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Physics 221A
Fall 2016
Notes 13
Representations of the Angular Momentum Operators and Rotations

1. Introduction

In Notes 12 we introduced the concept of rotation operators acting on the Hilbert space of some quantum mechanical system, and set down postulates (Eqs. (11.2)–(11.4)) that those operators should satisfy. From these we defined the angular momentum operators $\mathbf{J}$ (in Eq. (11.11)) and showed that the multiplication law for rotations implies that the components of $\mathbf{J}$ satisfy the commutation relations (11.24). Finally, we examined the case of spin-$\frac{1}{2}$ systems, for which $\mathbf{J} = (\hbar/2)\boldsymbol{\sigma}$, finding a double-valued representation $U = U(\mathsf{R})$ of the classical rotations by unitary operators, or, perhaps better, a single-valued representation of spin rotations by the classical rotations, $\mathsf{R} = \mathsf{R}(U)$.

In these notes we generalize to an arbitrary Hilbert space upon which unitary rotation operators act, either by a single-valued or double-valued representation $U(\mathsf{R})$ of the classical rotations. Equivalently, we can speak of a Hilbert space upon which a vector of Hermitian operators $\mathbf{J}$ acts, satisfying the commutation relations (11.24), since given $U(\mathsf{R})$ we can find $\mathbf{J}$ by differentiation (see Eq. (11.11)), while given $\mathbf{J}$ we can find $U(\mathsf{R})$ by exponentiation (see Eq. (12.18)). This is all we assume in these notes.

We summarize here the important conclusions from Notes 11. First, the angular momentum $\mathbf{J}$ must satisfy the commutation relations,

$$[J_i, J_j] = i\hbar\,\epsilon_{ijk}\,J_k. \tag{1}$$

Given such an angular momentum vector, we can find rotation operators in axis-angle form according to

$$U(\hat{\mathbf{n}}, \theta) = \exp\Big[-\frac{i}{\hbar}\theta(\hat{\mathbf{n}}\cdot\mathbf{J})\Big]. \tag{2}$$

Conversely, given $U(\hat{\mathbf{n}}, \theta) = U(\boldsymbol{\theta})$, where $\boldsymbol{\theta} = \theta\hat{\mathbf{n}}$, we can find $\mathbf{J}$ by

$$J_i = i\hbar \frac{\partial U(\boldsymbol{\theta})}{\partial \theta_i}\Big|_{\boldsymbol{\theta}=0}. \tag{3}$$

We will see that the angular momentum operators can be used to construct a particularly useful basis on the Hilbert space, what we will call a *standard angular momentum basis.* This is an example of a *symmetry adapted basis*, that is, a basis in terms of which symmetry operations (in this case, rotations) are most simply expressed. This basis will lead to a decomposition of our Hilbert space into an orthogonal set of *invariant, irreducible subspaces*, which are geometrical structures imposed on the Hilbert space by the rotation operators.

Although we will speak in these notes of a Hilbert space which is the ket space or state space of a quantum mechanical system, and we will use the Dirac notation for the (ket) vectors of this space, there are a wide variety of other vector spaces to which the same analysis applies. These include other types of ket spaces, such as subspaces of a given ket space, or tensor products of ket spaces. They also include spaces that are not ket spaces at all, such as vector spaces of operators (which we will take up in a later set of notes), or ordinary, three-dimensional, physical space (certainly a space upon which rotation operators act), or spaces of classical fields (for example, electric and magnetic), in which the standard angular momentum basis is related to the multipole expansion of those fields. Thus, the treatment of this set of notes is actually quite general.

2. The spectrum of J^2 and J_3

We will now explore the consequences of the angular momentum commutation relations (1) for the spectrum of various angular momentum operators. We use a variation of Dirac's algebraic method that was applied in Sec. 8.4 to the harmonic oscillator.

We begin by constructing the nonnegative definite operator J^2,

$$J^2 = J_1^2 + J_2^2 + J_3^2, \tag{4}$$

which, as an easy calculation shows, commutes with all three components of $\mathbf{J}$,

$$[J^2, \mathbf{J}] = 0. \tag{5}$$

Since J^2 commutes with $\mathbf{J}$, it commutes also with any function of $\mathbf{J}$, including the rotation operators $U(\theta, \hat{\mathbf{n}})$ (see Eq. (2)). An operator such as J^2 that commutes with all the generators of a group is called a *Casimir operator*. Since J^2 and $\mathbf{J}$ commute, we can construct simultaneous eigenkets of J^2 and any one of the components of $\mathbf{J}$. However, since these components do not commute with each other, we cannot find simultaneous eigenbasis of more than one component of $\mathbf{J}$. By convention we choose the 3-component, and look for simultaneous eigenkets of J^2 and J_3.

We denote the eigenvalues of J^2 and J_3 by $\hbar^2 a$ and $\hbar m$, respectively, so that a and m are dimensionless. We note that a and m must be real, since J^2 and J_3 are Hermitian, and that $a \geq 0$, since J^2 is nonnegative definite. Apart from this, we make no assumptions at this point about the allowed values of a and m.

We will begin by assuming for simplicity that the operators (J^2, J_3) form a complete set of commuting operators by themselves, so that their simultaneous eigenstates $|am\rangle$ are nondegenerate and form a basis in the Hilbert space. Later we will return to what happens when this is not so.

The eigenvalue equations determine the kets $|am\rangle$ to within a normalization and a phase. We assume the kets are normalized,

$$\langle am|am\rangle = 1, \tag{6}$$

and that some arbitrary (at this point) phase conventions have been chosen. The kets $|am\rangle$ satisfy

$$\begin{aligned} J^2|am\rangle &= \hbar^2 a|am\rangle, \\ J_3|am\rangle &= \hbar m|am\rangle. \end{aligned} \tag{7}$$

