Rotation operator and angular momentum

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date, September 23, 2014)

The commutation relations between the components of an angular momentum are actually the expression of the geometrical properties of rotation in ordinary three dimensional space. Here we discuss the relation between rotations and angular momentum operators. We consider a physical system whose quantum mechanical state is characterized by the ket $|\psi\rangle$ of the state space. We perform a rotation $\Re$ on this system. In this new position, the state of the system is described by a ket $|\psi'\rangle$. Given the geometrical transformation $\Re$, the problem is to determine the new state $|\psi'\rangle$ from $|\psi\rangle$. With every geometrical rotation $\Re$ can be associated a linear operator $\hat{R}$ acting such that

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

where $\hat{R}$ is related to the corresponding angular momentum $\hat{\boldsymbol{J}}$. We will show that

$$\hat{R}|\boldsymbol{r}\rangle = |\Re\boldsymbol{r}\rangle, \qquad \hat{R}^{+}|\boldsymbol{r}\rangle = |\Re^{-1}\boldsymbol{r}\rangle$$

where $\Re\boldsymbol{r}$ is the geometrical rotation in the three dimensional space.

1. Rotation operator in Quantum mechanics

After the geometrical rotation;

$$\boldsymbol{r} \rightarrow \Re\boldsymbol{r} = \boldsymbol{r}' \text{ (geometrical rotation)}$$

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

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

or

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

or

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

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),

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

Here we calculate

$$\hat{\boldsymbol{r}}\hat{R}|\boldsymbol{r}\rangle=\hat{R}\Re\hat{\boldsymbol{r}}|\boldsymbol{r}\rangle=\hat{R}\Re\boldsymbol{r}|\boldsymbol{r}\rangle=\Re\boldsymbol{r}\hat{R}|\boldsymbol{r}\rangle.$$

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

$$\hat{R}|\boldsymbol{r}\rangle=|\Re\boldsymbol{r}\rangle.$$

When

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

or

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

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

or

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

For any $\boldsymbol{r}$, we have

$$\left|\Re^{-1}\boldsymbol{r}\right\rangle = \hat{R}^{+}\left|\boldsymbol{r}\right\rangle$$

$$\hat{R}\hat{R}^{+}\left|\boldsymbol{r}\right\rangle = \hat{R}\left|\Re^{-1}\boldsymbol{r}\right\rangle = \left|\Re\Re^{-1}\boldsymbol{r}\right\rangle = \left|\boldsymbol{r}\right\rangle.$$

In summary, we have

1. $\hat{R}^{+}\hat{R} = \hat{R}\hat{R}^{+} = \hat{1}$.

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

3. $\left\langle\boldsymbol{r}\right|\hat{R}^{+} = \left\langle\Re\boldsymbol{r}\right|$.

4. $\hat{R}^{+}\left|\boldsymbol{r}\right\rangle = \left|\Re^{-1}\boldsymbol{r}\right\rangle$.

5. $\left\langle\boldsymbol{r}\right|\hat{R} = \left\langle\Re^{-1}\boldsymbol{r}\right|$.

2. Group properties of the rotation operator

Here we show that the operator $\hat{R}$ has the same group properties as $\Re$:

(a) Identity

$$\left|\Re\cdot 1\boldsymbol{r}\right\rangle = \left|\Re\boldsymbol{r}\right\rangle,$$

or

$$\hat{R}\cdot\hat{1}\left|\boldsymbol{r}\right\rangle = \hat{R}\left|\boldsymbol{r}\right\rangle,$$

or

$$\hat{R}\cdot\hat{1} = \hat{R}.$$

(b) Closure

$$\left|\Re_1\Re_2\boldsymbol{r}\right\rangle = \left|\Re_3\boldsymbol{r}\right\rangle,$$

