

Lecture 4

1. THE REPRESENTATIONS OF $o(3)$

The book *Principles of Quantum Mechanics* by R. Shankar has a more detailed discussion of this topic.

Symmetry transformations form a group. Infinitesimal transformations form a Lie algebra. In quantum mechanics, symmetry transformations are represented by unitary matrices: the states of the system change but their length must not. The same symmetry can have quite different consequences depending on how it is represented on the states. We will work out all the unitary representations of the Lie algebra of rotations. They can be broken up into direct sums of certain irreducible representations (indivisible pieces). Each irreducible representation is determined by the largest allowed value of angular momentum along some (say third) direction. The trivial case is when the angular momentum vanishes. The next is when the largest angular momentum is $\frac{\hbar}{2}$, then \hbar , after that $\frac{3\hbar}{2}$ and so on. Each elementary particle of nature falls into one of these irreducible representations.

The representation theory of $so(3)$ forms the template on which that of other Lie algebras is constructed. By now there is a complete understanding of unitary representation of all the compact Lie algebras: i.e., algebras which admit a positive scalar product such as $so(3)$. Modern theoretical physics also raises questions involving infinite dimensional Lie algebras about which very little is known as yet.

1.1. Infinitesimal rotations around the co-ordinate axes satisfy.

$$[S_{12}, S_{23}] = S_{13}, \quad [S_{23}, S_{13}] = S_{12}, \quad [S_{13}, S_{12}] = S_{13}$$

As we saw before, these infinitesimal rotations are 3×3 antisymmetric matrices

$$S_{12} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad S_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad S_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

1.1.1. A finite rotation is an orthogonal matrix of the form $e^{\theta_{12}S_{12} + \theta_{23}S_{23} + \theta_{13}S_{13}}$, the θ 's being the angles of rotation in each co-ordinate plane.

1.1.2. Any triplet of matrices (K_{12}, K_{23}, K_{13}) satisfying these commutation relations is a representation of the rotation algebra.

1.1.3. *The representation is unitary if the K 's are anti-hermitean.* In this case the exponentials $e^{\theta_{12}K_{12}+\theta_{23}K_{23}+\theta_{13}K_{13}}$ are a unitary representation of the group of rotation. It is always much easier to work with infinitesimal transformations instead of finite ones. Whenever possible we will work with the Lie algebra rather than the group. A representation of a Lie algebra that leads to a unitary representation for the group is called unitary representation.

Physicists like to work with hermitean rather than anti-hermitean matrices: they represent observables in quantum mechanics. This is easy to arrange, as a hermitean matrix is simply i times an anti-hermitean matrix. The corresponding observables are the components of angular momentum in the case of rotations. Thus, putting $iK_{12} = J_1$ etc. we get

1.1.4. *The components of angular momentum are hermitean matrices satisfying the commutation relations.*

$$[J_1, J_2] = iJ_3, \quad [J_2, J_3] = iJ_1, \quad [J_3, J_1] = iJ_2.$$

We will find all possible solutions to these conditions: all possible unitary representations of the rotation Lie algebra. Then we will know all possible ways a system can possess angular momentum. But a change of basis does not really give us a new set of angular momentum matrices.

1.1.5. *Two representations are equivalent if there is a unitary matrix U such that*

$$UJ_1U^\dagger = \tilde{J}_1, \quad UJ_2U^\dagger = \tilde{J}_2, \quad UJ_3U^\dagger = \tilde{J}_3$$

. We are interested in finding all possible representations up to this equivalence. Now, given two representations \mathbf{M} and \mathbf{N} , we can always find a third by taking the direct sum of matrices

$$\mathbf{J} = \begin{pmatrix} \mathbf{M} & 0 \\ 0 & \mathbf{N} \end{pmatrix}$$

or

$$\mathbf{J} = \mathbf{M} \oplus \mathbf{N}$$

The resulting representation is said to be reducible, as there is an *invariant subspace* (say states of the form $\begin{pmatrix} \psi \\ 0 \end{pmatrix}$) that by itself is a representation of the angular momentum algebra.