To analyze the spectrum of J^2 and J_3 we introduce the ladder or raising and lowering operators,

$$J_\pm = J_1 \pm iJ_2. \tag{8}$$

These are Hermitian conjugates of each other,

$$(J_\pm)^\dagger = J_\mp, \tag{9}$$

and they satisfy the commutation relations,

$$[J_3, J_\pm] = \pm\hbar J_\pm, \tag{10}$$

$$[J_+, J_-] = 2\hbar J_3, \tag{11}$$

$$[J^2, J_\pm] = 0. \tag{12}$$

They also satisfy the relations,

$$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_3^2, \tag{13}$$

$$J_-J_+ = J^2 - J_3(J_3 + \hbar), \tag{14}$$

$$J_+J_- = J^2 - J_3(J_3 - \hbar). \tag{15}$$

Let us take some normalized eigenket $|am\rangle$ of J^2 and J_3, for some as yet unknown values of a and m. Sandwiching $|am\rangle$ around Eqs. (14) and (15), we find

$$\langle am|J_-J_+|am\rangle = \hbar^2[a - m(m+1)] \geq 0, \tag{16}$$

$$\langle am|J_+J_-|am\rangle = \hbar^2[a - m(m-1)] \geq 0, \tag{17}$$

where the inequalities follow from the fact that the left hand sides are the squares of ket vectors (see Eq. (1.27)). Taken together, these imply

$$a \geq \max[m(m+1), m(m-1)]. \tag{18}$$

The functions $m(m\pm1)$ are plotted in Fig. 1, and the maximum of these two functions is plotted in Fig. 2. The maximum function is symmetric about $m = 0$, and ≥ 0 everywhere. A value of a is indicated by a horizontal line in Fig. 2, showing that for any $a \geq 0$ there is a maximum and minimum value of m within which Eq. (18) is true. Let us denote the maximum value of m for a given value of a by j, as shown in the figure, so that the minimum value is $-j$. Then we have

$$-j \leq m \leq +j. \tag{19}$$

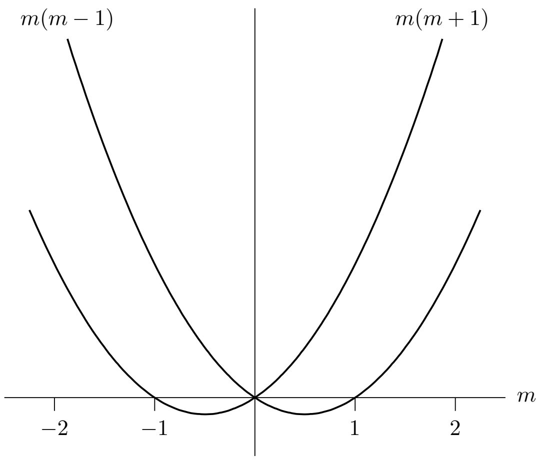

Fig. 1. Functions $m(m+1)$ and $m(m-1)$.

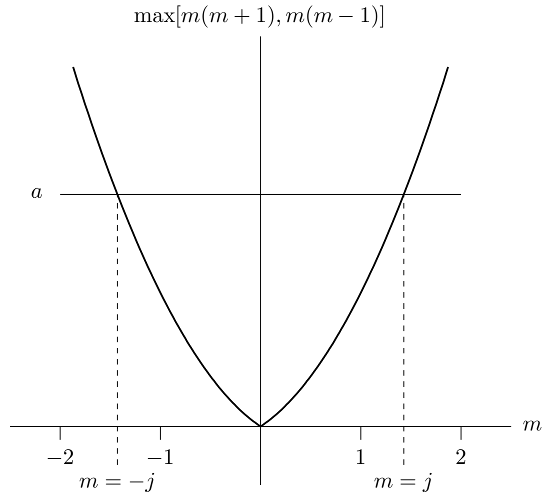

Fig. 2. Function $\max[m(m+1), m(m-1)]$, with maximum and minimum values of m for a given value of a.

Thus, knowing the eigenvalue a of J^2, there are bounds on the eigenvalue m of J_3. The quantity j specifying the bounds is a function of a, and, as is clear from the figure, $j \geq 0$ since $a \geq 0$.

From Fig. 2 we see that the quantities a and j are related by

$$a = j(j+1). \tag{20}$$

It turns out to be more convenient to parameterize the eigenvalues of J^2 by j instead of a, so henceforth let us write $j(j+1)$ for the eigenvalue of J^2 instead of a, and let us write $|jm\rangle$ instead of $|am\rangle$ for the eigenkets of J^2 and J_3. Then Eqs. (7) become

$$\begin{aligned} J^2|jm\rangle &= j(j+1)\hbar^2|jm\rangle, \\ J_3|jm\rangle &= m\hbar|jm\rangle. \end{aligned} \tag{21}$$

We also rewrite Eqs. (16) and (17) with this change of notation, noting that the right hand sides can be factored,

$$\langle jm|J_-J_+|jm\rangle = \hbar^2[j(j+1) - m(m+1)] = \hbar^2(j-m)(j+m+1) \geq 0, \tag{22}$$

$$\langle jm|J_+J_-|jm\rangle = \hbar^2[j(j+1) - m(m-1)] = \hbar^2(j+m)(j-m+1) \geq 0. \tag{23}$$

Let us consider the conditions under which these two inequalities become equalities, that is, when the matrix elements on the left hand sides vanish. For Eq. (22), we have $J_+|jm\rangle = 0$ if and only if

$$j - m = 0 \qquad \text{or} \qquad j+m+1 = 0, \tag{24}$$

that is,

$$m = j \qquad \text{or} \qquad m = -j-1. \tag{25}$$

But by Eq. (19), $m = -j-1$ is impossible, so we find

$$J_+|jm\rangle = 0 \qquad \text{iff} \qquad m = j. \tag{26}$$

Similarly analyzing Eq. (23), we find

$$J_-|jm\rangle = 0 \qquad \text{iff} \qquad m = -j. \tag{27}$$

Now we explore the raising and lowering properties of $J_\pm$. Let us assume that $|jm\rangle$ is a normalized eigenket of J^2 and J^3 with quantum numbers j and m. Then if ket $J_+|jm\rangle$ does not vanish, it is an eigenket of J^2 and J_3 with quantum numbers j and $m+1$, that is, J_+ does not change j but it raises m by one unit. This follows from the commutation relations (10) and (12),

$$\begin{aligned} J^2\big(J_+|jm\rangle\big) &= J_+J^2|jm\rangle = j(j+1)\hbar^2\big(J_+|jm\rangle\big), \\ J_3\big(J_+|jm\rangle\big) &= (J_+J_3 + \hbar J_+)|jm\rangle = (m+1)\hbar\big(J_+|jm\rangle\big). \end{aligned} \tag{28}$$

Similarly, if ket $J_-|jm\rangle$ does not vanish, then it is an eigenket of J^2 and J_3 with quantum numbers j and $m-1$, that is, J_- lowers m by one unit.

