II. *SU*(2) and *SO*(3)

The first interesting continuous group; that is, the first that is not commutative, has three generators. You have already encountered this group in quantum mechanics, and we now turn our attention to this group.

A. O(3) and SO(3)

The laws of physics, so far as we can tell, are invariant under rotations. A rotation is a linear transformation of the coordinates, $\mathbf{r} \rightarrow R\mathbf{r}$, where *R* is a 3×3 real matrix that preserves distance from the origin. In other words,

$$\mathbf{r}^{2} = \left(R\mathbf{r}\right)^{2} = \left(R\mathbf{r}\right)^{T} \left(R\mathbf{r}\right) = \mathbf{r}^{T} R^{T} R\mathbf{r}$$
(2.1)

for all vectors **r**. The only way this can work for arbitrary **r** is to have

$$R^T R = 1 \tag{2.2}$$

A square matrix satisfying (2.2) is called an *orthogonal* matrix and the set of all such 3×3 matrices is called O(3).

If we take the determinant of (2.2), keeping in mind that $|R^{T}| = |R|$, we see that $|R|^{2} = 1$, and this implies

$$|R| = \pm 1 \tag{2.3}$$

Thus the set of all such rotations naturally breaks into two groups, those with determinant 1, called *proper* rotations, and those with determinant -1, called *improper* rotations. If

we define the special element J = -1, the inversion matrix, then it's pretty easy to show that all improper rotations are of the form R = JR', where R' is a proper rotation. It follows that the group O(3) is really a direct product of the inversion group $\mathcal{J} = \{E, J\}$ and the group of all proper rotations, so that

$$O(3) = SO(3) \times \mathcal{J} \tag{2.4}$$

The group \mathcal{J} has irreps that are trivial to work out, as given in Fig. 2-1, so the problem of describing O(3) is just reduced to describing the connected group SO(3).¹

¹ The same rule applies, $O(n) = SO(n) \times \mathcal{J}$ in any odd number of dimensions. Even dimensions are more complicated, but we will simply disregard this case since we are mostly interested in connected groups anyway.



B. Irreps of SO(3)

The first step might seem logically to determine if SO(3) is compact, since if it does, it will have unitary representations. Fortunately, in this case (and every case we will focus on), this step is unnecessary, because we already *know* that SO(3) has a unitary representation, namely, $\Gamma(R) = R$ is an orthogonal representation of the group, and since any orthogonal matrix is also unitary, this so called *defining* representation is unitary. We'd now like to work out the generators and commutation relations for the group SO(3).

The generators take the form $\Gamma(R(\mathbf{x})) = R(\mathbf{x}) = \exp(-i\mathbf{x}\cdot\mathbf{T})$, but since $R(\mathbf{x})$ is always real, we must have $i\mathbf{x}\cdot\mathbf{T}$ real, which implies the generators T_a must be pure imaginary. They must also be Hermitian, which implies they are anti-symmetric. There are three linearly independent such matrices, which are normally chosen as

$$T_{1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad T_{2} = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad T_{3} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$
(2.5)

These are "orthonormal" in the sense that $tr(T_aT_b) = 2\delta_{ab}$. These three operators satisfy the commutation relations

$$\left[T_a, T_b\right] = i \sum_c \varepsilon_{abc} T_c \tag{2.6}$$

so the structure constants are $f_{abc} = \varepsilon_{abc}$. It is easy to demonstrate that, in fact, (2.5) is the adjoint representation, since $(T_a)_{bc} = -i\varepsilon_{abc}$. Equation (2.6) is reminiscent of the commutation relations for angular momentum operators in quantum mechanics, and this is no coincidence; apart from a factor of \hbar , angular momentum operators *are* the generators of rotations.

Our goal now is to determine all the irreps of the group SO(3), or at least as much as possible, from the structure constants, which is the same as the commutation relations (2.6). We already have one representation of the generators of this group, namely (2.5), but there are many others. We now let T_a stand for an arbitrary representation of these three generators. Now, no two of these generators commute with each other, but we can pick one of the three (normally chosen as T_3) and diagonalize it by performing an appropriate similarity transformation. In the new basis, our generator T_3 will now be diagonal, which we write as

$$T_3 \left| m \right\rangle = m \left| m \right\rangle \tag{2.7}$$

where $|m\rangle$ is a basis vector labeled by its eigenvalue under the now diagonal operator T_3 . We now define three new operators:²

$$\mathbf{\Gamma}^2 = T_1^2 + T_2^2 + T_3^2 \tag{2.8a}$$

$$T_{\pm} = T_1 \pm iT_2 \tag{2.8b}$$

² Georgi defines T_{\pm} to be (2.8b) divided by a factor of root 2.

The operators T_{\pm} are called raising and lowering operators respectively. These operators can be shown to have the following useful properties:

$$\begin{bmatrix} \mathbf{T}^2, T_a \end{bmatrix} = 0, \tag{2.9a}$$

$$\left[T_3, T_{\pm}\right] = \pm T_{\pm} \,, \tag{2.9b}$$

$$\mathbf{T}^{2} = T_{\pm}T_{\pm} + T_{3}^{2} \pm T_{3} \,. \tag{2.9c}$$

$$T_{+}^{\dagger} = T_{\pm} \tag{2.9d}$$

Since \mathbf{T}^2 commutes with all the generators of the group, it will commute with all the elements of the group, and hence by Schur's Lemma, for an irrep it must be a constant matrix. We will name its value $j^2 + j$, for reasons that will become apparent later on, so that

$$\mathbf{T}^{2} |m\rangle = (j^{2} + j) |m\rangle$$
(2.10)

Now, consider the vector $T_{\pm}|m\rangle$. It is easily demonstrated that

$$T_{3}(T_{\pm}|m\rangle) = ([T_{3},T_{\pm}] + T_{\pm}T_{3})|m\rangle = \pm T_{\pm}|m\rangle + T_{\pm}m|m\rangle = (m\pm1)(T_{\pm}|m\rangle)$$
(2.11)

