Physics 221A
Fall 2010
Notes 13
Representations of the Angular Momentum Operators
and Rotations

1. Introduction

In Notes 12, the angular momentum $\mathbf{J}$ of a quantum system was defined by Eq. (12.13) (equivalently, by Eq. (12.11)) as the infinitesimal generator of rotations, and it was shown that the components of $\mathbf{J}$ must satisfy the commutation relations (12.24) in order that the quantum rotation operators should provide a representation of the classical rotations. We repeat these commutation relations here:

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

Our strategy in finding a representation of the rotations is first to find a representation of the angular momentum commutation relations, that is, a set of three Hermitian operators (J_1, J_2, J_3) that satisfy Eq. (1), and then to exponentiate linear combinations of them according

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

(This repeats Eq. (12.18).) This gives the rotation operators $U(\hat{\mathbf{n}}, \theta)$ themselves. In Notes 12, we carried out this strategy in detail, working with the specific representation of the angular momentum commutation relations given by $\mathbf{J} = (\hbar/2)\boldsymbol{\sigma}$, which gave us rotation operators for spin-$\frac{1}{2}$ systems.

In these notes we will solve the representation problem for the angular momentum commutation relations in all generality. That is, we will seek and find the most general vector (J_1, J_2, J_3) of Hermitian operators that satisfy Eq. (1). After we have done this, we will explore the properties of the rotation operators that are generated from the angular momentum operators by Eq. (2). We will find that the rotation operators created in this manner sometimes form a double-valued representation of the classical rotations, just as we found in the case of spin-$\frac{1}{2}$ rotations in Notes 12, and sometimes form a genuine, single-valued representation.

2. Statement of the Problem

Let us assume that we have some vector space upon which three Hermitian operators (J_1, J_2, J_3) act, such that the commutation relations (1) are satisfied. We make no other assumptions about these operators or the vector space upon which they act, and, in particular, we make no assumptions about the dimensionality of the vector space. It pays to treat this problem in some generality, because there is a wide variety of circumstances in physical problems where such operators and commutation relations arise. For example, the vector space could be a ket space, in which case the operators (J_1, J_2, J_3) are ordinary operators in quantum mechanics. The ket space could belong to the spatial degrees of freedom for a quantum system (that is, it could be a wave function space); it could be a ket space for spin degrees of freedom; it could be the tensor product of such spaces, perhaps representing a multiparticle system; or it could be a subspace of such spaces.

In fact, the vector space need not be a ket space. It could be a vector space of operators, as will be discussed in later notes on irreducible tensor operators and the Wigner-Eckart theorem. It could be ordinary 3-dimensional space, in which case we could "rediscover" the theory of classical rotations as in Notes 11. It could be a space of wave fields for a classical wave system, as in the multipole expansion for classical electromagnetic fields. There are many possibilities. Nevertheless, to be specific, in the following discussion we will proceed as if the vector space is a ket space, and we will use bra-ket notation for the vectors of the space.

3. 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,

$$J^2 = J_1^2 + J_2^2 + J_3^2, \tag{3}$$

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

$$[J^2, \mathbf{J}] = 0. \tag{4}$$

Since J^2 commutes with $\mathbf{J}$, it commutes also with any function of $\mathbf{J}$. An operator with this property 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 in general find simultaneous eigenkets of more than one component of $\mathbf{J}$. By convention we choose the 3-component, and look for simulataneous 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 that a and m might take on.

For simplicity we assume that the eigenvalues $J^2 = \hbar^2 a$ and $J_3 = \hbar m$ are nondegenerate, so that the ket $|am\rangle$ is determined to within a normalization and a phase. We assume the kets are normalized,

$$\langle am|am\rangle = 1, \tag{5}$$

and that some arbitrary (at this point) phase conventions have been chosen. In effect, we are assuming that the set (J^2, J_3) by itself forms a complete set of commuting observables. Later we will relax this condition and allow for degeneracies. The kets $|am\rangle$ satisfy

$$\begin{aligned} J^2|am\rangle &= \hbar^2 a|am\rangle, \\ J_3|am\rangle &= \hbar m|am\rangle. \end{aligned} \tag{6}$$

