Matrix of Rotation Operator with S = 1

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We determine the eigenstates of $\hat{S}_x$ and $\hat{S}_y$ for a spin-1 particle in terms of the eigenstates $\left| j = 1, m \right\rangle$ (m = 1, 0, -1) of $\hat{S}_z$

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \hat{S}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

For simplicity, we use the unit of $\hbar = 1$.

1. Eigenvalue and eigenkets of $\hat{S}_x$

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

$$\left|1,1\right\rangle_x = \hat{U}_x\left|1,1\right\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix},$$

$$\left|1,0\right\rangle_x = \hat{U}_x\left|1,0\right\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix},$$

$$\left|1,-1\right\rangle_x = \hat{U}_x\left|1,-1\right\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix},$$

where $\hat{U}_x$ is a unitary operator.

Eigenvalue problem

$$\hat{S}_x\left|\psi\right\rangle = \lambda\hbar\left|\psi\right\rangle,$$

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C \end{pmatrix} = \lambda \begin{pmatrix} C_1 \\ C_2 \\ C \end{pmatrix},$$

or

$$\begin{pmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

For nontrivial solution, the determinant should be zero,

$$\begin{vmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{vmatrix} = 0,$$

or

$$\lambda(\lambda - 1)(\lambda + 1) = 0.$$

Note that

$$\hat{S}_x |1,1\rangle_x = \hbar |1,1\rangle_x, \qquad (\lambda = 1)$$

$$\hat{J}_x |1,0\rangle_x = 0 |1,0\rangle_x, \qquad (\lambda = 0)$$

$$\hat{J}_x |1,-1\rangle_x = -\hbar |1,-1\rangle_x, \qquad (\lambda = -1)$$

(a) $\hat{S}_x |1,1\rangle_x = \hbar |1,1\rangle_x$

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}, \qquad \text{or} \qquad \begin{pmatrix} -1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Then we have

$$U_{11} = \frac{1}{\sqrt{2}} U_{21}, \qquad U_{31} = \frac{1}{\sqrt{2}} U_{21}.$$

with the normalization condition

$$|U_{11}|^2 + |U_{21}|^2 + |U_{31}|^2 = 1.$$

So we get $|U_{21}| = \frac{1}{\sqrt{2}}$. Here we choose $U_{21} = \frac{1}{\sqrt{2}}$

$$U_{11} = \frac{1}{2}, \qquad U_{31} = \frac{1}{2}.$$

Finally we obtain the eigenket $|1,1\rangle_x$,

$$|1,1\rangle_x = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}(|1,1\rangle + \sqrt{2}|1,0\rangle + |1,-1\rangle).$$

(b) $\hat{S}_x |1,0\rangle_x = 0|1,0\rangle_x = 0$

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

Then we have

$$U_{22} = 0, \qquad U_{12} + U_{32} = 0,$$

with the normalization condition

$$|U_{12}|^2 + |U_{22}|^2 + |U_{32}|^2 = 1.$$

So we have $U_{12} = \frac{1}{\sqrt{2}}$, $U_{32} = -\frac{1}{\sqrt{2}}$.

In summary we get

$$.|1,0\rangle_x = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \sqrt{2} \\ 0 \\ -\sqrt{2} \end{pmatrix} = \frac{1}{2}(\sqrt{2}|1,1\rangle - \sqrt{2}|1,-1\rangle)$$

(c) $\hat{S}_x|1,-1\rangle_x = -\hbar|1,-1\rangle_x$

$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = -\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 1 \end{pmatrix}\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Then we have

$$U_{33} + \frac{1}{\sqrt{2}}U_{23} = 0, \qquad U_{13} + \frac{1}{\sqrt{2}}U_{23} = 0.$$

with the normalization condition

$$|U_{13}|^2 + |U_{23}|^2 + |U_{33}|^2 = 1.$$

So we get $|U_{23}| = \frac{1}{\sqrt{2}}$. Here we choose $U_{23} = -\frac{1}{\sqrt{2}}$

$$U_{13} = \frac{1}{2}, \qquad U_{33} = \frac{1}{2},$$

$$|1,-1\rangle_x = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2}(|1,1\rangle - \sqrt{2}|1,0\rangle + |1,-1\rangle).$$