or

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

or

$$\hat{R}_1\hat{R}_2|\boldsymbol{r}\rangle = \hat{R}_3|\boldsymbol{r}\rangle ,$$

Then for any $|\boldsymbol{r}\rangle$, we have

$$\hat{R}_1\hat{R}_2 = \hat{R}_3 .$$

(c) Inverse

$$|\Re\Re^{-1}\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle ,$$

or

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

or

$$\hat{R}\hat{R}^{-1}|\boldsymbol{r}\rangle = |\boldsymbol{r}\rangle ,$$

or

$$\hat{R}\hat{R}^{-1} = \hat{1} .$$

Similarly,

$$\hat{R}^{-1}\hat{R} = \hat{1} .$$

(d) Associative

$$|\Re_1(\Re_2\Re_3)\boldsymbol{r}\rangle = |(\Re_1\Re_2)\Re_3\boldsymbol{r}\rangle = |\Re_1\Re_2\Re_3\boldsymbol{r}\rangle$$

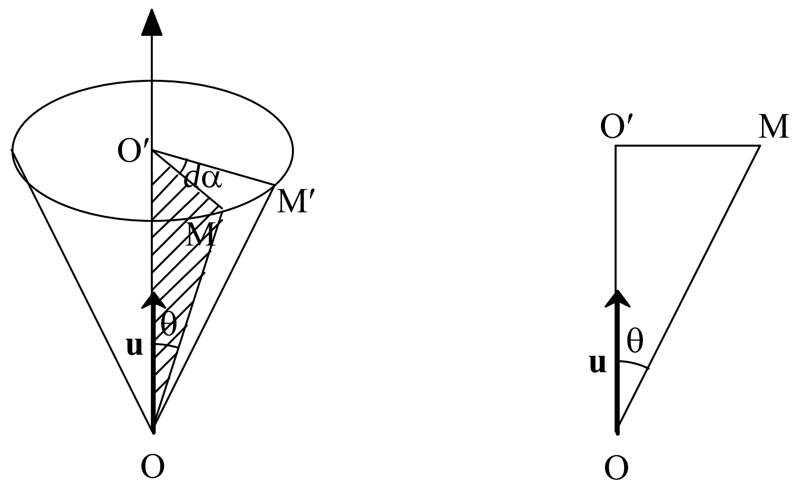
or

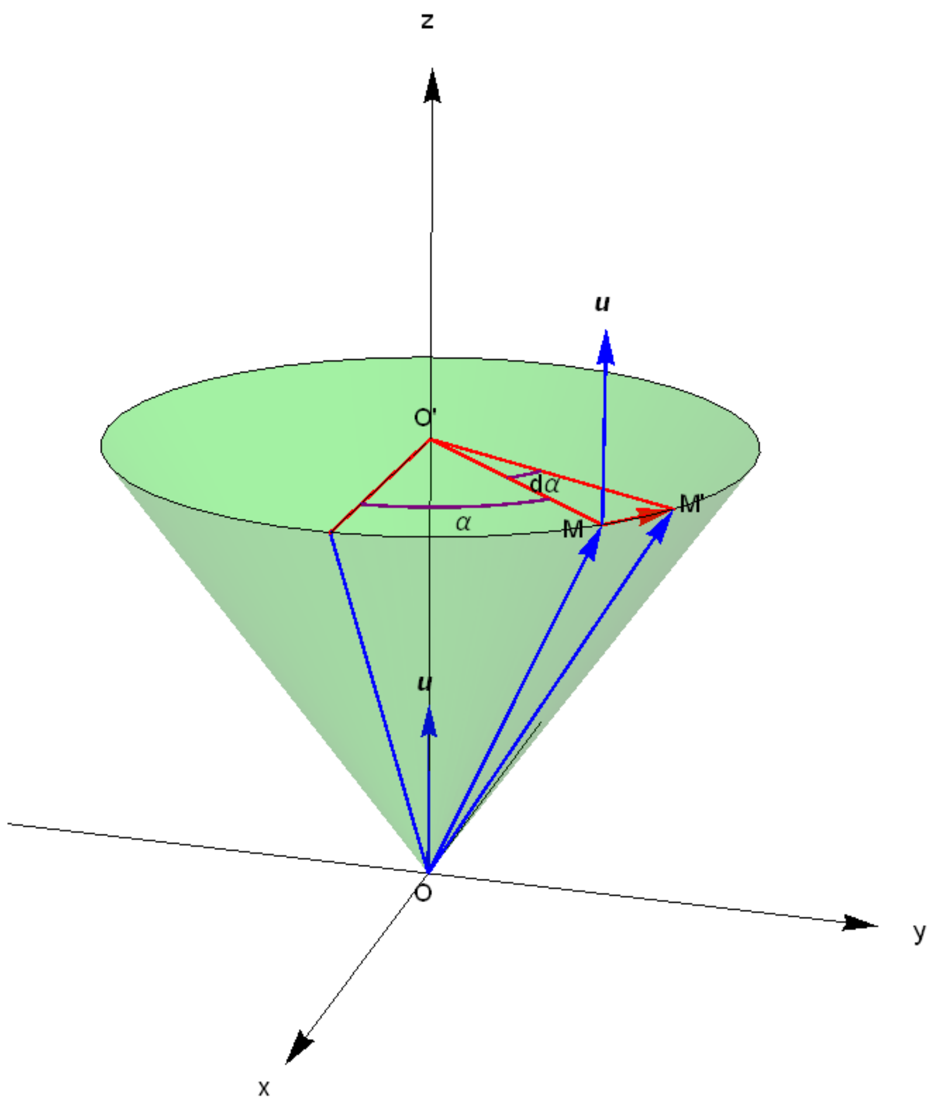
$$\hat{R}_1(\hat{R}_2\hat{R}_3)|\boldsymbol{r}\rangle = (\hat{R}_1\hat{R}_2)\hat{R}_3|\boldsymbol{r}\rangle = \hat{R}_1\hat{R}_2\hat{R}_3|\boldsymbol{r}\rangle$$