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

$$J_\pm = J_1 \pm iJ_2. \tag{7}$$

These are Hermitian conjugates of each other,

$$(J_\pm)^\dagger = J_\mp, \tag{8}$$

and they satisfy the commutation relations,

$$[J_3, J_\pm] = \pm\hbar J_\pm, \tag{9}$$

$$[J_+, J_-] = 2\hbar J_3, \tag{10}$$

$$[J^2, J_\pm] = 0. \tag{11}$$

They also satisfy the relations,

$$J^2 = \frac{1}{2}(J_+J_- + J_-J_+) + J_3^2, \tag{12}$$

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

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

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. (13) and (14), we find

$$\langle am|J_-J_+|am\rangle = \hbar^2[a - m(m+1)] \geq 0, \tag{15}$$

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

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

$$a \geq \max[m(m+1), m(m-1)]. \tag{17}$$

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. (17) 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

$$-j \leq m \leq +j. \tag{18}$$

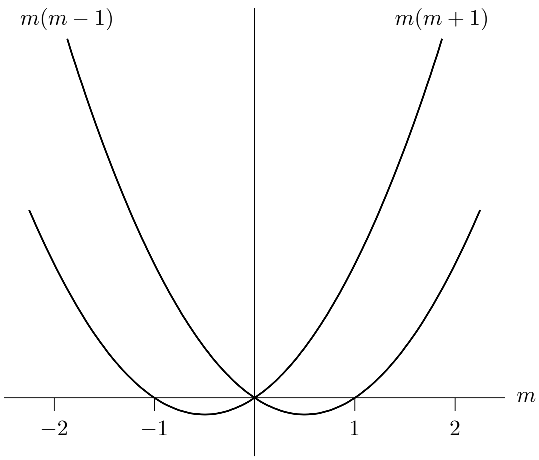

Fig. 1. Functions $m(m+1)$ and $m(m-1)$.

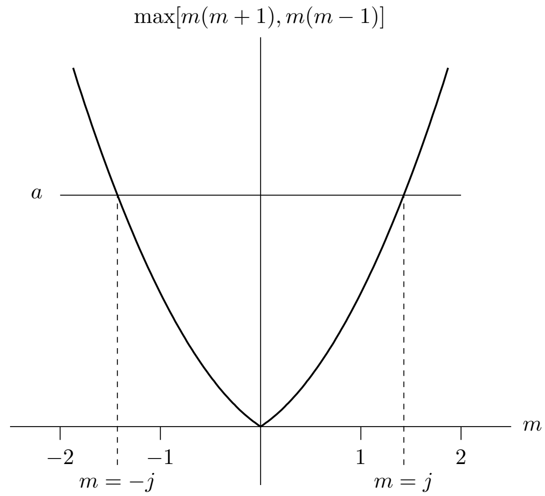

Fig. 2. Function $\max[m(m{+}1), m(m{-}1)]$, with maximum and minimum values of m for a given value of a.

As for j, it 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

$$a = j(j+1). \tag{19}$$

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. (6) become

$$\begin{aligned} J^2|jm\rangle &= j(j+1)\hbar^2|jm\rangle, \\ J_3|jm\rangle &= m\hbar|jm\rangle. \end{aligned} \tag{20}$$

We also rewrite Eqs. (15) and (16) with this change of notation, noting that the right hand sides can be factored,

$$\langle jm|J_-J_+|jm\rangle = \hbar^2[j(j+1) - m(m+1)] = \hbar^2(j-m)(j+m+1) \geq 0, \tag{21}$$

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

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. (21), we have $J_+|jm\rangle = 0$ if and only if

$$j - m = 0 \qquad \text{or} \qquad j + m + 1 = 0, \tag{23}$$

that is,

$$m = j \qquad \text{or} \qquad m = -j - 1. \tag{24}$$

But by Eq. (18), $m = -j - 1$ is impossible, so we find

$$J_+|jm\rangle = 0 \qquad \text{iff} \qquad m = j. \tag{25}$$

Similarly analyzing Eq. (22), we find

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

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 (9) and (11),

$$\begin{aligned} J^2\big(J_+|jm\rangle\big) &= J_+J^2|jm\rangle = j(j+1)\hbar^2\big(J_+|jm\rangle\big), \\ J_3\big(J_+|jm\rangle\big) &= (J_+J_3 + \hbar J_+)|jm\rangle = (m+1)\hbar\big(J_+|jm\rangle\big). \end{aligned} \tag{27}$$

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

$$m = j - n_1, \tag{28}$$

where $n_1 \geq 0$ 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 (18) was violated. Similarly, we show

$$m = -j + n_2, \tag{29}$$

where $n_2 \geq 0$ is another integer. But taken together, Eqs. (28) and (29) 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

$$j \in \{0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots\}. \tag{30}$$

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,

$$m = -j, -j+1, \ldots, +j, \tag{31}$$

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 (31) 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.

