

# Rotations in Quantum Mechanics

We have seen that physical transformations are represented in quantum mechanics by unitary operators acting on the Hilbert space. In this section, we'll think about the specific case of the three-dimensional rotations. Our setup is that we have a Hilbert space of some dimension, and this describes states of a physical system that has 3D rotations as a possible physical transformation; that is, given any state of the system, there should be some other state that is a rotated version of the original state.

For every possible rotation  $R$ , there should be some corresponding unitary operator  $\mathcal{T}(R)$  acting on our Hilbert space. Just like the Hamiltonian is different for different quantum systems, the rotation operators  $\mathcal{T}(R)$  will generally be different in different systems. However, the map from rotations to unitary operators can't just be anything; if  $R_1$  and  $R_2$  are two different rotations, and  $R = R_2 \circ R_1$  is the rotation we get by performing first  $R_1$  and then  $R_2$ , we must have that

$$\mathcal{T}(R) = \mathcal{T}(R_2)\mathcal{T}(R_1) . \tag{1}$$

This is just saying that if we perform the rotation  $R$  on the quantum system “all at once,” it should give the same result as performing the rotation in two steps, first rotation by  $R_1$  and then by  $R_2$ .

Since any rotation can be built up from infinitesimal rotations, we can use the relation (1) to find the unitary corresponding to any rotation as long as we know the unitary operators corresponding to the independent infinitesimal rotations. Let's think about any one of these infinitesimal transformations, for example the “right handed” rotation about axis  $\hat{n}$ . We know that this must take the form

$$\mathcal{T}(\epsilon) = 1 - \frac{i}{\hbar}\epsilon J_n + \dots . \tag{2}$$

Here, the operator  $J_n$  is Hermitian, and we know that the associated physical observable will be conserved if rotations are a symmetry. This quantity is what we normally call *angular momentum* about the axis  $\hat{n}$ , and we have included the constant  $\hbar$  so that the operator  $J$  will agree with the usual definition of angular momentum.

So once we understand what the angular momentum operators  $J_n$  are for our system, we will know how any rotation acts. We can actually simplify things further: it's not too hard to see that we can make any infinitesimal rotation by combining infinitesimal rotations about the  $x$ ,  $y$ , and  $z$  axes.<sup>1</sup> Specifically, we can write:

$$J_n = n_x J_x + n_y J_y + n_z J_z \tag{3}$$

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<sup>1</sup>To visualize this, pick up an object and imagine some axis through it. Call this the  $z$  axis. After any infinitesimal rotation, this will now be pointing in a slightly different direction, and the object might have rotated a bit about this axis. We can reproduce this combination first by doing a  $z$  rotation to reproduce the last effect, and then by doing a combination of little rotations around the  $x$  and  $y$  axes to make the axis point in the needed direction.

So we really only need to say what the operators  $J_x, J_y$ , and  $J_z$  are, and then we will know how any rotation acts.

There is one final piece of information that we can use. If you pick up an object, then rotate it a little about  $x$  axis, and then a little about the  $y$  axis, the result is not the same when you do those operations in the opposite order.<sup>2</sup> We can say that these operations don't commute with each other. This should be reflected in the fact that the operators  $J_x$  and  $J_y$  also don't commute with each other (otherwise, we would be able to perform those operations on the quantum system in any order and get the same result). In fact, there is a definite answer to what rotation we get when we rotate by angle  $\epsilon_1$  about the  $x$  axis, then a rotation by angle  $\epsilon_2$  about the  $y$  axis, then reverse these, but in the opposite order; in the limit where  $\epsilon_1$  and  $\epsilon_2$  are very small, it's exactly a rotation by angle  $-\epsilon_1\epsilon_2$  about the  $z$  axis.<sup>3</sup> If we do these operations on our quantum system, the relation (1) then implies that

