Angular momentum & spin

January 8, 2002

1 Angular momentum

Angular momentum appears as a very important aspect of almost any quantum mechanical system, so we need to briefly review some basic properties of this quantity.

1.1 Definitions

The classical definition of the angular momentum of a particle:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}.$$

Using the correspondence between classical and quantum linear momentum

$$\mathbf{p} \rightarrow -i\hbar\nabla,$$

the quantum mechanical operator for angular momentum becomes

$$\mathbf{L} = -i\hbar(\mathbf{r} \times \nabla),$$

for example

$$L_z = -i\hbar(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}).$$

The characteristic size of the quantum of angular momentum is $\hbar$.

1.2 Commutators

Recall that a quantum state may be an eigenstate of several operators if they commute. Let's look at commutators of components of $\mathbf{L}$.

$$\begin{aligned} [L_x, L_y] &= [(yp_z - zp_y), (zp_x - xp_z)] \\ &= [yp_z, zp_x] - [zp_y, zp_x] - [yp_z, xp_z] + [zp_y, xp_z] \end{aligned}$$

Evaluate these commutators with the usual rules:

$$\begin{aligned} [yp_z, zp_x] &= [yp_z, z]p_x + z[yp_z, p_x] \\ &= -[z, yp_z]p_x - z[p_x, yp_x] \\ &= -[z, y]p_zp_x - y[z, p_z]p_x - z[p_x, y]p_z - zy[p_x, p_z] \\ &= -0 - y[z, p_z]p_x - 0 - 0 \\ &= -i\hbar yp_x. \end{aligned}$$

Continuing in this way, we find

$$[L_x, L_y] = i\hbar L_z$$

and cyclically.

The operators L_i *do not commute* and we cannot find simultaneous eigenfunctions and eigenvalues of all three at once. Only one component of $\mathbf{L}$ has a definite value. By convention, we usually take this to be L_z.

Defining the total angular momentum as usual,

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$$

we find that

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

Thus, simultaneous eigenfunctions of L_z and $\mathbf{L}^2$ exist.

1.3 L in spherical polar coordinates

It is interesting to change to spherical polar coordinates,

$$x = r \sin\theta \cos\phi,$$

etc. In these coordinates,

$$L_z = -i\hbar \frac{\partial}{\partial \phi}.$$

The eigenfunctions of L_z satisfy

$$L_z \Phi(\phi) = -i\hbar \frac{\partial \Phi}{\partial \phi} = m\hbar \Phi(\phi).$$

Normalized solutions are

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} \exp(im\phi).$$

Since $\Phi(\phi)$ must be single-valued, $\Phi(2\pi) = \Phi(0)$, m must be an integer.

The operator $\mathbf{L}^2$ is given by

$$\mathbf{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right].$$

Simultaneous eigenfunctions of $\mathbf{L}^2$ and L_z are known as the spherical harmonics $Y_{lm}(\theta, \phi)$. They satisfy

$$\mathbf{L}^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi)$$

and

$$L_z Y_{lm}(\theta, \phi) = m\hbar Y_{lm}(\theta, \phi).$$

We'll see shortly why the eigenvalue of $\mathbf{L}^2$ has been written as $l(l+1)\hbar^2$. Assume we can separate variables (note that the function of θ depends both on its own eigenvalues and on m):

$$Y_{lm}(\theta,\phi) = \Theta_{lm}(\theta)\Phi_m(\phi);$$

the functions Θ_{lm} satisfy

$$\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{m^2}{\sin^2\theta}\right]\Theta_{lm}(\theta) = l(l+1)\Theta_{lm}(\theta).$$

Finite solutions of this equation exist only for $l = 0, 1, 2, ...$ and $m = -l, -(l-1), ... + l$ (explaining our choice of how to write the eigenvalues of the equation). The $Y_{lm}(\theta,\phi)$ are expressed in terms of the associated Legendre functions, which are defined using the Legendre polynomials (as explained by B & J, where many properties of these functions are summarized).

It is interesting to look at polar diagrams of a few spherical harmonics.