4. 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

$$\begin{aligned} J_+|jm\rangle &= c|j,m+1\rangle, \\ J_-|jm\rangle &= c'|j,m-1\rangle, \end{aligned} \tag{32}$$

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

$$\begin{aligned} \langle jm|J_-J_+|jm\rangle &= |c|^2 = \hbar^2(j-m)(j+m+1), \\ \langle jm|J_+J_-|jm\rangle &= |c'|^2 = \hbar^2(j+m)(j-m+1). \end{aligned} \tag{33}$$

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,

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

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 litte induction to express an arbitary state $|jm\rangle$ as a lowered version of the stretched state $|jj\rangle$,

$$|jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}\left(\frac{J_-}{\hbar}\right)^{j-m}|jj\rangle. \tag{35}$$

This may be compared to Eq. (8.38) for the harmonic oscillator.

5. Degeneracies and Multiplicities

Suppose now that the simultaneous eigenstates of J^2 and J_3 are degenerate. Let us denote the eigenspace of J^2 and J_3 with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$ by $\mathcal{E}_{jm}$, and let us write

$$N_{jm} = \dim\mathcal{E}_{jm} \tag{36}$$

for the dimensionality of this eigenspace. We wish to consider the case that $N_{jm}>1$.

Let us take the stretched eigenspace $\mathcal{E}_{jj}$ 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 $\mathcal{E}_{j,j-1}$, and, as one can show, they are also linearly independent. Thus, $\dim\mathcal{E}_{j,j-1} = N_{j,j-1} \ge N_{jj}$.

Now choose a set of $N_{j,j-1}$ linearly independent vectors in $\mathcal{E}_{j,j-1}$ and apply the raising operator J_+ to them. This creates a set of $N_{j,j-1}$ vectors that lie in the stretched eigenspace $\mathcal{E}_{jj}$, 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 $\mathcal{E}_{jm}$ for $m = -j, \ldots, +j$ have the same dimension. We denote this dimension 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 ∞.

6. The Standard Angular Momentum Basis

Now return to the stretched eigenspace $\mathcal{E}_{jj}$, and choose an orthonormal basis in this space indexed by an index γ, where $\gamma = 1, \ldots, N_j$. Denote these vectors by $|\gamma jj\rangle$. Then use Eq. (35) to define

$$|\gamma jm\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}} \left(\frac{J_-}{\hbar}\right)^{j-m} |\gamma jj\rangle. \tag{37}$$

By this construction, the raising and lowering operators change only the m values, not the j or γ values. Also, the resulting set of vectors is orthonormal,

$$\langle \gamma' j' m' | \gamma jm\rangle = \delta_{\gamma\gamma'}\, \delta_{jj'}\, \delta_{mm'}, \tag{38}$$

and the relations (34) become

$$\begin{aligned} J_+|\gamma jm\rangle &= \hbar\sqrt{(j-m)(j+m+1)}\,|\gamma j, m+1\rangle, \\ J_-|\gamma jm\rangle &= \hbar\sqrt{(j+m)(j-m+1)}\,|\gamma j, m-1\rangle. \end{aligned} \tag{39}$$

With these conventions, we will say that the eigenkets $|\gamma jm\rangle$ form a *standard angular momentum basis* on the full Hilbert space.

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 $|\gamma jm\rangle$. These are

$$\langle \gamma' j' m' | J_3 | \gamma jm\rangle = \delta_{\gamma'\gamma}\, \delta_{j'j} \times m\hbar\, \delta_{m'm}, \tag{40a}$$

$$\langle \gamma' j' m' | J_\pm | \gamma jm\rangle = \delta_{\gamma'\gamma}\, \delta_{j'j} \times \sqrt{(j \mp m)(j \pm m+1)}\,\hbar\, \delta_{m',m\pm1}, \tag{40b}$$

$$\langle \gamma' j' m' | J^2 | \gamma jm\rangle = \delta_{\gamma'\gamma}\, \delta_{j'j} \times j(j+1)\hbar^2\, \delta_{m'm}. \tag{40c}$$

The matrix elements of J_1 and J_2 follow trivially from those of $J_\pm$ by

$$J_1 = \frac{1}{2}(J_+ + J_-), \qquad J_2 = \frac{1}{2i}(J_+ - J_-). \tag{41}$$

The matrix elements (40) are diagonal in j and γ, and furthermore depend only on j and m but not on γ. They follow directly from the angular momentum commutation relations (1) and incorporate some phase and other conventions, but they do not depend in any way on the specific nature of the operators that satisfy those commutation relations. Thus, the same matrix elements apply to spin, orbital angular momentum, isospin, etc.