Therefore $T_{\pm} |m\rangle$ is proportional to some new vector which is also an eigenvector of T_3 , $T_{\pm} |m\rangle \propto |m\pm 1\rangle$ We can determine the proportionality constant by noting that

$$\left|T_{\pm}\left|m\right\rangle\right|^{2} = \left\langle m\left|T_{\pm}^{\dagger}T_{\pm}\right|m\right\rangle = \left\langle m\left|T_{\mp}T_{\pm}\right|m\right\rangle = \left\langle m\left|\left(\mathbf{T}^{2}-T_{3}^{2}\mp T_{3}\right)\right|m\right\rangle = j^{2}+j-m^{2}\mp m$$
(2.12)

It therefore follows that

$$T_{\pm} \left| m \right\rangle = \sqrt{j^2 + j - m^2 \mp m} \left| m \pm 1 \right\rangle \tag{2.13}$$

It is obvious from (2.12) that the expression $j^2 + j - m^2 \mp m$ must be non-negative. The problem is that (2.13) implies that we can apparently raise (or lower) *m* indefinitely, and therefore *m* should eventually become so large that $j^2 + j - m^2 \mp m < 0$. How can we avoid this catastrophe? The answer is that there was a flaw in our claim that $T_{\pm} |m\rangle$ is a new eigenvector of T_3 . Eigenvectors are, by definition, and it is possible that $T_{\pm} |m\rangle$ will vanish, hence producing nothing new. For $T_{+} |m\rangle$, we see this occurs when $j^2 + j - m^2 - m = 0$, or m = j, while for $T_{-} |m\rangle$, it occurs when m = -j. We therefore conclude that *m* takes on the values

$$m = -j, -j + 1, \dots, j - 1, j \tag{2.14}$$

Note that this implies that the highest value of m must differ form the lowest one by an integer, so 2j is an integer, implying that j is an integer or half-integer.

One detail that might be of concern is whether there might be two (or more) states with the same eigenvalue m in the same irrep of SO(3). Is it possible that if we start with

a state *m*, and then raise (or lower) it, and then lower (or raise) it, we end up with a different state? The answer is no. It is easy to show with the help of (2.9c), (2.7) and (2.10) that $T_{\mp}T_{\pm}|m\rangle = (j^2 + j - m^2 \mp m)|m\rangle$, so in fact we never get new states by this process.

We are now prepared to write our matrices T_3 and T_{\pm} explicitly. We need to pick an order to list our basis vectors, which is commonly chosen to be $\{|j\rangle, |j-1\rangle, ..., |-j\rangle\}$. In this basis, we can see from (2.7) and (2.13) that

$$\langle m' | T_3 | m \rangle = m \delta_{mm'}$$
 and $\langle m' | T_+ | m \rangle = \sqrt{j^2 + j - m^2 - m} \delta_{m,m'+1}$ (2.15)

Written as a matrix, this would be

$$T_{3}^{(j)} = \begin{pmatrix} j & 0 & \cdots & 0 \\ 0 & j-1 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & -j \end{pmatrix} \text{ and } T_{+}^{(j)} = \begin{pmatrix} 0 & \sqrt{2j} & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ \vdots & \vdots & \ddots & \sqrt{2j} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$
(2.16)

where the non-zero terms in T_+ are always just one off the diagonal. Note that the dimension of this representation is 2j + 1.³ We have added the superscript index $T_a^{(j)}$ because we will label our irreps by the value of *j*. The remaining matrices can then be determined from

$$T_{-}^{(j)} = \left(T_{+}^{(j)}\right)^{\dagger}, \quad T_{x}^{(j)} = \frac{1}{2}\left(T_{+}^{(j)} + T_{-}^{(j)}\right), \quad T_{y}^{(j)} = \frac{1}{2}i\left(T_{-}^{(j)} - T_{+}^{(j)}\right)$$
(2.17)

Once we have all these matrices, the representation is given by

$$\Gamma^{(j)}(R(\mathbf{x})) = \exp(-i\mathbf{x} \cdot \mathbf{T}^{(j)})$$
(2.18)

We will later be particularly interested in the first few of these irreps., for which the explicit form of T_+ is:

$$T_{+}^{(0)} = (0), \quad T_{+}^{(\frac{1}{2})} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad T_{+}^{(1)} = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}, \quad T_{+}^{(\frac{3}{2})} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$
(2.19)

Interestingly, the defining representation given by (2.5) does not seem to correspond to any of these irreps, but as you will demonstrate in a homework problem, in fact it is equivalent to the j = 1 irrep.

³ The irrep (*j*) is sometimes instead labeled by its dimension, 2j + 1. I will try to distinguish these two notations (both of which I actually use) by writing one like this: $(\frac{1}{2})$ and the other like this: 2.

<u>C. SU(2) and SO(3)</u>

Consider the $j=\frac{1}{2}$ irrep worked out in the previous section; that is, the set of all 2×2 matrices of the form (2.19) where the generators are given by

$$T_{a}^{\left(\frac{1}{2}\right)} = \frac{1}{2}\sigma_{a}, \quad \sigma_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(2.20)

The three matrices σ_a are called the Pauli matrices. Furthermore, these matrices are traceless. There is a well-known identity that says the determinant of an exponential of a matrix is the exponential of the trace,

$$|\exp(M)| = \exp[\operatorname{tr}(M)]$$
 (2.21)

This can be proven, for example, by first proving it for εM , where ε is small, and then multiplying it by itself many times to get to M. Applying this to (2.18) using (2.20), we see that

$$\left|\Gamma^{\left(\frac{1}{2}\right)}\left(R(\mathbf{x})\right)\right| = \exp\left(i\mathbf{x}\cdot\operatorname{tr}\left[\mathbf{T}^{\left(\frac{1}{2}\right)}\right]\right) = \exp\left(0\right) = 1$$
(2.22)

Of course, since the **T**'s are Hermitian, the representation will also be unitary. Hence, all of the matrices in this representation are elements of SU(2). Indeed, it isn't hard to see that the Pauli matrices represent a complete set of traceless Hermitian matrices, and therefore this representation includes *all* elements of SU(2). Thus the group we've been studying is not just SO(3), but SU(2) as well.

