Lecture 2 Highlights
Phys 402

Orbital Angular Momentum

We concluded our review of Phys 401 with a discussion of orbital and spin angular momentum. Angular momentum is defined as $\vec{L} = \vec{r} \times \vec{p}$, and as such depends on the choice of origin. We take the origin as the force center for the Coulomb central force in the "relative problem" that results from the 2-body problem (see problem 1 in HW 2). In quantum mechanics we consider the angular momentum to be an operator of the form $\vec{\hat{L}} = \hat{L}_x \hat{\imath} + \hat{L}_y \hat{\jmath} + \hat{L}_z \hat{k}$, where $\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$, etc. and the momentum operator is $\hat{p}_i = -i\hbar \frac{\partial}{\partial x_i}$, where $i = 1, 2, 3$ represent the 3 Cartesian coordinates $x_1 = x, x_2 = y, x_3 = z$. Recall that the linear position and momentum operators obey these commutation relations: $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$, where δ_{ij} is the Kronecker delta. Note that "i" appears in two different forms in the commutation relation. It appears as a subscript and also as the square root of -1. You are expected to know the meaning of "i" from the context! We also have $[\hat{x}_i, \hat{x}_j] = 0$ and $[\hat{p}_i, \hat{p}_j] = 0$. From these commutation relations you can derive those for the components of the angular momentum: $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$, and all cyclic permutations (i.e. x-y-z, y-z-x, z-x-y). These non-zero commutators mean that the components of $\vec{\hat{L}}$ are incompatible operators. One cannot form simultaneous eigenfunctions of $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$.

However, consider the angular momentum squared operator: $\hat{L}^2 = \vec{\hat{L}} \cdot \vec{\hat{L}} = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2$. This operator commutes with any of the three components: $[\hat{L}^2, \hat{L}_i] = 0$. Hence one can form simultaneous eigenfunctions of $\hat{L}^2$ and any one component of $\vec{\hat{L}}$. By convention we choose this to be the z-component operator. The eigenfunctions are the spherical harmonics: $\hat{L}^2 Y_{\ell,m} = \ell(\ell+1)\hbar^2 Y_{\ell,m}$ and $\hat{L}_z Y_{\ell,m} = m\hbar Y_{\ell,m}$.

In analogy with the quantum harmonic oscillator we can think of quantum angular momentum in terms of a *ladder of states*. We can define ladder operators as $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ and $\hat{L}_- = \hat{L}_x - i\hat{L}_y$. This can be written more compactly as $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$. One can examine the $\hat{L}^2$ and $\hat{L}_z$ eigenvalues of the ladder operators applied to the $Y_{\ell,m}$. The results are: $\hat{L}^2(\hat{L}_\pm |\ell,m\rangle) = \hbar^2\ell(\ell+1)(\hat{L}_\pm |\ell,m\rangle)$, and $\hat{L}_z(\hat{L}_\pm |\ell,m\rangle) = (m \pm 1)\hbar(\hat{L}_\pm |\ell,m\rangle)$, showing that the $\hat{L}_\pm$ moves the state up or down the ladder of states labeled by the z-component of angular momentum quantum number. (Note that we are using the ket $|\ell,m\rangle$ as a stand-in for the spherical harmonics $Y_{\ell,m}$) We expect this ladder of states to be finite, for a given ℓ, because the component of a vector can never exceed it's length. By calculating the length of the ket $\hat{L}_\pm |\ell,m\rangle$ we can find the relevant constraint on values of m for a given ℓ. One can show that the scalar quantity $\left|\hat{L}_\pm |\ell,m\rangle\right|^2$ is equal to $\hbar^2[\ell(\ell+1) - m(m \pm 1)] \geq 0$, and this must be either positive or zero. This is satisfied as long as the z-component quantum integer falls in this set of values: $-\ell \leq m \leq \ell$. Thus the ladder of states associated with orbital angular momentum has these important properties:

1) The ladder is centered on $m = 0$.
2) The ladder is symmetric about $m = 0$.

3) The ladder has steps in units of $\hbar$.

Note that there are total of $2\ell + 1$ steps in the ladder, which is an odd number for the allowed values of ℓ in the hydrogen atom. For example, a hydrogen atom making a transition from a 2p to 1s state will have its spectral line split into 3 lines in the presence of an external magnetic field. This splitting is proportional to the magnetic field. This Zeeman effect is due to the interaction between the external magnetic field and the magnetic moment created by the current loop of the electron in the 2p state. The z-component of that magnetic moment has three different values, depending on the magnetic quantum number m. We will study the Zeeman effect in detail later in the semester.

Note that the length of the angular momentum vector has the strange value of $|\vec{L}| = \sqrt{\ell(\ell+1)}\,\hbar$. The maximum z-component of $\vec{L}$, namely the $\hat{L}_z$ eigenvalue is $\ell\hbar$. Hence the angular momentum vector can never lie precisely in the z-direction (or any other direction for that matter!). If it did have a well-defined direction then it would imply that the electron orbit around the force center is exactly planar, violating the position-momentum uncertainty relation for the direction perpendicular to the plane. Consequently, the angular momentum vector can only be localized to somewhere (everywhere actually) on a cone defined by a vector of length $\sqrt{\ell(\ell+1)}\,\hbar$ with some quantized z-projection, $m\hbar$. Check out the example of the angular momentum states for $\ell = 2$.

