Matrix representation of the rotation operator for S = 1/2

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The matrix representation of the rotation operator

$$\hat{R}_x(\theta), \qquad \hat{R}_y(\theta), \qquad \hat{R}_z(\theta).$$

is discussed for the spin 1/2, using several methods using the Mathematica.

1. Calculation of the matrix representation of $\hat{R}_y(\theta)$ under the basis of $\left|\pm z\right\rangle$

The change of basis between $\{\left|\pm z\right\rangle\}$ and $\{\left|\pm y\right\rangle\}$ is defined by

$$\left|+y\right\rangle = \hat{U}\left|+z\right\rangle, \qquad \left|-y\right\rangle = \hat{U}\left|-z\right\rangle,$$

$$\left\langle +y\right| = \left\langle +z\right|\hat{U}^{+} \qquad \left\langle -y\right| = \left\langle -z\right|\hat{U}^{+},$$

using the unitary operator

$$\hat{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \qquad \hat{U}^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}.$$

We note that

$$\hat{J}_y\left|+y\right\rangle = \frac{\hbar}{2}\left|+y\right\rangle, \qquad \hat{J}_y\left|-y\right\rangle = -\frac{\hbar}{2}\left|-y\right\rangle, \qquad \text{(eigenvalue problem)}$$

and

$$\hat{R}_y(\theta)\left|+y\right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_y\theta)\left|+y\right\rangle = e^{-\frac{i\theta}{2}}\left|+y\right\rangle,$$

$$\hat{R}_y(\theta)\left|-y\right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_y\theta)\left|-y\right\rangle = e^{\frac{i\theta}{2}}\left|-y\right\rangle.$$

Using the closure relation, we get

$$\begin{aligned}\hat{R}_y(\theta) &= \hat{R}_y(\theta)(|+y\rangle\langle +y| + |-y\rangle\langle -y|) \\ &= e^{-\frac{i\theta}{2}}|+y\rangle\langle +y| + e^{\frac{i\theta}{2}}|-y\rangle\langle -y| \\ &= \hat{U}(e^{-\frac{i\theta}{2}}|+z\rangle\langle +z| + e^{\frac{i\theta}{2}}|-z\rangle\langle -z|)\hat{U}^+\end{aligned}$$

Under the basis of $\{|\pm z\rangle\}$, we have

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

where

$$e^{-\frac{i\theta}{2}}|+z\rangle\langle +z| + e^{\frac{i\theta}{2}}|-z\rangle\langle -z| = \begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix}.$$

2. Calculation of the matrix representation of $\hat{R}_x(\theta)$ under the basis of $|\pm z\rangle$

The change of basis between $\{|\pm z\rangle\}$ and $\{|\pm x\rangle\}$ is defined by

$$|+x\rangle = \hat{U}|+z\rangle, \qquad |-x\rangle = \hat{U}|-z\rangle,$$

$$\langle +x| = \langle +z|\hat{U}^+ \qquad \langle -x| = \langle -z|\hat{U}^+,$$

using the unitary operator,

$$\hat{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad \hat{U}^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We note that

$$\hat{J}_x \left| +x \right\rangle = \frac{\hbar}{2}\left| +x \right\rangle, \qquad \hat{J}_x \left| -x \right\rangle = -\frac{\hbar}{2}\left| -x \right\rangle, \qquad \text{(eigenvalue problem)}$$

and

$$\hat{R}_x(\theta)\left| +x \right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_x\theta)\left| +x \right\rangle = e^{-\frac{i\theta}{2}}\left| +x \right\rangle,$$

$$\hat{R}_x(\theta)\left| -x \right\rangle = \exp(-\frac{i}{\hbar}\hat{J}_x\theta)\left| -x \right\rangle = e^{\frac{i\theta}{2}}\left| -x \right\rangle.$$

Using the closure relation, we get

$$\begin{aligned}
\hat{R}_x(\theta) &= \hat{R}_x(\theta)(\left| +x \right\rangle\left\langle +x \right| + \left| -x \right\rangle\left\langle -x \right|) \\
&= e^{-\frac{i\theta}{2}}\left| +x \right\rangle\left\langle +x \right| + e^{\frac{i\theta}{2}}\left| -x \right\rangle\left\langle -x \right| \\
&= \hat{U}(e^{-\frac{i\theta}{2}}\left| +z \right\rangle\left\langle +z \right| + e^{\frac{i\theta}{2}}\left| -z \right\rangle\left\langle -z \right|)\hat{U}^{+}
\end{aligned}$$

Under the basis of $\{\left| \pm z \right\rangle\}$, we have

$$\begin{aligned}
\hat{R}_x(\theta) &= \hat{U}\begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix}\hat{U}^{+} \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}
\end{aligned}$$

where

$$e^{-\frac{i\theta}{2}}\left|+z\right\rangle\left\langle+z\right|+e^{\frac{i\theta}{2}}\left|-z\right\rangle\left\langle-z\right|=\begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix},$$

under the basis of between $\{\left|\pm z\right\rangle\}$.