There is one tricky point here that needs to be addressed. It is not hard to show that $R(\mathbf{x})$ represents a rotation by an angle $|\mathbf{x}|$ about an axis pointing in the direction of **x**. Consider, for the moment, $\mathbf{x} = (0, 0, 2\pi)$, a rotation about the *z*-axis by 2π . It isn't hard to see with the help of (2.16) that

$$\Gamma^{(j)}(R(0,0,2\pi)) = \exp(-i2\pi T_3^{(j)}) = \begin{pmatrix} e^{-2\pi i j} & 0 & \cdots & 0 \\ 0 & e^{2\pi i (1-j)} & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & e^{2\pi i j} \end{pmatrix} = e^{2\pi i j} \mathbf{1} \quad (2.23)$$

But since a rotation by 2π is the same as no rotation, surely $R(2\pi) = E$, and therefore we would want $\Gamma^{(j)}(R(0,0,2\pi)) = 1$, which would imply that *j* must be an integer. Hence the representations we worked out in section B do *not* all work. For the group SO(3), we are restricted to integer *j*, while for the group SU(2), we can use integer or half-integer. The two groups have the same structure constants, and for small elements they multiply exactly the same, but for large elements they are distinct. One way to state this, in the language of the first half of the semester, is that SU(2) is the double group of SO(3).

Now, that I've argued that they are different, let me argue that they are the same. As we already know, in quantum mechanics, when you perform a rotation, the wave functions get mixed in with their partners under some irrep. We know, experimentally, the universe looks exactly the same if we, say, rotate by 2π . If we allowed half-integer values of *j*, then this would not be the case, since rotating some object by 2π would cause its wave function to change sign. But wait! Two wave functions are physically identical if they differ only by a phase, so in fact, an object would *look* identical if we rotated it by 2π , even if the wave function had a half-integer value of *j*. So it really isn't clear that the rotational symmetry of the universe is described by the group SO(3), maybe SU(2) is the proper group to describe it after all.

The issue is beyond the scope of this lecture, but let's just say that in nonrelativistic quantum mechanics, the way it works out is that physical particles are described by wave functions $\Psi(\mathbf{r}, t)$ which often have multiple components. If you rotate this wave function, there will be two effects: the coordinate \mathbf{r} will get rotated, and the components of Ψ will get mixed up with each other. The rotation of the coordinate is always achieved by a representation of SO(3), so that j (or as it is usually called in this context, l) must be an integer, and the corresponding operators T_a are called angular momentum operators L_a .⁴ However, the way the components of Ψ get mixed up together is not restricted, and therefore j (or as it is usually called in this context, s) may be integer or half integer, and the corresponding operators are called spin operators S_a .

The distinction between SO(3) and SU(2) may be important to mathematicians, but I am going to be sloppy and generally not make such a distinction. We will define groups in terms of their structure constants, and hence whether I say SO(3) or SU(2), I am really referring to the group SU(2). Indeed, it is possible to demonstrate that the group Sp(1) is also the same as SU(2), and hence we will write

$$SO(3) = SU(2) = Sp(1)$$
 (2.24)

though strictly speaking, the equality on the left isn't really true.

The same problem actually came up before, but we swept it under the rug. We correctly stated in the previous chapter that SO(2) = U(1), but when discussing

representations, we mentioned that the representations $\Gamma^{(q)}$ should properly be restricted to integer values of q. However, just like with SO(3), when talking about U(1) we really mean some larger group defined by just the structure constants. Such a label is justified, for example, in SO(2), because when we rotate a system by 2π , there is no guarantee that the wave function might not be changed by some phase. Hence we will, in general, allow representations $\Gamma^{(q)}$ of the group U(1) where q takes on any value.

D. Tensor products and other combinations of representations

We have four different methods of taking representations and creating new ones. If we have a particular representation T_a of our generators, we can create a new generator by the transformation $T'_a = S^{-1}T_aS$, and if we pick S unitary, the new generators will also be Hermitian, and will generate a similar unitary representation of SU(2). It is easily

⁴ Actually, $L_a = \hbar T_a^{(l)}$, and the same applies to spin as well, $S_a = \hbar T_a^{(s)}$

demonstrated that the new generators will, however, have exactly the same eigenvalues as the old. Hence, it is easy to tell if two representations are equivalent, just check the eigenvalues of T_a . Indeed, as we will argue below, this is more work than is necessary, we can simply check the eigenvalues of T_3

Now, suppose we took two or more irreps of SU(2) and perform a direct sum, say $\Gamma^{(j_1 \oplus j_2)}$. As we can see from (1.57), the eigenvalues of the generators $T_a^{(j_1 \oplus j_2)}$ representation, which has dimension $2j_1 + 1 + 2j_2 + 1$, will simply be the eigenvalues of $T_a^{(j_1)}$ and $T_a^{(j_2)}$. For example, for T_3 , they will simply be the numbers running from $-j_1$ to $+j_1$, and then from $-j_2$ to $+j_2$. This will normally include a lot of duplicates, which means that $T_3^{(j_1 \oplus j_2)}$ has some degenerate eigenvalues.

This suggests a means for decomposing representations. Suppose we are given a representation Γ made from generators T_a which satisfy the correct commutation relations, and we are given the task of decomposing this representation into irreps. We will do so using only the generator T_3 , using a method called the highest weight decomposition. Find the eigenvalues of T_3 . Call its highest eigenvalue M. Now, if this representation contained any irrep $\Gamma^{(j)}$ with j > M, then it would have T_3 eigenvalues bigger than M, so this must not be the case. If, on the other hand, all the irreps had j < M, then all the T_3 eigenvalues would be smaller than M. The inescapable conclusion is that Γ contains at least one copy of $\Gamma^{(M)}$, where j = M. This implies eigenvalues of T_3 running from -M to +M. Cross these off the list. Look at the remaining eigenvalues. Find the new highest one M'. There must now be a copy of $\Gamma^{(M')}$. Continue until all eigenvalues are used up. You now know the decomposition of Γ into irreps.