From this it immediately follows that

$$m = j - n_1, \tag{29}$$

where $n_1 \ge 0$ is an integer, for if this were not so, we could successively apply J_+ to $|jm\rangle$ (which is nonzero), and generate nonzero kets with successively higher values of m until the rule (19) was violated. Similarly, we show

$$m = -j + n_2, \tag{30}$$

where $n_2 \ge 0$ is another integer. But taken together, Eqs. (29) and (30) imply $2j = n_1 + n_2$, that is, $2j$ is a nonnegative integer. Thus, the only values of j allowed by the commutation relations (1) are

$$j \in \{0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots\}. \tag{31}$$

When we say that j belongs to the indicated set of values (integers and half-integers), we mean that the commutation relations alone tell us that j can take on only these values. They do not tell us which of these values actually occur in a specific application.

For example, speaking of the spin of a spin-$\frac{1}{2}$ particle, j (that is, the spin) takes on only the value $j = \frac{1}{2}$. But in a central force problem, in which the energy eigenfunctions are $\psi_{n\ell m}(r,\theta,\phi)$ and j is identified with the orbital angular momentum ℓ, j (that is, ℓ) takes on all possible integer values $(0,1,2,\ldots)$ but none of the half-integer values.

But in any application, if some j value does occur, then all m values in the range,

$$m = -j, -j+1, \ldots, +j, \tag{32}$$

also occur, for if any one m value in this list occurs, that is, if a nonzero eigenket $|jm\rangle$ exists, then all other nonzero eigenkets with the same j value but other m values in the range (32) can be generated from the given one by raising and lowering operators. Thus, the eigenvalue $j(j+1)\hbar^2$ of J^2 is $(2j+1)$-fold degenerate.

3. Phase Conventions and Matrix Elements of $J_\pm$

Since by assumption the simultaneous eigenkets of J^2 and J_3 are nondegenerate, we must have

$$\begin{aligned} J_+|jm\rangle &= c|j,m+1\rangle, \\ J_-|jm\rangle &= c'|j,m-1\rangle, \end{aligned} \tag{33}$$

where c, c' are complex numbers. These numbers can be determined to within a phase by squaring both sides,

$$\begin{aligned} \langle jm|J_-J_+|jm\rangle &= |c|^2 = \hbar^2(j-m)(j+m+1), \\ \langle jm|J_+J_-|jm\rangle &= |c'|^2 = \hbar^2(j+m)(j-m+1). \end{aligned} \tag{34}$$

To determine the phases of c, c', we first choose an arbitrary phase convention for the stretched state $|jj\rangle$, and then link the phases of $|jm\rangle$ for $m<j$ to that of $|jj\rangle$ by using lowering operators and demanding that c' be real and positive. Having done this, we can raise the states back up with raising operators, and since the product J_+J_- is nonnegative definite, we find that c is also real and positive. Thus we obtain,

$$J_+|jm\rangle = \hbar\sqrt{(j-m)(j+m+1)}\,|j,m+1\rangle, \tag{35a}$$

$$J_-|jm\rangle = \hbar\sqrt{(j+m)(j-m+1)}\,|j,m-1\rangle. \tag{35b}$$

These phase conventions are standard in the theory of angular momentum and rotations, but there is no physics in such conventions.

With these phase conventions we can use a little induction to express an arbitrary state $|jm\rangle$ as a lowered version of the stretched state $|jj\rangle$,

$$|jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\left(\frac{J_-}{\hbar}\right)^{j-m}|jj\rangle. \tag{36}$$

This may be compared to Eq. (8.38) for the harmonic oscillator. The basis $\{|jm\rangle\}$ that we have constructed is the *standard angular momentum basis* for the Hilbert space in the case we are considering (where eigenkets $|jm\rangle$ of J^2 and J_3 are nondegenerate).

4. Structure of Matrices in the Standard Angular Momentum Basis

Equations (35) allow us to write down the matrix elements of $J_\pm$ in the standard angular momentum basis. By multiplying those equations by the bra $\langle j'm'|$ and using the orthonormality of the basis, we obtain

$$\langle j'm'|J_+|jm\rangle = \hbar\,\delta_{j'j}\,\delta_{m',m+1}\,\sqrt{(j-m)(j+m+1)}, \tag{37a}$$

$$\langle j'm'|J_-|jm\rangle = \hbar\,\delta_{j'j}\,\delta_{m',m-1}\,\sqrt{(j+m)(j-m+1)}. \tag{37b}$$

Similarly, Eqs. (21) allow us to write down the matrix elements of J^2 and J_3,

$$\langle j'm'|J_3|jm\rangle = \hbar\,\delta_{j'j}\,\delta_{m'm}\,m, \tag{38a}$$

$$\langle j'm'|J^2|jm\rangle = \hbar^2\,\delta_{j'j}\,\delta_{m'm}\,j(j+1). \tag{38b}$$

Since J_1 and J_2 can be expressed in terms of $J_\pm$,

$$J_1 = \frac{1}{2}(J_+ + J_-), \qquad J_2 = \frac{1}{2i}(J_+ - J_-), \tag{39}$$

it is also easy to write down the matrix elements of these operators. Note that since the matrix elements of $J_\pm$ are real, by Eq. (39) those of J_1 are real and those of J_2 are purely imaginary.

Thus we know the matrix elements of all three components of $\mathbf{J}$ in the standard angular momentum basis. From these one can find the matrix elements of any function of $\mathbf{J}$, such as the rotation operators $U(\hat{\mathbf{n}}, \theta)$. Notice that all these matrices are diagonal in j (the matrix elements are proportional to $\delta_{j'j}$), so the matrix elements themselves depend only on j, m' and m.

5. Invariant, Irreducible Subspaces

We have touched on the concept of an invariant subspace previously (see Sec. 1.23). Suppose we have a vector space, an operator that acts on that space, and a subspace that we are interested in. When can we think of the operator as acting on the subspace, and forget about the larger space in which the subspace lies? The simplest answer is, only when the operator maps every vector of that subspace into another vector of the same subspace. This is a special condition, in general an operator would map a vector of a given subspace into another vector that sticks out of that subspace. But if the condition is met, then we say that the subspace is *invariant* under the action of the operator. In that case we can forget about the larger space if we wish and speak of the *restriction* of the original operator to the subspace. This is really just a restriction of the domain of the original operator, the action of the restricted operator on vectors in the subspace is the same as that of the original operator.

