V. Symmetry In Quantum Mechanics

5.3. Spatial Rotations & Angular Momentum Operators

5.3-1. Geometry of rotations & the rotation group

Isotropy of space ⟺ equivalence of experiments performed in frames rotated relative to each other

Consider two observers whose Cartesian frames of reference are rotated relative to each other with their origins in common. Or alternatively, suppose we rotate our system and measuring apparatus from point $\vec{r}$ to point $\vec{r}'$. The coordinates of the two laboratories are related by the rotation transformation

$$x_i' = R_{ij} x_j \, . \quad \text{Since}$$

rotations about a common origin leave the length of a vector unchanged we have

$$\vec{r}'\cdot\vec{r}' = \vec{r}\cdot\vec{r} = x_j x_j = x_j \delta_{jk} x_k$$

$$= R_{ij} x_j R_{ik} x_k = x_j (R^T_{ji} R_{ik}) x_k$$

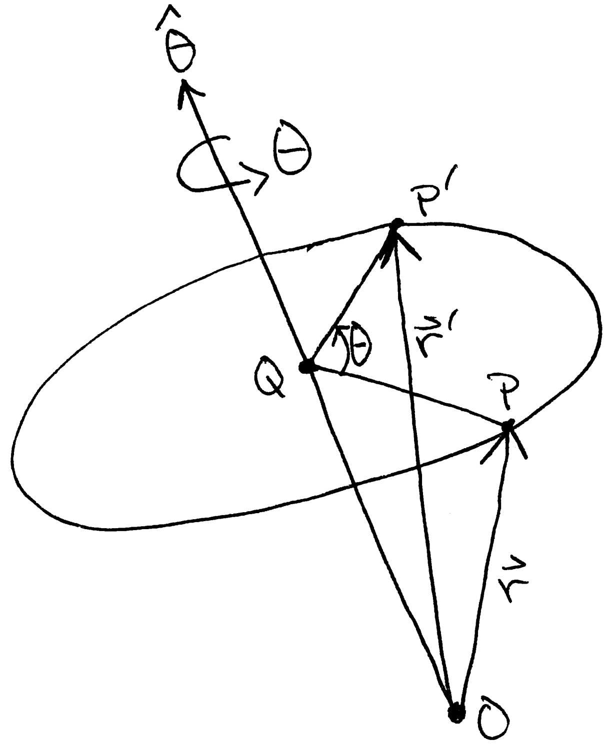
$$\Rightarrow R^T R = 1 \Rightarrow R^T = R^{-1}$$

Thus the rotation matrix R is a

real 3×3 orthogonal matrix. Further $\det(RR^T) = \det 1 = 1 \Rightarrow \det R = \pm 1$. Since we are interested in rotations connected to the identity rotation, we will restrict ourselves to $\det R = +1$ rotations only, these are called proper rotations. $\det R = -1$ rotations can be obtained by making a proper rotation followed by a parity transformation. In general R_{ij} has 9 independent matrix elements. However $R^T = R^{-1}$ reduces this to just 3 independent matrix elements. The choice of which 3 parameters specify the rotation in question is arbitrary.

According to Euler's Theorem (Goldstein Chapter 4.6) an arbitrary rotation can be specified in terms of a rotation thru angle θ about a fixed axis whose orientation is given by a unit vector denoted $\hat{\theta}$. Hence given the vector $\vec{\theta} = \theta\hat{\theta}$, the rotation between $\vec{r}$ and $\vec{r}'$ is specified $R_{ij} = R_{ij}(\vec{\theta})$.

Given $\vec{\theta}$ we can find $R_{ij}(\vec{\theta})$ by considering the geometry of the rotation