7. Matrices of Angular Momentum Operators in the Standard Basis

We have now completely solved the problem of finding all possible representations of operators $\mathbf{J}$ that satisfy the commutation relations (1), for we have shown that there exists a basis (the standard basis $|\gamma jm\rangle$) in which the matrix elements of (J_1, J_2, J_3) are given by Eqs. (40). It is useful to visualize the matrices representing the angular momentum operators in this basis. To do this, we order the basis kets $|\gamma jm\rangle$ in such a way that m varies most rapidly, γ next most rapidly, and j least rapidly. Then the matrices are block-diagonal, beginning with N_0 copies of the 1×1 matrices corresponding to $j=0$, followed by $N_{1/2}$ copies of the 2×2 matrices corresponding to $j=\frac{1}{2}$, etc. For example, if $N_0 = 3$, $N_{1/2} = 1$, $N_1 = 2$, etc., then the matrices will have the following structure:

$$\langle\gamma jm|X|\gamma' j' m'\rangle = \begin{pmatrix} \boxed{0} & & & & & & \\ & \boxed{0} & & & & & \\ & & \boxed{0} & & & & \\ & & & \boxed{\tfrac{1}{2}} & & & \\ & & & & \boxed{\;1\;} & & \\ & & & & & \boxed{\;1\;} & \\ & & & & & & \ddots \end{pmatrix}. \tag{42}$$

Here X stands for any of the operators, (J_1, J_2, J_3), or for any function of these operators, such as $J_\pm$, J^2, or the rotation operators $\exp(-i\theta\hat{\mathbf{n}}\cdot\mathbf{J}/\hbar)$. In all cases, all copies of the $j=0$ matrices are identical, all copies of the $j=\frac{1}{2}$ matrices are identical, etc, since their matrix elements depend on m and j but not on γ. The matrices that go into the blocks on the diagonal depend on which operator X is referred to, but the block structure itself is the same for all choices of X.

8. Invariant and Irreducible Subspaces

Whenever a matrix representing an operator has a block-diagonal form, it means that the operator possesses invariant subspaces; this is the abstract meaning of the block-diagonal structure. A subspace is considered *invariant* under the action of an operator if every vector in that subspace is mapped into another vector in the same subspace by the operator. In the present case, the invariant subspaces are the those spanned by the basis kets $|\gamma jm\rangle$ for fixed values of γ and j but variable m, since these are the values of (γjm) that correspond to one of the blocks. For example, the second $j=1$ block (a 3×3 block) in Eq. (42) corresponds to $\gamma=2$, $j=1$, $m=1,0,-1$. Any linear combination of the basis vectors $|\gamma jm\rangle$ for these three values of (γjm) is mapped into another such linear combination by any function of the angular momentum operators.

Let us denote the invariant subspaces by $\mathcal{E}_{\gamma j}$ (not to be confused with the spaces $\mathcal{E}_{jm}$ used above), so that

$$\mathcal{E}_{\gamma j} = \text{span}\{|\gamma jm\rangle | m = -j, -j+1, \ldots, +j\}, \tag{43}$$

and so that

$$\dim \mathcal{E}_{\gamma j} = 2j+1. \tag{44}$$

As it turns out, these subspaces are not only invariant under all the angular momentum and rotation operators, but they possess no smaller subspaces that are so invariant. As a result, they are called *invariant, irreducible* subspaces. Thus, they are invariant subspaces of minimal dimensionality, in a sense. We shall call them *irreducible subspaces* for short, and for our purposes their most important property is that they are invariant under the action of the rotation operators. As a simple rule, you may remember that an irreducible subspace is spanned by a set of $2j+1$ vectors linked by raising and lowering operators.