The fact that the matrix elements of the components of $\mathbf{J}$, and hence of any function of $\mathbf{J}$, are diagonal in j draws attention to certain subspaces of the original Hilbert space, namely,

$$\mathcal{E}_j = \text{span}\{|jm\rangle, m = -j, \ldots, +j\}. \tag{40}$$

These are otherwise the eigenspaces of J^2, which are labeled by the allowed j values in the given Hilbert space. The basis vectors in these subspaces are elements of the standard angular momentum basis $|jm\rangle$ with fixed values of j, while m ranges from $-j$ to $+j$. Thus,

$$\dim \mathcal{E}_j = 2j + 1. \tag{41}$$

The subspaces $\mathcal{E}_j$ are invariant under the action of the components of $\mathbf{J}$, and hence under the action of any function of $\mathbf{J}$, notably the rotation operators. If $\mathcal{E}$ is the entire Hilbert space with which we started, then it is decomposed by the action of the rotation operators into a set of orthogonal, invariant subspaces $\mathcal{E}_j$,

$$\mathcal{E} = \sum_j \oplus \mathcal{E}_j. \tag{42}$$

This is a geometrical structure imposed on the Hilbert space by the rotation operators.

The concept of invariant subspaces plays an important role in the representation theory of groups, which we are developing here in the special case of $SO(3)$ or $SU(2)$. Even more important is the concept of an *irreducible* invariant subspace. Although we will not pursue general aspects of representation theory, we will explain what this terminology means.

There are many subspaces that are invariant under rotations, for example, the entire Hilbert space $\mathcal{E}$ is invariant, as is the 0-dimensional (trivial) subspace containing only the zero vector. In general there are other invariant subspaces of intermediate dimensionality as well. If a vector space, invariant under rotations, possesses a smaller subspace (not counting the trivial subspace) that is also invariant under rotations, then it is said to be *reducible.* In that case, because of the unitarity of the rotation operators, the space orthogonal to the invariant subspace is also invariant. If it possesses no smaller invariant subspace that is invariant, then it is *irreducible.* If it possesses smaller, invariant subspaces, then these are either reducible or irreducible; if reducible, they can be broken into even smaller invariant subspaces. In this way ultimately any invariant vector space (such as the original space $\mathcal{E}$) can be decomposed into a set of orthogonal, invariant and irreducible subspaces. In fact, the subspaces $\mathcal{E}_j$ defined in Eq. (40) are irreducible, and the decomposition of $\mathcal{E}$ into irreducible subspaces is indicated by Eq. (42). We will not prove the irreduciblity of the $\mathcal{E}_j$ because we will not make explicit use of it, but we will refer to the subspaces $\mathcal{E}_j$ as *invariant, irreducible subspaces*, or *irreducible subspaces* for short.

6. Matrices for Angular Momentum and Operators

Let X be any function of $\mathbf{J}$, such as the components of $\mathbf{J}$, the operators $J_\pm$ and J^2, and the rotation operators $U(\hat{\mathbf{n}},\theta)$. The action of X on a vector of the standard angular momentum basis can be expanded as a linear combination of those same basis vectors,

$$X|jm\rangle = \sum_{j'm'} |j'm'\rangle\langle j'm'|X|jm\rangle, \tag{43}$$

where we have inserted a resolution of the identity. But the matrix element of X shown is diagonal in j,

$$\langle j'm'|X|jm\rangle = \delta_{j'j}\,\langle jm'|X|jm\rangle, \tag{44}$$

where the j values are the same on both sides of the final matrix element. Thus the j' sum in Eq. (43) can be done,

$$X|jm\rangle = \sum_{m'} |jm'\rangle\langle jm'|X|jm\rangle. \tag{45}$$

We see that the action of X on a basis vector in one of the invariant subspaces $\mathcal{E}_j$ produces a linear combination of the basis vectors in the same subspace. This is an explicit statement that the subspace is invariant under X. In effect, the final matrix element in Eq. (45) is a matrix element of X restricted to the subspace $\mathcal{E}_j$ (upon which j is a constant).

Let us work out some examples of these matrices. We label the rows and columns of matrices on $\mathcal{E}_j$ with m indices that start with $m = j$ and go to $m = -j$ (running down the columns or across the rows). We will present the matrices for J_3 and J_+. In view of Eq. (9) the matrix for J_- is the Hermitian conjugate of the matrix for J_+ (actually, just the transpose since by our phase conventions the matrices are real), so it need not be listed separately. Also, the matrices for J_1 and J_2 are easily computed by Eq. (39), so we will not present them separately, either. And by Eq. (38b), the matrix for J^2 on $\mathcal{E}_j$ is a multiple of the identity,

$$\langle jm'|J^2|jm\rangle = \delta_{m'm}\,\hbar^2\,j(j+1), \tag{46}$$

so we will not present it, either.

We list the matrices according to the j value. Not all j values occur in all applications, but when they do occur the matrices are the following.

First, in the case $j=0$, we have

$$J_3 = \hbar\,(\,0\,)\,, \tag{47}$$

and

$$J_+ = \hbar\,(\,0\,)\,. \tag{48}$$

In this case, the indices m, m' take on the single value 0, and all three components of $\mathbf{J}$ are represented by the 1×1 matrix containing the single element 0. We see that the operator $\mathbf{J}$ restricted to a subspace $\mathcal{E}_0$ is the zero operator.

In the case $j=\frac{1}{2}$, we have

$$J_3 = \hbar\begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \tag{49}$$

and

$$J_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{50}$$

If we compute the matrices also for J_1 and J_2, we find altogether $\mathbf{J} = (\hbar/2)\boldsymbol{\sigma}$, as in Notes 12.

In the case $j=1$, we have

$$J_3 = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{51}$$

and

$$J_+ = \hbar\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}. \tag{52}$$

These matrices would apply to a p-wave (a state with $\ell=1$) in a central force problem, or to the spin state of a spin-1 particle such as the deuteron or the photon.