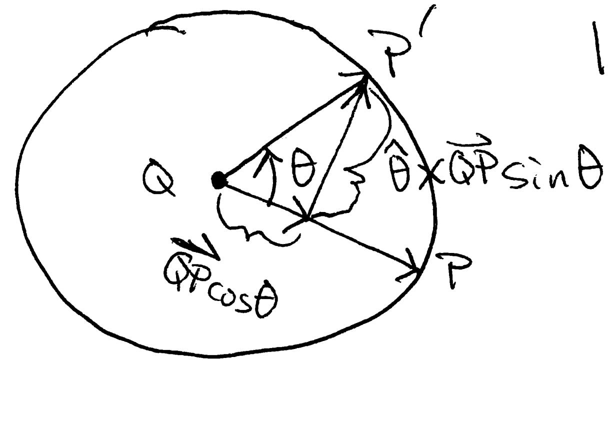


So

$$\vec{r}\,' = \overrightarrow{OQ} + \overrightarrow{QP}\,'$$

Now to find $\overrightarrow{QP}\,'$ look down the $\hat{\theta}$-axis from above

$$|\overrightarrow{QP}| = |\overrightarrow{QP}\,'|$$



$$\vec{r}\,' = \overrightarrow{OQ} + \overrightarrow{QP}\cos\theta + \hat{\theta}\times\overrightarrow{QP}\sin\theta$$

But vector $\overrightarrow{OQ} = (\vec{r}\cdot\hat{\theta})\hat{\theta}$ and

vector $\overrightarrow{QP} = \vec{r} - \overrightarrow{OQ} = \vec{r} - (\vec{r}\cdot\hat{\theta})\hat{\theta}$

So

$$\vec{r}\,' = (\vec{r}\cdot\hat{\theta})\hat{\theta} + \left(\vec{r}\cos\theta - (\vec{r}\cdot\hat{\theta})\hat{\theta}\cos\theta\right)$$
$$+ \left(\hat{\theta}\times\vec{r}\sin\theta - \underbrace{(\vec{r}\cdot\hat{\theta})\cancel{\hat{\theta}\times\hat{\theta}}\sin\theta}_{0}\right)$$

$$\boxed{\vec{r}\,' = \vec{r}\cos\theta + (\vec{r}\cdot\hat{\theta})\hat{\theta}(1-\cos\theta) + \hat{\theta}\times\vec{r}\sin\theta}$$

In terms of components this yields

$$x'_i = \left[\delta_{ij}\cos\theta + \hat{\theta}_i\hat{\theta}_j(1-\cos\theta) + \epsilon_{ikj}\hat{\theta}_k\sin\theta\right]x_j$$
$$= R_{ij}(\vec{\theta})\,x_j$$

Hence given $\vec{\theta}$ we have

$$\boxed{R_{ij}(\vec{\theta}) = \delta_{ij}\cos\theta + \hat{\theta}_i\hat{\theta}_j(1-\cos\theta) + \epsilon_{ikj}\hat{\theta}_k\sin\theta}$$

(Note: $\mathrm{Tr}\,R = R_{ii} = 3\cos\theta + (1-\cos\theta) = 1+2\cos\theta$
$\epsilon_{kij}R_{ij} = \epsilon_{kij}\epsilon_{ilj}\hat{\theta}_l\sin\theta = -2\hat{\theta}_k\sin\theta$).

We can simplify the writing of this matrix by introducing the 3×3 matrix generators of rotation matrices. Define the matrix

$$\Theta_{ij} \equiv \epsilon_{ikj}\hat{\theta}_k$$
$$= \begin{bmatrix} 0 & -\hat{\theta}_3 & \hat{\theta}_2 \\ \hat{\theta}_3 & 0 & -\hat{\theta}_1 \\ -\hat{\theta}_2 & \hat{\theta}_1 & 0 \end{bmatrix} \equiv \hat{\theta}\cdot\vec{I}_{ij}$$

where the 3-matrices $\vec{I}_{ij}$ are

$$(I_k)_{ij} \equiv \epsilon_{ikj}.$$

That is
$$I_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} (= I_x)$$

$$I_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} (= I_y)$$

$$I_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} (= I_z)$$

Since ϵ_{ijk} obeys the Jacobi identity
$$0 = \epsilon_{ijk}\epsilon_{mnk} + \epsilon_{jnk}\epsilon_{mik} + \epsilon_{nik}\epsilon_{mjk}$$
we have $[I_i, I_j] = \epsilon_{ijk} I_k$.