$$\left(1 + \frac{i}{\hbar}\epsilon_2 J_y\right)\left(1 + \frac{i}{\hbar}\epsilon_1 J_x\right)\left(1 - \frac{i}{\hbar}\epsilon_2 J_y\right)\left(1 - \frac{i}{\hbar}\epsilon_1 J_x\right) = \left(1 + \frac{i}{\hbar}\epsilon_1\epsilon_2 J_z + \dots\right) \quad (4)$$

where the dots indicate terms with higher powers of  $\epsilon_1$  or  $\epsilon_2$ . Keeping only the terms in this equation proportional to  $\epsilon_1\epsilon_2$ , we get  $[J_x, J_y] = i\hbar J_z$ . We could repeat this argument with  $y$  and  $z$  rotations or with  $x$  and  $z$  rotations. The final result is that if  $J_i$  are the Hermitian operators representing the rotation generators (i.e. the angular momentum operators) for any quantum system, they must obey the commutation relations

$$\begin{aligned} [J_x, J_y] &= i\hbar J_z \\ [J_y, J_z] &= i\hbar J_x \\ [J_z, J_x] &= i\hbar J_y \end{aligned} \quad (5)$$

in order for (1) to hold, i.e. in order that the rotation operations in quantum mechanics combine in the correct way. If we choose some basis for our Hilbert space, then  $J_x, J_y$ , and  $J_z$  will be represented by some matrices in this basis, and these matrices must also obey the commutation relations (5).

Understanding the possible operators/matrices that satisfy the commutation relations (5) is described mathematically as the problem of finding the possible *representations of the rotation group*.

### Example: particle in three dimensions

The form of the angular momentum operators differs depending on the quantum system we are talking about. For a particle moving in three-dimensional space, the familiar classical definition of angular momentum is  $\vec{L} = \vec{r} \times \vec{p}$ . Writing this out in components, we would

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<sup>2</sup>This is easiest to see if you actually rotate by a larger amount, like 90 degrees.

<sup>3</sup>This is just a basic fact about rotations; it doesn't have anything to do with quantum mechanics. To check it, we just need to carefully rotate an object (or do a calculation involving rotation matrices).

have

$$L_x = yp_z - zp_y \quad L_y = zp_x - xp_z \quad L_z = xp_y - yp_x . \quad (6)$$

In the quantum system, it is natural to guess that the angular momentum operators would be just the same, with positions and momenta replaced by the corresponding operators:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x . \quad (7)$$

Using the basic commutation relations  $[x_i, p_j] = i\hbar\delta_{ij}$  between positions and momenta, we can check that these quantum angular momentum operators satisfy the necessary relations (5) and so are a valid choice for the operators  $J_i$ . In this example, the angular momentum operators give the ordinary angular momenta of the particle about the origin. The fact that the various angular momentum operators don't commute means that a particle can't have a definite angular momentum about more than one axis.

### Example: spin half particle

The previous example was for an infinite dimensional Hilbert space. But there are also much simpler quantum systems that we can rotate. You are probably familiar with the simplest case, where the Hilbert space is two-dimensional and the angular momentum operators take the form  $J_i = S_i$  where the matrices representing  $S_i$  are the *Pauli matrices*  $\sigma_i$ , given by

$$\sigma_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \quad (8)$$

This quantum system describes the “internal” states of certain types of particles that we call spin 1/2. What this means is that even after we specify the position (i.e. the spatial wavefunction) of such a particle, we need to specify more information to say what state the particle is in. For a spin 1/2 particle, there are just two independent states that the particle can be in, with all other states obtained as linear combinations of these. We'll understand how to derive the Pauli matrices below.

### Example: combining representation

Any time we have two quantum systems, each one with some angular momentum operators, we can combine these into a single quantum system describing both parts. For example, when we think about an electron in a hydrogen atom, we need to describe both the electron's position and its spin state. The full quantum system is described by basis elements that are combinations of basis elements for the two systems. For example, we can use  $|\vec{x}, \uparrow\rangle$ ,  $|\vec{x}, \downarrow\rangle$  describing the electron with spin up at position  $\vec{x}$  and an electron with spin down at position  $\vec{x}$ . For this system, the full angular momentum operators will just be a sum of the operators for the two parts

$$J_i = L_i + S_i . \quad (9)$$

This says that the angular momentum of the full system is equal to the angular momentum from the electron's orbital motion plus the angular momentum from the electron's spin. Alternatively, it says that a rotation on the system affects both the electron's spin state and its position state.