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3. Derivation of the matrix representation using Mathematica

With the use of the Mathematica, we can derive the matrix representation of the rotation operators directly. The angular momentum for the spin 1/2 system can be written as

$$\hat{J}_x=\frac{\hbar}{2}\hat{\sigma}_x, \qquad \hat{J}_y=\frac{\hbar}{2}\hat{\sigma}_y, \qquad \hat{J}_z=\frac{\hbar}{2}\hat{\sigma}_z.$$

in terms of the Pauli matrices,

$$\hat{\sigma}_x=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_z=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The rotation operators are defined by

$$\hat{R}_x(\theta)=\exp(-\frac{i}{\hbar}\hat{J}_x\theta)=\exp(-\frac{i}{2}\hat{\sigma}_x\theta),$$

$$\hat{R}_y(\theta)=\exp(-\frac{i}{\hbar}\hat{J}_y\theta)=\exp(-\frac{i}{2}\hat{\sigma}_y\theta),$$

$$\hat{R}_z(\theta)=\exp(-\frac{i}{\hbar}\hat{J}_z\theta)=\exp(-\frac{i}{2}\hat{\sigma}_z\theta),$$

for the spin 1/2.

((**Mathematica**))

Matrices j = 1/2

```
Clear["Global`*"]; j = 1/2;
Jx[j_, n_, m_] := ħ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ħ/2 ⅈ Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 ⅈ Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jz[j_, n_, m_] := ħ m KroneckerDelta[n, m];
Jx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jy = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Ry[θ_] := MatrixExp[-ⅈ/ħ Jy θ] // Simplify ;
Rz[ϕ_] := MatrixExp[-ⅈ/ħ Jz ϕ] // Simplify;
```

```
R = (Rz[ϕ].Ry[θ]); R // MatrixForm
```

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

```
u1 = R.{1, 0} // Simplify
```

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

```
u2 = R.{0, 1} // Simplify
```

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

```
Rx[θ_] := MatrixExp[-(i/ħ) Jx θ] // Simplify;
```

```
Rx[θ] // MatrixForm
```

$$\begin{pmatrix} \text{Cos}\left[\frac{\theta}{2}\right] & -i\,\text{Sin}\left[\frac{\theta}{2}\right] \\ -i\,\text{Sin}\left[\frac{\theta}{2}\right] & \text{Cos}\left[\frac{\theta}{2}\right] \end{pmatrix}$$

```
Ry[θ] // MatrixForm
```

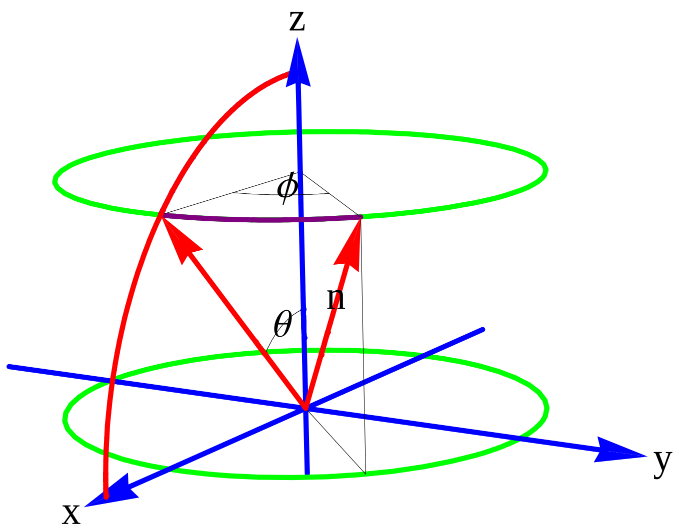
$$\begin{pmatrix} \text{Cos}\left[\frac{\theta}{2}\right] & -\text{Sin}\left[\frac{\theta}{2}\right] \\ \text{Sin}\left[\frac{\theta}{2}\right] & \text{Cos}\left[\frac{\theta}{2}\right] \end{pmatrix}$$

```
Rz[θ] // MatrixForm
```

$$\begin{pmatrix} e^{-\frac{i\theta}{2}} & 0 \\ 0 & e^{\frac{i\theta}{2}} \end{pmatrix}$$