1.1.6. *An irreducible representation is one that has no smaller representation contained in it.*

1.1.7. *Any unitary representation of the angular momentum algebra is a direct sum of irreducible representations.* Suppose a representation had an invariant subspace. Then its orthogonal complement would also be invariant. We can write the representation as a direct sum of these two subrepresentations. Then we repeat the argument on each of these spaces, until we get a situation with no invariant subspaces.

The projection operator to an invariant subspace commutes with \mathbf{J} .

$$\left[\mathbf{J}, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right] = 0.$$

This leads to an important criterion:

1.1.8. *Schur's Lemma: A representation is irreducible if and only if there is no operator that commutes with all the components of angular momentum (except a multiple of the identity).* In summary, it is enough to find all the irreducible representations (up to equivalence) of the angular momentum algebra. Any representation is equivalent to a sum of such irreducible representations. Remember that more than one copy of a given irreducible representation can appear in this sum.

1.2. **The Irreducible Representations of $o(3)$.** The operator

$$J^2 = J_1^2 + J_2^2 + J_3^2$$

has the classical meaning of the square of the magnitude of angular momentum. Being a scalar, it must be unchanged by rotations. In quantum mechanics it is a matrix, so it is hard to think of it as in general as the length of any vector. Still, it is true that

1.2.1.

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

Proof. Let us prove it for one component: the argument is the same for the others.

$$\begin{aligned} [J_1^2 + J_2^2 + J_3^2, J_3] &= J_1[J_1, J_3] + [J_1, J_3]J_1 + J_2[J_2, J_3] + [J_2, J_3]J_2 \\ &= -i(J_1J_2 + J_2J_1) + i(J_2J_1 + J_1J_2) = 0. \end{aligned}$$

□

Schur's Lemma this tells us that

1.2.2. In an irreducible representation, J^2 is a multiple of the identity. Being a hermitean matrix, there is a basis in which J_3 diagonal. We cannot diagonalize J_1 or J_2 in the same basis since they do not commute with J_3 . Let us denote the eigenvalues of J_3 by m . (Not to be confused with mass.)

$$J_3|m\rangle = m|m\rangle$$

We can choose these states to be orthonormal:

$$\langle m|m'\rangle = \delta_{mm'}$$

What effect do J_1 and J_2 have on these eigenstates? It is useful to form combinations

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

Because J_1, J_2 are hermitean, these two combinations are conjugates of each other:

$$J_{\pm} = J_{\mp}^{\dagger}.$$

The commutation relations of angular momentum can be written as

$$[J_3, J_{\pm}] = J_{\pm}$$

$$[J_+, J_-] = 2J_3$$

Moreover

$$J_-J_+ = J_1^2 + J_2^2 + i[J_1, J_2] = J_1^2 + J_2^2 - J_3$$

so that

$$(1.1) \quad J^2 = J_3(J_3 + 1) + J_-J_+.$$

These identities are about to become very useful.

1.2.3.

$$J_3J_+|m\rangle = (m+1)J_+|m\rangle.$$

Proof. Just calculate:

$$J_3J_+|m\rangle = J_+J_3|m\rangle + [J_3, J_+]|m\rangle = mJ_+|m\rangle + J_+|m\rangle.$$

□

This means that J_+ is a “raising operator”: it increases the eigenvalue of J_3 by one step, as long as $J_+|m\rangle \neq 0$. But we cannot increase the value of m forever: J^2 is equal to J_3^2 plus a positive operator:

$$J_3^2 \leq J^2.$$

Since J^2 is a multiple of the identity in an irreducible representation, J_3^2 is bounded by the value of J^2 . Repeated application of J_+ must eventually give zero, when it hits the state with the largest eigenvalue of J_3 . Let us call this largest eigenvalue j .