or

$$\hat{R}_1(\hat{R}_2\hat{R}_3) = (\hat{R}_1\hat{R}_2)\hat{R}_3 = \hat{R}_1\hat{R}_2\hat{R}_3$$

3. Theorem-I





$\Re_{\mathbf{u}}(d\alpha)$: 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 $\mathbf{u}\times\overrightarrow{OM}$. θ is the angle between ***u*** and $\overrightarrow{OM}$

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

4. Theorem II

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.

5. Proof of theorems by 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***, #]&

(the most important formula in Mathematica).

(5) Rotation:

R[***u***, *α*][***r***]

((**Mathematica-I**))

Geometrical rotation

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

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

Definition of geometrical rotation

```
R[u_, δ_] := # + δ Cross[u, #] &;

R[ez, dα][r]

{x - dα y, dα x + y, z}
```

Theorem 1

ℝ[ez,dα1]ℝ[ez,dα2]=ℝ[ez,dα2]ℝ[ez,dα1]=ℝ[ez,dα1+dα2]

where

ℝ is a geometrical rotation

dα1 and dα2 are infinitesimal rotation angles

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

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

```
eq11 = R[ez, dα2][R[ez, dα1][r]] // Simplify
```

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

```
eq12 = R[ez, dα1 + dα2][r] // Simplify
```

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

```
eq11 - eq12 // 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]

```
r1 = R[ex, -dα1][r]; r2 = R[ey, dα2][r1] // Simplify;
r3 = R[ex, dα1][r2] // Simplify;
```

```
eq21 = R[ey, -dα2][r3] // Simplify
```

$\{(1 + d\alpha 2^2)\, x - d\alpha 1\, d\alpha 2\, (y + d\alpha 1\, z),$
$d\alpha 1\, d\alpha 2\, x + y + d\alpha 1^2\, y,\ -d\alpha 1\, d\alpha 2^2\, y + z + d\alpha 1^2\, z + d\alpha 2^2\, z\}$

```
eq22 = R[ez, dα1 dα2][r] // Simplify
```

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

```
eq21 - eq22 // Simplify
```

$\{d\alpha 2\, (d\alpha 2\, x - d\alpha 1^2\, z),\ d\alpha 1^2\, y,\ -d\alpha 1\, d\alpha 2^2\, y + d\alpha 1^2\, z + d\alpha 2^2\, z\}$

Theorem 3

ℝ[-ez,dα]ℝ[ez,dα]=1

