Spin

Lecture 27

Physics 342
Quantum Mechanics I

Monday, April 5th, 2010

There is an intrinsic characteristic of "point" particles that has an analogue in (but no direct derivation from) classical rigid body rotation. On the classical side, the partitioning of kinetic energy into center of mass and rotational is just a matter of book-keeping. In quantum mechanics, we are forced to accept a fundamentally new descriptor of particles: Spin. The mathematical formulation of spin is just a copy of the commutators for orbital angular momentum (since spin *is* an angular momentum of sorts, and we must be able to add the spin representation to the orbital portion, it is almost required that it have identical form). While we can experimentally motivate/verify the existence of spin, it is natural to ask why, if electrons possess this property, there has been no discussion of it during our studies of Hydrogen.

27.1 Classical Description

Classically, there is a a natural separation between orbital (center of mass) angular momentum (the earth orbits around the sun), and "spin" angular momentum (the earth rotates about an axis). But in the classical setting, that's *all* it is, a separation. There is no new physics in the observation that the motion of a piece of mass consists of two parts. Indeed, if we think of the kinetic term in any Lagrangian for an extended body:

$$T = \frac{1}{2} \int \rho(\mathbf{r}') \, \mathbf{v} \cdot \mathbf{v} \, d\tau' \tag{27.1}$$

is the end of the story. We can, for computational reasons, distinguish between motion associated with a point $\dot{\mathbf{r}}_{cm}$ and a local "rotation" piece associated with motion about some dynamically determined axis $\mathbf{\Omega}$. The

rotation induces a change $d\mathbf{r}' = \mathbf{\Omega} \times \mathbf{r}'\, dt$ and then we can decompose the velocity of a parcel of mass into these two elements

$$\mathbf{v} = \mathbf{v}^{cm} + \mathbf{\Omega} \times \mathbf{r}'. \tag{27.2}$$

If we input this into the kinetic term from above:

$$T = \frac{1}{2} \int \rho(\mathbf{r}') \left(v_i^{cm} + \epsilon_{ijk}\, \Omega_j\, r'_k\right) \left(v_i^{cm} + \epsilon_{imn} \Omega_m\, r'_n\right)\, d\tau', \tag{27.3}$$

then this can be separated into pieces by expanding the quadratic:

$$T = \frac{1}{2}\, \mathbf{v}^{cm} \cdot \mathbf{v}^{cm} \underbrace{\int \rho(\mathbf{r}')\, d\tau'}_{=M} + \mathbf{v}^{cm} \cdot \left[\mathbf{\Omega} \times \underbrace{\int \rho\, \mathbf{r}'\, d\tau'}_{\equiv \mathbf{p}}\right] + \frac{1}{2}\, \Omega_j\, \Omega_m \underbrace{\int \rho \left(\delta_{jm}\, r'^2 - r'_j\, r'_m\right)\, d\tau'}_{=I_{jm}}. \tag{27.4}$$

We naturally associate these terms with the monopole (total mass), dipole and quadrupole of the mass distribution making up the rigid body. If we let $\mathbf{r}' = \mathbf{r} - \mathbf{r}^{cm}$, so that we are calculating the dipole moment about the center of mass, then

$$\mathbf{p} = \int \rho\, \mathbf{r}'\, d\tau' = \int \rho\, \mathbf{r}\, d\tau - \int \rho\, \mathbf{r}^{cm}\, d\tau = 0 \tag{27.5}$$

since the center of mass is defined to be: $\frac{1}{M} \int \rho\, \mathbf{r}\, d\tau$ (with respect to the original, non-center-of-mass origin). So the dipole term goes away provided we work in center of mass coordinates. The kinetic energy of the system is then

$$T = \frac{1}{2}\, M\, \mathbf{v}^{cm} \cdot \mathbf{v}^{cm} + \frac{1}{2}\, I_{jm}\, \Omega_j\, \Omega_m, \tag{27.6}$$

and this is the familiar breakup of center of mass and "rotational kinetic energy" ($\frac{1}{2}\, I\, \omega^2$) from introductory physics. But here, we emphasize the notion that this *comes from* the total kinetic energy in a natural way. All of the usual Newton's laws for center of mass and angular momentum of rigid bodies derive from a Lagrangian involving the above. In this way, "spin" or rigid body rotation, is truly just a bookkeeping device, and has no intrinsic physical meaning.

Not so, in quantum mechanics. We must consider a completely new property of matter, on a par with mass and electric charge, the spin defines experimentally verifiable physics that is not naturally associated with the macroscopic discussion above (being possessed by point particles, for example, which have no moment of inertia – the center of mass defines the particle position, and there is no extent over which to integrate for rigid body rotation).