Now let's tackle complex conjugation. What is the decomposition of the representation $\Gamma^{(j)*}$? As discussed in the previous chapter, the generators of $\Gamma^{(j)*}$ will be $-T_a^*$, and since T_a is Hermitian and has real eigenvalues, the eigenvalues of $-T_a^*$ will simply be the minuses of the eigenvalues of T_a . Clearly, since the eigenvalues of $T_a^{(j)}$ just run from -j to +j, they have the same eigenvalues, so by the highest weight decomposition algorithm, they will be similar representations, and we conclude

$$\left(j\right)^{*} = \left(j\right) \tag{2.25}$$

However, this does *not* mean that the representation is real, it merely means the complex conjugate is similar to the original representation. Indeed, if you use the explicit forms of the generators (2.16), it is not hard to see that the matrices you get are *not* real (except in the case j = 0). On the other hand, a "real representation" is not necessarily explicitly real, it might be only similar to a real representation. For example, the j = 1 representation is equivalent to the defining representation, (2.5), which *is* explicitly real, so j = 1 really is real. Without proof, I will simply state the ultimate result, which is

$$\Gamma^{(j)} \text{ is } \begin{cases} \text{real if } j \text{ is integer,} \\ \text{pseudo-real if } j \text{ is half-integer.} \end{cases}$$
(2.26)

Last, and most interesting, is the subject of taking tensor products of representations, a subject normally titled "addition of angular momentum" in quantum mechanics. The representation $\Gamma^{(j_1 \otimes j_2)}$ is produced by the generators $T_a^{(j_1 \otimes j_2)}$, which according to (1.58) take the form

$$T_{a}^{(j_{1}\otimes j_{2})} = T_{a}^{(j_{1})} \otimes \mathbf{1} + \mathbf{1} \otimes T_{a}^{(j_{2})}$$
(2.27)

The basis vectors of this representation will look like $|m_1\rangle \otimes |m_2\rangle = |m_1, m_2\rangle$, and when acted on by the generator T_3 have the eigenvalue

$$T_{3}^{(j_{1}\otimes j_{2})}|m_{1},m_{2}\rangle = \left[T_{3}^{(j_{1})}\otimes\mathbf{1} + \mathbf{1}\otimes T_{3}^{(j_{2})}\right]|m_{1},m_{2}\rangle = (m_{1}+m_{2})|m_{1},m_{2}\rangle$$
(2.28)

where m_1 and m_2 range from $-i_1$ to $+j_1$ (for m_1) and from $-j_2$ to $+j_2$ (for m_2). This is a total of $(2j_1+1)(2j_2+1)$ eigenvalues. We now simply decompose it using the highest weight decomposition. The highest weight is just $j_1 + j_2$, and this can be only made one way, so it must include a $(j_1 + j_2)$ irrep. We now remove the eigenvalues from $-j_1 - j_2$ to $j_1 + j_2$. The eigenvalue $j_1 + j_2 - 1$ will generally still be present, because it can be made two ways: $(m_1, m_2) = (j_1 - 1, j_2)$ or $(m_1, m_2) = (j_1, j_2 - 1)$, so we now conclude there is a $(j_1 + j_2 - 1)$ irrep. The process continues until we get down to $(|j_1 - j_2|)$, as illustrated in Fig. 2-2. At this



Figure 2-2: Grapical illustration of the highest weight decomposition of $(j_1 \otimes j_2)$ for $j_1 = 4$ and j_2 = 2. Each dot corresponds to an eigenvalue of T_3 ; the corresponding eigenvalue is $m_1 + m_2$. The highest eigenvalue is the dot in the upper right hand corner, which has m = 6. We therefore cross out all the eigenvalues for the (6) representation (red line), and now the highest weight has m = 5. We cross out the corresponding eigenvalues for m= 5 (blue line), then m = 4 (gold line), m = 3(green line) and finally m = 2 (plum line). At this point we have crossed them all out, and are done.

point we will discover that we have accounted for all the eigenvalues of T_3 , and we are done. Hence our final conclusion is

$$(j_1 \otimes j_2) = (j_1 + j_2) \oplus (j_1 + j_2 - 1) \oplus \cdots \oplus (|j_1 - j_2|)$$

$$(2.29)$$

It is useful to know how to explicitly demonstrate the decomposition given in (2.29). What we have demonstrated, in (2.29), is that the representations are similar; so,

$$\Gamma^{(j_1+j_2)} \oplus \Gamma^{(j_1+j_2-1)} \oplus \dots \oplus \Gamma^{(|j_1-j_2|)} = S^{\dagger} \Gamma^{(j_1 \otimes j_2)} S$$
(2.30)

We'd like to explicitly find the matrix *S* and; that is to say, we'd like to find its matrix elements. What will these matrix elements look like? The rows will bear the same labels

as $\Gamma^{(j_1 \otimes j_2)}$, so m_1 and m_2 . The columns will be labeled by the index j, labeling which of the $\Gamma^{(j)}$ we are dealing with, as well as by m, which component of that matrix (where m runs from j to -j). They will be given by the overlap between the corresponding eigenvectors, or $S_{m_1m_2,jm} = \langle m_1m_2 | jm \rangle$. It would be nice to tabulate, or come up with a formula for, these matrix elements, for every value of j_1 and j_2 . To avoid confusion, we will introduce these labels into the matrix element, writing them as⁵

$$S_{m_{1}m_{2},jm}^{(j_{1}\otimes j_{2})} = \left\langle j_{1}, j_{2}; m_{1}, m_{2} \, \big| \, j, m \right\rangle, \tag{2.31}$$

which are named *Clebsch-Gordan coefficients*, or Clebsch's for short. It is also common to drop much of the punctuation inside the matrix element when this does not cause confusion.

