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A Guide to Rotations in Quantum Mechanics

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Abstract

To lay a foundation for the study and use of rotation operators in graduate quantum mechanics and in research, a thorough discussion is presented of rotations in Euclidean three space ($\Re^3$) and of their effect on kets in the Hilbert space of a single particle. The Wigner D-matrices are obtained and used to rotate spherical harmonics. An extensive ready-reference appendix of the properties of these matrices, expressed in a consistent notation, is provided. Careful attention is paid throughout to various conventions (e.g. active *versus* passive viewpoints) that are used in the literature.

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Part I. INTRODUCTION

Rotation operators, their matrix representations, and their effect on quantum states are an essential part of the quantum mechanics of microscopic systems. In graduate-level treatments of this topic (cf. Gottfried 1966; Shankar 1980; Messiah 1966; Schiff 1968; Merzbacher 1970; Sakurai 1985; Böhm 1979; Cohen-Tannoudji *et al.* 1977) the introduction of the rotation operator in Hilbert space and the Euler angle parametrization of rotations leads in short order to the Wigner rotation matrices.* These matrices, in turn, are widely used in a variety of applications (cf. Weissbluth 1979).

In our experience, newcomers to the theory of angular momentum, be they students or practicing physicists, are frequently confused by differences in the conventions and viewpoints used by various authors and by the lack of clarity in many introductory texts. Moreover, many have difficulty relating their intuitive (classical) notion of a rotation to the quantum mechanics of rotations in Hilbert space — primarily, we think, because their training in rotations in $\Re^3$ is poor. Although a few recent papers have dealt with rotations in Euclidean three space ($\Re^3$) (Leubner 1980) and with rotation matrices (Bayha 1984), few have addressed the rotation operators *per se* (see, however, Wolf 1969).

Our objective is to lay a foundation for the study of rotations in quantum mechanics and to provide a compendium of essential results of the theory of angular momentum. We begin in § II by discussing geometrical rotations in $\Re^3$ and the corresponding rotation matrices, both for a general rotation and in the Euler angle parametrization. (Goldstein 1980). We also discuss the difference between active and passive rotation conventions — a notorious source of confusion.

There follows in § III an introduction to rotations in Hilbert space. This leads to the Wigner rotation matrices, which are illustrated by rotating the familiar spherical harmonics. We have not included proofs of the properties of these matrices, since such proofs can be found in many texts and treatises on angular momentum (Brink and Satchler 1962; Edmonds 1960; Rose 1957; Biedenharn and Louck 1981; Judd 1975; Normand 1980; Silver 1976; Cushing 1975; Wybourne 1970).† To compensate for this lack, we have listed the important properties of the Wigner matrices in a "ready-reference appendix." The material in this appendix was gathered from a wide range of sources, but is here presented in a consistent notation and viewpoint.

Part II. ROTATIONS IN $\Re^3$

1. Simple Rotations about an Arbitrary Axis

A rotation in $\Re^3$ is a geometrical transformation. A particular rotation can be fully specified by two parameters: a **rotation angle** δ and a **rotation axis** $\hat{e}_u$, the axis about which the rotation occurs. We shall denote a rotation in $\Re^3$ by $\mathcal{R}_u(\delta)$. Unless otherwise indicated, all rotations are in the *positive* sense, as illustrated in Fig. 1.

* Rotations are treated in several advanced undergraduate quantum mechanics texts, including Dicke and Wittke (1960), Saxon (1968), Liboff (1980), and Powell and Crasemann (1961).

† Group theory is applied to rotations in Tinkham (1964) and in Hammermesh (1962); see also Harter *et al.* (1978).

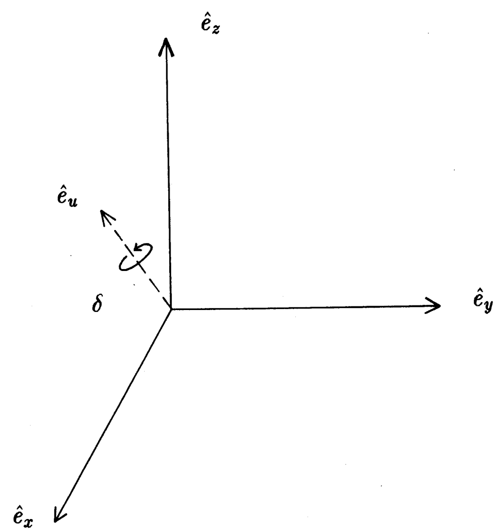

Fig. 1. A rotation in $\Re^3$ is defined by a rotation angle δ and a rotation axis $\hat{e}_u$. For $\delta > 0$, the rotation $\mathcal{R}_u(\delta)$ appears *counterclockwise* to an observer looking towards the origin.

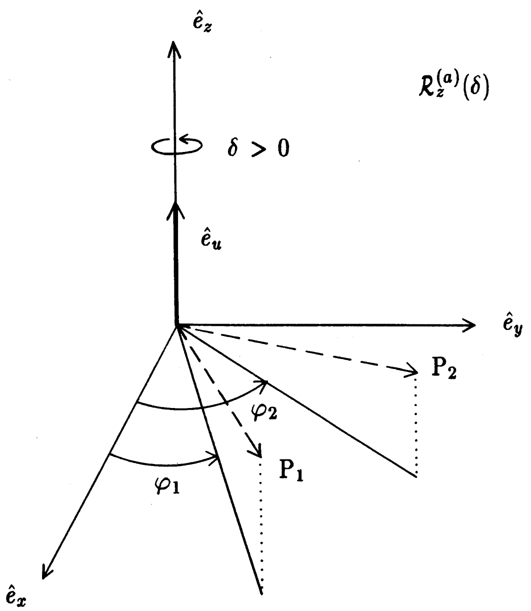

Fig. 2. An *active* rotation through a positive angle δ about the z axis. The operator that effects this rotation is $\mathcal{R}_z^{(a)}(\delta)$. Note that $\delta = \varphi_2 - \varphi_1$.

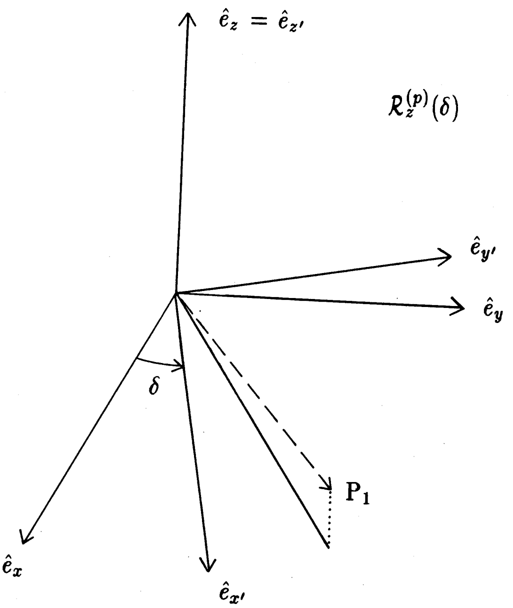

Fig. 3. A *passive* rotation through a positive angle δ about the z axis. The operator that effects this rotation is $\mathcal{R}_z^{(p)}(\delta)$. This rotation is *not* equivalent to the active rotation in Fig. 2.

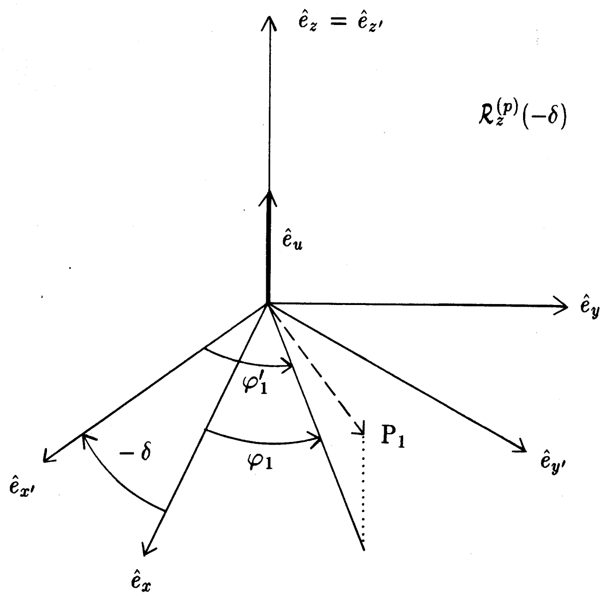

Fig. 4. The passive rotation that is equivalent to $\mathcal{R}_z^{(a)}(\delta)$ of Fig 1. The operator for this rotation is $\mathcal{R}_z^{(p)}(-\delta)$. Note that $\delta = \varphi_1' - \varphi_1$.

(a) Active and Passive Rotations

To describe the effect of a rotation in $\Re^3$, we first define a right-handed coordinate system, such as the one in Fig. 1. Because this system does not change its orientation, we call it the **space-fixed system**. The orthogonal unit vectors that define the space-fixed system are $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$.

A rotation in $\Re^3$ can be described using two viewpoints: active or passive. (Davydov 1976; Biedenharn and Louck 1981). **An active rotation** is a rotation *of a vector in a fixed coordinate frame.* We shall use a superscript (a) to emphasize that a rotation is active e.g. $\mathcal{R}_u^{(a)}(\delta)$. In the active rotation about the z axis ($\hat{e}_u = \hat{e}_z$) shown in Fig. 2, the vector $\boldsymbol{r}_1$ from the origin to point P_1 is rotated by $\mathcal{R}_z^{(a)}(\delta)$ into the vector $\boldsymbol{r}_2$ to point P_2:

$$\boldsymbol{r}_2 = \mathcal{R}_z^{(a)}(\delta)\,\boldsymbol{r}_1. \tag{1}$$

The inverse of an active rotation through angle δ about $\hat{e}_u$ is an active rotation through $-\delta$ about $\hat{e}_u$ or, equivalently, through δ about $-\hat{e}_u$:

$$\mathcal{R}_u^{(a)-1}(\delta) = \mathcal{R}_u^{(a)}(-\delta) = \mathcal{R}_{-u}^{(a)}(\delta). \tag{2}$$

Thus, the inverse of the rotation $\mathcal{R}_u^{(a)}(\delta)$ shown in Fig. 2 takes $\boldsymbol{r}_2$ into $\boldsymbol{r}_1$, i.e.

$$\boldsymbol{r}_1 = \mathcal{R}_u^{(a)-1}(\delta)\,\boldsymbol{r}_2. \tag{3}$$

In contrast, a **passive rotation** is a rotation *of the coordinate system.* In a particular reference frame, a point (the tip of a vector from the origin) is labelled by a triple of numbers — e.g. (x, y, z) or (r, θ, ϕ). Under a passive rotation, the vector remains fixed, but the point it defines receives new labels. That is, the numbers that describe the location of the point change from those appropriate to the (initial) unrotated frame to the (final) rotated frame. We shall use a superscript (p) to denote a passive rotation, e.g. $\mathcal{R}_u^{(p)}(\delta)$.

A passive rotation through a positive angle δ about the z axis is shown in Fig. 3. Denoting the location of the point P_1 in the fixed frame by unprimed coordinates and that of *the same point* in the rotated frame by primed coordinates, we can write the effect of a passive rotation as

$$\boldsymbol{r}_1' = \mathcal{R}_z^{(p)}(\delta)\,\boldsymbol{r}_1. \tag{4}$$

The rotations shown in Figs 2 and 3 are not equivalent. They differ because both are defined as *positive* rotations through a *positive* angle ($\delta > 0$). The *passive* rotation of coordinates that is equivalent to an active rotation through δ about $\hat{e}_u$ must do to the coordinate axes the *opposite* of what $\mathcal{R}_u^{(a)}(\delta)$ does to a vector. So the passive rotation that is equivalent to $\mathcal{R}_z^{(a)}(\delta)$ of Fig. 2 is $\mathcal{R}_z^{(p)}(-\delta)$, as illustrated in Fig. 4.

There is therefore an *equivalence* (an isomorphism) between active and passive rotations, i.e.

$$\mathcal{R}_u^{(a)}(\delta) \iff \mathcal{R}_u^{(p)}(-\delta), \tag{5a}$$

where $\iff$ stands for "is equivalent to". A similar argument establishes the corresponding equivalence

$$\mathcal{R}_u^{(p)}(\delta) \iff \mathcal{R}_u^{(a)}(-\delta). \tag{5b}$$

These equivalences will play an important role in the subsequent discussions of Euler angle rotations (§ II.2) and of rotation operators in Hilbert space (§ III).

To summarize: we can describe a rotation mathematically using either the active or passive convention, because according to Eqs (5), these rotations are equivalent *provided we remember to change the sign of the rotation angle.* The essential point is that $\mathcal{R}_u^{(a)}(\delta)$ and $\mathcal{R}_u^{(p)}(-\delta)$ are merely two ways to describe the same *geometrical* rotation. In an active rotation the "final" coordinate system is the same as the initial one; in a passive rotation the final system is $(\hat{e}_{x'}, \hat{e}_{y'}, \hat{e}_{z'})$. But the proximity of the physical system to the final coordinate system is the same regardless of whether we carry out the rotation in the active or the (equivalent) passive viewpoint.