```
r6 = R[-ez, dα][r]; eq3 = R[ez, dα][r6] // Simplify
```

$\{(1 + d\alpha^2)\, x,\ (1 + d\alpha^2)\, y,\ z\}$

Theorem 2

$\mathbb{R}[ey,-d\alpha 2]\mathbb{R}[ex,d\alpha 1]\mathbb{R}[ey,d\alpha 2]\mathbb{R}[ex,-d\alpha 1]=\mathbb{R}[ez,d\alpha 1 d\alpha 2]$

```
r1 = R[ex, -dα1][r]
{x, y + dα1 z, -dα1 y + z}

r2 = R[ey, dα2][r1] // Simplify
{x + dα2 (-dα1 y + z), y + dα1 z, -dα2 x - dα1 y + z}

r3 = R[ex, dα1][r2] // Simplify
{x + dα2 (-dα1 y + z), dα1 dα2 x + y + dα1^2 y, -dα2 x + z + dα1^2 z}

r4 = R[ey, -dα2][r3] // 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}

r5 = R[ez, dα1 dα2][r] // Simplify
{x - dα1 dα2 y, dα1 dα2 x + y, z}

r5 - r4 // Simplify
{dα2 (-dα2 x + dα1^2 z), -dα1^2 y, dα1 dα2^2 y - dα1^2 z - dα2^2 z}
```

Theorem 3

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

```
r6 = R[-ez, dα][r]
{x + dα y, -dα x + y, z}

r7 = R[ez, dα][r6] // Simplify
{(1 + dα^2) x, (1 + dα^2) y, z}
```

6. Summary for the geometrical rotation

The above calculations are summarized as follows.

(a) Theorem-1

$$\Re_z(d\alpha_1)\Re_z(d\alpha_2)\boldsymbol{r} = \Re_z(d\alpha_2)\Re_z(d\alpha_1)\boldsymbol{r} = \Re_z(d\alpha_1 + d\alpha_1)\boldsymbol{r}$$
$$= (x - yd\alpha_1 - yd\alpha_2, y + xd\alpha_1 + xd\alpha_2, z)$$

2. Theorem-2

$$\Re_y(-d\alpha_2)\Re_x(d\alpha_1)\Re_y(d\alpha_2)\Re_x(-d\alpha_1)\boldsymbol{r}$$
$$= (x + x(d\alpha_2)^2 - yd\alpha_1 d\alpha_2, y + (d\alpha_1)^2 y + xd\alpha_1 d\alpha_2, z + z(d\alpha_1)^2 + y(d\alpha_2)^2)$$
$$\approx (x - yd\alpha_1 d\alpha_2, y + xd\alpha_1 d\alpha_2, z)$$

$$\Re_z(d\alpha_1 d\alpha_2)\boldsymbol{r}$$
$$= (x - yd\alpha_1 d\alpha_2, y + xd\alpha_1 d\alpha_2, z)$$

3. Theorem-3

$$\Re_{-z}(d\alpha)\Re_z(d\alpha)\boldsymbol{r}$$
$$= (x + x(d\alpha)^2, y + x(d\alpha)^2, z)$$
$$\approx (x, y, z)$$

where the angle $d\alpha$ is infinitesimally small.

---

7. Expression of rotation operator

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

Using

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

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

((**Mathematica**))

```
Clear["Global`*"]; ex = {1, 0, 0}; ey = {0, 1, 0}; ez = {0, 0, 1};
r = {x, y, z}; R[u_, δ_] := # + δ CrossProduct[u, #] &;

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

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

R[-ez, dα][AP] // Simplify
{(1 + dα^2) x, (1 + dα^2) y, z}

R[ez, dα][AM] // Simplify
{(1 + dα^2) x, (1 + dα^2) y, z}

R[ey, dα][r]
{x + dα z, y, -dα x + z}

R[ex, dα][r]
{x, y - dα z, dα y + 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

$$x' = x - yd\alpha$$
$$y' = y + xd\alpha$$

for the rotation; $\boldsymbol{r}' = \Re_z(d\alpha)\,\boldsymbol{r}$

Therefore we have

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

$$= \langle \boldsymbol{r} | 1 - \frac{i}{\hbar} d\alpha \hat{L}_z | \psi \rangle$$