Finally, for $j=3/2$, we have

$$J_3 = \hbar\begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}, \tag{53}$$

and

$$J_+ = \hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{54}$$

In all these cases, the matrix for J_3 is diagonal, naturally because we are using an eigenbasis of the operator J_3. The matrices for $J_\pm$ are nonzero only on one diagonal above or below the main diagonal, and are real. Therefore by Eq. (39), the matrix for J_1 is real and that for J_2 is pure imaginary.

7. Rotation Matrices; Reduced Rotation Matrices

Let us now set $X = U(\hat{\mathbf{n}}, \theta)$ in Eq. (43), which we write in the form

$$U|jm\rangle = \sum_{m'} |jm'\rangle \, D^j_{m'm}(U), \tag{55}$$

where we have defined

$$D^j_{m'm}(U) = \langle jm'|U|jm\rangle. \tag{56}$$

If U is parameterized in various forms (axis-angle, Euler angles, classical rotation), that is, $U(\hat{\mathbf{n}}, \theta)$, $U(\alpha, \beta, \gamma)$, $U(\mathsf{R})$, then we will use the same parameters for the matrices D^j, writing, for example, $D^j_{m'm}(\hat{\mathbf{n}}, \theta)$, $D^j_{m'm}(\alpha, \beta, \gamma)$, $D^j_{m'm}(\mathsf{R})$. The matrices D^j contain the matrix elements of the corresponding rotation operator on an irreducible subspace $\mathcal{E}_j$, in the standard angular momentum basis. The symbol D stands for German *Drehung* ("rotation").

The matrices D^j are obtained by exponentiating linear combinations of the angular momentum matrices, according to Eq. (2), or by computing D^j matrices for rotations about the coordinate axes and using the Euler angle decomposition (see Eq. (11.58)). Rotations about the z-axis are especially simple, because the matrix for J_3 is diagonal,

$$\langle jm'|J_3|jm\rangle = m\hbar \, \delta_{m'm}. \tag{57}$$

The exponential of a diagonal matrix is also diagonal, so

$$D^j_{mm'}(\hat{\mathbf{z}}, \theta) = \langle jm|e^{-i\theta J_z/\hbar}|jm'\rangle = e^{-im\theta} \, \delta_{mm'}. \tag{58}$$

This means that two of the factors in the Euler angle representation of the rotation operators are diagonal, so that

$$\begin{aligned} D^j_{mm'}(\alpha, \beta, \gamma) &= \langle jm|e^{-i\alpha J_z/\hbar} \, e^{-i\beta J_y/\hbar} \, e^{-i\gamma J_z/\hbar}|jm'\rangle \\ &= \sum_{m_1, m_2} \langle jm|e^{-i\alpha J_z/\hbar}|jm_1\rangle\langle jm_1|e^{-i\beta J_y/\hbar}|jm_2\rangle\langle jm_2|e^{-i\gamma J_z/\hbar}|jm'\rangle \\ &= \sum_{m_1, m_2} e^{-i\alpha m_1} \, \delta_{mm_1} \langle jm_1|e^{-i\beta J_y/\hbar}|jm_2\rangle e^{-i\gamma m'} \, \delta_{m_2 m'} \\ &= e^{-i\alpha m - i\gamma m'} \, d^j_{mm'}(\beta), \end{aligned} \tag{59}$$

where

$$d^j_{mm'}(\beta) = \langle jm|e^{-i\beta J_y/\hbar}|jm'\rangle. \tag{60}$$

In Eq. (59), we only sum over m in the resolution of the identity, because we are working on a single irreducible subspace $\mathcal{E}_j$. The matrix $d^j_{mm'}(\beta)$ is called the *reduced* rotation matrix; we see that in the Euler angle decomposition of an arbitrary rotation, only the rotation about the y-axis is nontrivial, and it depends only on the one Euler angle β. Furthermore, since the matrix elements of J_y are purely imaginary under our conventions, the reduced matrix elements $d^j_{mm'}(\beta)$ are purely real. This is one of the conveniences of the zyz-convention for Euler angles in quantum mechanics.

Therefore when tabulating the D^j matrices in Euler angle form, it suffices to tabulate only the reduced rotation (or d^j-) matrices. The first few of these are easy to work out, and for more complicated cases, there exist tables or explicit formulas.

For the case $j = 0$, the result is trivial:

$$d^0_{mm'}(\beta) = (\,1\,)\,. \tag{61}$$

We see that a rotation does nothing to a state of zero angular momentum, such as that of a spin-0 particle, or an s-wave in a central force problem (you may recall, for example, that the $1s$ or ground state wave function of the hydrogen atom is rotationally invariant). All vectors of zero angular momentum are invariant under rotations.

For the case $j = 1/2$, we use the properties of the Pauli matrices to obtain

$$d^{1/2}_{mm'}(\beta) = \cos(\beta/2) - i\sigma_y \sin(\beta/2) = \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}, \tag{62}$$

which is a special case of Eq. (12.27) (see also Prob. 1.1).

For the case $j = 1$, we can find recursions among the powers of the matrix for J_y, and sum the exponential series to obtain

$$d^1_{mm'}(\beta) = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\sin\beta/\sqrt{2} & \frac{1}{2}(1-\cos\beta) \\ \sin\beta/\sqrt{2} & \cos\beta & -\sin\beta/\sqrt{2} \\ \frac{1}{2}(1-\cos\beta) & \sin\beta/\sqrt{2} & \frac{1}{2}(1+\cos\beta) \end{pmatrix}. \tag{63}$$

This calculation is repeated in Sakurai. For higher values of j it is most convenient to use recursion relations or other methods for calculating the matrices d^j. These matrices are tabulated in standard references on rotations in quantum mechanics.

The D^j-matrices form what we call a *representation* of the rotation group $SO(3)$ or $SU(2)$, that is, matrix multiplication reproduces the group multiplication laws. In fact, since they are the matrices on an irreducible subspace, these are called *irreducible representations*.

The matrix elements for J_3, given by Eq. (58), contain an important lesson. Since m is integral (half-integral) when j is integral (half-integral), and since the phases $e^{-im\theta}$ occur on the diagonal of the matrix elements for J_3, we see that the irreducible representations of the rotation operators form a double-valued representation of $SO(3)$ in the case of half-integral j, and a single-valued representation in the case of integral j. That is, if j is half-integral, then $U(\hat{\mathbf{z}}, 2\pi) = -1$, a generalization of Eq. (12.38), which applied in the special case $j = \frac{1}{2}$. In all cases, the D-matrices form a (proper, single-valued) irreducible representation of the group $SU(2)$.