1.4 The rigid rotator

A very simple system is interesting to study at this point. Consider a quantum particle held at a fixed distance R_0 from a central point, but free to move in all directions. Its moment of inertia is $I = mR_0^2$, and its classical total energy is given by $E_{\rm tot} = mv^2/2 = m^2R_0^2v^2/(mR_0^2) = \mathbf{L}^2/(2I)$. Its Schroedinger equation is thus

$$\frac{\mathbf{L}^2}{2I}\psi(\theta,\phi) = E\psi(\theta,\phi).$$

This is just the eigenvalue equation for total angular momentum, so we find that the eigenfunctions are the spherical harmonics, and the allowed energy levels are

$$E_l = \frac{\hbar^2}{2I}l(l+1),\ \ l = 0, 1, 2, ...$$

1.5 Spin angular momentum

Experiments indicate that electrons and other particles behave as though they have an intrinsic magnetic moment, which is quantized in direction like angular momentum. This suggests that magnetic moment may be due to an intrinsic (rather than orbital) angular momentum of the particle. We say that such particles possess **spin** angular momentum. Since this is an intrinsically quantum mechanical property of the particle, we must guess at the rules governing it. We assume that it will behave like orbital angular momentum, and will obey the same commutator relations and satisfy similar eigenvalue equations. Thus if S_x, S_y, and S_z are the components of the spin operator $\mathbf{S}$, the eigenfunctions of $\mathbf{S}^2$ and S_z satisfy

$$\mathbf{S}^2\chi_{s,m} = s(s+1)\hbar^2\chi_{s,m}$$

and

$$S_z\chi_{s,m} = m_s\hbar\chi_{s,m}.$$

Experimentally, we find only two spin states for an electron, so we must have $m = \pm 1/2$, and so $s = 1/2$. We say that the electron has spin one-half. Only two normalized spin eigenfunctions exist for this system:

$$\alpha \equiv \chi_{1/2,1/2}; \beta \equiv \chi_{1/2,-1/2}.$$

These two states are spin eigenstates with "spin up" and "spin down" respectively. A general spin state is a linear superposition of α and β:

$$\chi = \chi_+ \alpha + \chi_- \beta,$$

so that the probability of spin up is $|\chi_+^2|$. Note that the spin eigenfunctions contain only information about the spin state – they tell you nothing about space distributions.

The spin state may be represented as a two-component column vector, and the spin operators by two-by-two matrices, as discussed by B & J. For particles with spin larger than 1/2 (quite possible), the number of basic spin eigenstates and the dimensions of the matrices are larger. Like angular momentum, spin may be described qualitatively with the aid of a simple vector model.

1.6 Total angular momentum

As in classical physics, the total angular momentum of a particle is

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

$\mathbf{L}$ operates in ordinary space only; $\mathbf{S}$ operates only in spin space. All components of $\mathbf{L}$ commute with all components of $\mathbf{S}$, and both satisfy the same commutation relations. Thus $\mathbf{J}$ satisfies the same commutation relations as $\mathbf{L}$ and $\mathbf{S}$. It is shown by B & J (App 4) that simultaneous eigenfunctions of $\mathbf{J}^2$ and J_z satisfy

$$\mathbf{J}^2 \psi_{jm_j} = j(j+1)\hbar^2 \psi_{jm_j}$$

and

$$J_z \psi_{jm_j} = m_j \psi_{jm_j},$$

where j is an integer or half-integer, and m_j ranges between $-j$ and j. Because $\mathbf{L}^2$, L_z, $\mathbf{S}^2$, and S_z all commute, they have simultaneous eigenfunctions, given by

$$\psi_{lsm_lm_s} = Y_{lm_l}(\theta, \phi)\chi_{s,m_s}.$$

Alternatively, the four operators $\mathbf{L}^2$, $\mathbf{S}^2$, $\mathbf{J}^2$ and J_z form a commuting set. Their simultaneous eigenfunctions are linear combinations of the $\psi_{lsm_lm_s}$. For given l and s the values of j are $|l - s|$ up to $l + s$, and m_j can take on values from $-j$ to j.

