2, -3 / 2, -1}, {q, 3 / 2, -3 / 2, -1}] // MatrixForm
```

$$\begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}$$

```
Table[Jy[3 / 2, p, q], {p, 3 / 2, -3 / 2, -1}, {q, 3 / 2, -3 / 2, -1}] // MatrixForm
```

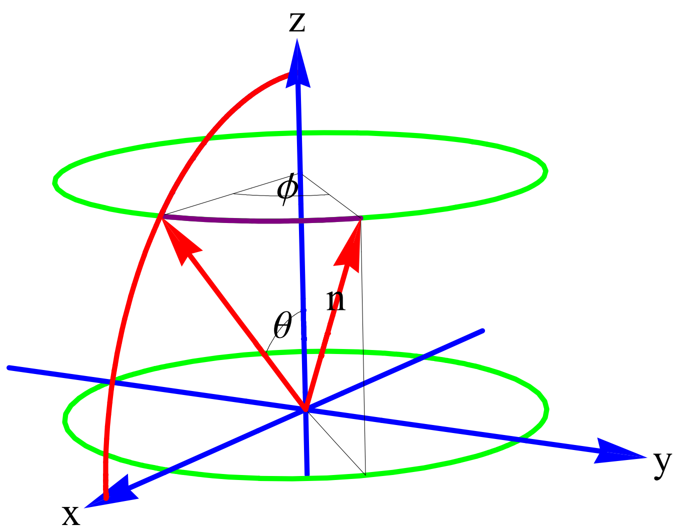
$$\begin{pmatrix} 0 & -\frac{i\sqrt{3}}{2} & 0 & 0 \\ \frac{i\sqrt{3}}{2} & 0 & -i & 0 \\ 0 & i & 0 & -\frac{i\sqrt{3}}{2} \\ 0 & 0 & \frac{i\sqrt{3}}{2} & 0 \end{pmatrix}$$

```
Table[Jz[3 / 2, p, q], {p, 3 / 2, -3 / 2, -1}, {q, 3 / 2, -3 / 2, -1}] // MatrixForm
```

$$\begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

27.18 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

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

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 $d_{m'm}^{(j)}(\theta)$.

27.19 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 $\left|+\right\rangle_n$ and $\left|-\right\rangle_n$ are obtained as

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

and

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

where **n** is the unit vector given by

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

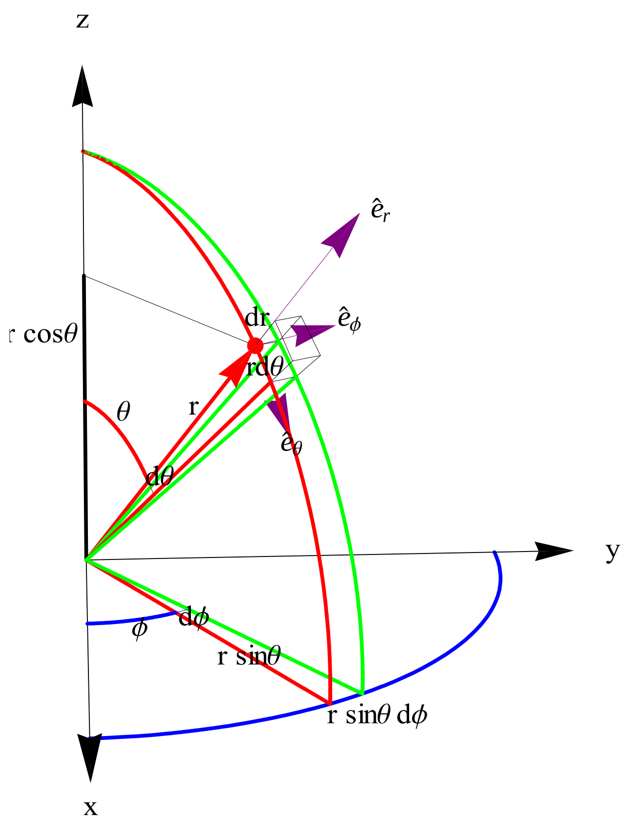
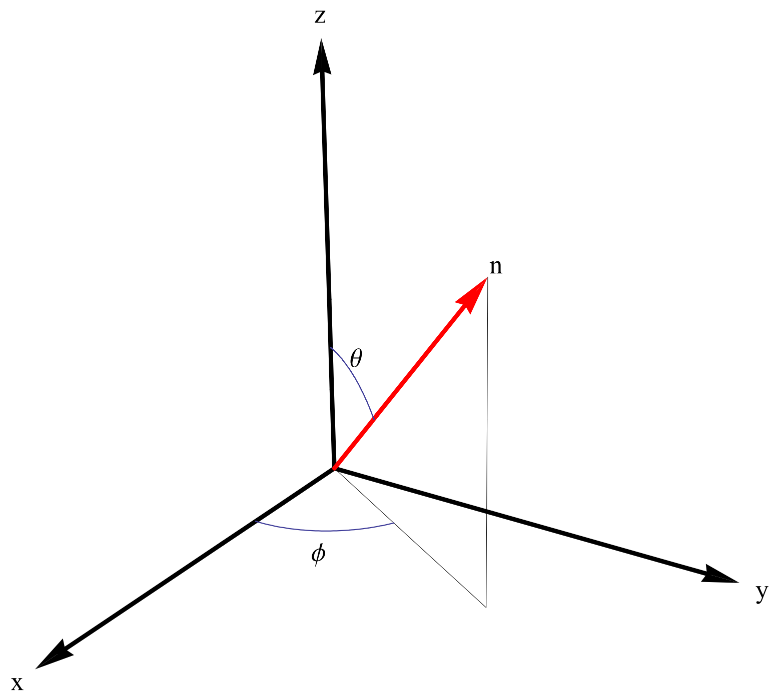


Fig. $r = 1$. $\hat{n} = \mathbf{e}_r$.



27.20 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 $\left|1\right\rangle_n$, $\left|0\right\rangle_n$, and $\left|-1\right\rangle_n$ 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
```