The D-matrices have many properties, of which we mention three. First, if U is a rotation operator and $D^j_{mm'}(U)$ the corresponding matrix, then the operator U^{-1} corresponds to the matrix D^{-1}. But since U is unitary, so is the matrix D, and we have

$$D^j_{mm'}(U^{-1}) = [D^j(U)^{-1}]_{mm'} = [D^j(U)^\dagger]_{mm'} = D^{j*}_{m'm}(U). \tag{64}$$

Next there is the representation property. If we think of the D-matrices as parameterized by the unitary rotation operators U, then

$$D^j(U_1)D^j(U_2) = D^j(U_1U_2). \tag{65}$$

If we think of D-matrices as parameterized by the classical rotations R, then in the case of integer j they form a representation of $SO(3)$,

$$D^j(\mathsf{R}_1)D^j(\mathsf{R}_2) = D^j(\mathsf{R}_1\mathsf{R}_2), \qquad (j \text{ integer}). \tag{66}$$

In the case of half-integral j they form a double valued representation of $SO(3)$, in which each classical R corresponds to two D-matrices, differing by a sign. In that case we can write

$$D^j(\mathsf{R}_1)D^j(\mathsf{R}_2) = \pm D^j(\mathsf{R}_1\mathsf{R}_2), \qquad (j \text{ half-integer}), \tag{67}$$

with the same understandings as in Eq. (12.41).

Finally, the transformation properties of angular momentum under time reversal, a topic we shall consider later, show that

$$D^j_{mm'}(U) = (-1)^{m'-m}\, D^{j*}_{-m,-m'}(U). \tag{68}$$

See Prob. 20.1.

8. Degeneracies and Multiplicities

Let us now consider the general case in which the simultaneous eigenstates of J^2 and J_3 are degenerate, that is, the operators (J^2, J_3) by themselves do not form a complete set of commuting operators, and their simultaneous eigenspaces are multidimensional. Let us denote the eigenspace of J^2 and J_3 with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ by $\mathcal{S}_{jm}$, and let us write

$$N_{jm} = \dim \mathcal{S}_{jm}. \tag{69}$$

We wish to consider the case that $N_{jm} > 1$.

Let us take the stretched eigenspace $\mathcal{S}_{jj}$ which has dimension N_{jj}, and let us choose a set of N_{jj} linearly independent vectors in this space. Applying J_- to these vectors, we obtain a set of N_{jj}

vectors that are eigenvectors of J^2 and J_3 with eigenvalues $j(j+1)\hbar^2$ and $(m-1)\hbar$ (that is, with a lowered value of m). These vectors must lie in the eigenspace $\mathcal{S}_{j,j-1}$, and, as one can show, they are also linearly independent. Thus, $\dim \mathcal{S}_{j,j-1} = N_{j,j-1} \geq N_{jj}$.

Now choose a set of $N_{j,j-1}$ linearly independent vectors in $\mathcal{S}_{j,j-1}$ and apply the raising operator J_+ to them. This creates a set of $N_{j,j-1}$ vectors that lie in the stretched eigenspace $\mathcal{S}_{jj}$, which, as one can show, are also linearly independent. Thus, $N_{jj} \geq N_{j,j-1}$. But this is consistent with $N_{j,j-1} \geq N_{jj}$ only if $N_{j,j-1} = N_{jj}$.

Continuing in this way, we see that all the eigenspaces $\mathcal{S}_{jm}$ for $m = -j, \ldots, +j$ have the same dimensionality. We denote this dimensionality by N_j, which we call the *multiplicity* of the given j value. The multiplicity can take on any value from 0 (in which case the j value does not occur) to ∞.

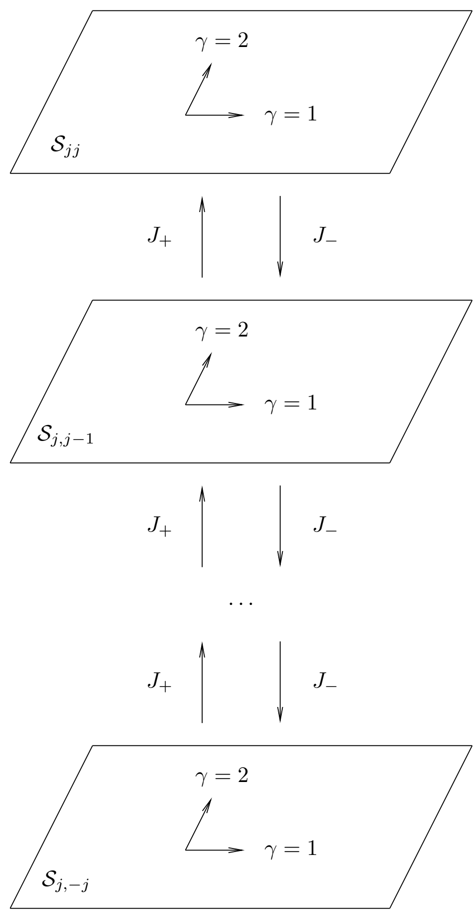

Fig. 3. The standard angular momentum basis $|\gamma jm\rangle$ is obtained by choosing an arbitrary orthonormal basis in the stretched space $\mathcal{S}_{jj}$, indexed by γ, and applying lowering operators.