In addition Θ_{ij} has simple multiplication properties
$$(\Theta^2)_{ij} = \hat{\theta}_i \hat{\theta}_j - \delta_{ij}$$
$$(\Theta^3)_{ij} = -\Theta_{ij}$$
$$(\Theta^4)_{ij} = -(\Theta^2)_{ij}, \text{ etc.}$$

So
$$(\Theta^{2n})_{ij} = (-1)^{n+1}(\Theta^2)_{ij}$$
$$(\Theta^{2n+1})_{ij} = (-1)^n \Theta_{ij}$$

Hence

$$\left(e^{\theta\Theta}\right)_{ij} = \delta_{ij} + \sum_{n=1}^{\infty} \frac{1}{n!}\theta^n (\Theta^n)_{ij}$$

$$= \delta_{ij} + \sum_{n=0}^{\infty} \frac{1}{(2n+1)!}\theta^{2n+1}(\Theta^{2n+1})_{ij}$$

$$+ \sum_{n=1}^{\infty} \frac{1}{(2n)!}\theta^{2n}(\Theta^{2n})_{ij}$$

$$= \delta_{ij} + \sum_{n=1}^{\infty} \frac{\theta^{2n}}{(2n)!}(-1)^{n+1}(\Theta^2)_{ij}$$

$$+ \sum_{n=0}^{\infty} \frac{\theta^{2n+1}}{(2n+1)!}(-1)^n \Theta_{ij}$$

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using $(-1)^{n+1} = -1(i)^{2n}$

$(-1)^n = -i(i)^{2n+1}$

$$(e^{\theta\boldsymbol{\Theta}})_{ij}$$

$$= \delta_{ij} + (\boldsymbol{\Theta}^2)_{ij}\sum_{n=1}^{\infty} \frac{-(i)^{2n}\,\theta^{2n}}{(2n)!}$$

$$+ \boldsymbol{\Theta}_{ij}\sum_{n=0}^{\infty} \frac{-i(i)^{2n+1}\,\theta^{2n+1}}{(2n+1)!}$$

$$= \delta_{ij} - (\boldsymbol{\Theta}^2)_{ij}(\cos\theta - 1) + \boldsymbol{\Theta}_{ij}\sin\theta$$

$$\boxed{\begin{aligned} &= \delta_{ij} + (\boldsymbol{\Theta})_{ij}\sin\theta - (\boldsymbol{\Theta}^2)_{ij}(\cos\theta - 1) \\ &= (e^{\theta\boldsymbol{\Theta}})_{ij} \end{aligned}}$$

On the other hand recall

$$R_{ij}(\vec{\theta}) = \delta_{ij}\cos\theta + \hat{\theta}_i\hat{\theta}_j(1-\cos\theta) + \epsilon_{ikj}\hat{\theta}_k\sin\theta$$

$$= \delta_{ij}\cancel{\cos\theta} + (\hat{\theta}_i\hat{\theta}_j - \delta_{ij})(1-\cos\theta) + \delta_{ij}(1-\cancel{\cos\theta}) + (\boldsymbol{\Theta})_{ij}\sin\theta$$

So

$$\boxed{\begin{aligned} R_{ij}(\vec{\theta}) &= \delta_{ij} + (\Theta^2)_{ij}(1-\cos\theta) \\ &\quad + (\Theta)_{ij}\sin\theta \\ &= \left(e^{\theta\Theta}\right)_{ij} \end{aligned}}$$

Clearly we see that the rotation thru θ can be built up by successive rotations about $\hat{\theta}$ since

$$R_{ij}(\theta\hat{\theta})R_{jk}(\theta'\hat{\theta}) = \left(e^{\theta\Theta}\right)_{ij}\left(e^{\theta'\Theta}\right)_{jk}$$

$$= \left(e^{(\theta+\theta')\Theta}\right)_{ik}$$

$$= R_{ik}((\theta+\theta')\hat{\theta})$$

since $[\Theta, \Theta] = 0$. (i.e. clearly we have

$$R(\vec{\theta}) = \lim_{n\to\infty}\Big[\underbrace{1 + \frac{\theta}{n}\Theta}_{=R(\frac{\vec{\theta}}{n})}\Big]^n = e^{\theta\Theta}$$

).