Whenever an operator has an invariant subspace, it is possible to restrict that operator to the subspace (see Sec. 1.16). For example, if we choose a basis in the invariant subspace, the operator restricted to the subspace becomes represented by a matrix whose size is the dimensionality of the subspace. In the present case, any of the operators X (any function of the angular momentum operators) can be restricted to the irreducible subspaces $\mathcal{E}_{\gamma j}$, whereupon it becomes represented by a $(2j+1) \times (2j+1)$ matrix, and in the standard basis the components of this matrix are independent of γ. These are the matrices sitting on the diagonal in Eq. (42). In the case that X stands for the components of $\mathbf{J}$, we obtain Hermitian matrices representing $\mathbf{J}$ that satisfy the angular momentum commutation relations (1); these matrices are said to form an *irreducible representation* of those commutation relations. In the case that X stands for the rotation operators $\exp(-i\theta\hat{\mathbf{n}} \cdot \mathbf{J}/\hbar)$, we obtain unitary matrices that reproduce the multiplication law for rotations; these matrices are said to form an *irreducible representation* of the rotations. In either case, there is a distinct irreducible representation for each value of j. We see that when studying the general problem of the representations of the angular momentum commutation relations or the rotation operators, it suffices to study the irreducible representations because an arbitrary representation consists of copies of irreducible representations as illustrated by Eq. (42).

Let us restrict the angular momentum operators to a single irreducible subspace, and record the matrix elements. We can suppress the index γ when writing the basis vectors of the irreducible subspace, since γ is constant on such a subspace and the matrix elements do not depend on γ. Thus, we write these basis vectors as $|jm\rangle$. Furthermore, j is fixed in a single irreducible subspace, and only m varies. The matrix elements themselves are simple transcriptions of Eq. (40):

$$\begin{aligned}
\langle jm'|J_3|jm\rangle &= m\hbar\, \delta_{m'm}, \\
\langle jm'|J_+|jm\rangle &= \hbar\sqrt{(j-m)(j+m+1)}\, \delta_{m',m+1}, \\
\langle jm'|J_-|jm\rangle &= \hbar\sqrt{(j+m)(j-m+1)}\, \delta_{m',m-1}, \\
\langle jm'|J^2|jm\rangle &= \hbar^2 j(j+1)\, \delta_{m'm}
\end{aligned} \tag{45}$$

These matrix elements do not depend on which irreducible subspace we work with, since they are independent of γ. Nor do they depend on the details of the physical interpretation of the operators $\mathbf{J}$ (orbital angular momentum, spin angular momentum, isospin, etc.). They are universal matrices applying to any problem involving angular momenta, and depend only on the commutation relations (1) plus the various conventions we have established.

9. Examples of Irreducible Representations of Angular Momentum Operators

Let us display some examples of the irreducible representations of the angular momentum operators. We will content ourselves with the matrices representing J_3 and J_+, since the matrix for J_- is the Hermitian conjugate of that for J_+, and the matrices for J_1 and J_2 can be obtained from Eq. (41). Nor do we bother with J^2, since by Eq. (45), its matrix representation on an irreducible subspace is a multiple of the identity.

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

$$J_3 = \hbar\,(\,0\,)\,, \tag{46}$$

and

$$J_+ = \hbar\,(\,0\,)\,. \tag{47}$$

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. In these equations and below, we are writing J_3 and J_+ for what are really the matrices representing these operators in the standard basis.

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

$$J_3 = \hbar \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \tag{48}$$

and

$$J_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{49}$$

Here and below we order the m values from largest to smallest as we move across rows or down columns, so that, for example, the upper right corner of these matrices correspond to row $m = \frac{1}{2}$ and column $m' = -\frac{1}{2}$. These matrices for the case $j = \frac{1}{2}$ are of course equivalent to $\mathbf{J} = (\hbar/2)\boldsymbol{\sigma}$.

In the case $j = 1$, we have

$$J_3 = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{50}$$

and

$$J_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}. \tag{51}$$

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

$$J_3 = \hbar \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}, \tag{52}$$

and

$$J_+ = \hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{53}$$

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. (41), the matrix for J_1 is real and that for J_2 is pure imaginary. As mentioned, the matrix for J^2 is a multiple of the identity.