(b) Rotation Matrices

Operationally, we describe the effect of a rotation in $\Re^3$ in terms of the components of the vector being rotated. For example, we can write $\boldsymbol{r}_1$ in terms of the unit vectors that define the fixed reference frame as

$$\boldsymbol{r}_1 = x_1\hat{e}_x + y_1\hat{e}_y + z_1\hat{e}_z. \tag{6}$$

The Cartesian components x_1, y_1, and z_1 are just the direction cosines of $\boldsymbol{r}_1$ with respect to the fixed axes, e.g. $x_1 = \hat{e}_x \cdot \boldsymbol{r}_1$. We can conveniently represent $\boldsymbol{r}_1$ by the column vector

$$\mathbf{r}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}. \tag{7}$$

To write Eq. (6) in matrix notation, we must first define the basis

$$\mathbf{e}_x = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{e}_y = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \mathbf{e}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{8}$$

Then the matrix counterpart of (6) is Eq. (7),

$$\mathbf{r}_1 = x_1\mathbf{e}_x + y_1\mathbf{e}_y + z_1\mathbf{e}_z. \tag{9}$$

The representation (7) depends critically on the coordinate system — this column vector is the correct representation of $\boldsymbol{r}_1$ only in the basis (8) which, in turn, pertains only to the fixed frame $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$.

A vector $\boldsymbol{r}_2$ that is obtained via an *active* rotation of $\boldsymbol{r}_1$ [Eq. (1)] can similarly be represented in the basis (8) by

$$\mathbf{r}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}. \tag{10}$$

How can the components of $\boldsymbol{r}_2$ in the fixed basis (8) be obtained directly from those of $\boldsymbol{r}_1$ in this basis? The components of a vector before and after rotation are related by a **rotation matrix**; for each rotation $\mathcal{R}_u^{(a)}(\delta)$ in $\Re^3$ there exists a matrix $\mathbf{R}_u(\delta)$ that appears in the matrix counterpart of Eq. (1),

$$\mathbf{r}_2 = \mathbf{R}_u(\delta)\, \mathbf{r}_1. \tag{11}$$

To find the elements of $\mathbf{R}_u(\delta)$ we first write both sides of (1) in the fixed frame and then translate the resulting equation into matrix notation using the basis (8). We begin by letting $\mathcal{R}_u^{(a)}(\delta)$ act on both sides of Eq. (6):

$$\boldsymbol{r}_2 = x_1\mathcal{R}_u^{(a)}(\delta)\hat{e}_x + y_1\mathcal{R}_u^{(a)}(\delta)\hat{e}_y + z_1\mathcal{R}_u^{(a)}(\delta)\hat{e}_z. \tag{12}$$

Let us denote the (orthogonal) unit vectors obtained when $\hat{e}_x$, $\hat{e}_y$, and $\hat{e}_z$ in (12) are rotated via $\mathcal{R}_u^{(a)}(\delta)$ by $\hat{f}_x$, $\hat{f}_y$, and $\hat{f}_z$:

$$\hat{f}_x = \mathcal{R}_u^{(a)}(\delta)\hat{e}_x, \tag{13a}$$

$$\hat{f}_y = \mathcal{R}_u^{(a)}(\delta)\hat{e}_y, \tag{13b}$$

$$\hat{f}_z = \mathcal{R}_u^{(a)}(\delta)\hat{e}_z. \tag{13c}$$

In terms of these rotated unit vectors, Eq. (12) is simply

$$\boldsymbol{r}_2 = x_1\hat{f}_x + y_1\hat{f}_y + z_1\hat{f}_z. \tag{14}$$

But our goal is to obtain the components of $\boldsymbol{r}_2$ in the *fixed* basis. To do so, we must write each unit vector in (13) in terms of $\hat{e}_x$, $\hat{e}_y$, $\hat{e}_z$; e.g.

$$\hat{f}_x = (\hat{e}_x \cdot \hat{f}_x)\,\hat{e}_x + (\hat{e}_y \cdot \hat{f}_x)\,\hat{e}_y + (\hat{e}_z \cdot \hat{f}_x)\,\hat{e}_z. \tag{15}$$

We now define the direction cosines in (15) to be elements *of the first* column of a 3×3 matrix $\mathbf{R}$:

$$R_{11} = (\hat{e}_x \cdot \hat{f}_x), \tag{16a}$$

$$R_{21} = (\hat{e}_y \cdot \hat{f}_x), \tag{16b}$$

$$R_{31} = (\hat{e}_z \cdot \hat{f}_x). \tag{16c}$$

The elements of the second and third columns of $\mathbf{R}$ are just the direction cosines of $\hat{f}_y$ and $\hat{f}_z$, respectively. Using the elements of the matrix $\mathbf{R}$, we can write the right-hand side of (14) in the fixed frame, viz.

$$\begin{aligned} \boldsymbol{r}_2 = {} & x_1\,R_{11}\,\hat{e}_x + x_1\,R_{21}\,\hat{e}_y + x_1\,R_{31}\,\hat{e}_z \\ & + y_1\,R_{12}\,\hat{e}_x + y_1\,R_{22}\,\hat{e}_y + y_1\,R_{32}\,\hat{e}_z \\ & + z_1\,R_{13}\,\hat{e}_x + z_1\,R_{23}\,\hat{e}_y + z_1\,R_{33}\,\hat{e}_z. \end{aligned} \tag{17}$$

When we translate (17) into matrix notation using the basis (8), we recognize $\mathbf{R}$ as the rotation matrix of Eq. (11):

$$\mathbf{R}_u(\delta) = \begin{pmatrix} (\hat{e}_x \cdot \hat{f}_x) & (\hat{e}_x \cdot \hat{f}_y) & (\hat{e}_x \cdot \hat{f}_z) \\ (\hat{e}_y \cdot \hat{f}_x) & (\hat{e}_y \cdot \hat{f}_y) & (\hat{e}_y \cdot \hat{f}_z) \\ (\hat{e}_z \cdot \hat{f}_x) & (\hat{e}_z \cdot \hat{f}_y) & (\hat{e}_z \cdot \hat{f}_z) \end{pmatrix}. \tag{18}$$

This matrix is orthogonal, because $\mathcal{R}_u^{(a)}(\delta)$ is an orthogonal transformation. In § II.2 we shall write down the rotation matrix for an arbitrary rotation in the (parametrized) Euler angle form.

To illustrate how one determines a rotation matrix, let us consider an active rotation through angle δ about the z axis (Fig. 2). For $\hat{e}_u = \hat{e}_z$, the rotation matrix (18) is

$$\mathbf{R}_z(\delta) = \begin{pmatrix} \cos\delta & -\sin\delta & 0 \\ \sin\delta & \cos\delta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{19}$$

For example, if $\delta = \sin^{-1}(\frac{4}{5}) \approx 53.1301°$, then

$$\mathbf{R}_z(\delta) = \begin{pmatrix} 3/5 & -4/5 & 0 \\ 4/5 & 3/5 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{20}$$

Suppose we rotate the vector $\boldsymbol{r}_1$ with components

$$\mathbf{r}_1 = \begin{pmatrix} 10 \\ 5 \\ 3 \end{pmatrix} \tag{21}$$

through 53.1301° about $\hat{e}_z$. To determine the resulting rotated vector, we multiply the matrix (20) by the column vector (21), viz.

$$\mathbf{r}_2 = \mathbf{R}_u(\delta)\,\mathbf{r}_1 = \begin{pmatrix} 2 \\ 11 \\ 3 \end{pmatrix}. \tag{22}$$

We could, of course, carry out the rotation $\mathcal{R}_u^{(a)}(\delta)$ using the *passive* viewpoint. To do so in $\Re^3$, we would have to use the *equivalent* passive rotation operator $\mathcal{R}_u^{(p)}(-\delta)$. But we can determine the components of $\boldsymbol{r}_1$ in the rotated frame using the rotation matrix $\mathbf{R}_u(\delta)$ of Eq. (18). To see why, let us act on $\boldsymbol{r}_1$ of (6) with $\mathcal{R}_u^{(p)}(-\delta)$:

$$\boldsymbol{r}_1' = \mathcal{R}_u^{(p)}(-\delta)\,\boldsymbol{r}_1 \tag{23a}$$
$$= x_1\mathcal{R}_u^{(p)}(-\delta)\,\hat{e}_x + y_1\mathcal{R}_u^{(p)}(-\delta)\,\hat{e}_y + z_1\mathcal{R}_u^{(p)}(-\delta)\,\hat{e}_z. \tag{23b}$$

Now, to work out the effect of $\mathcal{R}_u^{(p)}(-\delta)$ on the unit vectors in (23*b*), we replace this operator with its active equivalent, viz.

$$\boldsymbol{r}_1' = x_1\mathcal{R}_u^{(a)}(\delta)\,\hat{e}_x + y_1\mathcal{R}_u^{(a)}(\delta)\,\hat{e}_y + z_1\mathcal{R}_u^{(a)}(\delta)\,\hat{e}_z. \tag{24}$$

The right-hand side of (24) is now identical to that of (12). So $\mathbf{R}_u(\delta)$ of (18) gives us the components of $\boldsymbol{r}_1$ in the rotated frame, e.g.

$$x_1' = R_{11}(\delta)\,x_1 + R_{12}(\delta)\,y_1 + R_{13}(\delta)\,z_1. \tag{25}$$

The fact that the same rotation matrix is used in the active rotation (17) and in the passive rotation (25) should not come as a surprise, since *by construction of the equivalent passive rotation*, the components of $\boldsymbol{r}_1$ in the rotated frame are related to those of the rotated vector $\boldsymbol{r}_2$ in the fixed frame by

$$x_1' = x_2, \tag{26a}$$
$$y_1' = y_2, \tag{26b}$$
$$z_1' = z_2. \tag{26c}$$

Finally, we should note that the rotation matrix (18) differs from that found in texts that adopt the passive viewpoint. According to the equivalence (5*b*), the active rotation that is equivalent to $\mathcal{R}_u^{(p)}(\delta)$ is $\mathcal{R}_u^{(a)}(-\delta)$. Therefore the rotation matrix for a *passive* rotation through a *positive* angle δ about $\hat{e}_z$ is obtained from

(19) by replacing δ with $-\delta$, i.e.

$$\mathbf{R}_z(-\delta) = \begin{pmatrix} \cos\delta & \sin\delta & 0 \\ -\sin\delta & \cos\delta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{27}$$

2. Euler Angle Rotations in $\Re^3$

(a) Definitions of the Euler Angles

It is convenient to parametrize rotations in $\Re^3$, and the most widely used parametrization is that of Euler angles. In this formulation, an arbitrary rotation is carried out via three successive rotations about prescribed axes.

Euler angle rotations are often described in the **passive** viewpoint, in which *the fixed coordinate system ($\hat{e}_x$, $\hat{e}_y$, $\hat{e}_z$) is rotated through three positive angles, the Euler angles α, β, and γ.** Each rotation produces a new set of axes, which are labelled by successively more cumbersome sets of primes. The three stages of a passive Euler angle rotation are

PASSIVE EULER ANGLE ROTATION

- **Step 1:** Rotate the (unprimed) fixed axes through an angle α $(0 \le \alpha \le 2\pi)$ about $\hat{e}_z$, taking the $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$ coordinate system into the $(\hat{e}_{x'}, \hat{e}_{y'}, \hat{e}_{z'})$ system.

- **Step 2:** Rotate the primed axes from step 1 through β $(0 \le \beta \le \pi)$ about $\hat{e}_{y'}$, taking the $(\hat{e}_{x'}, \hat{e}_{y'}, \hat{e}_{z'})$ system into the $(\hat{e}_{x''}, \hat{e}_{y''}, \hat{e}_{z''})$ system.

- **Step 3:** Rotate the double primed axes from step 2 through γ $(0 \le \gamma \le 2\pi)$ about $\hat{e}_{z''}$, taking the $(\hat{e}_{x''}, \hat{e}_{y''}, \hat{e}_{z''})$ system into the $(\hat{e}_{x'''}, \hat{e}_{y'''}, \hat{e}_{z'''})$ system.

So the passive Euler angle rotation operator is

$$\mathcal{R}^{(p)}(\alpha,\beta,\gamma) \equiv \mathcal{R}^{(p)}_{z''}(\gamma)\,\mathcal{R}^{(p)}_{y'}(\beta)\,\mathcal{R}^{(p)}_{z}(\alpha). \tag{28}$$

(b) Active Euler Angle Rotation

As noted above, we have adopted the *active* viewpoint, in which the physical system, not the reference frame, is rotated. Conventionally, such an Euler angle rotation is performed as follows (cf. Goldstein 1980):

- **Step 1:** Rotate the system through an angle α $(0 \le \alpha \le 2\pi)$ about $\hat{e}_z$: $\mathcal{R}^{(a)}_z(\alpha)$.

- **Step 2:** Rotate the system through β $(0 \le \beta \le 2\pi)$ about $\hat{e}_{y'}$: $\mathcal{R}^{(a)}_{y'}(\beta)$.

- **Step 3:** Rotate the system through γ $(0 \le \gamma \le 2\pi)$ about $\hat{e}_{z''}$: $\mathcal{R}^{(a)}_{z''}(\gamma)$.