In olden days, eigenvalues of Lie algebra generators were called “weights”. So

1.2.4. A state satisfying $J_3|j\rangle = j|j\rangle$, $J_+|j\rangle = 0$ is called a “highest weight state”. Using (1.1) we see that

$$J^2|j\rangle = j(j+1)|j\rangle.$$

But, J^2 is a multiple of the identity:

$$J^2 = j(j+1).$$

In exactly the same way we can see that J_- is a lowering operator

$$J_3 J_- |m\rangle = (m-1) J_- |m\rangle$$

The lowest eigenvalue j' of J_3 occurs for a state annihilated by J_- ; i.e., a lowest weight state satisfies

$$J_- |j'\rangle = 0.$$

Using the identity

$$J^2 = J_3(J_3 - 1) + J_+ J_-$$

can show that

$$J^2 |j'\rangle = j'(j'-1) |j'\rangle.$$

Thus

$$j(j+1) = j'(j'-1)$$

or

$$j' = -j.$$

We just solved the eigenvalue problem for J_3 :

$$J_3|m\rangle = m|m\rangle, \quad \text{for } m = j, j-1, \dots, -j.$$

There are $2j+1$ such states, which form a basis in the Hilbert space of an irreducible representation. If the space is odd dimensional j is an integer. Other wise it is a half-integer. No other values are allowed.

1.2.5. *An irreducible representation of the angular momentum algebra is determined by a number j which can take values $0, \frac{1}{2}, 1, \frac{3}{2}, \dots$. The dimension of the representation is $2j+1$. An orthonormal basis is given by the eigenstates of J_3 .*

$$J_3|m\rangle = m|m\rangle, \quad \text{for } m = j, j-1, \dots, -j.$$

To complete the story we must determine the matrix elements of J_1, J_2 (or equivalently J_{\pm}) in this basis. Suppose

$$J_+|m\rangle = c_m|m+1\rangle.$$

From hermiticity

$$c_m = \langle m+1|J_+|m\rangle = \langle m|J_-|m+1\rangle^*$$

In other words

$$J_-|m+1\rangle = c_m^*|m\rangle$$

or

$$J_-|m\rangle = c_{m-1}^*|m-1\rangle.$$

Now

$$J^2|m\rangle = j(j+1)|m\rangle$$

since it is a multiple of the identity. Using (1.1)

$$j(j+1) = m(m+1) + |c_m|^2.$$

Or

$$|c_m| = \sqrt{j(j+1) - m(m+1)}.$$

It is possible to choose c_m to be real: the phase can be absorbed into the definition of the basis vectors $|m\rangle$. We get

Theorem 1. *There is an irreducible representation of the Lie algebra $o(3)$ for each value of the dimension $n = 0, 1, \dots$. The value of J^2 is $j(j+1)$ where $2j+1 = n$. There is an orthonormal basis $|m\rangle$, for $m = j, j-1, \dots, -j$ such that*

$$J_3|m\rangle = m|m\rangle,$$

$$J_+|m\rangle = \sqrt{j(j+1) - m(m+1)}|m+1\rangle, \quad J_-|m\rangle = \sqrt{j(j+1) - m(m-1)}|m-1\rangle$$

Let us work out special cases.

Corollary. *The case $j = 0$ is the trivial representation with zero angular momentum.*

Corollary. *When $j = \frac{1}{2}$ we get a representation in terms of Pauli matrices.*

$$J_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2} \sigma_3, \quad J_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2} \sigma_1, \quad J_2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2} \sigma_2.$$

Corollary. *When $j = 1$ we get*

$$J_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad J_- = \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \quad J_+ = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$$

This is in fact the representation in terms of rotation matrices we started with: the defining representation. It looks different only because we are using a different basis, which diagonalizes iS_{12} . Find a change of basis such that

$$J_3 = U(iS_{12})U^\dagger$$

and verify that $J_1 = U(iS_{23})U^\dagger$ and $J_2 = U(iS_{13})U^\dagger$.

Exercise. Find the matrices representing angular momentum for $j = \frac{3}{2}$ and for $j = 2$.

2. ORBITAL ANGULAR MOMENTUM

There is a representation of $o(3)$ on functions of position:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \mathbf{p} = -i\nabla.$$

This represents orbital angular momentum. It is clear that the distance r commutes with it. The components of \mathbf{L} depend only on the angular variables. For example,

$$L_3 = -i \frac{\partial}{\partial \phi}$$

The simultaneous eigenfunctions of L^2, L_3 are the spherical harmonics $Y_{lm}(\theta, \phi)$. More on this in Shankar's book.