4. Summary

Let the polar and the azimuthal angles that characterize ***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

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

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

The eigenkets $\left|+\boldsymbol{n}\right\rangle$ and $\left|-\boldsymbol{n}\right\rangle$ are obtained as

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

and

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

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

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

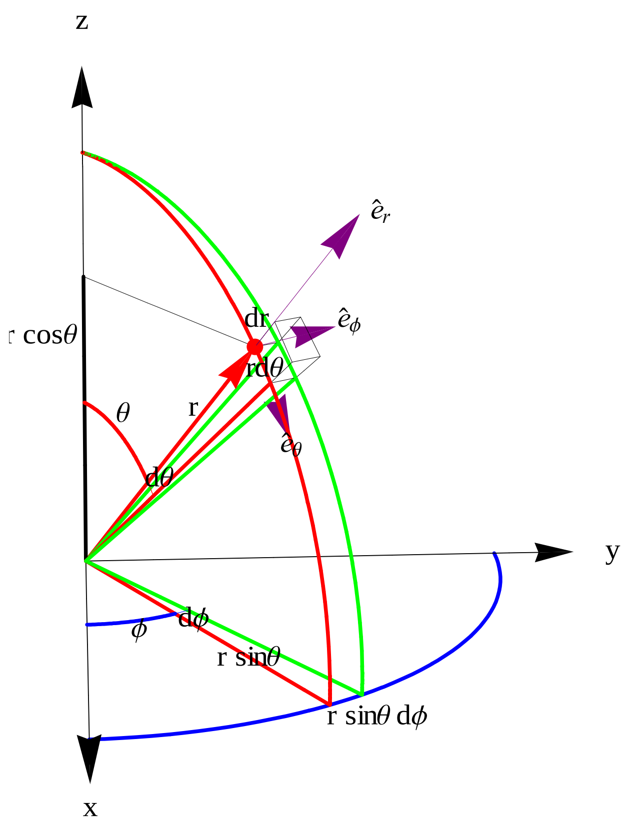


Fig. Spherical co-ordinate. $r = 1$. $\hat{n} = \mathbf{e}_r$.

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5. Properties of the rotation operators

We discuss a variety of properties of the matrices of the rotation operators under the basis of $\{|+z\rangle, |-z\rangle$, based on the Mathematica. The Mathematica programs are provided below. The following discussions are given in the textbook (D.C. Marinescu and G.M. Marinesscu, Approaching Quantum Computing, Pearson, Upper Saddle River, NJ 2004).

The matrices of the rotation operators for $S = 1/2$ about the x, y, and z axes with the same angle β are given by

$$\hat{R}_x(\beta) = \exp(-\frac{i}{2}\beta\hat{\sigma}_z) = \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix},$$

$$\hat{R}_y(\beta) = \exp(-\frac{i}{2}\beta\hat{\sigma}_y) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix},$$

$$\hat{R}_z(\beta) = \exp(-\frac{i}{2}\beta\hat{\sigma}_z) = \begin{pmatrix} e^{-i\frac{\beta}{2}} & 0 \\ 0 & {}^{-i\frac{\beta}{2}} \end{pmatrix}.$$

The composition of two rotations with angles δ and β is

$$\begin{aligned} \hat{R}_z(\delta)\hat{R}_y(\beta) &= \exp(-\frac{i}{2}\delta\hat{\sigma}_z)\exp(-\frac{i}{2}\beta\hat{\sigma}_y) \\ &= \begin{pmatrix} e^{-i\frac{\beta}{2}} & 0 \\ 0 & {}^{-i\frac{\beta}{2}} \end{pmatrix}\begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix} \\ &= \begin{pmatrix} e^{-i\frac{\beta}{2}}\cos\frac{\beta}{2} & -e^{-i\frac{\beta}{2}}\sin\frac{\beta}{2} \\ e^{i\frac{\beta}{2}}\sin\frac{\beta}{2} & e^{i\frac{\beta}{2}}\cos\frac{\beta}{2} \end{pmatrix} \end{aligned}$$

Any rotation on the Bloch sphere can be reduced to the previous expression for the angles δ and β. We note that

$$\hat{R}_x(\beta)\hat{R}_x(-\beta) = \hat{1}, \qquad \hat{R}_y(\beta)\hat{R}_y(-\beta) = \hat{1}, \qquad \hat{R}_z(\beta)\hat{R}_z(-\beta) = \hat{1}.$$