10. Rotation Matrices; Reduced Rotation Matrices

When we exponentiate the angular momentum operators in accordance with Eq. (2), we obtain the rotation operators. Similarly, when we exponentiate the irreducible matrix representations of the angular momentum operators, we obtain the irreducible representations of the rotation operators. These can be expressed in axis-angle form or in Euler angle form. The symbol D is a standard notation for these matrices, standing for German *Drehung* ("rotation"):

$$D^j_{mm'}(\hat{\mathbf{n}}, \theta) = \langle jm|U(\hat{\mathbf{n}}, \theta)|jm'\rangle, \tag{54}$$

or

$$D^j_{mm'}(\alpha, \beta, \gamma) = \langle jm|U(\alpha, \beta, \gamma)|jm'\rangle. \tag{55}$$

We note in particular that rotations about the z-axis are especially simple in the basis we have chosen, because the matrices are diagonal:

$$D^j_{mm'}(\hat{\mathbf{z}}, \theta) = \langle jm|e^{-i\theta J_z/\hbar}|jm'\rangle = e^{-im\theta}\,\delta_{mm'}. \tag{56}$$

This means that two of the factors in the Euler angle representation of the rotation operators (see Eq. (11.55)) are diagonal, so that

$$\begin{aligned} D^j_{mm'}(\alpha, \beta, \gamma) &= \langle m|e^{-i\alpha J_z/\hbar}\, e^{-i\beta J_y/\hbar}\, e^{-i\gamma J_z/\hbar}|m'\rangle \\ &= \sum_{m_1, m_2} \langle m|e^{-i\alpha J_z/\hbar}|m_1\rangle\langle m_1|e^{-i\beta J_y/\hbar}|m_2\rangle\langle m_2|e^{-i\gamma J_z/\hbar}|m'\rangle \\ &= \sum_{m_1, m_2} e^{-i\alpha m_1}\,\delta_{mm_1}\langle m_1|e^{-i\beta J_y/\hbar}|m_2\rangle e^{-i\gamma m'}\,\delta_{m_2 m'} \\ &= e^{-i\alpha m - i\gamma m'}\, d^j_{mm'}(\beta), \end{aligned} \tag{57}$$

where

$$d^j_{mm'}(\beta) = \langle m|e^{-i\beta J_y/\hbar}|m'\rangle. \tag{58}$$

In Eq. (57), we only sum over m in the resolution of the identity, because we are working on a single irreducible subspace. 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_2 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 irreducible matrix representations of the rotation operators in Euler angle form, it suffices to tabulate only the reduced rotation 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:

$$d^0_{mm'}(\beta) = (\,1\,)\,. \tag{59}$$

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 (which is rotationally invariant). For the case $j = 1/2$, we use the properties of the Pauli matrices to obtain

$$d^{1/2}_{mm'}(\beta) = \cos(\beta/2) - i\sigma_y \sin(\beta/2) = \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix}. \tag{60}$$

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

$$d^1_{mm'}(\beta) = \begin{pmatrix} \frac{1}{2}(1+\cos\beta) & -\sin\beta/\sqrt{2} & \frac{1}{2}(1-\cos\beta) \\ \sin\beta/\sqrt{2} & \cos\beta & -\sin\beta/\sqrt{2} \\ \frac{1}{2}(1-\cos\beta) & \sin\beta/\sqrt{2} & \frac{1}{2}(1+\cos\beta) \end{pmatrix}. \tag{61}$$

This calculation is repeated in Sakurai.

The matrix elements for J_3, given by Eq. (56), 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. In all cases, the D-matrices form a (proper, single-valued) irreducible representations of the group $SU(2)$.

The D-matrices have many properties, of which we mention only two here. 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

$$D^j_{mm'}(U^{-1}) = [D^j(U)^{-1}]_{mm'} = [D^j(U)^\dagger]_{mm'} = D^{j*}_{m'm}(U). \tag{62}$$

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

$$D^j_{mm'}(U) = (-1)^{m'-m}\, D^{j*}_{-m,-m'}(U). \tag{63}$$

11. Rotating Basis Vectors of the Standard Basis

Often in quantum mechanics we need to find the action of a rotation operator on some state. When the state is expanded in terms of the standard basis, the problem is equivalent to rotating a vector $|\gamma jm\rangle$ of the standard basis. That is, we seek an expression for $U|\gamma jm\rangle$, where U is a rotation operator. But since the irreducible subspaces are invariant under rotations, the vector $U|\gamma jm\rangle$ must be expressible as a linear combination of other basis vectors in the same irreducible subspace, that is,

$$U|\gamma jm\rangle = \sum_{m'} |\gamma jm'\rangle\langle\gamma jm'|U|\gamma jm\rangle = \sum_{m'} |\gamma jm\rangle\langle jm'|U|jm\rangle. \tag{64}$$

Notice that in the first sum we have effectively introduced a resolution of the identity, but only in the irreducible subspace. That is, there is no sum over γ or j, because U is diagonal in γ and j, which is the same as saying that the irreducible subspace is invariant under U. In the second sum we have suppressed the γ indices in the matrix elements of U, since these matrix elements do not depend on γ; the resulting matrix element is just a component of a D matrix. Thus, we have

$$\boxed{U|\gamma jm\rangle = \sum_{m'} |\gamma jm'\rangle D^j_{m'm}(U),} \tag{65}$$

which is often useful. Notice the positions of the indices m', m in this formula.