We'll also see examples where we want to keep track of the spin state of two different particles. For example, for an electron in the  $1s$  state of hydrogen, there is no orbital angular momentum (the wavefunction is rotationally symmetric), but the total angular momentum of the system is a combination of the angular momentum from the electron spin and the proton spin. The spin states of these two particles are described by a four-dimensional quantum system with basis elements  $|\uparrow, \uparrow\rangle$ ,  $|\downarrow, \uparrow\rangle$ ,  $|\downarrow, \uparrow\rangle$ , and  $|\downarrow, \uparrow\rangle$ , and angular momentum operators

$$J_i = S_i^{proton} + S_i^{electron} . \quad (10)$$

In these examples, the angular momentum operators for the different parts of the system commute with each other, since each part has its own independent angular momentum.

## 1 Finding the possible rotation matrices

There is a well-defined mathematical procedure to determine the possible forms of the angular momentum/rotation operators similar to how we found the states and energies of the harmonic oscillator. This is described in Griffiths section 4.3.1, so I won't go over it in detail here.

A key point is that the operator

$$J^2 = J_x J_x + J_y J_y + J_z J_z \quad (11)$$

commutes with all the rotation operators. This implies that if we have some eigenstate of  $J^2$ , we can act with any combination of  $J_i$  operators, and the result will still be an eigenstate of  $J^2$  with the same eigenvalue.

For any eigenstate of  $J^2$ , we can consider all the states that can be obtained from it by acting with the rotation and/or angular momentum operators. This forms some subspace of the whole system, and we can show that the size of the subspace is completely determined by the value of  $J^2$ . The possible eigenvalues of  $J^2$  are  $\hbar^2 j(j+1)$  where  $j$  is a nonnegative integer or half-integer, and the number of states in the subspace with this  $J^2$  eigenvalue is  $2j+1$ . We can choose a basis for this subspace where the basis elements are eigenvectors of  $J_z$  and show that the eigenvalues must be  $\hbar m$  where  $m = -j, -j+1, \dots, j-1, j$ .

In cases where the whole system has a rotation symmetry (i.e., the  $J_i$  matrices all commute with the Hamiltonian), then  $J^2$  also commutes with the Hamiltonian, so we can find a basis of states which are energy eigenstates and also eigenstates of  $J^2$  and  $J_z$ .

## 2 What you really need to know

For any quantum system that admits 3D rotations, there will be some set of angular momentum operators  $J_i$  satisfying the basic commutation relations (5). From these, we can build the infinitesimal rotation operators (2) or the general rotation operator

$$e^{-\frac{i}{\hbar}\theta n_i J_i} \quad (12)$$

which is a right-handed rotation by angle  $\theta$  about the axis described by unit vector  $n^i$ .

The full set of states of the Hilbert space splits up into subspaces, where the states in each subspace all have the same total angular momentum (i.e.  $J^2$  eigenvalue) and can all be obtained from each other by acting with  $J_i$  operators. We can choose a basis for such a subspace, where the basis elements are eigenstates of both  $J^2$  and  $J_z$ . These are labeled as  $|jm\rangle$  where  $j$  is a nonnegative integer or half-integer, and  $m$  runs over the  $2j + 1$  possible values  $(-j, -j + 1, \dots, j - 1, j)$ . For the state  $|jm\rangle$ , we have

$$\begin{aligned} J_z |jm\rangle &= \hbar m |jm\rangle \\ J^2 |jm\rangle &= \hbar^2 j(j+1) |jm\rangle \\ &\dots \end{aligned} \quad (13)$$

We can say how the other operators  $J_x$  and  $J_y$  act by defining

$$J_+ = J_x + iJ_y \quad J_- = J_x - iJ_y \quad (14)$$

Then these act a bit like creation and annihilation operators for the harmonic oscillator:

$$\begin{aligned} J_+ |jm\rangle &= \hbar \sqrt{j(j+1) - m(m+1)} |jm+1\rangle \\ J_- |jm\rangle &= \hbar \sqrt{j(j+1) - m(m-1)} |jm-1\rangle \\ &\dots \end{aligned} \quad (15)$$

Here, we note that  $J_+ |jj\rangle = J_- |j-j\rangle = 0$  so we only have  $2j + 1$  states in each group.