The unitary operator is obtained as

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

$$\hat{U}_x^{\ +} = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix},$$

$$\hat{U}_x^{\ +}\hat{J}_x\hat{U}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

We now calculate the rotation operator $\hat{R}_y(\alpha) = \exp(-\frac{i}{\hbar}\hat{J}_x\alpha)$

$$\exp(-\frac{i}{\hbar}\hat{J}_x\alpha) = \hat{U}_x\begin{pmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix}\hat{U}_x^{\ +}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} e^{-i\alpha} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix}\frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos^2\frac{\alpha}{2} & -\frac{i}{\sqrt{2}}\sin\alpha & -\sin^2\frac{\alpha}{2} \\ -\frac{i}{\sqrt{2}}\sin\alpha & \cos\alpha & -\frac{i}{\sqrt{2}}\sin\alpha \\ -\sin^2\frac{\alpha}{2} & -\frac{i}{\sqrt{2}}\sin\alpha & \cos^2\frac{\alpha}{2} \end{pmatrix}$$

2. Eigenvalues and eigenkets of $\hat{S}_y$

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

$$|1,1\rangle_y = \hat{U}_y|1,1\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix},$$

$$|1,0\rangle_y = \hat{U}_y|1,0\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix},$$

$$|1,-1\rangle_y = \hat{U}_y|1,-1\rangle = \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{21} & U_{22} & U_{23} \\ U_{31} & U_{32} & U_{33} \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix},$$

where $\hat{U}_y$ is a unitary operator. Note that

$$\hat{S}_y|1,1\rangle_y = \hbar|1,1\rangle_y,$$

$$\hat{S}_y|1,0\rangle_y = 0|1,0\rangle_y,$$

$$\hat{S}_y|1,-1\rangle_y = -1|1,-1\rangle_y,$$

(a) $\hat{S}_y|1,1\rangle_y = \hbar|1,1\rangle_y$

$$\begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix}, \text{ or } \qquad \begin{pmatrix} -1 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & -1 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & -1 \end{pmatrix}\begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Then we have

$$U_{11} = -\frac{i}{\sqrt{2}}U_{21}, \qquad U_{31} = \frac{i}{\sqrt{2}}U_{21}.$$

with the normalization condition

$$|U_{11}|^2 + |U_{21}|^2 + |U_{31}|^2 = 1,$$

So we get $|U_{21}| = \frac{1}{\sqrt{2}}$. Here we choose $U_{21} = \frac{i}{\sqrt{2}}$

$$U_{11} = \frac{1}{2}, \qquad U_{31} = -\frac{1}{2}.$$

Finally we obtain the eigenket $|1,1\rangle_y$,

$$|1,1\rangle_y = \begin{pmatrix} U_{11} \\ U_{21} \\ U_{31} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} = \frac{1}{2}(|1,1\rangle + i\sqrt{2}|1,0\rangle - |1,-1\rangle).$$

(b) $\hat{S}_y|1,0\rangle_y = 0|1,0\rangle_y = 0$

$$\begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

Then we have

$$U_{22} = 0, \qquad U_{12} = U_{32},$$

with the normalization condition

$$|U_{12}|^2 + |U_{22}|^2 + |U_{32}|^2 = 1.$$

So we have $U_{12} = \frac{1}{\sqrt{2}}$, $U_{32} = \frac{1}{\sqrt{2}}$.