The corresponding geometrical rotation operator is

$$\mathcal{R}^{(a)}(\alpha,\beta,\gamma) \equiv \mathcal{R}^{(a)}_{z''}(\gamma)\,\mathcal{R}^{(a)}_{y'}(\beta)\,\mathcal{R}^{(a)}_{z}(\alpha). \tag{29}$$

* The passive rotation operator is used, for example, in Rose (1957). Somewhat confusingly, Rose discussed Euler angle rotations from the passive viewpoint although his rotations in $\Re^3$ and in state space are active.

But this parametrization mixes the active and passive viewpoints, since steps 2 and 3 entail rotations of the system about *rotated axes.* So it is convenient, both conceptually and operationally, to rewrite (29) in terms of rotations solely about fixed axes. In Appendix A, we use the class angle relation — which shows how to change the axis with respect to which a rotation operator is defined — to rewrite (29) as

$$\mathcal{R}^{(a)}(\alpha,\beta,\gamma) = \mathcal{R}_z^{(a)}(\alpha)\,\mathcal{R}_y^{(a)}(\beta)\,\mathcal{R}_z^{(a)}(\gamma). \tag{30}$$

This result prescribes the following steps:

ACTIVE EULER ANGLE ROTATION

- **Step 1:** Rotate the system through an angle γ $(0 \le \gamma \le 2\pi)$ about $\hat{e}_z$.
- **Step 2:** Rotate the system through β $(0 \le \beta \le \pi)$ about $\hat{e}_y$.
- **Step 3:** Rotate the system through α $(0 \le \alpha \le 2\pi)$ about $\hat{e}_z$.

Notice that when we rotate about the fixed axes, we perform the rotation by γ first; when we rotate about the rotated axes, we perform this rotation last.

(c) Passive Euler Angle Rotations

The passive Euler angle rotation (28) can also be written as a product of rotations about the fixed axes, viz.

$$\mathcal{R}^{(p)}(\alpha,\beta,\gamma) = \mathcal{R}_z^{(p)}(\alpha)\,\mathcal{R}_y^{(p)}(\beta)\,\mathcal{R}_z^{(p)}(\gamma). \tag{31}$$

The effect on a vector of the equivalent *active* rotation operator must be the inverse of what $\mathcal{R}^{(p)}(\alpha,\beta,\gamma)$ does to the coordinate axes, i.e.

$$\begin{aligned}
\mathcal{R}^{(p)}(\alpha,\beta,\gamma) \Longleftrightarrow {} & \left[\mathcal{R}_z^{(a)}(\alpha)\mathcal{R}_y^{(a)}(\beta)\mathcal{R}_z^{(a)}(\gamma)\right]^{-1} && (32a)\\
&= \mathcal{R}_z^{(a)-1}(\gamma)\,\mathcal{R}_y^{(a)-1}(\beta)\,\mathcal{R}_z^{(a)-1}(\alpha) && (32b)\\
&= \mathcal{R}_z^{(a)}(-\gamma)\,\mathcal{R}_y^{(a)}(-\beta)\,\mathcal{R}_z^{(a)}(-\alpha). && (32c)
\end{aligned}$$

(d) The Euler Angle Rotation Matrix

To write down the rotation matrix that corresponds to $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$, we first use Eq. (30) to express this operator in terms of three, single angle, active rotations and write the result in terms of the matrices of § II.1(b), viz.

$$\mathbf{R}(\alpha,\beta,\gamma) = \mathbf{R}_z(\alpha)\mathbf{R}_y(\beta)\mathbf{R}_z(\gamma)\,. \tag{33}$$

We can now construct an explicit form for the **Euler angle rotation matrix** $\mathbf{R}(\alpha,\beta,\gamma)$ from the single angle rotation matrices (18) as

$$\mathbf{R}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{34}$$

(Notice the location of the minus sign in the second of these matrices.) We need not append a superscript (a) to $\mathbf{R}(\alpha,\beta,\gamma)$, because the matrix (34) applies to the active rotation $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$ and to the equivalent passive rotation. Note that in the passive convention, which is preferred by some authors (cf. Pack and Hirschfelder 1970) the Euler angle rotation matrix is $\mathbf{R}(-\alpha, -\beta, -\gamma)$.

Part III. ROTATION OPERATORS IN HILBERT SPACE

1. Single Angle Rotation of an Arbitrary Ket

Consider an active rotation $\mathcal{R}_u^{(a)}(\delta)$ of a physical system. Let $\mathcal{E}$ denote the state space of the system and $|\,\psi(t)\,\rangle$ the ket that describes a state of the system at time t. As a consequence of rotation of the system in $\Re^3$, the ket that describes its state in $\mathcal{E}$ will change; let $|\,\psi'(t)\,\rangle$ denote the "rotated ket", i.e. the ket in $\mathcal{E}$ that represents the state immediately after rotation.

Corresponding to the rotation $\mathcal{R}_u^{(a)}(\delta)$ in $\Re^3$, there is a unitary **rotation operator** that acts in $\mathcal{E}$ to map $|\,\psi(t)\,\rangle$ into $|\,\psi'(t)\,\rangle$:

$$\hat{R}_u(\delta) \;:\; |\,\psi(t)\,\rangle \;\mapsto\; |\,\psi'(t)\,\rangle, \tag{35a}$$

$$|\,\psi'(t)\,\rangle = \hat{R}_u(\delta)\,|\,\psi(t)\,\rangle. \tag{35b}$$

The rotation operator that corresponds to $\mathcal{R}_u^{(a)}(\delta)$ is an exponential* involving the projection on the rotation axis $\hat{e}_u$ of the total angular momentum operator $\hat{\boldsymbol{J}}$, i.e.

$$\hat{R}_u^{(a)}(\delta) = \exp(-i\,\delta\,\hat{J}_u), \tag{36}$$

where we have used atomic units ($\hbar = 1$). [This operator is derived from the operator for an infinitesimal rotation by considering $\mathcal{R}_u^{(a)}(\delta)$ as an infinite succession of infinitesimal rotations (cf. Cohen-Tannoudji *et al.* 1977).] Hence the basic Hilbert space transformation (35b) is

$$|\,\psi'(t)\,\rangle = \exp(-i\,\delta\,\hat{J}_u)\,|\,\psi(t)\,\rangle. \tag{37}$$

The *equivalent* passive rotation is $\mathcal{R}_u^{(p)}(-\delta)$. For this rotation, the final ket is $|\,\psi'(t)\,\rangle$ of (35b), so the appropriate rotation operator is just the one used for the active rotation in Eq. (36).

For a *passive rotation through a positive angle* δ, the rotation operator is determined by the fundamental correspondence (5b), which requires that we change the sign of the angle in (36):

$$\hat{R}_u^{(p)}(\delta) = \exp(i\,\delta\,\hat{J}_u). \tag{38}$$

This convention is used by many authors.

2. Euler Angle Rotation of an Arbitrary Ket

Let us now write down the Hilbert space operator that corresponds to an arbitrary active rotation in the Euler angle parametrization. Recall that for (positive) Euler angles α, β, and γ, the rotation operator in $\Re^3$ is

$$\mathcal{R}^{(a)}(\alpha,\beta,\gamma) = \mathcal{R}_z^{(a)}(\alpha)\,\mathcal{R}_y^{(a)}(\beta)\,\mathcal{R}_z^{(a)}(\gamma). \tag{39}$$

* The exponential of an operator is defined by a series that has the same coefficients as the exponential of a function, i.e. $\exp(\hat{A}) = \sum_{n=0}^{\infty} A^n/(n!)$.

The quantum mechanical rotation operator corresponding to $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$ is the product of three, single angle, rotation operators, each of the form (36):

$$\hat{R}^{(a)}(\alpha,\beta,\gamma) = \hat{R}_z^{(a)}(\alpha)\,\hat{R}_y^{(a)}(\beta)\,\hat{R}_z^{(a)}(\gamma) \tag{40a}$$

$$= \exp(-i\,\alpha\,\hat{J}_z)\,\exp(-i\,\beta\,\hat{J}_y)\,\exp(-i\,\gamma\,\hat{J}_z). \tag{40b}$$

[We cannot write (40*b*) as a single exponential, because $\hat{J}_z$ and $\hat{J}_y$ do not commute.] Using this operator, we can express the effect on a ket $|\,\psi(t)\,\rangle$ in $\mathcal{E}$ of the rotation (39):

$$|\,\psi'(t)\,\rangle = \hat{R}^{(a)}(\alpha,\beta,\gamma)\,|\,\psi(t)\,\rangle. \tag{41}$$

3. Euler Angle Rotations of a Position Eigenket

Some of the most important applications of rotation operators in quantum mechanics are made in the position representation (cf. Weissbluth 1979). It is therefore important to know the effect on a position eigenket in $\mathcal{E}$ of an active rotation $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$ of a vector $\boldsymbol{r}_1$ in $\Re^3$, such as

$$\boldsymbol{r}_2 = \mathcal{R}^{(a)}(\alpha,\beta,\gamma)\,\boldsymbol{r}_1. \tag{42}$$

Using the rotation operator (40*b*), we can exhibit the relationship between the rotation in $\Re^3$ and its effect in $\mathcal{E}$; denoting the "rotated ket" by $|\,\boldsymbol{r}_2\,\rangle$, we have

$$|\,\boldsymbol{r}_2\,\rangle = \hat{R}^{(a)}(\alpha,\beta,\gamma)\,|\,\boldsymbol{r}_1\,\rangle = |\mathcal{R}^{(a)}(\alpha,\beta,\gamma)\,\boldsymbol{r}_1\rangle\,. \tag{43}$$

In § III.6, we shall need the dual of this result. Since the rotation operator is unitary, i.e.

$$\hat{R}^{(a)\,-1}(\alpha,\beta,\gamma) = \hat{R}^{(a)\dagger}(\alpha,\beta,\gamma), \tag{44}$$

the bra corresponding to $|\,\boldsymbol{r}_2\,\rangle$ is

$$\langle\,\boldsymbol{r}_2\,| = \langle\,\boldsymbol{r}_1\,|\,\hat{R}^{(a)\dagger}(\alpha,\beta,\gamma), \tag{45a}$$

whence

$$\langle\,\boldsymbol{r}_1\,| = \langle\,\boldsymbol{r}_2\,|\,\hat{R}^{(a)}(\alpha,\beta,\gamma). \tag{45b}$$

4. Euler Angle Rotations of an Angular Momentum Eigenket

The mathematical manipulations required to rotate an arbitrary ket in $\mathcal{E}$ can be simplified by first expanding the ket in an angular momentum basis. If we denote by $\hat{J}^2$ and $\hat{J}_z$ the square and z projection of the total angular momentum $\hat{\boldsymbol{J}}$, we can write this basis as $\{\,|\,(k),j,m\,\rangle\,\}$. [Note carefully that $\hat{J}_z$ is the projection of $\hat{\boldsymbol{J}}$ on the *fixed* $\hat{e}_z$ axis.] The quantum numbers j and m are defined by the eigenvalue equations for the basis kets,

$$\hat{J}^2\,|\,(k),j,m\,\rangle = j\,(j+1)\,|\,(k),j,m\,\rangle, \tag{46a}$$

$$\hat{J}_z|\,(k),j,m\rangle = m\,|\,(k),j,m\,\rangle, \tag{46b}$$

where j and m obey the usual restrictions (Cohen-Tannoudji *et al.* 1977):

$$j = 0,\tfrac{1}{2},1,\tfrac{3}{2},\ldots,$$

$$m = -j,-j+1,-j+2,\ldots,j-2,j-1,j.$$

The symbol (k) represents the set of quantum numbers that, together with j and m, completely specify a particular state; i.e. the quantum numbers (k) correspond to the eigenvalues of a set of operators $\hat{A}$ that, together with $\hat{J}^2$ and $\hat{J}_z$, comprise a complete set of commuting operators (CSCO).

The expansion of a ket $|\psi(t)\rangle$ in this basis is

$$|\psi(t)\rangle = \sum_{(k)} \sum_{j} \sum_{m} |(k), j, m\rangle \langle (k), j, m \,|\, \psi(t)\rangle. \tag{47}$$

We are here concerned with the angular momentum properties of quantum states, so from now on we shall suppress the indices (k), e.g. for $|(k), j, m\rangle$ we shall write $|j, m\rangle$.

Using the expansion (47), we can rotate an arbitrary ket if we know the effect of a rotation operator $\hat{R}^{(a)}(\alpha, \beta, \gamma)$ on an eigenket. This result will eventually lead us to the Wigner D-matrices.

To develop a general result for the "rotated ket" $\hat{R}^{(a)}(\alpha, \beta, \gamma)\,|j, m\rangle$, we use closure of the angular momentum basis $\{\,|j, m\rangle\,\}$ to write

$$\hat{R}^{(a)}(\alpha, \beta, \gamma)\,|j, m\rangle = \sum_{\mu=-j}^{+j} |j, \mu\rangle \langle j, \mu \,|\, \hat{R}^{(a)}(\alpha, \beta, \gamma) \,|\, j, m\rangle. \tag{48}$$

[In writing Eq. (48) we used the fact that the eigensubspace defined by the quantum number j, which we denote by $\overline{\mathcal{E}}(k, j) \equiv \overline{\mathcal{E}}(j)$, is globally invariant under any operator function of the components of $\hat{\boldsymbol{J}}$, and hence is invariant under $\hat{R}^{(a)}(\alpha, \beta, \gamma)$.]