Now let us choose an arbitrary, orthonormal basis in the stretched space $\mathcal{S}_{jj}$, indexed by an index γ, where $\gamma = 1, \ldots, N_j$. See Fig. 3. Let us call these vectors $|\gamma jj\rangle$. If we apply J_- to these, we obtain vectors in the next space down, $\mathcal{S}_{j,j-1}$. One can easily show that the orthogonality of these vectors is preserved under the action of J_-. As for the normalization, it is changed by J_-, that is the meaning of the square root factor in Eq. (35b), but if we compensate for this we obtain an orthonormal basis in $\mathcal{S}_{j,j-1}$. Let us call the new vectors $|\gamma j, j-1\rangle$, that is, let us *define* $|\gamma j, j-1\rangle$ by

$$J_-|\gamma jj\rangle = \hbar\,\sqrt{(j+j)(j-j+1)}\,|\gamma j, j-1\rangle. \tag{70}$$

Continuing in this way, we propagate an orthonormal basis from $\mathcal{S}_{jj}$ all the way down to $\mathcal{S}_{j,-j}$, as in Fig. 3. We call the basis vectors $|\gamma jm\rangle$, and by their construction they satisfy

$$\begin{aligned} J_+|\gamma jm\rangle &= \hbar\sqrt{(j-m)(j+m+1)}\,|\gamma j, m+1\rangle, \\ J_-|\gamma jm\rangle &= \hbar\sqrt{(j+m)(j-m+1)}\,|\gamma j, m-1\rangle. \end{aligned} \tag{71}$$

Equivalently, using recursion as in Eq. (36), we can write

$$|\gamma jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\,\Big(\frac{J_-}{\hbar}\Big)^{j-m}|\gamma jj\rangle. \tag{72}$$

By this construction, the raising and lowering operators change only the m values, not the j or γ values. The resulting set of vectors forms an orthonormal on the entire Hilbert space $\mathcal{E}$,

$$\langle\gamma' j' m'|\gamma jm\rangle = \delta_{\gamma\gamma'}\,\delta_{jj'}\,\delta_{mm'}. \tag{73}$$

We call the basis $\{|\gamma jm\rangle\}$ a *standard angular momentum basis* on $\mathcal{E}$ in the general case in which (J^2, J_3) by themselves do not form a complete set. It is still an eigenbasis of J^2 and J_3,

$$\begin{aligned} J^2|\gamma jm\rangle &= \hbar^2\,j(j+1)|\gamma jm\rangle, \\ J_3|\gamma jm\rangle &= \hbar\,m|\gamma jm\rangle, \end{aligned} \tag{74}$$

in which the index γ resolves the degeneracies.

The spaces $\mathcal{E}_{j\gamma}$ defined by

$$\mathcal{E}_{j\gamma} = \mathrm{span}\{|\gamma jm\rangle, m = -j, \ldots, +j\} \tag{75}$$

are the invariant, irreducible subspaces in this general case. The index j runs over all j values in the set (31) that occur in the particular problem, and the index γ runs over $1, \ldots, N_j$. The entire Hilbert space is broken up into a set of mutually orthogonal irreducible subspaces,

$$\mathcal{E} = \sum_{j\gamma} \oplus\,\mathcal{E}_{j\gamma}, \tag{76}$$

which generalizes Eq. (42).

We can now write down the matrix elements of the raising and lowering operators, as well as those of J^2 and J_3, in the standard angular momentum basis $|\gamma jm\rangle$. Multiplying Eqs. (71) or (74) on the left by $\langle\gamma' j' m'|$ and using the orthonormality, we obtain

$$\langle\gamma' j' m'|J_3|\gamma jm\rangle = \delta_{\gamma'\gamma}\,\delta_{j'j} \times m\hbar\,\delta_{m'm}, \tag{77a}$$

$$\langle\gamma' j' m'|J_\pm|\gamma jm\rangle = \delta_{\gamma'\gamma}\,\delta_{j'j} \times \sqrt{(j\mp m)(j\pm m+1)}\,\hbar\,\delta_{m',m\pm 1}, \tag{77b}$$

$$\langle\gamma' j' m'|J^2|\gamma jm\rangle = \delta_{\gamma'\gamma}\,\delta_{j'j} \times j(j+1)\hbar^2\,\delta_{m'm}. \tag{77c}$$

The matrix elements are diagonal in both γ and j, and depend only on j, m' and m. This means that the spaces $\mathcal{E}_{j\gamma}$ are invariant under the action of any function of $\mathbf{J}$, including the rotations operators.

Letting X be any function of $\mathbf{J}$, we can repeat the analysis of Sec. 6, showing the action of X on a vector of the standard angular momentum basis, but now with the index γ. That is, starting with an insertion of a resolution of the identity, we have

$$\begin{aligned} X|\gamma jm\rangle &= \sum_{\gamma' j' m'} |\gamma' j' m'\rangle\langle\gamma' j' m'|X|\gamma jm\rangle = \sum_{\gamma' j' m'} |\gamma' j' m'\rangle\,\delta_{\gamma'\gamma}\,\delta_{j'j}\,\langle jm'|X|jm\rangle \\ &= \sum_{m'} |\gamma jm'\rangle\langle jm'|X|jm\rangle. \end{aligned} \tag{78}$$

Here the notation $\langle jm'|X|jm\rangle$ can be regarded as a simplified notation for $\langle\gamma jm'|X|\gamma jm\rangle$, useful since this matrix element is independent of γ. But a better point of view is to regard it as the matrix element of X restricted to the irreducible subspace $\mathcal{E}_{j\gamma}$. These are the same matrix elements we had earlier when there was no index γ. Equation (78) shows that X acting on a vector of $\mathcal{E}_{j\gamma}$ produces another vector in $\mathcal{E}_{j\gamma}$, showing explicitly that these spaces are invariant under the action of X.

In particular, identifying X with a rotation operator U, we have

$$U|\gamma jm\rangle = \sum_{m'} |\gamma jm'\rangle D^j_{m'm}(U), \tag{79}$$

showing how basis vectors of the standard angular momentum basis transform under rotations. This is the same as Eq. (55), with the index γ added.

9. Generalized Adjoint Formula

We recall that we derived a version of the adjoint formula for classical rotations in Eq. (11.48), and later we found an analogous formula, Eq. (12.34), for spin-$\frac{1}{2}$ rotations. We now generalize this to arbitrary representations of the rotation operators. The generalization is obvious; it is

$$\boxed{U\mathbf{J}U^\dagger = \mathsf{R}^{-1}\mathbf{J},} \tag{80}$$

where $U = U(\hat{\mathbf{n}},\theta)$ and $\mathsf{R} = \mathsf{R}(\hat{\mathbf{n}},\theta)$. Notice that the left hand side is quadratic in U, so in the case of double-valued representations of $SO(3)$, it does not matter which U operator we choose to represent the rotation R.