And that is angular momentum ... whew!

2 Central forces

Central forces (or approximately central forces) occur in many systems, and it is worthwhile to review some of the general properties of a system in which the force is described by a potential $V(r)$.

Consider a particle in a potential well that depends only on r, not on $\mathbf{r}$, so $V = V(r)$. Then using the expression for ∇^2 in spherical coordinates and that of the operator $\mathbf{L}^2$ in these coordinates, we easily find that the Schroedinger equation becomes

$$\begin{aligned} E\psi(\mathbf{r}) &= H\psi(\mathbf{r}) \\ &= \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right\}\psi(\mathbf{r}) \\ &= \left\{-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r)\right\}\psi(\mathbf{r}) \\ &= \left\{-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\mathbf{L}^2}{\hbar^2 r^2}\right] + V(r)\right\}\psi(\mathbf{r}). \end{aligned}$$

Now $\mathbf{L}^2$ and L_z commute, and operate only on θ and ϕ, so both commute with H and we may look for simultaneous eigenfunctions of H, $\mathbf{L}^2$ and L_z. Thus we have

$$\psi_{E,l,m}(r,\theta,\phi) = R_{E,l}(r)Y_{lm}(\theta,\phi).$$

Substituting into the Schroedinger equation and replacing the effect of the operator $\mathbf{L}^2$ by its eigenvalue, and then dividing by the $Y_{lm}(\theta,\phi)$, we get an equation for the radial function:

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l(l+1)}{r^2}\right] + V(r)\right\}R_{E,l}(r) = ER_{E,l}(r).$$

$R_{E,l}(r)$ does not depend on m.

We can simplify by choosing a new radial function

$$u_{E,l}(r) = rR_{E,l}(r)$$

which leads to the radial equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]u_{E,l}(r) = Eu_{E,l}(r).$$

This equation is very similar to the familiar one-dimensional Schroedinger equation with an effective potential

$$V_{\text{eff}}(r) = V(r) + \frac{l(l+1)\hbar^2}{2mr^2},$$

containing a centrifugal barrier term (but recall that r must be greater than 0).

2.1 Parity

Can quantum states have some kind of space symmetry? Consider the **parity** operator $\mathbf{P}$, which reflects space coordinates through the coordinate origin:

$$\mathbf{P}f(\mathbf{r}) = f(-\mathbf{r}).$$

It is Hermitian operator, and hence has real eigenvalues, so it may be observable. We can easily find its eigenvalues

$$\mathbf{P}\psi_\alpha(\mathbf{r}) = \alpha\psi_\alpha(\mathbf{r}),$$

since

$$\mathbf{P}\mathbf{P}f(\mathbf{r}) = \mathbf{P}f(-\mathbf{r}) = f(\mathbf{r}),$$

and hence $\alpha^2 = 1$, or $\alpha = +1$ or -1. We often denote the two eigenfunctions of $\mathbf{P}$ as $\psi_+(\mathbf{r})$ and $\psi_-(\mathbf{r})$; they are respectively symmetric and anti-symmetric under reflections through the origin. Any function may be written as a sum of even and odd parts:

$$\psi(\mathbf{r}) = \frac{1}{2}[\psi(\mathbf{r}) + \psi(-\mathbf{r})] + \frac{1}{2}[\psi(\mathbf{r}) - \psi(-\mathbf{r})].$$

Under the parity operation, spherical polar coordinates (r, θ, ϕ) become $(r, \pi - \theta, \phi + \pi)$. It is easily seen that this transformation does not alter the Hamiltonian for a central force, so $\mathbf{P}$ commutes with H and simultaneous eigenfunctions of both operators may be found. In fact the spherical harmonics have definite parity already, that of l, and so

$$\mathbf{P}[R_{E,l}Y_{lm}(\theta, \phi)] = R_{E,l}(-1)^l Y_{lm}(\theta, \phi),$$

so central force wave functions have the parity of l: even for even l and odd for odd l.