The quantity $\langle j, \mu \mid \hat{R}^{(a)}(\alpha, \beta, \gamma) \mid j, m\rangle$ in Eq. (48) is the famous **Wigner D-matrix**: *the matrix element of the unitary rotation operator $\hat{R}^{(a)}(\alpha, \beta, \gamma)$ on the eigensubspace $\overline{\mathcal{E}}(j)$ with respect to the angular momentum basis:**

$$\mathcal{D}^{j}_{\mu,m}(\alpha, \beta, \gamma) \equiv \langle j, \mu \mid \hat{R}^{(a)}(\alpha, \beta, \gamma) \mid j, m\rangle. \tag{49}$$

Using the definition of the D-matrix, we can write the transformation equation (48) as

$$\hat{R}^{(a)}(\alpha, \beta, \gamma)\,|j, m\rangle = \sum_{\mu=-j}^{+j} |j, \mu\rangle\, \mathcal{D}^{j}_{\mu,m}(\alpha, \beta, \gamma). \tag{50}$$

To obtain the D-matrix appropriate to a passive rotation, we can use the relationship between active and passive rotation operators, Eqs (36) and (38), to transform our equations into the passive viewpoint. According to Eq. (38),

$$\hat{R}^{(p)}(\alpha, \beta, \gamma) = \hat{R}^{(a)\dagger}(\alpha, \beta, \gamma), \tag{51}$$

so the D-matrix element for a passive rotation, $\langle j, \mu \mid \hat{R}^{(p)}(\alpha, \beta, \gamma) \mid j, m\rangle$, is simply related to the corresponding element for an active rotation:

$$\begin{aligned} \langle j, \mu \mid \hat{R}^{(p)}(\alpha, \beta, \gamma) \mid j, m\rangle &= \langle j, \mu \mid \hat{R}^{(a)\dagger}(\alpha, \beta, \gamma) \mid j, m\rangle && (52a) \\ &= \Big(\langle j, m \mid \hat{R}^{(a)}(\alpha, \beta, \gamma) \mid j, \mu\rangle\Big)^{*} && (52b) \\ &= \mathcal{D}^{j\,*}_{m,\mu}(\alpha, \beta, \gamma). && (52c) \end{aligned}$$

* Useful methods for calculation of the D-matrices can be found in Walker (1975) and Caride and Zanette (1979); see also Appendix B.

Thus, *to transform an equation written in the active convention to its counterpart in the passive convention, we merely replace $\mathcal{D}^j_{\mu,m}(\alpha,\beta,\gamma)$ everywhere by $\mathcal{D}^{j\,*}_{m,\mu}(\alpha,\beta,\gamma)$.* Not only must we take the complex conjugate of the D-matrix element, we must also switch the indices.*

5. Physical Significance of a Rotated Angular Momentum Eigenket

The "rotated" ket $\hat{R}^{(a)}(\alpha,\beta,\gamma)\,|\,j,m\,\rangle$ in (50) is an eigenvector of $\hat{J}^2$ but not of $\hat{J}_z$, the component of the total angular momentum along the *fixed* z axis. But this ket is an eigenket of the component of $\hat{\boldsymbol{J}}$ along a different quantization axis.

The axis of quantization of the *unrotated* ket is $\hat{e}_z$. Let $\hat{e}_{z'}$ denote the vector in $\Re^3$ into which $\hat{e}_z$ is rotated by $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$, i.e.

$$\hat{e}_{z'} = \mathcal{R}^{(a)}(\alpha,\beta,\gamma)\,\hat{e}_z. \tag{53}$$

To rotate $\hat{e}_z$ is to rotate the axis of quantization of the unrotated ket $|\,j,m\,\rangle$. Therefore, *the rotated axis $\hat{e}_{z'}$ is the axis of quantization for the rotated eigenket $\hat{R}^{(a)}(\alpha,\beta,\gamma)\,|\,j,m\,\rangle$.* If we denote the rotated eigenket by $|\,j,m\,\rangle'$, we have

$$|\,j,m\,\rangle' = \hat{R}^{(a)}(\alpha,\beta,\gamma)\,|\,j,m\,\rangle = \sum_{\mu=-j}^{+j} |\,j,\mu\,\rangle\,\mathcal{D}^j_{\mu,m}\,(\alpha,\beta,\gamma). \tag{54}$$

The eigenvalue equations for the rotated ket are

$$\hat{J}^2\,|\,j,m\,\rangle' = j\,(j+1)\,|\,j,m\,\rangle', \tag{55a}$$

$$\hat{J}_{z'}|\,j,m\,\rangle' = m\,|\,j,m\,\rangle'. \tag{55b}$$

Note that the *eigenvalues* are unchanged by this rotation — the eigenvalue of $|\,j,m\,\rangle$ with respect to $\hat{J}_z$ is m which, according to (55*b*), is also the eigenvalue of $|\,j,m\,\rangle'$ with respect to $\hat{J}_{z'}$. Equation (54) is a unitary transformation from the basis $\{\,|\,j,m\,\rangle\,\}$ of the CSCO $\{\hat{A},\hat{J}^2,\hat{J}_z\}$, to the basis $\{\,|\,j,m\,\rangle'\,\}$ of the CSCO $\{\hat{A},\hat{J}^2,\hat{J}_{z'}\}$.

6. Transformation of the Spherical Harmonics

As an application of the D-matrices, we shall transform spherical harmonics between two coordinate systems (Steinborn and Ruedenberg 1973). Such transformations are important in, for example, the theory of electron-molecule scattering (Lane 1980; Morrison 1983, 1987). The relative orientation of the two reference frames is described by the Euler angles α, β, and γ.

The spherical harmonics are the position representation of the eigenkets of the orbital angular momentum. More precisely, if $\hat{\boldsymbol{L}}$ is the orbital angular momentum operator, then $|\,\ell,m\,\rangle$ is a simultaneous eigenket of $\hat{L}^2$ and $\hat{L}_z$ with quantum numbers ℓ and m, respectively. In the position representation, the angular dependence of the scalar product of $|\,\ell,m\,\rangle$ and a position eigenket $|\,\boldsymbol{r}\,\rangle$ is given by the spherical harmonic $Y_\ell^m(\theta,\varphi)$.

* Authors such as Pack and Hirschfelder (1970) who work in the passive convention use D-matrices that are the Hermitian adjoint of the matrices in this section; see Appendix B.

First we write the basic relationships between "rotated" and fixed kets, Eq. (54), in terms of the eigenkets $|\ell, m\rangle$:

$$|\ell, m\rangle' = \hat{R}^{(a)}(\alpha, \beta, \gamma)\,|\ell, m\rangle = \sum_{\mu=-\ell}^{+\ell} |\ell, \mu\rangle\, \mathcal{D}^{\ell}_{\mu,m}(\alpha, \beta, \gamma). \tag{56}$$

The ket $|\ell, m\rangle$ is an eigenket of $\{\hat{A}, \hat{L}^2, \hat{L}_z\}$ (where $\hat{A}$ completes the CSCO) with eigenvalues $\ell(\ell+1)$ and m, and $|\ell, m\rangle'$ is an eigenket of $\{\hat{A}, \hat{L}^2, \hat{L}_{z'}\}$ with the same eigenvalues.

Now, let $\boldsymbol{r}$ be a vector to a point P in the fixed frame. Consider a second coordinate system whose z axis is coincident with the quantization axis of the rotated ket $|\ell, m\rangle'$. We shall denote this rotated system* by a single set of primes, $(\hat{e}_{x'}, \hat{e}_{y'}, \hat{e}_{z'})$. The vector to P in the rotated system will be denoted $\boldsymbol{r}'$.

The position eigenkets that correspond to these two vectors are related by a *passive* rotation, i.e.

$$|\boldsymbol{r}'\rangle = \hat{R}^{(p)}(\alpha, \beta, \gamma)\,|\boldsymbol{r}\rangle = \hat{R}^{(a)-1}(\alpha, \beta, \gamma)\,|\boldsymbol{r}\rangle. \tag{57}$$

The dual of this result is

$$\langle \boldsymbol{r}'| = \langle \boldsymbol{r}|\,\hat{R}^{(a)}(\alpha, \beta, \gamma). \tag{58}$$

Now, to express Eq. (56) in the position representation, we operate on the left with the bra $\langle \boldsymbol{r}|$, viz.

$$\langle \boldsymbol{r} \mid \ell, m\rangle' = \sum_{\mu=-\ell}^{+\ell} \langle \boldsymbol{r} \mid \ell, \mu\rangle \mathcal{D}^{\ell}_{\mu,m}(\alpha, \beta, \gamma). \tag{59}$$

But

$$\langle \boldsymbol{r} \mid \ell, m\rangle' = \langle \boldsymbol{r} \mid \hat{R}^{(a)}(\alpha, \beta, \gamma) \mid \ell, m\rangle, \tag{60}$$

so we can write (59) as

$$\langle \boldsymbol{r} \mid \hat{R}^{(a)}(\alpha, \beta, \gamma) \mid \ell, m\rangle = \sum_{\mu=-\ell}^{+\ell} \langle \boldsymbol{r} \mid \ell, \mu\rangle \mathcal{D}^{\ell}_{\mu,m}(\alpha, \beta, \gamma). \tag{61}$$

Now, using Eq. (58) for $\langle \boldsymbol{r} \mid \hat{R}^{(a)}(\alpha, \beta, \gamma)$, we obtain

$$\langle \boldsymbol{r}' \mid \ell, m\rangle = \sum_{\mu=-\ell}^{+\ell} \langle \boldsymbol{r} \mid \ell, \mu\rangle \mathcal{D}^{\ell}_{\mu,m}(\alpha, \beta, \gamma). \tag{62}$$

Writing this result in terms of the spherical harmonics we obtain the basic transformation relation

$$Y_{\ell}^{m}(\theta', \varphi') = \sum_{\mu=-\ell}^{+\ell} Y_{\ell}^{\mu}(\theta, \varphi)\, \mathcal{D}^{\ell}_{\mu,m}(\alpha, \beta, \gamma). \tag{63}$$

This equation is a special case of the general Hilbert space transformation (54).

* This frame is non-inertial; this fact need not concern us, since we consider its spatial orientation only at fixed time.

Part IV. CONCLUDING REMARKS

The rotation operators $\hat{R}_u^{(a)}(\delta)$ and the Wigner rotation matrices $\mathcal{D}^j_{\mu,m}(\alpha,\beta,\gamma)$ find application in a wide range of fields, including molecular spectroscopy, the theory of irreducible tensor operators, nuclear structure, and scattering theory. The tables in Appendix B provide most commonly-used formulas involving these operators and matrices, expressed in the notation and conventions of this paper, together with some guidance to other notations used in the vast literature of angular momentum theory.

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Appendix A: The Class Angle Proof

Let $\mathcal{R}_u^{(a)}(\delta)$ represent a rotation in $\Re^3$ through δ about $\hat{e}_u$. We can use the class angle relation (Biedenharn and Louck 1981) to determine the operator for a rotation through the same angle about a different axis, say $\hat{e}_v$.

There exists an active rotation that carries a vector that lies along $\hat{e}_u$ into a vector that lies along $\hat{e}_v$. Let ϕ be the angle and $\hat{n}$ the axis for this rotation, i.e.

$$\mathcal{R}_n^{(a)}(\phi) \;:\; \hat{e}_u \quad\mapsto\quad \hat{e}_v . \tag{A1}$$

According to the class angle relation, the operator for rotation through δ about the *rotated* axis $\hat{e}_v$ is given in terms of $\mathcal{R}_u^{(a)}(\delta)$ by

$$\mathcal{R}_v^{(a)}(\delta) = \mathcal{R}_n^{(a)}(\phi)\,\mathcal{R}_u^{(a)}(\delta)\,\mathcal{R}_n^{(a)\,-1}(\phi). \tag{A2}$$

We want to use this result to express the active Euler angle rotation (29),

$$\mathcal{R}^{(a)}(\alpha,\beta,\gamma) = \mathcal{R}_{z''}^{(a)}(\gamma)\,\mathcal{R}_{y'}^{(a)}(\beta)\,\mathcal{R}_z^{(a)}(\alpha), \tag{A3}$$

in terms of rotations about the fixed axes. To do so, we use the following theorem (Biedenharn and Louck 1981), which follows from Eq. ($A2$):

■ <u>*Theorem*</u>: Let $\mathcal{R}_k = \mathcal{R}_{n_k}(\phi_k)$, where $k = 1, 2, 3, \ldots, N$ labels a set of N rotations through angles ϕ_k about axes $\hat{n}_k$ in $\Re^3$. Define N new rotation axes by

$$\hat{n}'_k = \left[\mathcal{R}_{k-1}\,\mathcal{R}_{k-2}\ldots\mathcal{R}_2\,\mathcal{R}_1\right]^{-1}\hat{n}_k, \qquad k = 2, 3, \ldots N, \tag{A4a}$$

$$\hat{n}'_1 = \hat{n}_1 . \tag{A4b}$$

Then

$$\mathcal{R}_n\,\mathcal{R}_{n-1}\,\mathcal{R}_{n-2}\ldots\mathcal{R}_2\,\mathcal{R}_1 = \mathcal{R}'_1\,\mathcal{R}'_2\ldots\mathcal{R}'_{n-1}\,\mathcal{R}'_n. \quad ■ \tag{A5}$$