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**))

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

We have the relation

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

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

and

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

Then we have

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

or

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

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

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

---

8. Finite rotation

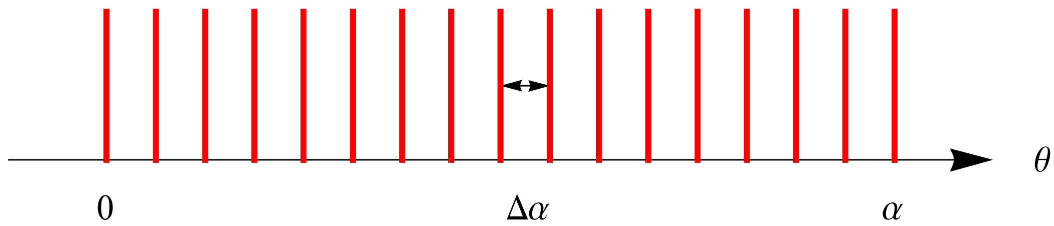


Fig. $\alpha = N\Delta\alpha$.

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

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

((**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 $\hat{\boldsymbol{J}}$ instead of $\hat{\boldsymbol{L}}$:

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

9. Commutation relations of the components of the angular momentum

The following discussion on this topics is seen in the book [C. Cohen-Tannoudji et al., Quantum Mechanics (John Wiley & Sons, New York, 1977].

We start from the relation for the geometrical operators

$$\Re_y(-d\alpha')\Re_x(d\alpha)\Re_y(d\alpha')\Re_x(-d\alpha) = \Re_z(d\alpha d\alpha') \qquad (1)$$

Note

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

Similarly

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

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

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

Correspondingly, we have

$$\hat{R}_y(-d\alpha')\hat{R}_x(d\alpha)\hat{R}_y(d\alpha')\hat{R}_x(-d\alpha) = \hat{R}_z(d\alpha d\alpha') \qquad (2)$$

Using the expression of the infinitesimal rotation operators, the commutation relation

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

can be derived as follows,

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

The left-hand side $= \hat{1} - \frac{d\alpha d\alpha'}{\hbar^2}(\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x) + \ldots$. 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

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

10. Commutation relations of the components of the angular momentum

The following discussion on this topics is seen in the book [M. Tinkham, Group Theory and Quantum Mechanics (McGraw-Hill Company, New York, 1964)].

When the angles θ_x and θ_y are very small, it is found that

$$\Re_x(\theta_x)\Re_y(\theta_y) = \Re_z(\theta_x\theta_y)\Re_y(\theta_y)\Re_x(\theta_x) .$$

(the proof is given later using the Mathematica). We note that

$$\Re_x(\theta_x)\Re_y(\theta_y)\boldsymbol{r} = (x + z\theta_y, y - z\theta_x + x\theta_x\theta_y, z + y\theta_x - x\theta_y)$$

and

$$\Re_z(\theta_x\theta_y)\Re_y(\theta_y)\Re_x(\theta_x)\boldsymbol{r} = (x + z\theta_y, y - z\theta_x + x\theta_x\theta_y, z + y\theta_x - x\theta_y)$$

where $\boldsymbol{r} = (x, y, z)$ in the 3D real space. Then we have

$$\left|\Re_x(\theta_x)\Re_y(\theta_y)\boldsymbol{r}\right\rangle = \left|\Re_z(\theta_x\theta_y)\Re_y(\theta_y)\Re_x(\theta_x)\boldsymbol{r}\right\rangle$$

or

$$\hat{R}_x(\theta_x)\hat{R}_y(\theta_y)\left|\boldsymbol{r}\right\rangle = \hat{R}_z(\theta_x\theta_y)\hat{R}_y(\theta_y)\hat{R}_x(\theta_x)\left|\boldsymbol{r}\right\rangle$$

leading to the relation for the rotation operators,

$$\hat{R}_x(\theta_x)\hat{R}_y(\theta_y) = \hat{R}_z(\theta_x\theta_y)\hat{R}_y(\theta_y)\hat{R}_x(\theta_x).$$