To prove Eq. (80), we define the operator vector,

$$\mathbf{X}(\theta) = U(\hat{\mathbf{n}}, \theta)\, \mathbf{J}\, U(\hat{\mathbf{n}}, \theta)^\dagger, \tag{81}$$

and we note the initial condition,

$$\mathbf{X}(0) = \mathbf{J}. \tag{82}$$

Next we obtain a differential equation for $\mathbf{X}(\theta)$:

$$\begin{aligned} \frac{d\mathbf{X}(\theta)}{d\theta} &= \frac{dU}{d\theta}\mathbf{J}U^\dagger + U\mathbf{J}\frac{dU^\dagger}{d\theta} = -\frac{i}{\hbar}U[\hat{\mathbf{n}}\cdot\mathbf{J}, \mathbf{J}]U^\dagger \\ &= -\hat{\mathbf{n}}\times(U\mathbf{J}U^\dagger) = -(\hat{\mathbf{n}}\cdot\mathsf{J})\mathbf{X}. \end{aligned} \tag{83}$$

The solution is

$$\mathbf{X}(\theta) = \exp\bigl(-\theta\hat{\mathbf{n}}\cdot\mathsf{J}\bigr)\mathbf{X}(0) = \mathsf{R}(\hat{\mathbf{n}}, \theta)^{-1}\mathbf{J}, \tag{84}$$

which is equivalent to the adjoint formula (80).

Finally, we can dot both sides of Eq. (80) by $-i\theta\hat{\mathbf{n}}/\hbar$ and exponentiate, to obtain a formula analogous to Eq. (11.51). After placing 0 subscripts on U and R for clarity, the result is

$$U_0 U(\hat{\mathbf{n}}, \theta) U_0^\dagger = U(\mathsf{R}_0\hat{\mathbf{n}}, \theta), \tag{85}$$

where U_0 and R_0 are corresponding quantum and classical rotations. Notice again that the left hand side is quadratic in U_0, so that in the case of double-valued representations it does not matter which U_0 operator we choose to represent the rotation R_0.

Problems

1. A molecule is approximately a rigid body. Consider a molecule such as H_2O, NH_3, or CH_4, which is not a diatomic. First let us talk classical mechanics. Then the kinetic energy of a rigid body is

$$H = \frac{L_x^2}{2I_x} + \frac{L_y^2}{2I_y} + \frac{L_z^2}{2I_z}, \tag{86}$$

where $\mathbf{L} = (L_x, L_y, L_z)$ is the angular momentum vector with respect to the body frame, and (I_x, I_y, I_z) are the principal moments of inertia. The body frame is assumed to be the principal axis frame in Eq. (86). The angular velocity $\boldsymbol{\omega}$ of the rigid body is related to the angular momentum $\mathbf{L}$ by

$$\mathbf{L} = \mathsf{I}\boldsymbol{\omega}, \tag{87}$$

where I is the moment of inertia tensor. When Eq. (87) is written in the principal axis frame, it becomes

$$\omega_i = \frac{L_i}{I_i}, \qquad i = x, y, z. \tag{88}$$

Finally, the equations of motion for the angular velocity or angular momentum in the body frame are the *Euler equations*,

$$\dot{\mathbf{L}} + \boldsymbol{\omega}\times\mathbf{L} = 0. \tag{89}$$

By using Eq. (88) to eliminate either $\boldsymbol{\omega}$ or $\mathbf{L}$, Eq. (89) can be regarded as an equation for either $\mathbf{L}$ or $\boldsymbol{\omega}$. The Euler equations are trivial for a spherical top ($I_x = I_y = I_z$), they are easily solvable in terms of trigonometric functions for a symmetric top ($I_x = I_y = I_\perp \neq I_z$), and they are solvable in terms of elliptic functions for an asymmetric top (I_x, I_y, I_z all unequal). The symmetric top is studied in all undergraduate courses in classical mechanics.

(a) In quantum mechanics, it turns out that the Hamiltonian operator for a rigid body has exactly the form (86). The angular momentum $\mathbf{L}$ satisfies the commutation relations,

$$[L_i, L_j] = -i\hbar\, \epsilon_{ijk}\, L_k, \tag{90}$$

with a minus sign relative to the familiar commutation relations because the components of $\mathbf{L}$ are (in this problem) measured relative to the body frame. (We will not justify this. If the components of $\mathbf{L}$ were measured with respect to the space or inertial frame, then there would be the usual plus sign in Eq. (90).) Compute the Heisenberg equations of motion for $\mathbf{L}$, and compare them with the classical Euler equations. You may take Eq. (87) or (88) over into quantum mechanics, in order to define an operator $\boldsymbol{\omega}$ to make the Heisenberg equations look more like the classical Euler equations. (Just get the equation for L_x, then cycle indices to get the others.) Make your answer look like Eq. (89) as much as possible.

(b) It is traditional in the theory of molecules to let the quantum number of L_z (referred to the body frame) be k. Write the rotational energy levels of a symmetric top ($I_x = I_y = I_\perp \neq I_z$) in terms of a suitable set of quantum numbers. Indicate any degeneracies. How is the oblate case ($I_z > I_\perp$) qualitatively different from the prolate case ($I_\perp > I_z$)? Hint: In order to deal with standard commutation relations, you may wish to write $\tilde{\mathbf{L}} = -\mathbf{L}$, so that $[\tilde{L}_i, \tilde{L}_j] = i\hbar\, \epsilon_{ijk}\, \tilde{L}_k$.

2. A spin-1 particle has the component of its spin in the direction

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{3}}(1,1,1), \tag{91}$$

measured, and the result is $\hbar$. Subsequently S_z is measured, with various probabilities of the three possible outcomes.

Let R be a rotation that maps the $\hat{\mathbf{z}}$ axis into $\hat{\mathbf{n}}$, that is, let

$$\mathsf{R}\hat{\mathbf{z}} = \hat{\mathbf{n}}. \tag{92}$$

Express the aforementioned probabilities in terms of the matrix, $D^1_{mm'}(\mathsf{R})$. Work out this matrix to find the probabilities explicitly. You may use tables of d-matrices.

3. The adjoint formula (80) is important in applications. The proof above uses a differential equation in the angle θ. The following is a more pictorial approach. It is based on the idea that finite rotations can be built up as the product of a large number of small rotations.

First show that if Eq. (80) is true for two rotation operators U_1 and U_2, and the corresponding classical rotations R_1 and R_2, then it is true for the products $U = U_1 U_2$ and $\mathsf{R} = \mathsf{R}_1 \mathsf{R}_2$. Then show that Eq. (80) is true for infinitesimal rotations. This is sufficient to prove the formula.