To apply this theorem to the Euler angle rotation ($A3$), we must consider three rotations:

$$\mathcal{R}_1 = \mathcal{R}_z^{(a)}(\alpha) \implies \phi_1 = \alpha,\ \hat{n}_1 = \hat{e}_z, \tag{A6a}$$

$$\mathcal{R}_2 = \mathcal{R}_{y'}^{(a)}(\beta) \implies \phi_2 = \beta,\ \hat{n}_2 = \hat{e}_{y'}, \tag{A6b}$$

$$\mathcal{R}_3 = \mathcal{R}_{z''}^{(a)}(\gamma) \implies \phi_3 = \gamma,\ \hat{n}_3 = \hat{e}_{z''}. \tag{A6c}$$

Since $\hat{n}_1 = \hat{n}'_1$, the first rotation operator on the right-hand side of ($A5$) is simply

$$\mathcal{R}'_1 = \mathcal{R}_z^{(a)}(\alpha). \tag{A7}$$

The new rotation axis for the second rotation $\mathcal{R}'_2$ is

$$\hat{n}'_2 = \mathcal{R}_z^{(a)\,-1}(\alpha)\,\hat{e}_{y'}\,. \tag{A8}$$

But $\hat{e}_{y'}$ was obtained from $\hat{e}_y$ via $\mathcal{R}_z^{(a)}(\alpha)$, so the second operator in ($A5$) is $\hat{n}'_2 = \hat{e}_y$, and we have

$$\mathcal{R}'_2 = \mathcal{R}_y^{(a)}(\beta)\,. \tag{A9}$$

Lastly, we must contend with $\mathcal{R}_3 = \mathcal{R}_{z''}^{(a)}(\gamma)$. To determine the corresponding new rotation axis, we must, according to ($A4$), evaluate

$$\hat{n}'_3 = [\mathcal{R}_2\,\mathcal{R}_1]^{-1}\,\hat{e}_{z''} = \left[\mathcal{R}_{y'}^{(a)}(\beta)\,\mathcal{R}_z^{(a)}(\alpha)\right]^{-1}\hat{e}_{z''}. \tag{A10}$$

Using

$$\left[\mathcal{R}_{u_1}^{(a)}(\delta_1)\,\mathcal{R}_{u_2}^{(a)}(\delta_2)\right]^{-1} = \mathcal{R}_{u_2}^{(a)-1}(\delta_2)\,\mathcal{R}_{u_1}^{(a)-1}(\delta_1), \tag{A11}$$

we can expand the inverse product in ($A10$) to obtain

$$\hat{n}'_3 = \mathcal{R}_z^{(a)-1}(\alpha)\,\mathcal{R}_{y'}^{(a)-1}(\beta)\,\hat{e}_{z''} = \hat{e}_z\,. \tag{A12}$$

Therefore the third operator in ($A5$) is

$$\mathcal{R}'_3 = \mathcal{R}_z^{(a)}(\gamma)\,. \tag{A13}$$

Now, if we use Eqs ($A7$), ($A9$), and ($A13$) in the theorem ($A5$), we find that the *active* Euler angle rotation $\mathcal{R}^{(a)}(\alpha,\beta,\gamma)$ can be written in two equivalent ways, depending on which set of axes we choose for the rotations: either as ($A3$) or as

$$\mathcal{R}^{(a)}(\alpha,\beta,\gamma) = \mathcal{R}_z^{(a)}(\alpha)\,\mathcal{R}_y^{(a)}(\beta)\,\mathcal{R}_z^{(a)}(\gamma)\,. \tag{A14}$$

Appendix B: The Wigner Rotation Matrices

In this appendix we give a partial list (without proofs) of some of the important properties of the Wigner rotation matrices. Detailed proofs and more elaborate discussions of these results can be found in Brink and Satchler (1962), Edmonds (1960), Rose (1957), Biedenharn and Louck (1981), Judd (1975), Normand (1980), Silver (1976), Cushing (1975), and Wybourne (1970). These properties assume use of the active convention, the choice made in the text of this paper. But they can easily be translated into the passive convention by replacing each D-matrix with its Hermitian adjoint and each rotation operator with the equivalent passive operator; see Eqs (32) and (34) and Appendix C.

List of Symbols

$\hat{e}_x, \hat{e}_y, \hat{e}_z$	Unit vectors in the fixed frame
$\hat{e}_{x'}, \hat{e}_{y'}, \hat{e}_{z'}$	Unit vectors in the rotated frame
α, β, γ	Euler rotation angles
$\hat{\mathcal{J}}_x, \hat{\mathcal{J}}_y, \hat{\mathcal{J}}_z$	Space-fixed angular momentum operators
$\hat{\mathcal{J}}_\pm$	Space-fixed raising and lowering operators
$\hat{\mathcal{J}}_{x'}, \hat{\mathcal{J}}_{y'}, \hat{\mathcal{J}}_{z'}$	Body-fixed angular momentum operators
$\hat{\mathcal{J}}_{\pm'}$	Body-fixed raising and lowering operators
$\hat{\boldsymbol{\mathcal{J}}}_x^{(j)}, \hat{\boldsymbol{\mathcal{J}}}_y^{(j)}, \hat{\boldsymbol{\mathcal{J}}}_z^{(j)}$	Space-fixed angular momentum matrix operators
$\|jm\rangle$	Eigenket of the angular momentum operators
$Y_j^m(\theta, \phi)$	Spherical harmonic (Condon-Shortley phase convention)
$\hat{T}_{kq}$	Spherical tensor operator
${}_2F_1$	Hypergeometric function
$\hat{R}^{(a)}$	Active rotation operator
$\hat{R}^{(p)}$	Passive rotation operator
$\mathbf{R}_u(\delta)$	Rotation matrix
$\hat{\boldsymbol{\mathcal{D}}}^j(\alpha, \beta, \gamma)$	Wigner rotation matrix
$\hat{\mathbf{d}}^j$	Reduced Wigner rotation matrix operator
$P_n^{(n_1, n_2)}$	Jacobi polynomial
P_l^m	Associated Legendre polynomial
P_l	Legendre polynomial
$\boldsymbol{\mathcal{I}}^j$	Identity matrix
$C(j_1, j_2, j; m_1, m_2, m)$	Clebsch-Gordan coefficient
$\boldsymbol{\mathcal{C}}$	Orthogonal Clebsch-Gordan matrix
χ^j	Character or trace of the Wigner rotation matrix
$\alpha_0, \alpha_1, \alpha_2, \alpha_3$	Euler-Rodrigues parameters
$\delta(x - x')$	Dirac delta function
$\Delta(j_1 j_2 j_3)$	Triangle relation
$\hat{\boldsymbol{\mathcal{P}}}_m^j$	Angular momentum matrix projection operator
I_x, I_y, I_z	Principal moments of inertia

Definitions

The Wigner rotation matrix $\hat{\mathcal{D}}^j(\alpha,\beta,\gamma)$ transforms a set of kets $|j\mu\rangle$ according to Eq. (54),

$$\begin{aligned} |j,m\rangle' &= \hat{R}^{(a)}|jm\rangle \\ &= \exp(-i\alpha\hat{\mathcal{J}}_z)\exp(-i\beta\hat{\mathcal{J}}_y)\exp(-i\gamma\hat{\mathcal{J}}_z)|jm\rangle \\ &= \exp(-i\delta\hat{\mathcal{J}}_u)|jm\rangle \\ &= \sum_{\mu=-j}^{j}\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma)|j\mu\rangle. \end{aligned} \tag{B1}$$

The ranges of the Euler angles are

$$0\le\alpha\le 2\pi,\quad 0\le\beta\le\pi,\quad 0\le\gamma\le 2\pi. \tag{B2}$$

The projection quantum numbers in $(B1)$ must satisfy

$$\begin{aligned} -j\le m\le j, \\ -j\le\mu\le j. \end{aligned} \tag{B3}$$

The angular momentum operators satisfy the usual commutation relations

$$\hat{\mathcal{J}}\times\hat{\mathcal{J}} = i\hat{\mathcal{J}}, \tag{B4}$$

i.e.

$$[\hat{\mathcal{J}}_i,\hat{\mathcal{J}}_j] = i\hat{\mathcal{J}}_k, \tag{B5}$$

where the subscripts i,j,k are any cyclic permutation of x,y,z.

Relations between Commonly-used Notations

$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = R^j_{\mu m}(\phi,\theta,\psi)$	Messiah (1966): Appendix C.10 Eq. (C.54)
$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = D^j_{\mu m}(\phi,\theta,\psi)$	Normand (1980): Eq. (6-21)
$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = D^j_{\mu m}(\alpha,\beta,\gamma)$	Rose (1957): Eq. (4.12)
	Biedenharn and Louck (1981): Eq. (3.59)
	Tinkham (1964): Eq. (5.35)
	Cushing (1975): Eq. (9.140)
	Judd (1975): Eq. (1.11)
$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = D^{j*}_{\mu m}(\alpha,\beta,\gamma)$	Bohr and Mottelson (1969): Eq. (1A-35)
$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = D^j_{\mu m}(-\alpha,-\beta,-\gamma)$	Edmonds (1960): Eq. (4.1.12)
	Weissbluth (1979): Eq. (4.5-2)
	Hammermesh (1962): Eq. (9.76)
	Fano and Racah (1959): Eq. (D.2)
	Wigner (1959): Eq. (15.27)
$\mathcal{D}^j_{\mu m}(\alpha,\beta,\gamma) = D^{j*}_{m\mu}(\alpha,\beta,\gamma)$	Pack and Hirschfelder (1970): Eq. (B1)

Explicit Expressions

The elements of the Wigner rotation matrix are matrix elements of the rotation operator (Rose 1957) (see § III.4)

$$\begin{aligned}\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) &= \langle j\mu|\exp(-i\alpha\hat{\mathcal{J}}_z)\exp(-i\beta\hat{\mathcal{J}}_y)\exp(-i\gamma\hat{\mathcal{J}}_z)|jm\rangle \\ &= \exp(-i\mu\alpha)\langle j\mu|\exp(-i\beta\hat{\mathcal{J}}_y)|jm\rangle\exp(-im\gamma) \\ &= \exp(-i\mu\alpha)d^j_{\mu m}(\beta)\exp(-im\gamma),\end{aligned} \tag{B6}$$

where

$$\begin{aligned}d^j_{\mu m}(\beta) = \left[\frac{(j-m)!(j+\mu)!}{(j+m)!(j-\mu)!}\right]^{1/2} &\frac{(\cos\beta/2)^{2j+m-\mu}(-\sin\beta/2)^{\mu-m}}{(\mu-m)!} \\ \times\ {}_2F_1\left(\mu-j,-m-j;\mu-m+1;-\tan^2\frac{\beta}{2}\right), &\qquad m'\geq m.\end{aligned} \tag{B7}$$

The hypergeometric function ${}_2F_1(a,b,c;z)$ is

$${}_2F_1(a,b,c;z) = 1+\frac{ab}{c}z+\frac{a(a+1)b(b+1)}{2!\,c(c+1)}z^2+\cdots \tag{B8}$$

In $(B8)$, a and b are negative integers or zero, so the hypergeometric function is a finite polynomial of degree $\min(|\mu-j|,|m+j|)$. The Wigner rotation matrix elements can also be expressed in terms of the Jacobi polynomials (Biedenharn and Louck 1981) $P_j^{(m,\mu)}$, viz.

$$\begin{aligned}d^j_{\mu m}(\beta) = \left[\frac{(j-m)!(j+m)!}{(j+\mu)!(j-\mu)!}\right]^{1/2} &\left(\cos\frac{\beta}{2}\right)^{m+\mu}\left(\sin\frac{\beta}{2}\right)^{m-\mu} \\ \times\ &P_{j-m}^{(m-\mu,m+\mu)}(\cos\beta).\end{aligned} \tag{B9}$$

The Jacobi polynomials in $(B9)$ can be written

$$\begin{aligned}P_n^{(n_1,n_2)}(\cos\beta) &= (n+n_1)!(n+n_2)! \\ &\times\sum_s\frac{1}{s!(n+n_1-s)!(n_2+s)!(n-s)!}\left(-\sin^2\frac{\beta}{2}\right)^{n-s}\left(\cos^2\frac{\beta}{2}\right)^s,\end{aligned} \tag{B10}$$

where n_1, n_2, and n are integers and the summation over s extends over all integers for which the arguments of the factorials are nonnegative. The Jacobi polynomials are orthogonal on the interval $-1\leq\cos\beta\leq 1$ with weighting factor $(1-\cos\beta)^{n_1}(1+\cos\beta)^{n_2}$.