$$\begin{pmatrix} e^{-i\phi}\cos\left[\frac{\theta}{2}\right]^2 & -\frac{e^{-i\phi}\sin[\theta]}{\sqrt{2}} & e^{-i\phi}\sin\left[\frac{\theta}{2}\right]^2 \\ \frac{\sin[\theta]}{\sqrt{2}} & \cos[\theta] & -\frac{\sin[\theta]}{\sqrt{2}} \\ e^{i\phi}\sin\left[\frac{\theta}{2}\right]^2 & \frac{e^{i\phi}\sin[\theta]}{\sqrt{2}} & e^{i\phi}\cos\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

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

$$\left\{e^{-i\phi}\cos\left[\frac{\theta}{2}\right]^2, \frac{\sin[\theta]}{\sqrt{2}}, e^{i\phi}\sin\left[\frac{\theta}{2}\right]^2\right\}$$

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

$$\left\{-\frac{e^{-i\phi}\sin[\theta]}{\sqrt{2}}, \cos[\theta], \frac{e^{i\phi}\sin[\theta]}{\sqrt{2}}\right\}$$

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

$$\left\{e^{-i\phi}\sin\left[\frac{\theta}{2}\right]^2, -\frac{\sin[\theta]}{\sqrt{2}}, e^{i\phi}\cos\left[\frac{\theta}{2}\right]^2\right\}$$

27.21 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
```

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

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

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

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

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

27.22 Mathematica for the rotation operator with *J*=2

Matrices j = 2

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

$$\texttt{Jx}[\ell\_, n\_, m\_] := \frac{1}{2}\sqrt{(\ell - m)\ (\ell + m + 1)}\ \texttt{KroneckerDelta}[n, m + 1] + \frac{1}{2}\sqrt{(\ell + m)\ (\ell - m + 1)}\ \texttt{KroneckerDelta}[n, m - 1]$$

$$\texttt{Jy}[\ell\_, n\_, m\_] := -\frac{1}{2}\, i\, \sqrt{(\ell - m)\ (\ell + m + 1)}\ \texttt{KroneckerDelta}[n, m + 1] + \frac{1}{2}\, i\, \sqrt{(\ell + m)\ (\ell - m + 1)}\ \texttt{KroneckerDelta}[n, m - 1]$$

$$\texttt{Jz}[\ell\_, n\_, m\_] := m\ \texttt{KroneckerDelta}[n, m]$$

```
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
```

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

27.23 Spherical Harmonics as rotator matrices

Using the relation

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

we have

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

Then

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

Here note that

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

or

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

We also note that

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

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

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

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

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

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

REFERENCES

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