27.2 Spin in Quantum Mechanics

Nevertheless, the intrinsic spin of a body is built out of an angular-momentum-like structure. Spin is naturally a vector, it gives a direction of sorts to a point particle, and the theory of spin is modeled precisely on the theory of angular momentum (also a vector operator). This is accomplished by defining the commutators of the spin operators to be structurally identical to those of $\mathbf{L}$. These new spin operators, being Hermitian, represent the act of measuring this new property of matter, and we define $\mathbf{S}$ with three components, satisfying

$$\boxed{[S_i, S_j] = i\,\hbar\,\epsilon_{kij}\,S_k.} \tag{27.7}$$

The eigenstates of the spin operator are indexed by s and m, and we choose S_z as the component that will commute with S^2 in defining the numbers s and m (with s playing the role of ℓ from angular momentum), and have, in bra-ket notation now (since we do not yet have a natural representation for the eigenstates – in the case of the orbital angular momentum, the wavefunction itself provided the representation):

$$S^2\,|s\,m\rangle = \hbar^2\,s\,(s+1)\,|s\,m\rangle \qquad S_z\,|s\,m\rangle = \hbar\,m\,|s\,m\rangle\,. \tag{27.8}$$

As with the angular momentum, we take $m = -s \ldots s$ in integer steps, so that s is integer or half-integer. We can define spin raising and lowering operators $S_\pm$ analagous to $L_\pm$:

$$S_\pm = S_x \pm i\,S_y. \tag{27.9}$$

These act as we expect: $S_+\,|s\,m\rangle \sim |s\,(m+1)\rangle$, and we can get the normalization constant in the same manner as for the raising and lowering operators from the harmonic oscillator or orbital angular momentum (they are, modulo the letter name, identical to $L_\pm$). Assume the state $|s\,m\rangle$ is normalized (i.e. $\langle s\,m|s\,m\rangle = 1$), then

$$S_\pm\,|s\,m\rangle = \alpha_\pm\,|s\,(m\pm 1)\rangle\,. \tag{27.10}$$

Since $S_+^\dagger = S_-$, the magnitude squared of the altered state is:

$$(S_\pm\,|s\,m\rangle)^\dagger\,S_\pm\,|s\,m\rangle = \langle s\,m|\;S_\mp S_\pm\,|s\,m\rangle \tag{27.11}$$

but just as for angular momentum, we have

$$S_\pm\,S_\mp = S^2 - S_z^2 \pm \hbar\,S_z \tag{27.12}$$

The normalization condition then reads

$$\alpha_\pm^2 = \hbar^2 \left(s\left(s+1\right) - m^2 \mp m \right) \longrightarrow \alpha_\pm = \hbar \sqrt{s\left(s+1\right) - m\left(m \pm 1\right)}, \quad (27.13)$$

so the operators act as

$$\boxed{S_\pm \left| s\, m \right\rangle = \hbar \sqrt{s\left(s+1\right) - m\left(m \pm 1\right)} \left| s\left(m \pm 1\right) \right\rangle .} \quad (27.14)$$

27.3 Spin and Representation

The angular momentum of a state is related to classical, orbital angular momentum, and it is possible to change ℓ by interacting with the system. In contrast, the spin of a particle is a fundamental property of the particle, it cannot change. We know that half-integer steps are allowed, so in theory we can study spin 0 (no spin at all), spin $\frac{1}{2}$, spin 1 etcetera. Unlike angular momentum ℓ, there are a finite number of interesting spins: all electrons, for example, are spin $\frac{1}{2}$, so to understand the spin of an electron, we need only understand $s = \frac{1}{2}$.

For $s = \frac{1}{2}$, we have $m = \pm\frac{1}{2}$, so there are only two states: "up" or "down" with spin S_z eigenvalues: $\frac{1}{2}\,\hbar$ and $-\frac{1}{2}\,\hbar$. We can represent these two options in vector format:

$$\left| s = \frac{1}{2}\, m = \frac{1}{2} \right\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \left| s = \frac{1}{2}\, m = -\frac{1}{2} \right\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (27.15)$$

χ_+ and χ_- in the book's language. Now the operators $\mathbf{S}$ and those derived from them can be represented as two-by-two matrices, those act via matrix-vector multiplication.