12. Generalized Adjoint Formula

We consider one final topic in the theory of rotation operators, namely, the generalized adjoint formula. This topic is somewhat disjoint from the rest of the material in these notes, since it does not depend on the theory of irreducible representations.

We recall that we derived a version of the adjoint formula for classical rotations in Eq. (11.45), 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

$$\boxed{U\mathbf{J}U^\dagger = \mathsf{R}^{-1}\mathbf{J},} \tag{66}$$

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. (66), we define the operator vector,

$$\mathbf{X}(\theta) = U(\hat{\mathbf{n}}, \theta)\,\mathbf{J}\,U(\hat{\mathbf{n}}, \theta)^\dagger, \tag{67}$$

and we note the initial condition,

$$\mathbf{X}(0) = \mathbf{J}. \tag{68}$$

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

$$\frac{d\mathbf{X}(\theta)}{d\theta} = \frac{dU}{d\theta}\mathbf{J}U^\dagger + U\mathbf{J}\frac{dU^\dagger}{d\theta} = -\frac{i}{\hbar}U[\hat{\mathbf{n}}\cdot\mathbf{J},\mathbf{J}]U^\dagger$$
$$= -\hat{\mathbf{n}}\times(U\mathbf{J}U^\dagger) = -(\hat{\mathbf{n}}\cdot\mathbf{J})\mathbf{X}. \tag{69}$$

The solution is

$$\mathbf{X}(\theta) = \exp\bigl(-\theta\hat{\mathbf{n}}\cdot\mathbf{J}\bigr)\mathbf{X}(0) = \mathsf{R}(\hat{\mathbf{n}},\theta)^{-1}\mathbf{J}, \tag{70}$$

which is equivalent to the adjoint formula (66).

Finally, we can dot both sides of Eq. (66) by $-i\theta\hat{\mathbf{n}}/\hbar$ and exponentiate, to obtain a formula analogous to Eq. (11.48). After placing 0 subscripts on U and R for clarity, the result is

$$U_0 U(\hat{\mathbf{n}},\theta)U_0^\dagger = U(\mathsf{R}_0\hat{\mathbf{n}},\theta), \tag{71}$$

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

$$H = \frac{L_x^2}{2I_x} + \frac{L_y^2}{2I_y} + \frac{L_z^2}{2I_z}, \tag{72}$$

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. (72). The angular velocity $\boldsymbol{\omega}$ of the rigid body is related to the angular momentum $\mathbf{L}$ by

$$\mathbf{L} = \mathsf{I}\boldsymbol{\omega}, \tag{73}$$

where I is the moment of inertia tensor. When Eq. (73) is written in the principal axis frame, it becomes

$$\omega_i = \frac{L_i}{I_i}, \qquad i = x, y, z. \tag{74}$$

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

$$\dot{\mathbf{L}} + \boldsymbol{\omega}\times\mathbf{L} = 0. \tag{75}$$

By using Eq. (74) to eliminate either $\boldsymbol{\omega}$ or $\mathbf{L}$, Eq. (75) 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 (72). The angular momentum $\mathbf{L}$ satisfies the commutation relations,

$$[L_i, L_j] = -i\hbar\, \epsilon_{ijk}\, L_k, \tag{76}$$

with a minus sign relative to the familar commutation relations because the components of $\mathbf{L}$ are (in this problem) measured relative to the body frame. (We will not justifiy 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. (76).) Compute the Heisenberg equations of motion for $\mathbf{L}$, and compare them with the classical Euler equations. You may take Eq. (73) or (74) 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 equataion for L_x, then cycle indices to get the others.) Make your answer look like Eq. (75) 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

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{3}}(1, 1, 1), \tag{77}$$

measured, and the result is $\hbar$. Find the probabilities for the various outcomes in a subsequent measurement of S_z. Do not diagonalize any matrices; use rotation operators.