### Addition of angular momentum

Finally, we sometimes need to know how angular momenta combine with each other in a multipart system. Say we have a system with two parts (e.g. an electron spin and a proton spin). Then everything we just said applies for each of the parts but also for the individual parts. We have rotation/angular momentum operators  $J_i^{(1)}, (J^{(1)})^2, J_i^{(2)}, (J^{(2)})^2$  for the individual parts but also the angular momentum operators  $J_i = J_i^{(1)} + J_i^{(2)}$  and  $J^2 = (J_i^{(1)} + J_i^{(2)})^2$  for the whole system.

Let's say we consider a subspace of the full system where the two parts have total angular momentum described by  $j_1$  and  $j_2$ . Then we can show that the  $J$  for the full system must

be somewhere in the range  $J = |j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2 - 1, j_1 + j_2$ . But not every state with definite values for  $j_1$  and  $j_2$  has a definite value for  $J$ .

The operators  $J_z^{(1)}, (J^{(1)})^2, J_z^{(2)}, (J^{(2)})^2$  all commute with each other, so we can find a basis of states which are eigenstates of all of these; we can write these as  $|j_1 m_1 j_2 m_2\rangle$ . But these won't be eigenstates of  $J^2$ , since  $J^2$  doesn't commute with  $J_z^{(1)}$  or  $J_z^{(2)}$ . Thus, if we want to talk about states of a definite total  $J^2$ , we need to use another basis. Since  $J^2, (J^{(1)})^2, (J^{(2)})^2, J_z$  all commute with each other, we can choose a basis of eigenstates of all of these; we label these basis elements by  $|j_1 j_2 JM\rangle$ .

Since we now have two bases for our states, it must be possible to express any basis element in one basis in terms of a basis element in another basis. That is, we can write

$$|j_1 j_2 JM\rangle = \sum_{m_1+m_2=M} C_{m_1 m_2 M}^{j_1 j_2 J} |j_1 m_1 j_2 m_2\rangle \quad (16)$$

for some coefficients  $C_{m_1 m_2 M}^{j_1 j_2 J}$ , which are known as the *Clebsch-Gordon coefficients* and can be looked up in tables (table 4.8 in Griffiths). We can also go the other direction and write

$$|j_1 m_1 j_2 m_2\rangle = \sum_{J, M=m_1+m_2} C_{m_1 m_2 M}^{j_1 j_2 J} |j_1 j_2 JM\rangle \quad (17)$$

where exactly the same coefficients appear.

The details of how to figure out the Clebsch-Gordon coefficients are in Griffiths 4.4.3.

### 3 Reading/review questions

- 1) For a state in some quantum system described in the notation above by  $|jm\rangle = |2\ 1\rangle$ , what is  $J_x|2\ 1\rangle$ ?
- 2) For a hydrogen atom (if we ignore all spin effects), there are various energy levels that we usually label by  $n$  with  $n$  a positive integer. For the states in level  $n$ , what are the possible values of total angular momentum  $L^2$ ? What is the total dimension of the subspace of states in the level  $n$  (again ignoring spin)? What is the total dimension if we include electron spin?
- 3) Suppose we have an electron ( $j_1 = 1/2$ ) in a rotationally invariant wavefunction (i.e. angular momentum 0) about a nucleus with  $j_2 = 3/2$ . What are the possible values for the total angular momentum of this system? List the allowed values of  $(J, M)$  for the total system.