The composition of two rotations with angles β_1 and β_2 is rotation with angle $\beta_1 + \beta_2$ about the same axis

$$\hat{R}_x(\beta_1)\hat{R}_x(\beta_2) = \hat{R}_x(\beta_1 + \beta_2),$$

$$\hat{R}_z(\beta_1)\hat{R}_x(\beta_2) = \hat{R}_z(\beta_1 + \beta_2) ,$$

$$\hat{R}_z(\beta_1)\hat{R}_z(\beta_2) = \hat{R}_z(\beta_1 + \beta_2) ,$$

$$\hat{\sigma}_x \hat{R}_y(\theta)\hat{\sigma}_x = \hat{R}_y(-\theta) ,$$

$$\hat{\sigma}_x \hat{R}_z(\theta)\hat{\sigma}_x = \hat{R}_z(-\theta) .$$

((**Theorem**))

If $\hat{U}$ is a unitary 2 x 2 matrix, then there exist unitary matrices $\hat{A}$, $\hat{B}$, and $\hat{C}$ such that $\hat{A}\hat{B}\hat{C} = \hat{1}$ and $\hat{U} = \hat{A}\hat{\sigma}_x\hat{B}\hat{\sigma}_x\hat{C}$.

In order to show we consider matrices $\hat{A}$, $\hat{B}$, and $\hat{C}$ defined by

$$\hat{A} = \hat{R}_z(\beta)\hat{R}_y\left(\frac{\gamma}{2}\right), \qquad \hat{B} = \hat{R}_y\left(-\frac{\gamma}{2}\right)\hat{R}_z(-\frac{\delta + \beta}{2}), \qquad \hat{C} = \hat{R}_z(\frac{\delta - \beta}{2}) .$$

then we have

$$\hat{U} = \hat{A}\hat{\sigma}_x\hat{B}\hat{\sigma}_x\hat{C} = \hat{R}_z(\beta)\hat{R}_y(\gamma)\hat{R}_z(\delta) .$$

((**Mathematica**))

```
Clear["Global`*"]; σx = PauliMatrix[1]; σy = PauliMatrix[2];
σz = PauliMatrix[3]; Sx = ℏ/2 σx; Sy = ℏ/2 σy; Sz = ℏ/2 σz;
Rx[β_] := MatrixExp[-ⅈ/ℏ Sx β] // Simplify ;
Ry[β_] := MatrixExp[-ⅈ/ℏ Sy β] // Simplify ;
Rz[β_] := MatrixExp[-ⅈ/ℏ Sz β] // Simplify;
```

```
Rx[β] // Simplify // MatrixForm
```

$$\begin{pmatrix} \cos\left[\frac{\beta}{2}\right] & -i \sin\left[\frac{\beta}{2}\right] \\ -i \sin\left[\frac{\beta}{2}\right] & \cos\left[\frac{\beta}{2}\right] \end{pmatrix}$$

```
Ry[β] // Simplify // MatrixForm
```

$$\begin{pmatrix} \cos\left[\frac{\beta}{2}\right] & -\sin\left[\frac{\beta}{2}\right] \\ \sin\left[\frac{\beta}{2}\right] & \cos\left[\frac{\beta}{2}\right] \end{pmatrix}$$

```
Rz[β] // Simplify // MatrixForm
```

$$\begin{pmatrix} e^{-\frac{i\beta}{2}} & 0 \\ 0 & e^{\frac{i\beta}{2}} \end{pmatrix}$$

```
Rz[ϕ].Ry[θ] // Simplify // MatrixForm
```

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

```
Rx[β].Rx[-β] // Simplify
```

{{1, 0}, {0, 1}}

```
Ry[β].Ry[-β] // Simplify
```

```
{{1, 0}, {0, 1}}
```

```
Rz[β].Rz[-β] // Simplify
```

```
{{1, 0}, {0, 1}}
```

```
Rx[β1].Rx[β2] - Rx[β1 + β2] // Simplify
```

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

```
Ry[β1].Ry[β2] - Ry[β1 + β2] // Simplify
```

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

```
Rz[β1].Rz[β2] - Rz[β1 + β2] // Simplify
```

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

$$A1 = Rz[\beta].Ry\left[\frac{\gamma}{2}\right];\ B1 = Ry\left[\frac{-\gamma}{2}\right].Rz\left[\frac{-(\delta+\beta)}{2}\right];\ C1 = Rz\left[\frac{(\delta-\beta)}{2}\right];$$

```
A1.B1.C1 // Simplify
```

```
{{1, 0}, {0, 1}}
```

```
A1.σx.B1.σx.C1 - Rz[β].Ry[γ].Rz[δ] // Simplify
```

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