Computing these coefficients by hand is straightforward but tedious. We first note that

$$T_{a} \left| j_{1} j_{2} m_{1} m_{2} \right\rangle = \sum_{m_{1}'} \left| j_{1} j_{2} m_{1}' m_{2} \right\rangle \left(T_{a}^{(j_{1})} \right)_{m_{1}' m_{1}} + \sum_{m_{2}'} \left| j_{1} j_{2} m_{1} m_{2}' \right\rangle \left(T_{a}^{(j_{2})} \right)_{m_{2}' m_{2}}, \qquad (2.32a)$$

$$T_a^{\dagger} \left| jm \right\rangle = \sum_{m'} \left| jm \right\rangle \left(T_a^{(j)\dagger} \right)_{m'm} = \sum_{m'} \left| jm \right\rangle \left(T_a^{(j)} \right)_{mm'}^{*}$$
(2.32b)

These relations are true not only for the three T_a 's for a = 1, 2, and 3, but also for T_{\pm} . Taking the Hermitian conjugate of the latter expression, we find

$$\left\langle jm \middle| T_a = \sum_{m'} \left\langle jm' \middle| \left(T_a^{(j)} \right)_{mm'} \right\rangle$$
(2.33)

We can use these together to find two expressions for $\langle jm | T_a | j_1 j_2 m_1 m_2 \rangle$, namely

$$\sum_{m'} \left(T_a^{(j)} \right)_{mm'} \left\langle jm' \right| j_1 j_2 m_1 m_2 \right\rangle = \sum_{m'_1} \left\langle jm \right| j_1 j_2 m'_1 m_2 \right\rangle \left(T_a^{(j_1)} \right)_{m'_1 m_1} + \sum_{m'_2} \left\langle jm \right| j_1 j_2 m_1 m'_2 \right\rangle \left(T_a^{(j_2)} \right)_{m'_2 m_2}$$
(2.34)

These relationships turn out to be sufficient to find proportionality constants between all non-vanishing matrix elements $\langle jm | j_1 j_2 m_1 m_2 \rangle$ for fixed *j*, j_1 , and j_2 . For further details, consult my quantum mechanics notes, posted <u>here</u>. For each value of *j*, they are therefore determined up to a normalization constant and a phase. The normalization constant can be worked out from the demand that $\langle jj | jj \rangle = 1$. The phase is arbitrary, but it is not hard to see from (2.34) that the Clebsch's can be chosen all real, in which case there is still a sign ambiguity that remains, which must be simply chosen arbitrarily.

From the construction, Clebsch's are meaningful only if j is in the range given by (2.29), and furthermore since the T_3 eigenvalues of the tensor product representation are

⁵ Unfortunately, the notation for Clebsch-Gordan coefficients is far from universal. They are also sometimes labeled as $\langle j_1, m_1; j_2, m_2 | j, m \rangle$ or $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \rangle$. Also, there are sign conventions. If you actually need to use Clebsch's and are looking them up their values or properties from sources, you should make sure your sources are consistent.

just the sums of the eigenvalues of the separate T_3 eigenvalues, we must have $m = m_1 + m_2$. Therefore,

$$\langle j_1 j_2; m_1 m_2 | jm \rangle \neq 0$$
 only if $m = m_1 + m_2$ and $| j_1 - j_2 | \le j \le j_1 + j_2$ (2.35)

They also satisfy some other simple identities:

$$\langle j_2 j_1; m_2 m_1 | jm \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 j_2; m_1 m_2 | jm \rangle$$
 (2.36a)

$$\langle j_1 j_2; -m_1, -m_2 | j, -m \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 j_2; m_1 m_2 | jm \rangle$$
 (2.36b)

$$\langle j_1 0; m0 | jm \rangle = \langle 0 j_2; 0m | jm \rangle = 1$$
 (2.36c)

Fortunately, because of their importance, Clebsch-Gordan coefficients can be looked up in tables; however, to save space, tables normally only include $j_1 \ge j_2 > 0$ and $m \ge 0$; other values can then be obtained using eqs. (2.36). There is also a straightforward formula for them.

$$\langle j_{1}, j_{2}; m_{1}, m_{2} | j, m \rangle = \delta_{m, m_{1} + m_{2}} \sqrt{\frac{(2j+1)(j+j_{1}-j_{2})!(j-j_{1}+j_{2})!(j_{1}+j_{2}-j!)}{(j_{1}+j_{2}+j+1)!}} \times \sum_{k} \frac{(-1)^{k} \sqrt{(j+m)!(j-m)!(j_{1}-m)!(j_{1}+m)!(j_{2}-m)!(j_{2}+m)!}}{k!(j_{1}+j_{2}-j-k)!(j_{1}-m_{1}-k)!(j_{2}+m_{2}-k)!(j-j_{2}+m_{1}+k)!(j-j_{1}-m_{2}+k)!}$$

$$(2.37)$$

The sum is taken over all integers k such that all the factorials in the denominator are non-negative. Fortunately, it is rarely necessary to *use* equation (2.37). I have written a Maple subroutine, available from the web page <u>here</u>, which can compute these for you.