The infinitesimal rotation operators are defined by

$$\hat{R}_x(\theta_x) = \exp(-\frac{i}{\hbar}\theta_x\hat{J}_x) \approx \hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x,$$

$$\hat{R}_y(\theta_y) = \exp(-\frac{i}{\hbar}\theta_y\hat{J}_y) \approx \hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y$$

$$\hat{R}_z(\theta_x\theta_y) = \exp(-\frac{i}{\hbar}\theta_x\theta_y\hat{J}_z) \approx \hat{1} - \frac{i}{\hbar}\theta_x\theta_y\hat{J}_z$$

The substitution of these operators into the above relation, we get the relation

$$(\hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x)(\hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y) = (\hat{1} - \frac{i}{\hbar}\theta_x\theta_y\hat{J}_z)(\hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y)(\hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x).$$

We expand this relation up to the term proportional to $\theta_x\theta_y$.

Left hand side = $(\hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x)(\hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y) = \hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x + \hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y + \left(\frac{i}{\hbar}\right)^2\theta_x\theta_y\hat{J}_x\hat{J}_y + ...$

Right hand side== $\hat{1} - \frac{i}{\hbar}\theta_x\hat{J}_x + \hat{1} - \frac{i}{\hbar}\theta_y\hat{J}_y + \left(\frac{i}{\hbar}\right)^2\theta_x\theta_y\hat{J}_y\hat{J}_x - \frac{i}{\hbar}\theta_x\theta_y\hat{J}_z. + ...$

Then we have

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

Similarly we get

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

11. Derivation of the geometrical operators (Tinkham)

We show that

$$\Re_x(\theta_x)\Re_y(\theta_y)\mathbf{r} = (x + z\theta_y, y - z\theta_x + x\theta_x\theta_y, z + y\theta_x - x\theta_y)$$

and

$$\Re_z(\theta_x\theta_y)\Re_y(\theta_y)\Re_x(\theta_x)\mathbf{r} = (x + z\theta_y, y - z\theta_x + x\theta_x\theta_y, z + y\theta_x - x\theta_y)$$

by using the Mathematica.

((**Mathematica**)) Proof of the theorems 1, 2, and 3

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

Geometrical rotation

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

```
{x, y, z}
```

Definition of geometrical rotation

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

```
R[ez, dα][r]
```

```
{x - dα y, dα x + y, z}
```

Theorem 1
ℝ[ez,dα1] ℝ[ez,dα2] = ℝ[ez,dα2] ℝ[ez,dα1] = ℝ[ez,dα1+dα2]
where
ℝ is a geometrical rotation
dα1 and dα2 are infinitesimal rotation angles

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

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

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

{x − dα1 dα2 x − (dα1 + dα2) y,
 dα2 x + y + dα1 (x − dα2 y), z}

```
R[ez, dα1 + dα2][r] // Simplify
```

{x − (dα1 + dα2) y, (dα1 + dα2) x + y, z}

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

```
r1 = R[ex, -dα1][r]
```

{x, y + dα1 z, −dα1 y + z}

```
r2 = R[ey, dα2][r1] // Simplify
```

{x + dα2 (−dα1 y + z), y + dα1 z, −dα2 x − dα1 y + z}

```
r3 = R[ex, dα1][r2] // Simplify
```

$\{x + d\alpha 2\,(-d\alpha 1\, y + z),$
$d\alpha 1\, d\alpha 2\, x + y + d\alpha 1^2\, y,\ -d\alpha 2\, x + z + d\alpha 1^2\, z\}$

```
r4 = R[ey, -dα2][r3] // Simplify
```

$\{(1 + d\alpha 2^2)\ x - d\alpha 1\ d\alpha 2\ (y + d\alpha 1\ z),$
$d\alpha 1\ d\alpha 2\ x + y + d\alpha 1^2\ y,\ -d\alpha 1\ d\alpha 2^2\ y + z + d\alpha 1^2\ z + d\alpha 2^2\ z\}$

```
r5 = R[ez, dα1 dα2][r] // Simplify
```