In fact for infinitesimal rotations where

$$\vec{\theta} = \omega \hat{\theta} \equiv \vec{\omega} \quad ; \quad \omega \text{ infinitesimal, we have}$$

$$R_{ij}(\vec{\omega}) = \left(e^{\omega \Theta}\right)_{ij} = \delta_{ij} + \omega \Theta_{ij}$$

$$= \delta_{ij} + \omega_{ij} \quad \text{with } \omega_{ij} \equiv \omega \Theta_{ij}$$

$$= -\epsilon_{ijk} \omega_k$$

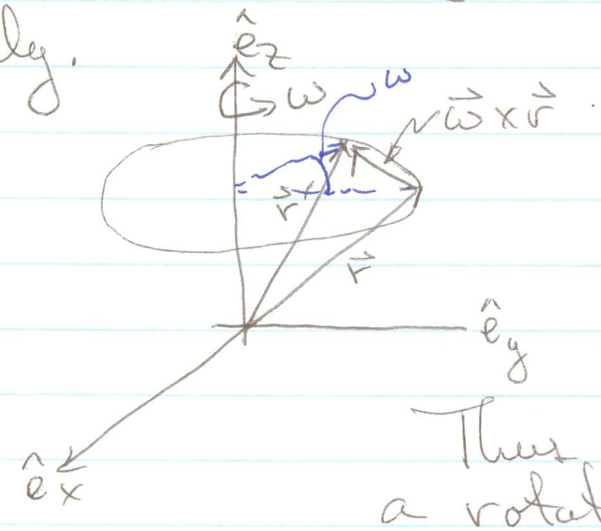
Thus $x_i' = R_{ij}(\vec{\omega}) x_j = x_i + \omega_{ij} x_j$

(i.e. $\vec{r}\,' = \vec{r} + \vec{\omega} \times \vec{r}$)

For example a rotation about the z-axis has

$$\vec{\omega} = \omega \hat{e}_z \Rightarrow \omega_{12} = -\omega = -\omega_{21}$$

only.



$$\vec{r}\,' = \vec{r} + \vec{\omega} \times \vec{r}$$
$$x' = x - \omega y$$
$$y' = y + \omega x$$
$$z' = z.$$

Thus ω_{ij} corresponds to a rotation in the $x_i - x_j$ plane.

Finally we consider sequential rotations

$$\begin{tikzcd} \vec{r} \arrow[r, "R(\vec{\theta}_1)"] \arrow[rr, bend right, "R(\vec{\theta}_3)"'] & \vec{r}\,' \arrow[r, "R(\vec{\theta}_2)"] & \vec{r}\,'' \end{tikzcd}$$

Then if

$$x_i'' = R_{ij}(\vec{\theta}_2)\, x_j'$$

$$x_j' = R_{jk}(\vec{\theta}_1)\, x_k$$

$$\Rightarrow \quad x_i'' = R_{ij}(\vec{\theta}_2) R_{jk}(\theta_1)\, x_k$$

$$= R_{ik}(\vec{\theta}_3)\, x_k$$

$$\Rightarrow R_{ij}(\vec{\theta}_2) R_{jk}(\vec{\theta}_1) = R_{ik}(\vec{\theta}_3)$$

So the composition law for rotations is matrix multiplication. Since $R(\vec{\theta}_1)$ and $R(\vec{\theta}_2)$ are orthogonal with determinant $= 1$ so is the product

$$\det\left(R(\vec{\theta}_2) R(\vec{\theta}_1)\right) = \det R(\vec{\theta}_2) \det R(\vec{\theta}_1) = 1$$

$$\left(R(\vec{\theta}_2) R(\vec{\theta}_1)\right)^T = R(\vec{\theta}_1)^T R(\vec{\theta}_2)^T$$

$$= R^{-1}(\vec{\theta}_1) R^{-1}(\vec{\theta}_2) = \left(R(\vec{\theta}_2) R(\vec{\theta}_1)\right)^{-1}$$

Hence $R(\vec{\theta}_3) = R(\vec{\theta}_2)R(\vec{\theta}_1)$ is also a determinant $=1$ orthogonal matrix, and hence a rotation. Since $R(\vec{0}) = \mathbb{1}$ and $R^{-1}(\vec{\theta}) = R(-\vec{\theta})$ and matrix multiplication is associative we see that the set of all rotations forms a group – the group of 3×3 orthogonal matrices with determinant one. This group is denoted $SO(3)$, the Special ($\det = 1$), Orthogonal ($R^{-1} = R^T$) group of 3×3 matrices. It is a group whose elements $R(\vec{\theta})$ depend continuously on 3 parameters given by $\vec{\theta}$.