E. Atoms

We'd now like to apply our understanding of group theory to the subject of atomic physics. An atom consists of a nucleus surrounded by one or more electrons. A typical Hamiltonion would look something like

$$H = H_0 + H', \text{ where } H_0 = \sum_i \frac{\mathbf{P}_i^2}{2m} - \sum_i \frac{Zk_e e^2}{|\mathbf{r}_i|} + \sum_{i < j} \frac{k_e e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$
(2.38)

where *H*'contains various effects that are typically quite small, such as external fields, spin-orbit coupling, etc. Actually *solving* (2.38) is quite difficult. All we want to notice is that all the terms included are invariant under rotations of coordinates. Hence if $|\psi(\mathbf{r}_i)\rangle$ is an eigenstate of *H*, so also will be $P_R |\psi(\mathbf{r}_i)\rangle = |\psi(R^T \mathbf{r}_i)\rangle$, where *R* is any element of O(3) and P_R is the rotation operator. In general, eigenstates will be accompanied by partners with the same energy, and when we perform a rotation, the wave functions will mix with corresponding partners according to

$$P_{R}\left|\psi_{m}^{(a)}\right\rangle = \sum_{m'}\left|\psi_{m'}^{(a)}\right\rangle\Gamma_{m'm}^{(a)}\left(R\right)$$
(2.39)

where (*a*) denotes the irreps of the group $O(3) = SO(3) \times \mathcal{J}$, Hence all atomic states can be labeled $|\psi_m^{(l,\pm)}\rangle$, where *l* denotes the rotations under SO(3) and \pm the inversion properties. Because our rotations are only of coordinates, *l* will be restricted to be an integer. These wave functions will have an automatic 2l + 1 degeneracy.

However, electrons are not described exclusively by their spatial wave functions; they also have *spin*, an intrinsic property of the electron. A single electron is described by a wave function $|\psi_{\alpha}(\mathbf{r})\rangle$, such that, under a rotation, the wave function changes to

$$P_{R}\left|\psi_{\alpha}\left(\mathbf{r}\right)\right\rangle = \sum_{\beta}\left|\psi_{\beta}\left(R^{T}\mathbf{r}\right)\right\rangle\Gamma_{\beta\alpha}^{\left(\frac{1}{2}\right)}\left(R\right)$$
(2.40)

Hence when performing rotations, we must rotate both the coordinate and the spin index. Multiple electrons will be described by products of these individual wave functions, and hence will have multiple spin indices. The total spin *s* will then be described by tensor product representations, of the form $(\frac{1}{2}) \otimes (\frac{1}{2}) \otimes \cdots \otimes (\frac{1}{2})$, which, depending on the number of electrons, can be as large as half the number of electrons.⁶

Note that the unperturbed Hamiltonian does not contain spin at all. It follows that we can perform *separately* rotations on the electronic wave functions and the spin indices; both commute with the Hamiltonian. Hence the symmetry of H_0 is

$$O(3) \times SU(2) = \mathcal{J} \times SO(3) \times SU(2)$$
(2.41)

States of this operator can be labeled $|\psi_{m,m'}^{(l,s,\pm)}\rangle$, and will have degeneracy (2l+1)(2s+1).

Of course, there may be various other interactions, as signified in *H*'. In particular, there will be *spin-orbit coupling*, a relativistic correction that causes an interaction between the angular dependence of the wave function and the spin. Nonetheless, since physics is invariant under rotations, we expect the full Hamiltonian to remain invariant if we rotate *both* the coordinates. This means the full symmetry (2.41) will break down to the smaller group $\mathcal{J} \times SU(2)$. The representations (l, s, \pm) will be combined via the rules (2.29) into representations (j, \pm) with only 2j+1 degeneracy, with *j* running from l+s down to |l-s|.

⁶ In fact, the spin can be shown to cancel out in all but the outermost "valence" electrons, so low spin states are more common than high spin states. However, the total spin will always be a half-integer if the number of electrons is odd, and an integer if it is even. One issue that might puzzle you is why the spins "interact" at all; that is, why can't we just rotate every spin separately, making the symmetry group much bigger, with one factor of SU(2) for each electron. Basically, because electrons are fermions, we must keep the wave function anti-symmetric. Rotating the spin indices of one electron while leaving the rest unchanged destroys this anti-symmetry, so we need to rotate them simultaneously.

Other external perturbations may cause further splittings of these states. In the presence of a magnetic field, say in the z-direction, our perturbation H'will no longer be rotationally invariant, except around the z-axis. As a consequence, the 2j+1 states will be further split, leaving no degeneracy at all. In some cases, the splitting due to strong magnetic fields may be more important than the spin-orbit coupling, but this will not normally be the case. A typical situation is illustrated in Fig. 2-3 for the sodium *D*-line.

$$\frac{l=1}{s=1/2} \longrightarrow \begin{cases} \frac{j=3/2}{} \longrightarrow \{ \frac{j=1/2}{} \\ \frac{j=1/2}{} \longrightarrow \{ \frac{j=1/2}{} \end{bmatrix}$$

Figure 2-3: Illustration of energy splittings in the Sodium *D*-line. If you ignore spin orbit coupling, there are 6 degenerate quantum states, all in the l = 1 and $s = \frac{1}{2}$ representation. Spin orbit coupling reduces the symmetry, breaking these six states into the two cases $j = \frac{3}{2}$ and $j = \frac{1}{2}$. In the presence of a magnetic field, the states are split completely.

If you place the atom in a crystal, there will generally be a nearly complete breakdown of spherical symmetry, reducing the group O(3) to some finite subgroup. At this point, we must return to using characters. We need to work out the characters for a finite rotation of an arbitrary element of SO(3). It is not hard to show that all rotations by the same angle are in the same conjugacy class, and hence must have the same

character. It is easiest to work out the character for rotations around the z-axis, for which we find

$$\chi^{(j)} \Big[R(\mathbf{x}) \Big] = \operatorname{tr} \Big[\exp \left(i x T_3^{(j)} \right) \Big] = \operatorname{tr} \Big[\operatorname{diag} \left(e^{i j x}, e^{i (j-1) x}, \dots, e^{-i j x} \right) \Big] = \sum_{m=-j}^{j} e^{i m x},$$
$$\chi^{(j)} \Big[R(\mathbf{x}) \Big] = \frac{\sin \Big[\frac{1}{2} (j+1) x \Big]}{\sin \big(\frac{1}{2} x \big)}, \tag{2.42}$$

A formula Dr. Holzwarth already derived. This formula can then be used to efficiently work out how the representation $\Gamma^{(j)}$ breaks down under some smaller subgroup.