$\{x - d\alpha 1\ d\alpha 2\ y,\ d\alpha 1\ d\alpha 2\ x + y,\ z\}$

```
r5 - r4 // Simplify
```

$\{d\alpha 2\ (-d\alpha 2\ x + d\alpha 1^2\ z),$
$-d\alpha 1^2\ y,\ d\alpha 1\ d\alpha 2^2\ y - d\alpha 1^2\ z - d\alpha 2^2\ z\}$

Theorem 3
ℝ[-ez, dα] ℝ[ez, dα] = 1

```
r6 = R[-ez, dα][r]
```

$\{x + d\alpha\ y,\ -d\alpha\ x + y,\ z\}$

```
r7 = R[ez, dα][r6] // Simplify
```

$\{(1 + d\alpha^2)\ x,\ (1 + d\alpha^2)\ y,\ z\}$

12. Derivation of the commutation relation [Sakurai, Townsend]

We start from the geometrical relation

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

where ε is the infinitesimally small angle. The rotation analogue for the rotation operators in the quantum mechanics, would read as

$$\hat{R}_x(\varepsilon)\hat{R}_y(\varepsilon) - \hat{R}_y(\varepsilon)\hat{R}_x(\varepsilon) = \hat{R}_z(\varepsilon^2) - \hat{1}$$

without proof. Then we get

$$(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_x-\frac{\varepsilon^2}{2\hbar^2}\hat{J}_x{}^2)(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_y-\frac{\varepsilon^2}{2\hbar^2}\hat{J}_y{}^2)-(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_y-\frac{\varepsilon^2}{2\hbar^2}\hat{J}_y{}^2)(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_x-\frac{\varepsilon^2}{2\hbar^2}\hat{J}_x{}^2)$$
$$=(\hat{1}-\frac{i}{\hbar}\varepsilon^2\hat{J}_z-\frac{\varepsilon^4}{2\hbar^2}\hat{J}_x{}^2)-\hat{1}$$

or

$$(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_x)+(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_x)(-\frac{i}{\hbar}\varepsilon\hat{J}_y)-(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_y)-(\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_y)(-\frac{i}{\hbar}\varepsilon\hat{J}_x)$$
$$=-\frac{i}{\hbar}\varepsilon^2\hat{J}_z$$

or

$$\hat{1}-\frac{i}{\hbar}\varepsilon\hat{J}_x-\frac{i}{\hbar}\varepsilon\hat{J}_y+(\frac{i}{\hbar})^2\varepsilon^2\hat{J}_x\hat{J}_y-\hat{1}+\frac{i}{\hbar}\varepsilon\hat{J}_y+\frac{i}{\hbar}\varepsilon\hat{J}_x-(\frac{i}{\hbar})^2\varepsilon^2\hat{J}_y\hat{J}_x$$
$$=-\frac{i}{\hbar}\varepsilon^2\hat{J}_z$$

or

$$(\frac{i}{\hbar})^2\varepsilon^2\hat{J}_x\hat{J}_y-(\frac{i}{\hbar})^2\varepsilon^2\hat{J}_y\hat{J}_x=-\frac{i}{\hbar}\varepsilon^2\hat{J}_z$$

This leads to the commutation relation

$$[\hat{J}_x,\hat{J}_y]=\hat{J}_x\hat{J}_y-\hat{J}_y\hat{J}_x=i\hbar\hat{J}_z \qquad \text{(commutation relation)}$$

Similarly we get

$$\left[\hat{J}_y,\hat{J}_z\right]=i\hbar\hat{J}_x, \qquad \left[\hat{J}_z,\hat{J}_x\right]=i\hbar\hat{J}_y. \qquad \text{(cyclic)}$$