Symmetry Relations

The reduced rotation matrices $\hat{\mathbf{d}}^j$ are real and satisfy the symmetry relations (Rose 1957)

$$d^j_{\mu m}(-\beta) = (-1)^{\mu-m}d^j_{\mu m}(\beta) = d^j_{m\ \mu}(\beta) = d^j_{-\mu\ -m}(\beta) = (-1)^{m-\mu}d^j_{-m\ -\mu}(\beta). \tag{B11}$$

Therefore the $\hat{\mathcal{D}}^j(\alpha,\beta,\gamma)$ matrices satisfy

$$\mathcal{D}^j_{\mu\ m}(-\gamma,-\beta,-\alpha) = \mathcal{D}^{j*}_{m\ \mu}(\alpha,\beta,\gamma), \tag{B12}$$

$$\mathcal{D}^{j*}_{\mu\ m}(\alpha,\beta,\gamma) = (-1)^{\mu-m}\mathcal{D}^{j}_{-\mu\ -m}(\alpha,\beta,\gamma), \tag{B13}$$

$$\mathcal{D}^{j}_{\mu m}(\alpha+\pi n_\alpha, \beta+2\pi n_\beta, \gamma+\pi n_\gamma) = (-1)^{2jn_\beta+\mu n_\alpha+mn_\gamma}\mathcal{D}^{j}_{\mu\ m}(\alpha,\beta,\gamma), \tag{B14}$$

where n_α, n_β and n_γ are integers. Equation (B14) shows that $\hat{\mathcal{D}}^{j}(\alpha,\beta,\gamma)$ has periodicity 4π in β and 2π in α and γ for all half integral j, and periodicity 2π in β and π in α and γ for all integral j.

Special Values

The matrix elements $\hat{\mathbf{d}}^{l}$ are related to the associated Legendre polynomials P_l^m by (Rose 1957)

$$d^{l}_{m0}(\beta) = (-1)^m \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\beta) \tag{B15}$$

and to the Legendre polynomials P_l by

$$d^{l}_{00}(\beta) = P_l(\cos\beta). \tag{B16}$$

For $m=\mu=j$ or $m=\mu=-j$ Eq. (B16) becomes

$$d^{j}_{jj}(\beta) = d^{j}_{-j-j}(\beta) = \cos^{2j}\frac{\beta}{2}. \tag{B17}$$

The matrix elements $\hat{\mathcal{D}}^{l}(\alpha,\beta,\gamma)$ are also related to the spherical harmonics Y_{lm} by

$$\mathcal{D}^{l}_{m\ 0}(\alpha,\beta,\gamma) = \left(\frac{4\pi}{2l+1}\right)^{1/2} Y^{*}_{lm}(\beta,\alpha), \tag{B18}$$

$$\mathcal{D}^{l}_{0\ m}(\alpha,\beta,\gamma) = \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{l-m}(\beta,\gamma), \tag{B19}$$

where we have used the phase convention of Condon and Shortley (1953).

Unitarity Relations

The Wigner rotation matrices are unitary (Brink and Satchler 1962), i.e.

$$\sum_{\mu=-j}^{j} \mathcal{D}^{j*}_{\mu\ m}(\alpha,\beta,\gamma)\mathcal{D}^{j}_{\mu\ m'}(\alpha,\beta,\gamma) = \delta_{m\ m'}, \tag{B20}$$

$$\sum_{m=-j}^{j} \mathcal{D}^{j}_{\mu\ m}(\alpha,\beta,\gamma)\mathcal{D}^{j*}_{\mu'\ m}(\alpha,\beta,\gamma) = \delta_{\mu\ \mu'}. \tag{B21}$$

In matrix notation, Eqs (B20) and (B21) are written

$$\hat{\mathcal{D}}^{j\dagger}(\alpha,\beta,\gamma)\hat{\mathcal{D}}^{j}(\alpha,\beta,\gamma) = \hat{\mathcal{D}}^{j}(\alpha,\beta,\gamma)\hat{\mathcal{D}}^{j\dagger}(\alpha,\beta,\gamma) = \mathcal{I}^{j} \tag{B22}$$

or

$$\hat{\mathcal{D}}^{j\dagger}(\alpha,\beta,\gamma) = \left[\hat{\mathcal{D}}^{j}(\alpha,\beta,\gamma)\right]^{-1} = \mathcal{D}^{j}(-\gamma,-\beta,-\alpha), \tag{B23}$$

where $\mathcal{I}^{j}$ is the $(2j+1)$ by $(2j+1)$ identity matrix. The determinant of a rotation matrix is (Biedenharn and Louck 1981)

$$\det\left[\hat{\mathcal{D}}^{j}(\alpha,\beta,\gamma)\right] = 1. \tag{B24}$$

Relation to Irreducible Tensor Operators

A spherical tensor operator (or irreducible tensor operator) transforms under a rotation as (Biedenharn and Louck 1981)

$$\hat{R}^{(a)}\hat{T}_{jm}\left[\hat{R}^{(a)}\right]^{-1} \equiv \sum_{\mu=-j}^{j} \mathcal{D}^{j}_{\mu\ m}(\alpha,\beta,\gamma)\hat{T}_{j\mu}, \tag{B25}$$

where $\hat{T}_{jm}$ is a spherical tensor operator. This tensor has rank j and $2j+1$ components. The product of two rotation matrix elements can be written as a linear combination of these matrix elements (the Clebsch-Gordan series) (Rose 1957):

$$\begin{aligned}\mathcal{D}^{j_1}_{\mu_1\ m_1}\mathcal{D}^{j_2}_{\mu_2\ m_2} = &\sum_{j=|j_1-j_2|}^{j_1+j_2} C(j_1,j_2,j;\mu_1,\mu_2,\mu_1+\mu_2)C(j_1,j_2,j;m_1,m_2,m_1+m_2)\\ &\times \mathcal{D}^{j}_{\mu_1+\mu_2\ m_1+m_2}.\end{aligned} \tag{B26}$$

The inverse of this series is

$$\begin{aligned}\mathcal{D}^{j}_{\mu\ m} = &\sum_{\mu_1=-j}^{j}\sum_{m_1=-j}^{j} C(j_1,j_2,j;\mu_1,\mu-\mu_1,\mu)C(j_1,j_2,j;m_1,m-m_1,m)\\ &\times \mathcal{D}^{j_1}_{\mu_1\ m_1}\mathcal{D}^{j_2}_{\mu-\mu_1\ m-m_1},\end{aligned} \tag{B27}$$

where $C(j_1,j_2,j;\mu_1,\mu_2,\mu)$ is a Clebsch-Gordan coefficient in the notation of Rose (1957). In matrix notation these transformations become

$$\begin{aligned}\mathcal{C}\,[\hat{\mathcal{D}}^{j_1}\otimes\hat{\mathcal{D}}^{j_2}]\mathcal{C}^t &= \hat{\mathcal{D}}^{j_1+j_2}\oplus\hat{\mathcal{D}}^{j_1+j_2-1}\oplus\cdots\oplus\hat{\mathcal{D}}^{|j_1-j_2|}\\ &= \begin{pmatrix} \hat{\mathcal{D}}^{j_1+j_2} & 0 & \dots & 0\\ 0 & \hat{\mathcal{D}}^{j_1+j_2-1} & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & \hat{\mathcal{D}}^{|j_1-j_2|}\end{pmatrix},\end{aligned} \tag{B28}$$

where $\otimes$ stands for a direct product and $\oplus$ for a direct sum. The dimensions of the matrices in ($B28$) are $(2j_1+1)(2j_2+1)$ by $(2j_1+1)(2j_2+1)$, and the matrix on right-hand side of this equation is block diagonal, with blocks consisting of the Wigner rotation matrices. Finally, the elements of the orthogonal transformation matrix $\mathcal{C}$ are

$$\mathcal{C}_{jm;m_1m_2} = C(j_1,j_2,j;m_1,m_2,m), \tag{B29}$$

where the pairs of indices j,m and m_1,m_2 label rows and columns respectively. These relations show that the Wigner rotation matrices constitute an irreducible representation of the groups $O^+(3)$ and $SU(2)$ (cf. Tinkham 1964). The character or trace of these matrices is (Weissbluth 1979)

$$\chi^j(\delta) \equiv Tr\left[\hat{\mathcal{D}}^j(\alpha,\beta,\gamma)\right] = \sum_{m=-j}^{j}\mathcal{D}^j_{m\ m}(\alpha,\beta,\gamma) = \frac{\sin(j+1/2)\delta}{\sin\delta/2}, \tag{B30}$$

where δ is a rotation about an arbitrary axis. For $\delta = 0$ the character of the Wigner rotation matrix must equal its dimension, i.e.

$$\chi^j(0) = 2j + 1 = \lim_{\delta \to 0} \frac{\sin(j + 1/2)\delta}{\sin \delta/2}. \tag{B31}$$

Using explicit expressions for the rotation matrix elements and Eq. ($B30$), we find a simple relation between the rotation angle δ about an arbitrary axis and the Euler angles:

$$\cos\left(\frac{\delta}{2}\right) = \cos\left[\frac{\alpha + \beta}{2}\right] \cos\left(\frac{\beta}{2}\right).$$

The product of two rotations is a rotation, so (Biedenharn and Louck 1981)

$$\hat{\mathcal{D}}^j(\alpha', \beta', \gamma')\hat{\mathcal{D}}^j(\alpha, \beta, \gamma) = \hat{\mathcal{D}}^j(\alpha'', \beta'', \gamma''). \tag{B32}$$

The Euler angles are related to the Euler-Rodrigues parameters $(\alpha_0, \hat{\alpha})$ where $\hat{\alpha} \equiv (\alpha_1, \alpha_2, \alpha_3)$. These parameters, which are the Cartesian components of a point on a unit sphere in four space, are related to the Euler angles by

$$\alpha_0 = \cos\left(\frac{\beta}{2}\right) \cos\left(\frac{\gamma + \alpha}{2}\right) = \cos\chi, \tag{B33}$$

$$\alpha_1 = \sin\left(\frac{\beta}{2}\right) \sin\left(\frac{\gamma - \alpha}{2}\right) = \sin\theta \cos\phi \sin\chi, \tag{B34}$$

$$\alpha_2 = \sin\left(\frac{\beta}{2}\right) \cos\left(\frac{\gamma - \alpha}{2}\right) = \sin\theta \sin\phi \sin\chi, \tag{B35}$$

$$\alpha_3 = \cos\left(\frac{\beta}{2}\right) \sin\left(\frac{\gamma + \alpha}{2}\right) = \cos\theta \sin\chi, \tag{B36}$$

where $0 \leq \phi \leq 2\pi$, $0 \leq \theta \leq \pi$ and $0 \leq \chi \leq \pi$ are the spherical polar coordinates in four space. The Euler angles in Eq. ($B32$) satisfy the quaternionic composition rule

$$\alpha_0'' = \alpha_0'\alpha - \hat{\alpha}' \cdot \hat{\alpha}, \tag{B37}$$

$$\hat{\alpha}'' = \alpha_0\hat{\alpha}' + \alpha_0'\hat{\alpha} + \hat{\alpha}' \times \hat{\alpha}. \tag{B38}$$

For small β the reduced rotation matrix elements are

$$\begin{aligned} d^j_{m\ \mu}(\beta) &\approx \delta_{m\,\mu} - i\beta\langle jm|\hat{\mathcal{J}}_y|j\mu\rangle \\ &\approx \delta_{m\,\mu} + \frac{\beta}{2}\{-\delta_{\mu,m+1}[j(j+1) - m(m+1)]^{1/2} \\ &\quad + \delta_{\mu,m-1}[j(j+1) - m(m-1)]^{1/2}\}. \end{aligned} \tag{B39}$$

Orthogonality and Normalization Relations

The Wigner rotation matrix elements are orthogonal but not normalized (Rose 1957):

$$\int \mathcal{D}^{j_1 *}_{\mu_1\ m_1}(\alpha, \beta, \gamma)\mathcal{D}^{j_2}_{\mu_2\ m_2}(\alpha, \beta, \gamma) d\Omega = \frac{8\pi^2}{2j_1 + 1}\delta_{\mu_1\mu_2}\delta_{m_1m_2}\delta_{j_1j_2}, \tag{B40}$$

where

$$\int d\Omega = \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma = 8\pi^2 \tag{B41}$$

is the integral over the surface of a four sphere.

Integrals

The integral of the product of three Wigner rotation matrix elements is (Rose 1957)

$$\int \mathcal{D}^{j_3^*}_{\mu_3\ m_3}(\alpha,\beta,\gamma)\mathcal{D}^{j_2}_{\mu_2\ m_2}(\alpha,\beta,\gamma)\mathcal{D}^{j_1}_{\mu_1\ m_1}(\alpha,\beta,\gamma)\, d\Omega$$

$$= \frac{8\pi^2}{2j_3+1} C(j_1,j_2,j_3;\mu_1,\mu_2,\mu_3)C(j_1,j_2,j_3;m_1,m_2,m_3). \tag{B42}$$

This integral is zero unless $m_1+m_2=m_3$, $\mu_1+\mu_2=\mu_3$ and the triangle rule $\Delta(j_1j_2j_3)$ is satisfied. Equation $(B42)$ leads to the Gaunt formula for spherical harmonics:

$$\int Y_{l_3}^{m_3^*}(\beta,\alpha)\, Y_{l_2}^{m_2}(\beta,\alpha)\, Y_{l_1}^{m_1}(\beta,\alpha) d\alpha \sin\beta d\beta$$

$$= \left[\frac{(2l_1+1)(2l_2+1)}{4\pi(2l_3+1)}\right]^{1/2} C(l_1,l_2,l_3;m_1,m_2,m_3)C(l_1,l_2,l_3;0,0,0), \tag{B43}$$

which is zero unless $l_1+l_2+l_3$ is even, $m_1+m_2=m_3$, and $\Delta(l_1l_2l_3)$ is satisfied.

