

Notes on transformations of Spherical Harmonic functions

These notes use the convention of M. E. Rose, *Elementary Theory of Angular Momentum*, John Wiley & Sons, Inc. 1957 which seems to be consistent with your Tinkham text. Consider a transformation of the spherical harmonic functions:

$$Y_{lm}(\widehat{\mathcal{R}\mathbf{r}}) = \sum_{m'} Y_{lm'}(\hat{\mathbf{r}}) \mathcal{D}_{m'm}^l(\mathcal{R}) \quad (1)$$

Here the transformation $\mathcal{R}\mathbf{r}$ might be a rotation through the 3 Euler angles (α about the $\hat{\mathbf{z}}$ axis, β about the new $\hat{\mathbf{y}}'$ axis, and γ about the new $\hat{\mathbf{z}}''$ axis) so that

$$\mathcal{R}\mathbf{r} = M_{z''}(\gamma)M_{y'}(\beta)M_z(\alpha)\mathbf{r}. \quad (2)$$

$$M_{z''}(\gamma) = \begin{pmatrix} \cos \gamma & \sin \gamma & 0 \\ -\sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (3)$$

$$M_{y'}(\beta) = \begin{pmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{pmatrix}, \quad (4)$$

and

$$M_z(\alpha) = \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (5)$$

By multiplying these three matrices, we find the 9 components of the rotation matrix to be:

$$\mathcal{R}_{xx} = \cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma \quad (6)$$

$$\mathcal{R}_{xy} = \sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma \quad (7)$$

$$\mathcal{R}_{xz} = -\sin \beta \cos \gamma \quad (8)$$

$$\mathcal{R}_{yx} = -\cos \alpha \cos \beta \sin \gamma - \sin \alpha \cos \gamma \quad (9)$$

$$\mathcal{R}_{yy} = -\sin \alpha \cos \beta \sin \gamma + \cos \alpha \cos \gamma \quad (10)$$

$$\mathcal{R}_{yz} = \sin \beta \sin \gamma \quad (11)$$

$$\mathcal{R}_{zx} = \cos \alpha \sin \beta \quad (12)$$

$$\mathcal{R}_{zy} = \sin \alpha \sin \beta \quad (13)$$

$$\mathcal{R}_{zz} = \cos \beta \quad (14)$$

It can be shown that the spherical harmonic transformation representation takes the form:

$$\mathcal{D}_{m'm}^l(\mathcal{R}) \equiv \mathcal{D}_{m'm}^l(\alpha, \beta, \gamma) = e^{-i\alpha m'} d_{m'm}^l(\cos \beta) e^{-i\gamma m}, \quad (15)$$

For $m' \geq m$,

$$d_{m'm}^l(\cos \beta) = \sqrt{\frac{(l-m)!(l+m')!}{(l+m)!(l-m')!}} \frac{1}{(m'-m)!} \left(\cos \frac{\beta}{2}\right)^{2l-(m'-m)} \left(\sin \frac{\beta}{2}\right)^{m'-m} \times {}_2F_1(m'-l; -m-l; m'-m+1; -\tan^2 \frac{\beta}{2}) \quad (16)$$

The hypergeometric function is defined to be

$${}_2F_1(a, b; c; z) \equiv 1 + \frac{ab}{c}z + \frac{1}{2} \frac{a(a+1)b(b+1)}{c(c+1)}z^2 + \dots \quad (17)$$

This equation can generate all the rotation matrices needed by use of some of the following identities:

$$d_{m'm}^l(\cos \beta) = d_{mm'}^l(-\cos \beta) \quad (18)$$

$$\mathcal{D}_{m'm}^l(\mathcal{R}) = (-1)^l \mathcal{D}_{m'm}^l(\bar{\mathcal{R}}), \quad (19)$$

where $\mathcal{R} \equiv (\text{inversion}) \times \bar{\mathcal{R}}$.

We can determine the Euler angles α , β , and γ for a given rotation matrix \mathcal{R} from the form of the nine components of the rotation matrix given above.

Therefore, given the rotation matrix \mathcal{R} , we can determine the Euler angles using

$$\cos \beta = \mathcal{R}_{zz} \quad (20)$$

$$\sin \beta = \sqrt{1 - \mathcal{R}_{zz}^2} \quad (21)$$

If $\sin \beta \neq 0$, then

$$e^{-i\alpha} = \frac{\mathcal{R}_{zx} - i\mathcal{R}_{zy}}{\sin \beta} \quad (22)$$

and

$$e^{-i\gamma} = \frac{\mathcal{R}_{xz} + i\mathcal{R}_{yz}}{-\sin \beta}. \quad (23)$$

If $\sin \beta = 0$, then we can choose $\gamma = 0$, and

$$e^{-i\alpha} = \frac{\mathcal{R}_{xx} - i\mathcal{R}_{xy}}{\mathcal{R}_{zz}} \quad (24)$$

When there is inversion symmetry, we can find α , β , and γ for $\bar{\mathcal{R}}$ and then use Eq. 19 to determine the complete transformation of \mathcal{R} .