Lecture 22

Relevant sections in text: §3.1, 3.2

Rotations in quantum mechanics

Now we will discuss what the preceding considerations have to do with quantum mechanics. In quantum mechanics transformations in space and time are "implemented" or "represented" by unitary transformations on the Hilbert space for the system. The idea is that if you apply some transformation to a physical system in 3-d, the state of the system is changed and this should be mathematically represented as a transformation of the state vector for the system. We have already seen how time translations and spatial translations are described in this fashion. Following this same pattern, to each rotation R we want to define a unitary transformation, $D(R)$, such that if $|\psi\rangle$ is the state vector for the system, then $D(R)|\psi\rangle$ represents the state vector after the system has undergone a rotation characterized by R. The key requirement here is that the pattern for combining two rotations to make a third rotation is "mimicked" by the unitary operators. For this we require that the unitary operators $D(R)$ depend continuously upon the rotation axis and angle and satisfy

$$D(R_1)D(R_2) = e^{i\omega_{12}}D(R_1R_2),$$

where ω_{12} is a real number, which may depend upon the choice of rotations R_1 and R_2, as its notation suggests. This phase freedom is allowed since the state vector $D(R_1R_2)|\psi\rangle$ cannot be *physically* distinguished from $e^{i\omega_{12}}D(R_1R_2)|\psi\rangle$.

If we succeed in constructing this family of unitary operators $D(R)$, we say we have constructed a "unitary representation of the rotation group up to a phase", or a "projective unitary representation of the rotation group". You can think of all the ω parameters as simply specifying, in part, some of the freedom one has in building the unitary representatives of rotations. (If the representation has all the ω parameters vanishing we speak simply of a "unitary representation of the rotation group".)

This possible phase freedom in the combination rule for representatives of rotations is a purely quantum mechanical possibility and has important physical consequences. Incidentally, your text book fails to allow for this phase freedom in the general definition of representation of rotations. This is a pedagogical error, and an important one at that. This error is quite ironic: the first example the text gives of the $D(R)$ operators is for a spin 1/2 system where the phase factors are definitely non-trivial, as we shall see.

Infinitesimal Rotations and Angular Momentum

Since $D(R)$ depends continuously upon an axis and angle, we can consider its infinitesimal form. For a fixed axis $\hat{n}$ and infinitesimal rotation angle ϵ we have

$$D(R) \approx I - \frac{i}{\hbar}\epsilon\hat{n}\cdot\vec{J},$$

where

$$\vec{J} = (J_1, J_2, J_3) = (J_x, J_y, J_z)$$

are self-adjoint operators, $J_i^\dagger = J_i$ with dimensions of angular momentum (in the sense that their matrix elements and eigenvalues have these dimensions). The operator J_i generates transformations on the Hilbert space corresponding to rotations of the system about the x^i axis. We identify the operators J_i with the angular momentum observables for the system. Of course, the physical justification of this mathematical model of angular momentum relies upon the unequivocal success of this strategy in describing physical systems. In particular, the J_i will (under appropriate circumstances) be conserved.

By demanding that the unitary transformations on the Hilbert space properly "mimic" (more precisely, "projectively represent") the rotations of 3-d space, it can be shown (see text for a version in which the phase factors are omitted) that the angular momentum operators satisfy the commutation relations

$$[J_k, J_l] = i\hbar\epsilon_{klm}J_m.$$

While the proof takes a little work and is omitted here, the result is very reasonable. Indeed, the commutation relations of infinitesimal generators in 3-d space encode the geometrical relationship between various rotations. It is therefore not surprising that the generators of rotations on the space of state vectors must obey the same commutation relations as the generators of rotations in 3-d space (up to the $i\hbar$, which is there because of the way we defined $\vec{J}$).

You have seen in your homework that the spin observables for a spin 1/2 system satisfy these commutation relations. Thus we identify the spin observables as a kind of angular momentum. This is not just a matter of terminology. In a closed system (*e.g.,* an atomic electron and a photon), angular momentum is conserved. However the angular momentum of a subsystem (*e.g.,* the electron) need not be conserved since it can exchange angular momentum with the rest of the system (*e.g.,* the photon) so long as the total angular momentum is conserved. The "bookkeeping" thus provided by conservation of angular momentum requires the spin angular momentum contribution to be included in order to "balance the books". Spin angular momentum provides a contribution to the conserved angular momentum of a closed system.

Using the same mathematical technology as we did for time and space translations, it is not hard to see that a finite (as opposed to infinitesimal) rotation can formally be built out of "many" infinitesimal rotations, leading to the formula:

$$D(\hat{n}, \theta) = \lim_{N\to\infty} (I - \frac{i}{\hbar}\frac{\theta}{N}\hat{n}\cdot\vec{J}) = e^{-\frac{i}{\hbar}\theta\hat{n}\cdot\vec{J}}.$$

The detailed form of this exponential operator, like that of the J_i depends upon the specific physical system being studied. The most familiar form of angular momentum is probably that of a particle moving in 3-d. However, spin also is a form of angular momentum (according to the above type of analysis) and it is the simplest, mathematically speaking, so we shall look at it first.

Spin as angular momentum

You will recall that the spin 1/2 observables S_i have the dimensions of angular momentum and satisfy the angular momentum commutation relations:

$$[S_k, S_l] = i\hbar\epsilon_{klm}S_m.$$

We therefore have that rotations of the spin 1/2 system are accomplished by unitary operators of the form

$$D(\hat{n}, \theta) = e^{-\frac{i}{\hbar}\theta\hat{n}\cdot\vec{S}}.$$

Let us have a look at an example.