In summary we get

$$|1,0\rangle_y = \begin{pmatrix} U_{12} \\ U_{22} \\ U_{32} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \sqrt{2} \\ 0 \\ \sqrt{2} \end{pmatrix} = \frac{1}{2}(\sqrt{2}|1,1\rangle + \sqrt{2}|1,-1\rangle).$$

(c) $S_y|1,-1\rangle_y = -\hbar|1,-1\rangle_y$

$$\begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = -\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix}, \qquad \text{or} \qquad \begin{pmatrix} 1 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 1 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 1 \end{pmatrix}\begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

Then we have

$$U_{13} - \frac{i}{\sqrt{2}} U_{23} = 0, \qquad U_{33} + \frac{i}{\sqrt{2}} U_{23} = 0,$$

with the normalization condition

$$|U_{13}|^2 + |U_{23}|^2 + |U_{33}|^2 = 1.$$

So we get $|U_{23}| = \frac{1}{\sqrt{2}}$. Here we choose $U_{23} = -\frac{i}{\sqrt{2}}$.

$$U_{13} = \frac{1}{2}, \qquad U_{33} = -\frac{1}{2},$$

$$|1,-1\rangle_y = \begin{pmatrix} U_{13} \\ U_{23} \\ U_{33} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ -i\sqrt{2} \\ -1 \end{pmatrix} = \frac{1}{2}(|1,1\rangle - i\sqrt{2}|1,0\rangle - |1,-1\rangle).$$

The unitary operator is obtained as

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

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

$$\hat{U}_y{}^+\hat{J}_y\hat{U}_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

3. Rotation operator $\hat{R}_y(\theta)$

Here we discuss the matrix of the rotation operator with j = 1. The rotation operator is defined by

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

$$\begin{aligned}
\hat{R}_y(\theta) &= \exp(-\frac{i}{\hbar}\hat{J}_y\theta)(|1,1;y\rangle\langle 1,1;y| + |1,0;y\rangle\langle 1,0;y| + |1,-1;y\rangle\langle 1,-1;y|) \\
&= \exp(-\frac{i}{\hbar}\hat{J}_y\theta)|1,1;y\rangle\langle 1,1;y| + \exp(-\frac{i}{\hbar}\hat{J}_y\theta)|1,0;y\rangle\langle 1,0;y| \\
&\quad + \exp(-\frac{i}{\hbar}\hat{J}_y\theta)|1,-1;y\rangle\langle 1,-1;y| \\
&= e^{-i\theta}|1,1;y\rangle\langle 1,1;y| + e^{0}|1,0;y\rangle\langle 1,0;y| + e^{i\theta}|1,-1;y\rangle\langle 1,-1;y| \\
&= \hat{U}_y(e^{-i\theta}|1,1;z\rangle\langle 1,1;z| + e^{0}|1,0;z\rangle\langle 1,0;z| + e^{i\theta}|1,-1;z\rangle\langle 1,-1;z|)\hat{U}_y{}^+ \\
&= \hat{U}_y\begin{pmatrix} e^{-i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\theta} \end{pmatrix}\hat{U}_y{}^+
\end{aligned}$$

or

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

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

4. The matrix of $\hat{R}_z(\phi)$

$$\hat{R}_z(\phi) = \exp(-\frac{i}{\hbar}\hat{J}_z\phi)(|1,1;z\rangle\langle 1,1;z| + |1,0;z\rangle\langle 1,0;z| + |1,-1;z\rangle\langle 1,-1;z|)$$
$$= e^{-i\phi}|1,1;z\rangle\langle 1,1;z| + e^{0}|1,0;z\rangle\langle 1,0;z| + e^{i\phi}|1,-1;z\rangle\langle 1,-1;z|$$
$$= \begin{pmatrix} e^{-i\phi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\phi} \end{pmatrix}$$

5. The matrix of $\hat{R} = \hat{R}_z(\phi)\hat{R}_y(\theta)$

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

((**Mathematica**))

Matrices j = 1

```
Clear["Global`*"]; j = 1;
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
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}];
```

```
Jx // MatrixForm
```

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

```
Jy // MatrixForm
```

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

```
Jz // MatrixForm
```

$$\begin{pmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{pmatrix}$$

```
eq1 = Eigensystem[Jx]
```

$$\left\{\{-\hbar, \hbar, 0\}, \left\{\left\{1, -\sqrt{2}, 1\right\}, \left\{1, \sqrt{2}, 1\right\}, \{-1, 0, 1\}\right\}\right\}$$

```
ψ1x = Normalize[eq1[[2, 2]]]; ψ1x // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix}$$