Matrix Elements of the Angular Momentum Operators

The nonvanishing matrix elements of the raising and lowering operators $\hat{\mathcal{J}}_\pm = \hat{\mathcal{J}}_x \pm i\hat{\mathcal{J}}_y$ are (Rose 1957)

$$\begin{aligned}\langle j\ m\pm 1|\hat{\mathcal{J}}_\pm|j\ m\rangle &= [j(j+1)-m(m\pm 1)]^{1/2}\\ &= [(j\mp m)(j\pm m+1)]^{1/2}.\end{aligned} \tag{B44}$$

The raising and lowering operators are not Hermitian; instead, $\hat{\mathcal{J}}_+^\dagger = \hat{\mathcal{J}}_-$. By inverting the definitions of these operators, we obtain $\hat{\mathcal{J}}_x = \frac{1}{2}(\hat{\mathcal{J}}_+ + \hat{\mathcal{J}}_-)$ and $\hat{\mathcal{J}}_y = -\frac{i}{2}(\hat{\mathcal{J}}_+ - \hat{\mathcal{J}}_-)$ and the corresponding matrix elements

$$\begin{aligned}\left[\hat{\mathcal{J}}_x^{(j)}\right]_{\mu m} = \langle j\mu|\hat{\mathcal{J}}_x|jm\rangle = \frac{1}{2}\{&\delta_{\mu,m+1}[j(j+1)-m(m+1)]^{1/2}\\ &+\delta_{\mu,m-1}[j(j+1)-m(m-1)]^{1/2}\},\end{aligned} \tag{B45}$$

$$\begin{aligned}\left[\hat{\mathcal{J}}_y^{(j)}\right]_{\mu m} = \langle j\mu|\hat{\mathcal{J}}_y|jm\rangle = \frac{i}{2}\{&-\delta_{\mu,m+1}[j(j+1)-m(m+1)]^{1/2}\\ &+\delta_{\mu,m-1}[j(j+1)-m(m-1)]^{1/2}\}.\end{aligned} \tag{B46}$$

The Wigner-Eckhart Theorem

The Wigner rotation matrices can be used to develop an elegant proof of the Wigner-Eckhart theorem,

$$\langle j'\mu|\hat{\mathcal{T}}_{kq}|jm\rangle = C(j,k,j';m,q,\mu)\langle j'||\hat{\mathcal{T}}_{(k)}||j\rangle, \tag{B47}$$

where $\langle j'||\hat{\mathcal{T}}_{(k)}||j\rangle$ is a reduced matrix element; for details, see Cushing (1975).

Differential Equations

The operators

$$\hat{\mathcal{J}}_x = i\cos\alpha\cot\beta\frac{\partial}{\partial\alpha} + i\sin\alpha\frac{\partial}{\partial\beta} - i\frac{\cos\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}, \tag{B48}$$

$$\hat{\mathcal{J}}_y = i\sin\alpha\cot\beta\frac{\partial}{\partial\alpha} - i\cos\alpha\frac{\partial}{\partial\beta} - i\frac{\sin\alpha}{\sin\beta}\frac{\partial}{\partial\gamma}, \tag{B49}$$

$$\hat{\mathcal{J}}_z = -i\frac{\partial}{\partial\gamma} \tag{B50}$$

satisfy the relation (Biedenharn and Louck 1981)

$$\hat{\boldsymbol{\mathcal{J}}}_i^{(j)}\hat{\boldsymbol{\mathcal{D}}}^j(\alpha,\beta,\gamma) = -\hat{\mathcal{J}}_i\hat{\boldsymbol{\mathcal{D}}}^j(\alpha,\beta,\gamma). \tag{B51}$$

The the operator on the left-hand side of Eq. ($B50$) is a matrix operator, but the operator on the right-hand side is a differential operator. The minus sign in Eq. ($B50$) is essential so that the differential and matrix operators satisfy the same commutation relations $\hat{\mathcal{J}} \times \hat{\mathcal{J}} = i\hat{\mathcal{J}}$ and $\hat{\mathcal{J}}^{(j)} \times \hat{\mathcal{J}}^{(j)} = i\hat{\mathcal{J}}^{(j)}$. The operators ($B49$)–($B51$) are the angular momentum operators associated with a space-fixed coordinate system. It should be noted that

$$\hat{\mathcal{J}}_i = \hat{e}_i \cdot \hat{\mathcal{J}} \qquad \text{and} \qquad \hat{\mathcal{J}}_{i'} = \hat{f}_i \cdot \hat{\mathcal{J}}.$$

The differential operators satisfy the commutation relations

$$[\hat{\mathcal{J}}_i, \hat{\mathcal{J}}_j] = i\hat{\mathcal{J}}_k. \tag{B52}$$

The space-fixed raising $\hat{\mathcal{J}}_+$ and $\hat{\mathcal{J}}_-$ operators are

$$\hat{\mathcal{J}}_+ = \hat{\mathcal{J}}_x + i\hat{\mathcal{J}}_y, \tag{B53}$$

$$\hat{\mathcal{J}}_- = \hat{\mathcal{J}}_x - i\hat{\mathcal{J}}_y. \tag{B54}$$

The corresponding operators associated with the body-fixed coordinate system are

$$\hat{\mathcal{J}}_{x'} = (\cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma)\hat{\mathcal{J}}_x + (\sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma)\hat{\mathcal{J}}_y - \sin\beta\cos\gamma\hat{\mathcal{J}}_z, \tag{B55}$$

$$\hat{\mathcal{J}}_{y'} = -(\cos\alpha\cos\beta\sin\gamma + \sin\alpha\cos\gamma)\hat{\mathcal{J}}_x + (-\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma)\hat{\mathcal{J}}_y + \sin\beta\sin\gamma\hat{\mathcal{J}}_z, \tag{B56}$$

$$\hat{\mathcal{J}}_{z'} = \sin\beta\cos\alpha\hat{\mathcal{J}}_x + \sin\beta\sin\alpha\hat{\mathcal{J}}_y + \cos\beta\hat{\mathcal{J}}_z, \tag{B57}$$

or, equivalently,

$$\hat{\mathcal{J}}_{j'} = \sum_i R_{ij'}(\alpha,\beta,\gamma)\hat{\mathcal{J}}_i = \sum_i \hat{\mathcal{J}}_i R_{ij'}(\alpha,\beta,\gamma) \qquad \begin{cases} i = x, y, z; \\ j' = x', y', z'. \end{cases} \tag{B58}$$

These body-fixed operators satisfy an equation analogous to Eq. ($B49$),

$$\hat{\boldsymbol{\mathcal{D}}}^j(\alpha,\beta,\gamma)\,\hat{\boldsymbol{\mathcal{J}}}_{i'}^{(j)} = -\hat{\mathcal{J}}_{i'}\hat{\boldsymbol{\mathcal{D}}}^j(\alpha,\beta,\gamma) \tag{B59}$$

and the commutation relations

$$[\hat{\mathcal{J}}_{i'}, \hat{\mathcal{J}}_{j'}] = -i\hat{\mathcal{J}}_{k'}. \qquad (B60)$$

[Note: The commutation relation for the body-fixed operators have a factor of $-i$, but the space-fixed operators (Eq. B53) have a factor of $+i$.] The body-fixed raising and lowering operators are

$$\hat{\mathcal{J}}_{+'} = \hat{\mathcal{J}}_{x'} - i\hat{\mathcal{J}}_{y'}, \qquad (B61)$$

$$\hat{\mathcal{J}}_{-'} = \hat{\mathcal{J}}_{x'} + i\hat{\mathcal{J}}_{y'}. \qquad (B62)$$

[Note: As a result of the minus sign in Eq. ($B61$) the equations that define the body-fixed raising and lowering operators differ from the equations that define the space-fixed raising and lowering operators; see Eqs ($B54$) and ($B55$)]. The body-fixed and space-fixed components of the angular momentum operators commute, i.e.

$$[\hat{\mathcal{J}}_i, \hat{\mathcal{J}}_{j'}] = 0. \qquad (B63)$$

The total angular momentum of the system is a constant of the motion, so

$$\hat{\mathcal{J}}^2 = \hat{\mathcal{J}}_{x'}^2 + \hat{\mathcal{J}}_{y'}^2 + \hat{\mathcal{J}}_{z'}^2 = \hat{\mathcal{J}}_x^2 + \hat{\mathcal{J}}_y^2 + \hat{\mathcal{J}}_z^2. \qquad (B64)$$

The operators $\hat{\mathcal{J}}^2$, $\hat{\mathcal{J}}_z$ and $\hat{\mathcal{J}}_{z'}$ form a complete set of commuting operators. Their eigenvalue equations are

$$\hat{\mathcal{J}}^2 \mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma) = j(j+1)\mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma), \qquad (B65)$$

$$\hat{\mathcal{J}}_z \mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma) = \mu\mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma), \qquad (B66)$$

$$\hat{\mathcal{J}}_{z'} \mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma) = m\mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma). \qquad (B67)$$

In ($B66$) $\hat{\mathcal{J}}_z$ is the component of the angular momentum operator along the space-fixed z axis; $\hat{\mathcal{J}}_{z'}$ in ($B67$) is the component of the angular momentum operator along the body-fixed z axis (symmetry axis).

The raising and lowering operators satisfy the following relations:

$$\hat{\mathcal{J}}_\pm \mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma) = [(j \mp \mu)(j \pm \mu + 1)]^{1/2}\, \mathcal{D}^{j^*}_{\mu\pm 1 m}(\alpha, \beta, \gamma), \qquad (B68)$$

$$\hat{\mathcal{J}}_{\pm'} \mathcal{D}^{j^*}_{\mu\, m}(\alpha, \beta, \gamma) = [(j \mp m)(j \pm m + 1)]^{1/2}\, \mathcal{D}^{j^*}_{\mu m\pm 1}(\alpha, \beta, \gamma). \qquad (B69)$$

The following relation is useful for determining the elements of the Wigner rotation matrix (Biedenharn and Louck 1981):

$$\mathcal{D}^{j^*}_{\mu m}(\alpha, \beta, \gamma) = \left[\frac{(j+\mu)!(j+m)!}{(2j)!(j-\mu)!(2j)!(j-m)!}\right]^{1/2} \left(\hat{\mathcal{J}}_-\right)^{j-\mu} \left(\hat{\mathcal{J}}_{-'}\right)^{j-m} \mathcal{D}^{j^*}_{jj}(\alpha, \beta, \gamma), \qquad (B70)$$

where

$$\mathcal{D}^{j^*}_{jj}(\alpha, \beta, \gamma) = \exp(ij\alpha)\left(\cos\frac{\beta}{2}\right)^{2j} \exp(ij\gamma). \qquad (B71)$$

The spherical components of the angular momentum operators are related to the raising and lowering operators (Weissbluth 1979) by

$$\hat{\mathcal{J}}_{+1} = -\frac{1}{\sqrt{2}}\hat{\mathcal{J}}_+, \qquad \hat{\mathcal{J}}_{-1} = \frac{1}{\sqrt{2}}\hat{\mathcal{J}}_-, \qquad \text{and} \qquad \hat{\mathcal{J}}_0 = \hat{\mathcal{J}}_z. \qquad (B72)$$

Hence the square of the total angular momentum operator is

$$\begin{aligned}\hat{\mathcal{J}}^2 &= \sum_{q=-1}^{1} (-1)^q \hat{\mathcal{J}}_q \hat{\mathcal{J}}_{-q} \\ &= -2\hat{\mathcal{J}}_{+1}\hat{\mathcal{J}}_{-1} + \hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 - 1) \\ &= -2\hat{\mathcal{J}}_{-1}\hat{\mathcal{J}}_{+1} + \hat{\mathcal{J}}_0(\hat{\mathcal{J}}_0 + 1).\end{aligned} \tag{B73}$$

Eigenfunctions of the Symmetric Top

The Wigner rotation matrix elements are proportional to the orthonormal eigenfunctions $R_{j\mu m}(\alpha, \beta, \gamma)$ of the symmetric top Hamiltonian (Biedenharn and Louck 1981)

$$\begin{aligned}&\left[\frac{1}{2I_{x'}}(\hat{\mathcal{J}}_{x'}^2 + \hat{\mathcal{J}}_{y'}^2) + \frac{1}{2I_{z'}}\hat{\mathcal{J}}_{z'}^2\right] \mathcal{D}^{j^*}_{\mu\ m}(\alpha, \beta, \gamma) \\ &\qquad = \left[\frac{1}{2I_{x'}}j(j+1) + \frac{1}{2}\left(\frac{1}{I_{z'}} - \frac{1}{I_{x'}}\right) m^2\right] \mathcal{D}^{j^*}_{\mu\ m}(\alpha, \beta, \gamma),\end{aligned} \tag{B74}$$

where $I_{x'} = I_{y'}$, and $I_{z'}$ are the principal moments of inertia, μ is the component of angular momentum along the space-fixed z axis and m is the component of angular momentum along the body-fixed symmetry axis. In particular, the normalized symmetric top eigenfunctions are (Burke and Chandra 1972)

$$R_{j\mu m}(\alpha, \beta, \gamma) = \left(\frac{2j+1}{8\pi^2}\right)^{1/2} \mathcal{D}^{j^*}_{\mu\ m}(\alpha, \beta, \gamma).$$

Because the Wigner rotation matrix in the passive convention (Steinborn and Ruedenberg 1973) is the Hermitian conjugate of the Wigner rotation matrix in this appendix, the matrix elements $\mathcal{D}^{j}_{\mu\ m}(\alpha, \beta, \gamma)$ are (unnormalized) eigenfunctions of the symmetric top Hamiltonian when the passive convention is used.