3. SPIN

In quantum mechanics it is possible for a particle to have angular momentum even when its momentum is zero. The total angular momentum is the sum of orbital angular momentum and an intrinsic angular momentum, also called spin.

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

$$[L_i, S_j] = 0$$

$$[S_1, S_2] = iS_3$$

etc. Because \mathbf{S} is by itself a representation of the angular momentum algebra,

$$S^2 = s(s+1)$$

in an irreducible representation of spin.

The simplest case is when $s = \frac{1}{2}$:

$$S_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The electron, proton, neutron are all examples of this.

4. SPIN-ORBIT COUPLING

An electron orbiting the nucleus of a hydrogen atom produces a small magnetic field. Also, it has an intrinsic magnetic moment that points along its spin. Thus there is a small correction to the energy of an electron due to the coupling of its magnetic moment to its own magnetic field.

$$H_1 = \mu \boldsymbol{\sigma} \cdot \mathbf{L}$$

which must be added to the usual hamiltonian H_0 of the atom. Since

$$[H_0, \mathbf{L}] = 0 = [H_0, \boldsymbol{\sigma}]$$

the correction term can be diagonalized separately and added to the eigenvalues of H_0 . Now

$$\boldsymbol{\sigma} \cdot \mathbf{L} = \frac{1}{2} (\boldsymbol{\sigma} + \mathbf{L})^2 - \frac{\boldsymbol{\sigma}^2}{2} - \frac{L^2}{2} = \frac{j(j+1) - l(l+1)}{2} - \frac{3}{4}$$

Although \mathbf{L} is not conserved any more, L^2 still is conserved. Thus the energies are

$$E_n + \mu \left[\frac{j(j+1) - l(l+1)}{2} - \frac{3}{4} \right]$$

where E_n are the usual Rydberg energies which only depend on the principal quantum number. The constant μ is proportional to the fine structure constant $\frac{e^2}{\hbar c}$.

5. LIE ALGEBRAS OF COMPACT SIMPLE TYPE

It is crucial that there is a positive operator $L^2 = L_1^2 + L_2^2 + L_3^2$ which commutes with all the L_i . Algebras of this type are much easier to understand.

5.1. A Lie algebra in which there is a positive quadratic form that commutes with all the basis elements is said to be of compact type.

5.2. A compact Lie algebra L is simple if it cannot be written as the sum of two other non-trivial Lie algebras. Simple does not mean easy to understand here: it means instead that the Lie algebra cannot be broken up into smaller pieces.

5.3. Any compact Lie algebra is a sum of simple Lie algebras. We won't prove this fact here.

5.4. Cartan found all the compact simple Lie algebras. $su(n), o(n)$ form two infinite series of such Lie algebras. There is one more infinite series (called D_n) that are related to matrices with quaternionic entries. We won't say much about the last sequence in this course. But they do have various uses in physics. We will develop the theory of representations of unitary and orthogonal algebras later.

5.4.1. The Exceptionals. In addition there are some exceptional Lie algebras that do not fall into such an infinite sequence of matrices (with names like G_2, F_4, E_6, E_7, E_8). Many mathematicians and physicists love them precisely because they do not fall into a pattern: every so often someone has a theory unifying everything in terms of one of these exceptional Lie algebras. None of them have worked so far.

5.5. Rank of a Lie Algebra. The maximum number of basis elements that commute with each other is called the rank. $o(3)$ is rank one, as only J_3 qualifies. For $su(3)$ the rank is 2; more generally for $su(n)$ the rank is $n - 1$.

The rank determines the number of labels such as m (the magnetic quantum number) that are needed to label a basis in an irreducible representation.

5.6. Casimir Operators. In a compact Lie algebra there is always one operator like L^2 which commutes with all generators. But there may be others that commute which are cubic or higher order. Such polynomials in the basis elements that commute with all of them are called Casimir operators. Their eigenvalues are constant within an irreducible representation.

5.7. The representation theory of non-compact Lie algebras is much deeper. The works of Harish-Chandra and later Kirillov have almost completely settled this subject. But there are still occasional surprises. This theory is beyond the scope of this course.