```
ψ2x = -Normalize[eq1[[2, 3]]]; ψ2x // MatrixForm
```

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

```
ψ3x = Normalize[eq1[[2, 1]]]; ψ3x // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix}$$

```
UxT = {ψ1x, ψ2x, ψ3x}; Ux = Transpose[UxT]; Ux // MatrixForm
```

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

```
UxH = UxT*; UxH // MatrixForm
```

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

```
UxH.Ux
```

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

```
eq2 = Eigensystem[Jy]
```

$\left\{\{-\hbar, \hbar, 0\}, \left\{\left\{-1, i\sqrt{2}, 1\right\}, \left\{-1, -i\sqrt{2}, 1\right\}, \{1, 0, 1\}\right\}\right\}$

```
ψ1y = -Normalize[eq2[[2, 2]]]; ψ1y // MatrixForm
```

$$\begin{pmatrix} \frac{1}{2} \\ \frac{i}{\sqrt{2}} \\ -\frac{1}{2} \end{pmatrix}$$

```
UyH.Uy // Simplify
```

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

$$Ry = Uy.\begin{pmatrix} \text{Exp}[-i\,\theta] & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \text{Exp}[i\,\theta] \end{pmatrix}.UyH \text{ // ExpToTrig // FullSimplify;}$$

```
Ry // MatrixForm
```

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

$$Rz = \begin{pmatrix} \text{Exp}[-i\,\phi] & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \text{Exp}[i\,\phi] \end{pmatrix};$$

```
R = Rz.Ry // Simplify; R // MatrixForm
```

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

Direct calculation of the rotation matrix

```
R1 = MatrixExp[-(-i/ħ) Jz ϕ].MatrixExp[(-i/ħ) Jy θ] // TrigFactor;
R1 // MatrixForm
```

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

```
R1.{1, 0, 0} // MatrixForm
```

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

```
R1.{0, 1, 0} // MatrixForm
```

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

7. Useful formula for J = 1

We note that these kets are the eigenket of $\hat{J}_n = \hat{\boldsymbol{J}}\cdot\boldsymbol{n}$, where $\boldsymbol{n}$ is the unit vector given by

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

and

$$\hat{J}_n = \hat{\boldsymbol{J}}\cdot\boldsymbol{n} = \hat{J}_x n_x + \hat{J}_y n_y + \hat{J}_z n_z = \hbar\begin{pmatrix} \cos\theta & \frac{\sin\theta}{\sqrt{2}}e^{-i\phi} & 0 \\ \frac{\sin\theta}{\sqrt{2}}e^{i\phi} & 0 & \frac{\sin\theta}{\sqrt{2}}e^{-i\phi} \\ 0 & \frac{\sin\theta}{\sqrt{2}}e^{i\phi} & -\cos\theta \end{pmatrix}.$$

One can use S = 1 instead of J = 1.

The eigenvalue problem can be written as

$$(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})|1,1;\boldsymbol{n}\rangle_n = \hbar|1,1;\boldsymbol{n}\rangle\,,$$

$$(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})|1,0;\boldsymbol{n}\rangle = 0\,,$$

$$(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})|1,-1;\boldsymbol{n}\rangle = -\hbar|1,-1;\boldsymbol{n}\rangle\,.$$

We calculation the rotation matrix with $J = 1$ without the use of **Mathematica**. First we consider the Taylor expansion:

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

where

$$\hat{J}_y = \frac{\hat{J}_+ - \hat{J}_-}{2i}.$$

Note that

$$\hat{J}_+|1,1\rangle = 0\,,\qquad \hat{J}_+|1,0\rangle = \sqrt{2}\hbar|1,1\rangle\,,\qquad \hat{J}_+|1,-1\rangle = \sqrt{2}\hbar|1,0\rangle\,,$$

$$\hat{J}_-|1,1\rangle = \sqrt{2}\hbar|1,0\rangle\,,\qquad \hat{J}_-|1,0\rangle = \sqrt{2}\hbar|1,-1\rangle\,,\qquad \hat{J}_-|1,-1\rangle = 0\,,$$

$$\hat{J}_y|1,1\rangle = \frac{i\hbar}{\sqrt{2}}|1,0\rangle\,,\qquad \hat{J}_y|1,0\rangle = \frac{-i\hbar}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle)\,,\qquad \hat{J}_y|1,-1\rangle = -\frac{i\hbar}{\sqrt{2}}|1,0\rangle\,.$$

Using the matrix

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

we have

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

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

Therefore the Taylor expansion can be rewritten as

$$\begin{aligned}\exp(-\frac{i}{\hbar}\theta\hat{J}_y) &= \hat{1} + \frac{\hat{J}_y}{\hbar}[(-\theta) + \frac{1}{3!}(-i\theta)^3 + \frac{1}{5!}(-i\theta)^5 + ..] \\ &+ \frac{\hat{J}_y{}^2}{\hbar^2}[\frac{1}{2!}(-i\theta)^2 + \frac{1}{4!}(-i\theta)^4 + ..] \\ &= \hat{1} - \frac{\hat{J}_y}{\hbar}(i\sin\theta) + \frac{\hat{J}_y{}^2}{\hbar^2}(\cos\theta - 1) \\ &= \begin{pmatrix} \frac{1+\cos\theta}{2} & -\frac{\sin\theta}{\sqrt{2}} & \frac{1-\cos\theta}{2} \\ \frac{\sin\theta}{\sqrt{2}} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}} \\ \frac{1-\cos\theta}{2} & \frac{\sin\theta}{\sqrt{2}} & \frac{1+\cos\theta}{2} \end{pmatrix}\end{aligned}$$

For $J = 1$, we have the following formula

$$\exp[-\frac{i}{\hbar}\alpha(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})] = \hat{1} - i\sin\alpha\frac{\hat{\boldsymbol{J}}\cdot\boldsymbol{n}}{\hbar} + (\cos\alpha - 1)\frac{(\hat{\boldsymbol{J}}\cdot\boldsymbol{n})^2}{\hbar^2}.$$

((**Proof**)) The proof for this formula is given in terms of Mathematica.

Matrix j = 1

```
Clear["Global`*"]; j = 1; I3 = IdentityMatrix[3];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
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}];

Jn = n1 Jx + n2 Jy + n3 Jz;

rule1 = {n3^2 → 1 - n1^2 - n2^2};

f1 = MatrixExp[-ⅈ Jn/ħ α] //. rule1 // FullSimplify;

f2 = I3 - Jn/ħ ⅈ Sin[α] + Jn.Jn/ħ^2 (Cos[α] - 1) //. rule1 // Simplify;
f1 - f2 // Simplify
```

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

((**Note**)) For $J = 1/2$, we have similar formula

$$\exp[-\frac{i}{2}\alpha(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})] = \hat{1}\cos(\frac{\alpha}{2}) - i(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\sin(\frac{\alpha}{2}).$$

Matrix j = 1/2

```
Clear["Global`*"]; j = 1/2; I2 = IdentityMatrix[2];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
σx = PauliMatrix[1]; σy = PauliMatrix[2];
σz = PauliMatrix[3];

σn = n1 σx + n2 σy + n3 σz;

rule1 = {n1 → Sin[θ] Cos[ϕ], n2 → Sin[θ] Sin[ϕ], n3 → Cos[θ]};
```

$$f1 = \text{MatrixExp}\left[-i \frac{\sigma n}{2} \alpha\right] \text{ //. rule1 // FullSimplify;}$$

$$f2 = \text{I2 Cos}\left[\frac{\alpha}{2}\right] - i\, \sigma n\, \text{Sin}\left[\frac{\alpha}{2}\right] \text{ //. rule1 // FullSimplify;}$$

```
f1 - f2 // Simplify

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