Recursion Relations

The following recursion relations, which can be derived from the Clebsch-Gordan series ($B26$), are useful for calculating Wigner rotation matrices (Biedenharn and Louck 1981):

$$\begin{aligned}&[(j-m)(j+m+1)]^{1/2} \sin\beta \, d^j_{\mu,m+1}(\beta) \\ &+[(j+m)(j-m+1)]^{1/2} \sin\beta \, d^j_{\mu,m-1}(\beta) = 2(m\cos\beta - \mu) d^j_{\mu,m}(\beta),\end{aligned} \tag{B75}$$

$$\begin{aligned}&[(j+m)(j-m+1)]^{1/2} d^j_{\mu,m-1}(\beta) \\ &\qquad +[(j+\mu)(j-\mu+1)]^{1/2} d^j_{\mu-1,m}(\beta) = (m-\mu)\cot\frac{\beta}{2} d^j_{\mu,m}(\beta).\end{aligned} \tag{B76}$$

Projection Operators

The operators $\hat{\mathcal{P}}^{j}_{m}$ defined by (Biedenharn and Louck 1981)

$$\hat{\mathcal{P}}^{j}_{m} \equiv \prod_{\substack{\mu=-j \\ \mu\neq m}}^{j} \frac{\hat{\mathcal{J}}^{(j)}_{y} - \mu I^{j}}{m-\mu} \tag{B77}$$

are idempotent, i.e.

$$\hat{\mathcal{P}}^{j}_{m}\hat{\mathcal{P}}^{j}_{m} = \hat{\mathcal{P}}^{j}_{m}. \tag{B78}$$

They are also mutually exclusive,

$$\hat{\mathcal{P}}^{j}_{m}\hat{\mathcal{P}}^{j}_{m'} = 0 \qquad \text{for} \qquad m \neq m', \tag{B79}$$

and form a resolution of the identity, i.e.

$$\sum_{m=-j}^{j} \hat{\mathcal{P}}^{j}_{m} = I^{j}. \tag{B80}$$

Therefore the matrices $\hat{\mathcal{P}}^{j}_{m}$ are projection operators.

Using these operators, we can write the spectral resolution (Cushing 1975) of $\hat{\mathcal{J}}^{(j)}_{y}$ as

$$\hat{\mathcal{J}}^{(j)}_{y} = \sum_{m=-j}^{j} m\hat{\mathcal{P}}^{j}_{m}. \tag{B81}$$

For any well-defined function F, one has

$$F[\hat{\mathcal{J}}^{(j)}_{y}] = \sum_{m=-j}^{j} F(m)\hat{\mathcal{P}}^{j}_{m}. \tag{B82}$$

Therefore one can determine $\hat{\mathbf{d}}^{j}(\beta)$ as

$$\hat{\mathbf{d}}^{j}(\beta) = \exp(-i\beta\hat{\mathcal{J}}^{(j)}_{y}) = \sum_{\mu=-j}^{j} \exp(-i\mu\beta)\hat{\mathcal{P}}^{j}_{m}. \tag{B83}$$

Solution of Laplace's Equation in Four Space

The elements of the Wigner rotation matrix elements are eigenfunctions of the Laplacian in four space (Judd 1975)

$$\nabla_4^2 \mathcal{D}^{j}_{\mu\, m}(\alpha,\beta,\gamma) = 0, \tag{B84}$$

where

$$\nabla_4^2 = \frac{\partial^2}{\partial x_0^2} + \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}. \tag{B85}$$

$\boldsymbol{J}^{(j)}_{i=x,y,z}$ **matrices for** $j = 1/2,\ j = 1,\ j = 3/2,\ j = 2$

$$\mathrm{d}^j = \exp(-i\beta \boldsymbol{J}^{(j)}_y)$$

$$\boldsymbol{J}^{(1/2)}_x = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(1/2)}_y = \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(1/2)}_z = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}$$

$$\boldsymbol{J}^{(1)}_x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(1)}_y = \begin{pmatrix} 0 & -\frac{i}{\sqrt{2}} & 0 \\ \frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(1)}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$\boldsymbol{J}^{(3/2)}_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(3/2)}_y = \begin{pmatrix} 0 & -i\frac{\sqrt{3}}{2} & 0 & 0 \\ i\frac{\sqrt{3}}{2} & 0 & -i & 0 \\ 0 & i & 0 & -i\frac{\sqrt{3}}{2} \\ 0 & 0 & i\frac{\sqrt{3}}{2} & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(3/2)}_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

$$\boldsymbol{J}^{(2)}_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(2)}_y = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad \boldsymbol{J}^{(2)}_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}$$

Wigner rotation matrices for $j = 1/2$, $j = 1$, $j = 3/2$, $j = 2$

$$d^{1/2}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}$$

$$d^{1}(\beta) = \begin{pmatrix} \frac{1+\cos\beta}{2} & -\frac{\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & -\frac{\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2} \end{pmatrix}$$

$$d^{3/2}(\beta) = \begin{pmatrix} \cos^3\frac{\beta}{2} & -\sqrt{3}\cos\frac{\beta}{2}\sin\frac{\beta}{2} & \sqrt{3}\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} & -\sin^3\frac{\beta}{2} \\ \sqrt{3}\cos^2\frac{\beta}{2}\sin\frac{\beta}{2} & \cos^3\frac{\beta}{2} - 2\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} & \sin^3\frac{\beta}{2} - 2\cos^2\frac{\beta}{2}\sin\frac{\beta}{2} & \sqrt{3}\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} \\ \sqrt{3}\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} & 2\cos^2\frac{\beta}{2}\sin\frac{\beta}{2} - \sin^3\frac{\beta}{2} & \cos^3\frac{\beta}{2} - 2\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} & -\sqrt{3}\cos^2\frac{\beta}{2}\sin\frac{\beta}{2} \\ \sin^3\frac{\beta}{2} & \sqrt{3}\cos\frac{\beta}{2}\sin^2\frac{\beta}{2} & \sqrt{3}\cos^2\frac{\beta}{2}\sin\frac{\beta}{2} & \cos^3\frac{\beta}{2} \end{pmatrix}$$

$$d^{2}(\beta) = \begin{pmatrix} \frac{1}{4}(1+\cos\beta)^2 & -\frac{1}{2}\sin\beta(1+\cos\beta) & \sqrt{\frac{3}{8}}\sin^2\beta & -\frac{1}{2}\sin\beta(1-\cos\beta) & \frac{1}{4}(1-\cos\beta)^2 \\ \frac{1}{2}\sin\beta(1+\cos\beta) & \frac{1}{2}(2\cos^2\beta + \cos\beta - 1) & -\sqrt{\frac{3}{2}}\sin\beta\cos\beta & -\frac{1}{2}(2\cos^2\beta - \cos\beta - 1) & -\frac{1}{2}\sin\beta(1-\cos\beta) \\ \sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3}{2}\cos^2\beta - \frac{1}{2} & -\sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\ \frac{1}{2}\sin\beta(1-\cos\beta) & -\frac{1}{2}(2\cos^2\beta - \cos\beta - 1) & -\sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{1}{2}(2\cos^2\beta + \cos\beta - 1) & -\frac{1}{2}\sin\beta(1+\cos\beta) \\ \frac{1}{4}(1-\cos\beta)^2 & \frac{1}{2}\sin\beta(1-\cos\beta) & \sqrt{\frac{3}{8}}\sin^2\beta & \frac{1}{2}\sin\beta(1+\cos\beta) & \frac{1}{4}(1+\cos\beta)^2 \end{pmatrix}$$

Calculation of the Wigner Rotation Matrices

There are several methods that one can use to obtain $d^j_{\mu m}(\beta)$, including

(i) explicit expressions in terms of the hypergeometric function or Jacobi polynomials ($B7$ or $B9$);

(ii) differential equations ($B71$);

(iii) recursion relations ($B76$ and $B77$);

(iv) projection operators ($B84$);

(v) boson operator techniques (Biedenharn and Louck 1981, Chapter 5).

Appendix C: The Passive Convention

In the text of this paper and in Appendix B, we used predominantly the active convention for rotations. For the convenience of readers who prefer the passive convention, we here express some of the most important results from this paper in this convention. *The equation numbers in this appendix refer to the corresponding equation (in the active convention) in the text or in Appendix B.*

- The passive Euler angle rotation matrix:

$$\mathsf{R}^{(p)}(\alpha,\beta,\gamma) = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{34}$$

- Definition of the Wigner rotation matrix:

$$\begin{aligned} \mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) &= \langle j\mu|\exp(i\gamma\hat{\mathcal{J}}_{z''})\exp(i\beta\hat{\mathcal{J}}_{y'})\exp(i\alpha\hat{\mathcal{J}}_z)|jm\rangle \\ &= \exp(i\mu\gamma)\langle j\mu|\exp(i\beta\hat{\mathcal{J}}_y)|jm\rangle\exp(im\alpha) \\ &= \exp(i\mu\gamma)d^j_{\mu m}(\beta)\exp(im\alpha). \end{aligned} \tag{B6}$$

Note that $d^j_{\mu m}(\beta)$ in the passive convention can be determined from Eqs ($B7$) or ($B8$) by replacing β by $-\beta$ in the right-hand side of these equations.

- Effect of the passive rotation operator on an angular momentum eigenket:

$$|\,j,m\,\rangle_2 \;=\; \hat{R}^{(p)}(\alpha,\beta,\gamma)\,|\,j,m\,\rangle_1 \;=\; \sum_{\mu=-j}^{+j} |\,j,\mu\,\rangle_1\,\mathcal{D}^j_{\mu,m}(\alpha,\beta,\gamma). \tag{54}$$

- Rotation of spherical harmonics:

$$Y^m_\ell(\theta_2,\varphi_2) \;=\; \sum_{\mu=-\ell}^{+\ell} Y^\mu_\ell(\theta_1,\varphi_1)\,\mathcal{D}^\ell_{\mu,m}(\alpha,\beta,\gamma). \tag{63}$$

- Relation of the elements of $\hat{\mathcal{D}}^l(\alpha,\beta,\gamma)$ to the spherical harmonics:

$$\mathcal{D}^l_{m\ 0}(\alpha,\beta,\gamma) \;=\; \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}(\beta,\gamma), \tag{B18}$$

$$\mathcal{D}^l_{0\ m}(\alpha,\beta,\gamma) \;=\; \left(\frac{4\pi}{2l+1}\right)^{1/2} Y^*_{l-m}(\beta,\alpha), \tag{B19}$$

using the phase convention of Condon and Shortley (1953).

- Eigenvalue equations for the Wigner rotation matrices:

$$\hat{\mathcal{J}}^2\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) = j(j+1)\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma), \tag{B65}$$

$$\hat{\mathcal{J}}_z\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) = m\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) \qquad \text{space-fixed } z \text{ axis}, \tag{B66}$$

$$\hat{\mathcal{J}}_{z'}\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) = \mu\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) \qquad \text{body-fixed } z \text{ axis}. \tag{B67}$$

- Effect of the raising and lowering operators on the rotation matrices:

$$\hat{\mathcal{J}}_{\pm}\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) = [(j\mp\mu)(j\pm\mu+1)]^{1/2}\,\mathcal{D}^j_{\mu\pm1 m}(\alpha,\beta,\gamma), \tag{B68}$$

$$\hat{\mathcal{J}}_{\pm'}\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma) = [(j\mp m)(j\pm m+1)]^{1/2}\,\mathcal{D}^j_{\mu m\pm1}(\alpha,\beta,\gamma). \tag{B69}$$

- The time-independent Schrödinger equation for a symmetric top:

$$\left[\frac{1}{2I_{x'}}(\hat{\mathcal{J}}^2_{x'}+\hat{\mathcal{J}}^2_{y'})+\frac{1}{2I_{z'}}\hat{\mathcal{J}}^2_{z'}\right]\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma)$$

$$= \left[\frac{1}{2I_{x'}}j(j+1)+\frac{1}{2}\left(\frac{1}{I_{z'}}-\frac{1}{I_{x'}}\right)m^2\right]\mathcal{D}^j_{\mu\ m}(\alpha,\beta,\gamma). \tag{B74}$$

- Normalized eigenfunctions of the symmetric top:

$$R_{j\mu m}(\alpha,\beta,\gamma) = \left(\frac{2j+1}{8\pi^2}\right)^{1/2}\mathcal{D}^j_{m\ \mu}(\alpha,\beta,\gamma).$$

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