Finally to complete the specification of the group multiplication law, we would like to specify $\vec{\theta}_3$ in terms of $\vec{\theta}_1$ and $\vec{\theta}_2$. Clearly this is somewhat messy. Since we can build up finite rotations from successive infinitesimal ones, it will suffice to consider the group product for the transformation

$$\begin{tikzcd}
\vec{r} \arrow[r, "R^{-1}(\vec{\theta})"] \arrow[d, "(1+\omega')"'] & \vec{r}\,' \arrow[r, "(1+\omega)"] & \vec{r}\,'' \arrow[dll, bend left, "R(\vec{\theta})"] \\
\vec{r}\,''' & &
\end{tikzcd}$$

Thus

$$x_i''' = R_{ij}(\vec{\theta})\, x_j''$$

$$x_j'' = (\delta_{jk} + \omega_{jk})\, x_k'$$

$$x_k' = R^{-1}_{kl}(\vec{\theta})\; x_l$$

$\Rightarrow$

$$x_i''' = R_{ij}(\vec{\theta})(\delta_{jk} + \omega_{jk}) R^{-1}_{kl}(\vec{\theta})\; x_l$$

equivalently $\quad x_i''' = (\delta_{il} + \omega'_{il})\, x_l$

$\Rightarrow$

$$\delta_{il} + \omega'_{il} = R_{ij}(\vec{\theta})(\delta_{jk} + \omega_{jk}) R^{-1}_{kl}(\vec{\theta})$$

$$= \delta_{il} + \left(R(\vec{\theta})\,\omega\, R^{-1}(\vec{\theta})\right)_{il}$$

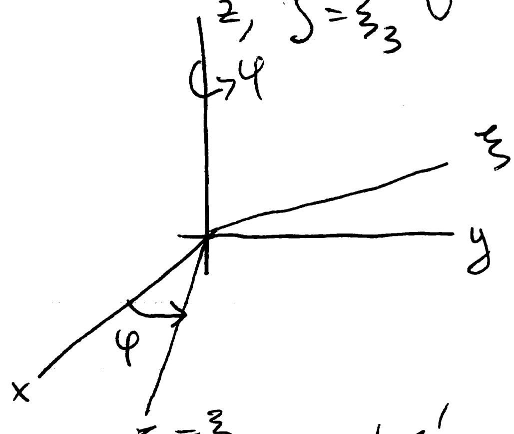
Hence given $\vec{\theta}$ and $\vec{\omega}$ we have the composite rotation resulting from the above sequence of transformations is

$$\boxed{\omega'_{ij} = \left(R(\vec{\theta})\,\omega\, R^{-1}(\vec{\theta})\right)_{ij}}$$

i.e. $R_{ij}(\vec{\omega}') = \delta_{ij} + \omega'_{ij}$

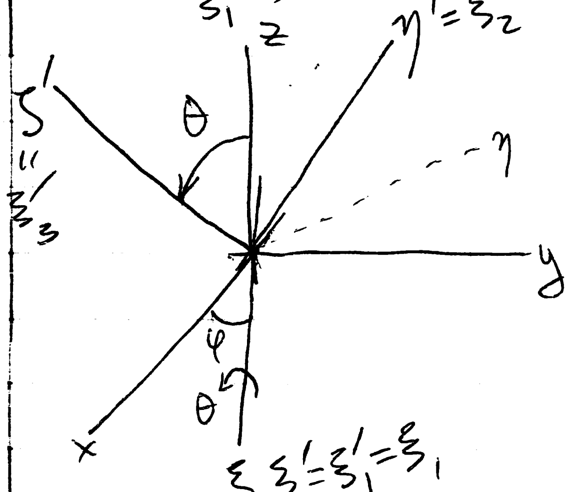
(Note: we have found $R(\vec{\omega}') = R(\vec{\theta}) R(\vec{\omega}) R^{-1}(\vec{\theta})$ that is
$$R(\vec{\omega}') R(\vec{\theta}) = R(\vec{\theta}) R(\vec{\omega}) \Big).$$

Of course we could specify our rotations by means of other parameterizations. For instance we could use the Euler angles to specify the orientation of the rotated frame.