Our job now is to construct a matrix representation for the operators that is a manifestation of the defining relation (27.7). The first step in our ansatz is that of Hermiticity, each of the matrices must be Hermitian in the matrix sense (conjugate transpose equal to the matrix itself). The most general form of a Hermitian matrix is

$$S_i \doteq \begin{pmatrix} u_i & v_i + i\, w_i \\ v_i - i\, w_i & z_i \end{pmatrix} \quad (27.16)$$

with u_i, z_i, w_i and v_i real. We can adapt our choice to the representation of the up and down states – remember that we want: $S_z \left| \frac{1}{2}\, \frac{1}{2} \right\rangle = \frac{1}{2}\,\hbar \left| \frac{1}{2}\, \frac{1}{2} \right\rangle$,

and similarly for the down state, then

$$\begin{pmatrix} u_3 & v_3 + i\,w_3 \\ v_3 - i\,w_3 & z_3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} u_3 \\ v_3 - i\,w_3 \end{pmatrix}, \tag{27.17}$$

from which we learn that $u_3 = \frac{1}{2}\,\hbar$ and $v_3 = w_3 = 0$. From the down constraint, we find $z_3 = \frac{1}{2}\,\hbar$, and our matrix representation of the S_z operator is

$$S_z \doteq \frac{1}{2}\,\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{27.18}$$

Now consider the commutator:

$$[S_x, S_z] = -i\,\hbar\,S_y. \tag{27.19}$$

From the matrix multiplication:

$$[S_x, S_z] = \begin{pmatrix} 0 & -\hbar\,(v_1 + i\,w_1) \\ \hbar\,(v_1 - i\,w_1) & 0 \end{pmatrix} \tag{27.20}$$

and we can set the components of S_y appropriately:

$$S_y = \begin{pmatrix} 0 & w_1 - i\,v_1 \\ w_1 + i\,v_1 & 0 \end{pmatrix}. \tag{27.21}$$

Finally, we can use the commutator $[S_x, S_y] = i\,\hbar\,S_z$

$$\begin{pmatrix} 2\,i\,(v_1^2 + w_1^2) & (u_1 - z_1)\,(w_1 - iv_1) \\ -i\,(u_1 - z_1)\,(v_1 - iw_1) & -2\,i\,(v_1^2 + w_1^2) \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\,i\,\hbar^2 & 0 \\ 0 & -\frac{1}{2}\,i\,\hbar^2 \end{pmatrix} \tag{27.22}$$

to set $u_1 = z_1 = 0$ (the last equality actually follows from consistency with the $[S_y, S_z]$ commutation relation) and $v_1^2 + w_1^2 = \frac{\hbar^2}{4}$. At this point, we have three matrices satisfying our commutation relations, and "normalized" so that $S_z\,|sm\rangle = \hbar\,m\,|sm\rangle$. In addition, the operator S^2 is independent of the particulars of v_1 and w_1 (besides the constraint above) and has the form:

$$S^2 \doteq \frac{3\,\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{27.23}$$

How to select the ratio of v_1 to w_1? This comes, in the end, from our raising and lowering relations:

$$S_+ \left|\frac{1}{2}\ -\frac{1}{2}\right\rangle = \hbar\,\sqrt{3/4 - (-1/2)\,(-1/2+1)}\,\left|\frac{1}{2}\,\frac{1}{2}\right\rangle = \hbar\,\left|\frac{1}{2}\,\frac{1}{2}\right\rangle. \tag{27.24}$$

When we construct S_+ in matrix representation, and act on $\left|\frac{1}{2}\ -\frac{1}{2}\right\rangle$, we get

$$S_+\,\chi_- = (S_x + i\,S_y)\,\chi_- \doteq \begin{pmatrix} 0 & 2\,(v_1 + i\,w_1) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 2\,(v_1 + i\,w_1) \\ 0 \end{pmatrix} \tag{27.25}$$

so that we need $w_1 = 0$ and then $v_1 = \frac{1}{2}\,\hbar$ (notice that then $v_1^2 + w_1^2 = \frac{\hbar^2}{4}$ as it must.

Our final set of matrices is completely fixed:

$$\boxed{\begin{aligned} S_x &\doteq \frac{1}{2}\,\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &\doteq \frac{1}{2}\,\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ S_z &\doteq \frac{1}{2}\,\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}} \tag{27.26}$$

There is no further freedom, and we have an appropriate representation for spin $\frac{1}{2}$ vectors and operators. The matrices in the above are the Pauli "sigma" matrices.

27.4 Comments

While we are being careful to distinguish between the classical and quantum forms of spin, the fact is, terms involving spin show up in Hamiltonian's in much the same way as classical spin. For example, a macroscopic, charged spinning body has a net magnetic dipole moment that can interact with magnetic fields in the usual way, via the potential $-\mathbf{m}\cdot\mathbf{B}$. A similar term arises for quantum spin – that is, even though it is a real, separate physical quantity, it couples to magnetic fields *as if* it were the dipole moment of a macroscopic body. This leads to measurable effects that establish both the eigenvalues for spin and the quantum mechanical theory of measurement.