Consider a rotation about the z-axis. Using the S_z eigenvectors as a basis we have the matrix elements

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

so that the matrix elements of the rotation operator are (exercise)

$$D(\hat{z}, \theta) = \begin{pmatrix} e^{-\frac{i}{2}\theta} & 0 \\ 0 & e^{\frac{i}{2}\theta} \end{pmatrix}.$$

You can do this calculation by using the power series definition of the exponential – you will quickly see the pattern. You can also use the spectral decomposition definition. Recall that for any self-adjoint operator A we have

$$A = \sum_i a_i |i\rangle\langle i|,$$

where $A|i\rangle = a_i|i\rangle$. Similarly, as you saw in the homework,

$$f(A) = \sum_i f(a_i)|i\rangle\langle i|.$$

Let

$$A = S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|),$$

and let f be the appropriate exponential function and you will get

$$D(\hat{z}, \theta) = e^{-\frac{i}{\hbar}\theta S_z} = e^{-\frac{i}{2}\theta}|+\rangle\langle+| + e^{\frac{i}{2}\theta}|-\rangle\langle-|.$$

Notice that this family of unitary operators satisfies

$$D(\hat{z}, \theta_1)D(\hat{z}, \theta_2) = D(\hat{z}, \theta_1 + \theta_2),$$

as it should. On the other hand, right away you should notice that something interesting has happened. The unitary transformation of a spin 1/2 system corresponding to a rotation by 2π is not the identity, but rather minus the identity! Thus, if you rotate a spin 1/2 system by 2π its state vector $|\psi\rangle$ transforms to

$$|\psi\rangle \to e^{-\frac{i}{\hbar}(2\pi)S_z}|\psi\rangle = -|\psi\rangle.$$

Indeed, it is only after a rotation by 4π that the spin 1/2 state vector returns to its original value. This looks bad; how can such a transformation rule agree with experiment? Actually, everything works out fine since the expectation values are insensitive to this change in sign:

$$\langle\psi|A|\psi\rangle \to \langle\psi|e^{\frac{i}{\hbar}(2\pi)S_z}Ae^{-\frac{i}{\hbar}(2\pi)S_z}|\psi\rangle = \langle\psi|(-1)A(-1)|\psi\rangle = \langle\psi|A|\psi\rangle.$$

What is happening here is that the spin 1/2 system is taking advantage of the phase freedom in the projective representation. On the one hand we have

$$R(\hat{n}, \theta)R(\hat{n}, 2\pi - \theta) = R(\hat{n}, 2\pi) = R(\hat{n}, 0) = I.$$

For the spin 1/2 representation we have

$$D(\hat{n}, \theta)D(\hat{n}, 2\pi - \theta) = -I = -D(\hat{n}, 0).$$

Let us note that the phase freedom in the representation of rotations is a rather subtle, intricate feature of the way in which quantum mechanics describes the physical world. Because of this subtlety in the theory we are able to properly accommodate spin 1/2 systems. This is one of the great successes of quantum mechanics.

How do observable quantities change in general when we make a rotation about z? Under a rotation about z the expectation value transforms via

$$\langle A\rangle = \langle\psi|A|\psi\rangle \to \langle\psi|e^{\frac{i}{\hbar}\theta S_z}Ae^{-\frac{i}{\hbar}\theta S_z}|\psi\rangle$$

Choose, for example, $A = S_x$. By expanding the exponentials in a Taylor series or by using the spectral decompositions, and using

$$S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|), \quad S_x = \frac{\hbar}{2}(|+\rangle\langle-| + |-\rangle\langle+|),$$

we have that (exercise)

$$\begin{aligned} e^{\frac{i}{\hbar}\theta S_z} S_x e^{-\frac{i}{\hbar}\theta S_z} &= \frac{\hbar}{2}(e^{i\theta}|+\rangle\langle-| + e^{-i\theta}|-\rangle\langle+|) \\ &= \cos\theta S_x - \sin\theta S_y. \end{aligned}$$

Note that this is exactly how the x-component of a vector transforms under a rotation about z. Because of this we get

$$\langle S_x\rangle \to \cos\theta\langle S_x\rangle - \sin\theta\langle S_y\rangle.$$

Similarly, it follows that

$$\langle S_y\rangle \to \cos\theta\langle S_y\rangle + \sin\theta\langle S_x\rangle,$$

and you can easily see that

$$\langle S_z\rangle \to \langle S_z\rangle$$

when the state vector is transformed. You can see that the unitary representative of rotations does indeed do its job as advertised.

Rotations represented on operators

Let us follow up on one result from above. We saw that

$$e^{\frac{i}{\hbar}\theta S_z} S_x e^{-\frac{i}{\hbar}\theta S_z} = \cos\theta S_x - \sin\theta S_y.$$

In the above equation the left hand side has the product of 3 Hilbert space operators appearing, corresponding to what happens to the spin vector observable when you change the state of the system via a unitary transformation corresponding to a rotation. The operator on the right hand side of the equation the linear combination of spin operators that you get by rotating them as if they are components of a vector in 3-d space.. This reflects a general rule which connects the rotations of 3-d space and their unitary representatives on the space of state vectors:

$$D^\dagger(\hat{n},\theta)\vec{S}D(\hat{n},\theta) = R(\hat{n},\theta)\vec{S}.$$

You can see immediately from this relation that the expectation values of $\vec{S}$ will behave like the components of a vector. More generally, if $\vec{V}$ is any trio of self-adjoint operators on Hilbert space representing a vector observable, then

$$D^\dagger(\hat{n},\theta)\vec{V}D(\hat{n},\theta) = R(\hat{n},\theta)\vec{V}.$$

You can think of this as analogous to the Heisenberg picture, but now for rotations. A rotation of the system can be mathematically viewed as a transformation of the state vector or, equivalently, as a transformation of the observables (but not both!).