((**Mathematica**)) Proof for the expression, $\Re_x(\varepsilon)\Re_y(\varepsilon)-\Re_y(\varepsilon)\Re_x(\varepsilon)=\Re_z(\varepsilon^2)-I$

```
Clear["Global`*"]; ex = {1, 0, 0}; ey = {0, 1, 0};
ez = {0, 0, 1}; I2 = IdentityMatrix[2];
r = {x, y, z}; R[u_, δ_] := # + δ Cross[u, #] &;
```

```
ry = R[ey, ϵ][r]
```

$\{x + z\epsilon, y, z - x\epsilon\}$

```
rx = R[ex, ϵ][r]
```

$\{x, y - z\epsilon, z + y\epsilon\}$

```
R1 = R[ex, ϵ][ry] // Simplify
```

$\{x + z\epsilon, y + \epsilon(-z + x\epsilon), z + (-x + y)\epsilon\}$

```
R2 = R[ey, ϵ][rx] // Simplify
```

$\{x + \epsilon(z + y\epsilon), y - z\epsilon, z + (-x + y)\epsilon\}$

```
R3 = R[ez, ϵ^2][r] // Simplify
```

$\{x - y\epsilon^2, y + x\epsilon^2, z\}$

```
R1 - R2 // Simplify
```

$\{-y\epsilon^2, x\epsilon^2, 0\}$

```
R1 - R2 - R3 // Simplify
```

$\{-x, -y, -z\}$

13. Invariance of $\hat{H}$ 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

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

or

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

or

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

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

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

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

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

REFERENCES

J.J. Sakurai and J. Napolitano, Modern Quantum Mechanics, second edition (Addison-Wesley, New York, 2011).

J.S. Townsend, A Modern Approach to Quantum Mechanics second edition (University

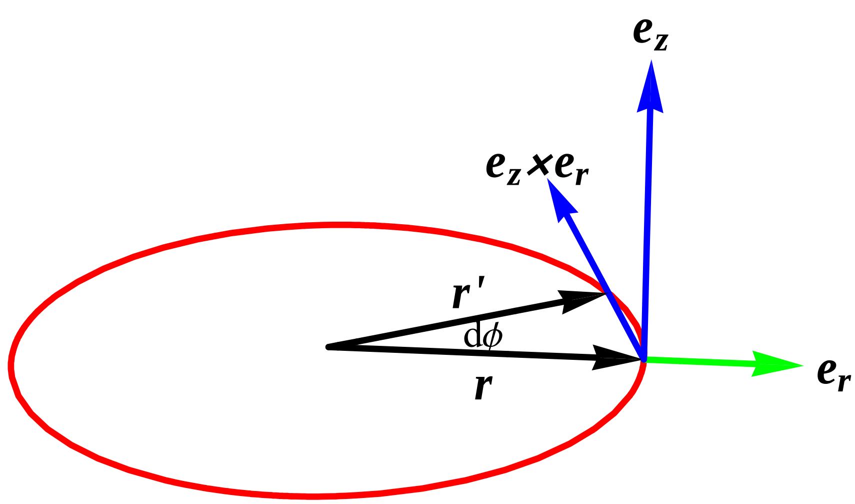
. Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics*, volume I and volume II (John Wiley & Sons, New York, 1977).

M. Tinkham, Group Theory and Quantum Mechanics (McGraw-Hill, New York, 1964).

D.H. McIntyre, Quantum Mechanics: A paradigms Approach (Pearson, 2012).

APPENDIX

The 2D rotation (infinitesimal angle)



In this figure we get the relation for the infinitesimal rotation

$$\begin{aligned} \boldsymbol{r}' &= \boldsymbol{r} + (r d\phi)(\boldsymbol{e}_z \times \boldsymbol{e}_r) \\ &= \boldsymbol{r} + d\phi(\boldsymbol{e}_z \times \boldsymbol{r}) \end{aligned}$$

where

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

Then we have

$$x' = x - y d\phi, \qquad y' = y + x d\phi, \qquad z' = z$$

Note that this relation can be also derived as follows.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \Re_z(d\phi) \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 & -d\phi & 0 \\ d\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x - y d\phi \\ y + x d\phi \\ z \end{pmatrix}$$

using the expression of $\Re_z(d\phi)$, where $d\phi$ is infinitesimally small.