Finally, we record the interpretation here – for a particle in a spin state $\chi = \alpha\,\chi_+ + \beta\,\chi_-$, we obtain a z-component of spin measurement of either $\frac{1}{2}\,\hbar$ or $-\frac{1}{2}\,\hbar$. The probabilities are as usual, $|\alpha|^2$ and $|\beta|^2$ (this is a finite discrete basis – our "usual" infinite sums over basis functions like sin are replaced by a simple sum of weighted components). We cannot yet talk about the temporal evolution of a generic spin state, since we have no Hamiltonian, but

we will find the usual sort of separation applies (provided the Hamiltonian is time-independent). Schrödinger's equation is, as always, $i\,\hbar\,\frac{d\chi}{dt} = H\,\chi$ and if we have a Hamiltonian that commutes with S^2 (as the spherically symmetric Hamiltonian does with L^2), then we would have

$$H\chi = E_+\,\alpha\,\chi_+ + E_2\,\beta\,\chi_- \longrightarrow \chi(t) = \alpha\,e^{\frac{i\,E_+\,t}{\hbar}}\,\chi_+ + \beta\,e^{\frac{i\,E_-\,t}{\hbar}}\,\chi_- \qquad (27.27)$$

where E_+ and E_- are the energies associated with the up and down spins respectively.

Expectation values and variances proceed as usual, with $\langle Q\rangle = \langle s|\,Q\,|s\rangle$ equal to the vector-matrix-vector form for the Hermitian operator Q represented as a matrix. For generic Q

$$Q \doteq \begin{pmatrix} q_0 & q_1 + i\,q_2 \\ q_1 - i\,q_2 & q_3 \end{pmatrix} \qquad (27.28)$$

and $|s\rangle$ given by

$$|s\rangle \doteq \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \qquad (27.29)$$

we have

$$\langle s|\,Q\,|s\rangle \doteq \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} \begin{pmatrix} q_0 & q_1 + i\,q_2 \\ q_1 - i\,q_2 & q_3 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \qquad (27.30)$$

with the side-constraint that $\langle s|s\rangle = 1$.

Keep in mind that it is possible to have a Hamiltonian with both spatial terms (our usual one) and spin terms, so it must also be possible to describe a wavefunction for an electron, say, that combines the position or momentum space functional form with the spin state. We can take the "full" wavefunction (barring any surprising new electron properties) to be $\bar{\psi}_{n\ell m} = \psi_{n\ell m}\,\chi$, where we have just combined the spatial wavefunction $\psi_{n\ell m}$ with the spin portion, χ.

Homework

Reading: Griffiths, pp. 171–178.

Problem 27.1

Griffiths 4.24. A quantum mechanical "rigid rotor" (no radial motion).

Problem 27.2

Given that spin combines with the orbital angular momentum $\mathbf{L}$ to form a "total" angular momentum operator $\mathbf{J} = \mathbf{L} + \mathbf{S}$, and that $\mathbf{J}$ is itself "an angular momentum" (meaning that it is a set of three operators that satisfy the commutators $[J_i, J_j] = i\,\hbar\,\epsilon_{kij}\,J_k$ and has all the usual properties familiar from the L_i), find the allowed values of J_z for a particle that has spin $s = \frac{1}{2}$ and orbital angular momentum $\ell = 1$ (an electron in an $\ell = 1$ state of Hydrogen, for example).

Problem 27.3

Here, we will establish the correctness of the infinitesimal rotation expression $d\mathbf{r}' = \mathbf{\Omega} \times \mathbf{r}$. Referring to the figure below, we have a vector $\mathbf{r}$ lying in the $x - z$ plane with $\mathbf{r} = R\,\hat{\mathbf{x}} + z\,\hat{\mathbf{z}}$. We rotate through an angle ϕ about the $\hat{\mathbf{z}}$ axis as shown to obtain $\mathbf{r}'$. Write all three components of $\mathbf{r}'$ in terms of $\sin\phi$ and $\cos\phi$, then make the small angle approximation for these trigonometric quantities, and show that $\mathbf{r}' - \mathbf{r} = \mathbf{\Omega} \times \mathbf{r}$ with $\mathbf{\Omega} \equiv \phi\,\hat{\mathbf{z}}$.

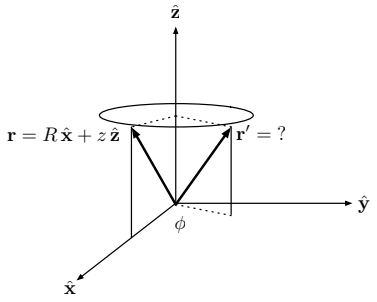

Figure 27.1: Establishing that infinitesimal rotation is given by $\mathbf{\Omega} \times \mathbf{r}$.