F. Spherical Tensor Operators

Consider the action of a rotation on a quantum state. In a manner very similar to how we defined the matrices T_a for a representation, let us define the operators T_a as

$$\mathcal{T}_{a} \equiv i \frac{\partial}{\partial x_{a}} P_{R(\mathbf{x})} \Big|_{\mathbf{x}=0}$$
(2.43)

In a straightforward manner, we then can show that

$$P_{R(\mathbf{x})} = \exp\left(-i\sum_{a} x_{a} \mathcal{T}_{a}\right)$$
(2.44)

Under a rotation, a set of wave functions $\left|\psi_{m}^{(j)}\right\rangle$ changes to

$$P_{R(\mathbf{x})} \left| \psi_{m}^{(j)} \right\rangle = \sum_{m'} \left| \psi_{m'}^{(j)} \right\rangle \Gamma_{m'm}^{(j)} \left(R(\mathbf{x}) \right),$$

$$\exp\left(-i\sum_{a} x_{a} T_{a} \right) \left| \psi_{m}^{(j)} \right\rangle = \sum_{m'} \left| \psi_{m'}^{(j)} \right\rangle \exp\left(-i\sum_{a} x_{a} T_{a}^{(j)} \right)_{m'm}$$
(2.45)

It therefore follows that

$$\mathcal{T}_{a}\left|\psi_{m}^{(j)}\right\rangle = \sum_{m'}\left|\psi_{m'}^{(j)}\right\rangle \left(\mathcal{T}_{a}^{(j)}\right)_{m'm} \tag{2.46}$$

It will prove useful to discuss how *operators* change when we perform a rotation on them. Suppose we have a state vector $|\psi\rangle$ which is acted on by an operator *O*, so we have $O|\psi\rangle$. When we perform a rotation *R*, we want this state to change to

$$P_{R}(O|\psi\rangle) = (P_{R}OP_{R}^{\dagger})(P_{R}|\psi\rangle)$$
(2.47)

it follows that under rotation, an operator changes to

$$P_{R}OP_{R}^{\dagger} = \exp\left(-i\sum_{a} x_{a}\mathcal{T}_{a}\right)O\exp\left(i\sum_{a} x_{a}\mathcal{T}_{a}\right)$$
(2.48)

Now, suppose we have a set of operators that get mixed into each other when we perform a rotation. For example, suppose we have a set of three vector operators $\mathbf{V} = (V_1, V_2, V_3)$ that rotate when you perform rotations, so that

$$P_R \mathbf{V} P_R^{\dagger} = R^T \mathbf{V}, \quad i.e. \quad P_R V_b P_R^{\dagger} = \sum_c V_c R_{cb} , \qquad (2.49)$$

Some examples are the position, momentum, orbital angular momentum, spin, and total angular momentum operators of quantum mechanics.

Now, write out (2.49) for small rotations, using (2.48) together with $R(\mathbf{x}) = \exp(-i\mathbf{x} \cdot \mathbf{T})$ with the explicit matrices \mathbf{T} given by (2.5), which as discussed there is the same as $(T_a)_{bc} = -i\varepsilon_{abc}$. We therefore have

$$(1-i\sum_{a} x_{a} \mathcal{T}_{a}) \mathbf{V} (1+i\sum_{a} x_{a} \mathcal{T}_{a}) = (1-i\sum_{a} x_{a} \mathcal{T}_{a})^{T} \mathbf{V},$$

$$\mathbf{V} - i\sum_{a} x_{a} (\mathcal{T}_{a} \mathbf{V} - \mathbf{V} \mathcal{T}_{a}) = \mathbf{V} - i\sum_{a} x_{a} \mathcal{T}_{a}^{T} \mathbf{V},$$

$$[\mathcal{T}_{a}, \mathbf{V}] = \mathcal{T}_{a}^{T} \mathbf{V},$$

$$[\mathcal{T}_{a}, V_{b}] = (\mathcal{T}_{a}^{T} \mathbf{V})_{b} = \sum_{c} V_{c} (\mathcal{T}_{a})_{cb} = -i\sum_{c} \varepsilon_{acb} V_{c} = i\sum_{c} \varepsilon_{abc} V_{c}$$

$$(2.50)$$

Now, let's define three new operators $V_m^{(1)}$ for m = +1, 0, -1:

$$V_0^{(1)} = V_3, \quad V_{\pm 1}^{(1)} = \frac{1}{\sqrt{2}} \left(\mp V_1 - iV_2 \right)$$
 (2.51)

Then it can be shown by simple computation that

$$\left[\mathcal{T}_{a}, V_{m}^{(1)}\right] = \sum_{m'} V_{m'}^{(1)} \left(\mathcal{T}_{a}^{(1)}\right)_{m'm}$$
(2.52)

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As we will demonstrate shortly, we can use this fact to help us compute matrix elements of the type $\langle n'j'm'|V_a^{(1)}|njm\rangle$.

We want to generalize this concept. Let us define *spherical tensor* operators $O_m^{(k)}$, where *m* runs from *k* to -k to be a set of operators that have the following commutation relations with our rotation generators \mathcal{T}_a :

$$\left[\mathcal{T}_{a}, O_{m}^{(k)}\right] = \sum_{m'} O_{m'}^{(k)} \left(\mathcal{T}_{a}^{(k)}\right)_{m'm}$$
(2.53)

The number k is called the *rank* of the spherical tensor. A scalar operator, for example, is an operator that commutes with \mathcal{T}_a , and corresponds to k = 0, and the vector operators $V_q^{(1)}$ are simply k = 1. We can build up higher tensors out of simpler ones, such as vectors. For example, if **V** and **W** are vector operators, it isn't hard to show that by multiplying them in all nine possible combinations, we can produce tensor operators of rank k = 0, 1, or 2. The rank 0 (scalar) is just produced by the dot product, $\mathbf{V} \cdot \mathbf{W}$, the rank 0 (vector) is just the cross-product, and the rank 2 part works out to correspond to the traceless symmetric tensor product. For more details, see my quantum notes <u>here</u>.