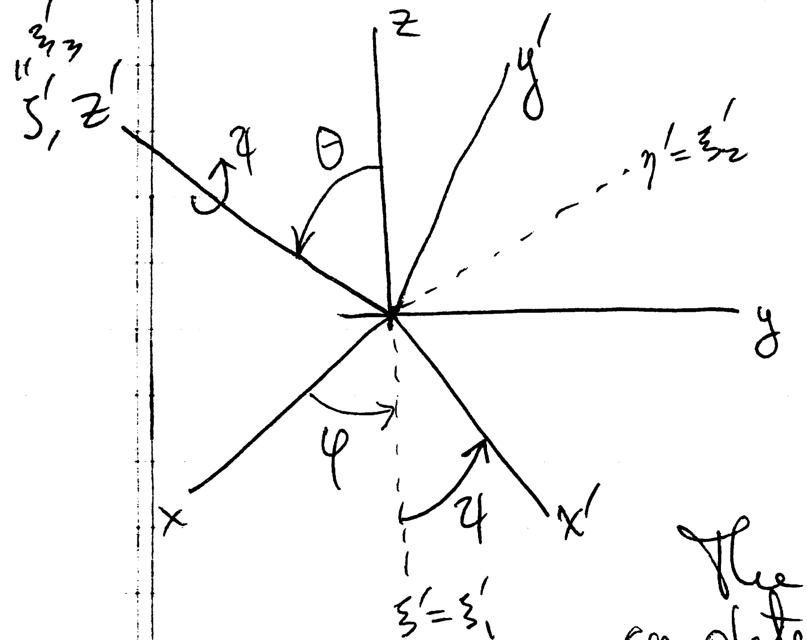
First rotate about the z-axis by $\measuredangle \varphi$

$$\xi_i = R_{ij}(\varphi \hat{e}_z)\, x_j$$



Second rotate about the ξ-axis by $\measuredangle \theta$

$$\xi_i' = R_{ij}(\theta \hat{e}_\xi)\, \xi_j$$



Finally rotate about the ξ'-axis by $\measuredangle\psi$

$$x'_i = R_{ij}(\psi \hat{e}_{z'})\, \xi'_j$$

The Euler angles (θ, φ, ψ) completely specify the rotation.

Thus we can label R by $R_{ij}(\theta, \varphi, \psi)$.

So we have

$$x'_i = R_{ij}(\theta, \varphi, \psi)\, x_j$$

where we made $R_{ij}(\theta, \varphi, \psi)$ by 3 successive rotations

$$R_{ij}(\theta, \varphi, \psi) = \Big(R(\psi \hat{e}_{z'})\, R(\theta \hat{e}_{3})\, R(\varphi \hat{e}_{z})\Big)_{ij}$$

But these are simple rotations about one of the coordinate axes. Hence

$$R(\varphi \hat{e}_z) = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(\theta \hat{e}_\xi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{pmatrix}$$

$$R(\psi \hat{e}_{z'}) = \begin{pmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Thus we find

$$R(\theta, \varphi, \psi) =$$

$$\begin{bmatrix} c\psi c\varphi - c\theta s\varphi s\psi & c\psi s\varphi + c\theta c\varphi s\psi & s\psi s\theta \\ -s\psi c\varphi - c\theta s\varphi c\psi & -s\psi s\varphi + c\theta c\varphi c\psi & c\psi s\theta \\ s\theta s\varphi & -s\theta c\varphi & c\theta \end{bmatrix}$$

(The inverse transformation $R^{-1} = R^T$ gives the transformation of the active view.)

S.3.2. <u>The Angular momentum operators and their commutation relations.</u>

Isotropy of space

If the state of the system is given by $|\psi\rangle$ before the system and the measuring apparatus is rotated, it is given by $|\psi'\rangle$ after it is rotated by $R(\vec{\theta})$ where

$$|\psi'\rangle = U(R(\vec{\theta}))\,|\psi\rangle .$$

Since any proper rotation can be written as a square $R(\vec{\theta}) = R^2(\tfrac{1}{2}\vec{\theta})$ we have

$$U(R(\vec{\theta})) = U^2(R(\tfrac{1}{2}\vec{\theta})),$$

hence $U(R)$ is unitary because the product of two unitary or two anti-unitary operators is unitary. So

$$U^\dagger(R(\vec{\theta})) = U^{-1}(R(\vec{\theta})) .$$