We have discussed how operators transform under rotation, but it is also helpful to discuss how they behave under parity. For the rotation R = J, inversion, we can classify operators based on how they behave, as one of two cases $P_J O P_J^{\dagger} = \pm O$. It isn't hard to show that P_J commutes with \mathcal{T}_a , and therefore all of the components of a spherical tensor $O_m^{(k)}$ will have the same type of parity, so we can classify them as $O_m^{(k,\pm)}$. Hence operators can be subcategorized based on parity. For example, position and momentum are each $O_m^{(1-)}$ operators, while orbital angular momentum, spin, and total angular momentum are each $O_m^{(1+)}$ operators.

G. The Wigner-Eckart Theorem

Our goal is to find all matrix elements of the form

$$\langle n'j'm' | O_q^{(k)} | njm \rangle,$$
 (2.54)

Consider the combination $O_q^{(k)} | njm \rangle$. Let one of our three operators \mathcal{T}_a act on it. The result is

$$\mathcal{T}_{a}O_{q}^{(k)}|njm\rangle = \left[\mathcal{T}_{a},O_{q}^{(k)}\right]|njm\rangle + O_{q}^{(k)}\mathcal{T}_{a}|njm\rangle$$

$$= \sum_{q'}O_{q'}^{(k)}\left(T_{a}^{(k)}\right)_{q'q}|njm\rangle + O_{q}^{(k)}\sum_{m''}|njm''\rangle \left(T_{a}^{(j)}\right)_{m''m}$$
(2.55)

Also, consider

$$\mathcal{T}_{a}^{\dagger} | n'j'm' \rangle = \sum_{m''} | n'j'm'' \rangle \left(T_{a}^{(j')\dagger} \right)_{m''m'} = \sum_{m''} | n'j'm'' \rangle \left(T_{a}^{(j')} \right)_{m'm''}^{*}$$
(2.56)

Taking the Hermitian conjugate of (2.56) and combining it with (2.55) then gives two ways to write the expression $\langle n'j'm' | \mathcal{T}_a O_q^{(k)} | njm \rangle$:

$$\sum_{m'} \left(T_{a}^{(j')} \right)_{m''m'} \left\langle n'j'm'' \left| O_{q}^{(k)} \right| njm \right\rangle = \begin{cases} \sum_{q'} \left\langle n'j'm' \left| O_{q'}^{(k)} \right| njm \right\rangle \left(T_{a}^{(k)} \right)_{q'q} \\ + \sum_{m''} \left\langle n'j'm' \left| O_{q}^{(k)} \right| njm'' \right\rangle \left(T_{a}^{(j)} \right)_{m''m} \end{cases}$$
(2.57)

Stop a moment, and compare (2.57) with (2.34). They are virtually the same equation! In the discussion after (2.34), I argued that (2.34) completely determined the Clebsch-Gordan coefficients, save for a normalization and phase that would depend on *j*. It follows that these matrix elements will be proportional to the Clebsch-Gordan coefficients:

$$\left\langle n'j'm' \left| O_q^{(k)} \right| njm \right\rangle \propto \left\langle j'm' \left| kj;qm \right\rangle.$$
 (2.58)

The proportionality constant can depend on n, j, n', j', and the operator, but they cannot depend on q, m, or m'. For reasons that are for the moment obscure, we also add a factor of $1/\sqrt{2j'+1}$ to the right side of (2.57). The remaining proportionality constant is then given the name $\langle n'j' || O || nj \rangle$, and we have

$$\left\langle n'j'm' \left| O_q^{(k)} \right| njm \right\rangle = \frac{1}{\sqrt{2j'+1}} \left\langle n'j' \left\| O \right\| nj \right\rangle \left\langle kj; qm \right| j'm' \right\rangle,$$
(2.59)

the Wigner-Eckart theorem. The Clebsch-Gordan coefficient seems to have had the bra and ket mysteriously interchanged; this is acceptable since these matrix elements are always chosen real. The nasty "reduced" matrix element $\langle n'j' || O || nj \rangle$ is not something you compute directly; instead, you measure or compute one matrix element on the left side of (2.59), then use the Wigner-Eckart theorem to immediately deduce the value of all the remaining matrix elements. For fixed n', j', n, and j, there is only one $\langle n'j' || O || nj \rangle$, but there are (2j+1)(2j'+1)(2k+1) matrix elements on the left side, all related to each other. They can be non-vanishing only if the Clebsch-Gordan coefficients are nonvanishing, so we must have m+q=m' and $|j-k| \leq j' \leq j+k$, for example.

It is not hard to show using (2.37) that if $O_0^{(k)}$ is a Hermitian operator, then

$$\left\langle n'j' \left\| O \right\| nj \right\rangle = \left\langle nj \left\| O \right\| n'j' \right\rangle^*$$
(2.60)

Hence these reduced matrix elements act a lot like ordinary matrix elements. This was the reason for including the factor of $1/\sqrt{2j'+1}$.

Let's use the Wigner-Eckart theorem to learn what we can about spontaneous emission from atoms. To leading order, these emissions tend to be dominated by the electric dipole approximation, such that the amplitude for decay of an atom from a state $|njm\rangle$ to a state $|n'j'm'\rangle$ is dominated by a term proportional to $\langle n'j'm' | \mathbf{r} | njm \rangle$, where **r** is the position operator. Like any other vector, **r** is a rank one spherical tensor, and

therefore this matrix element will vanish unless $|j-1| \le j' \le j+1$. To second order, the emission is governed primarily by either the electric quadrupole emission (a rank two spherical tensor) or by magnetic dipole emission (another vector).

In addition to rotational symmetry, parity can also be useful in determining which transitions take place. For example, because the position operator \mathbf{r} is a true vector, the initial and final states must have opposite parity.