Spin Angular Momentum

The electron orbiting the nucleus creates a current loop and a corresponding magnetic moment $\vec{\mu}$. In the presence of an external magnetic field $\vec{B}_{ext}$ (defining the z-direction), the atom has an energy depending on the relative orientation of the field and magnetic moment. This energy is given by $U_{Zeeman} = -\vec{\mu}\cdot\vec{B}_{ext}$. The lowest energy state is the one in which the magnetic field and magnetic moment are aligned (the dot product is positive), and the highest energy state is when they are anti-aligned. Note that if $\vec{B}_{ext}$ is perpendicular to $\vec{\mu}$ then this additional energy is zero. If one studies the transition from the 2p state to the 1s state of Hydrogen in zero magnetic field, there is a single spectral line. In the presence of a strong magnetic field on the hydrogen atom this spectral line is observed to 'split' in to three closely spaced spectral lines. These arise from the 3 different energies of the 2p state of Hydrogen, depending on the m quantum number (the 1s state is un-split because $\ell = m = 0$ and the atom has no magnetic moment in that state). This splitting of the spectral lines in a magnetic field is known as the Zeeman effect. Our theory of angular momentum predicts that the states will split in to an *odd* number. However, sometimes it is observed that there is an *even* number of states, and this is called the anomalous Zeeman effect.

The Stern-Gerlach (SG) device uses an inhomogeneous magnetic field to exert a force on neutral atoms in a manner that depends on the sign and magnitude of the "z-component" of magnetic moment (anti-parallel to the spin of the electron) of the atom. The z-direction is defined by the direction of the gradient in magnetic field of the SG device (see Griffiths page 181). The SG takes un-polarized atoms as input and produces spin-polarized beams as output. Again the SG machine can create either an odd number of output beams, or an even number of beams.

Wolfgang Pauli tried to explain these results by positing the existence of a "two-valuedness not describable classically." In other words he proposed a new quantized entity in the hydrogen atom that could take one of only two states. This entity became known as "spin" and is crudely thought to be the quantized rotational angular momentum of the electron.

The electron intrinsic angular momentum is denoted as $\vec{S}$. We take as a postulate that it has essentially the same properties as the quantum angular momentum. We describe the eigenstates using a ket notation: $|s, m_s\rangle$, satisfying the eigenvalue equations: $\hat{S}^2|s, m_s\rangle = s(s+1)\hbar^2|s, m_s\rangle$, and $\hat{S}_z|s, m_s\rangle = m_s\hbar|s, m_s\rangle$. We expect that the spin component operators will obey the commutation relations $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$, and all cyclic permutations. There is an associated ladder of states with properties:

1) The ladder is symmetric about $m_s = 0$.
2) The ladder has steps in units of $\hbar$.

Note that there are total of $2s+1$ steps in the ladder, which is an even number for the allowed values of s in the hydrogen atom. In general though, s can be integer or half-integer.

We can also define raising and lowering operators for moving on the ladder of states. These are defined as $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$, and they have this effect on the spin eigenstates: $\hat{S}_\pm|s, m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}\,|s, m_s \pm 1\rangle$. Note that trying to promote to a state above the top of the ladder, or below the bottom of the ladder, results in a 0 wavefunction (verified by putting in $m_s = \pm s$ in the pre-factor).

The spin-1/2 system is the prototype of all 2-level quantum systems. It is the quintessential quantum system that is the basis for quantum information science. A two-level system has basis states $|0\rangle$ and $|1\rangle$, and an arbitrary superposition is represented by $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$. In the spin-1/2 case we have basis states $\left|\frac{1}{2}, +\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, representing the states with $s = \frac{1}{2}$ and $m_s = \pm\frac{1}{2}$. The arbitrary super-position is given by $|\Psi\rangle = \alpha\left|\frac{1}{2}, +\frac{1}{2}\right\rangle + \beta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, or going over to a column vector format, $|\Psi\rangle = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}$. In this column vector format, all operators become matrices. You can verify that the following matrix versions of the operators give the correct eigenvalues,

$$\hat{S}^2 = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} = \frac{\hbar}{2}\sigma_x$$

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\i & 0\end{pmatrix} = \frac{\hbar}{2}\sigma_y$$

Where the σ_i are the famous Pauli spin matrices. The Pauli spin matrices obey the commutation relations like the spin components. One can define a vector of Pauli spin matrices as $\hat{\vec{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$, which can be used to represent the spin operator as $\hat{\vec{S}} = \frac{\hbar}{2}\hat{\vec{\sigma}}$.

Perturbation Theory

The point of perturbation theory is to form an approximate solution for the eigenvalues and eigenfunctions of a complicated problem that is closely related to an exactly solved problem. In perturbation theory we start with an 'unperturbed' Hamiltonian H^0 for which we can find the exact eigenvalues E_n^0 and eigenfunctions ψ_n^0:

$$\mathrm{H}^0\psi_n^0 = E_n^0\psi_n^0 \tag{1}$$

All of the QM problems that we solved in Phys401 are now going to be called "zeroth-order problems/solutions." We are interested in solving another problem with a very similar Hamiltonian $\mathrm{H} = \mathrm{H}^0 + \lambda\mathrm{H}'$, where H' is called the perturbing Hamiltonian, and $\lambda << 1$ is a small parameter to remind us that the perturbation should be "small." (Later we will take $\lambda = 1$ and replace it with a "smallness" condition on the perturbing Hamiltonian H'.) The exact solution to this problem involves new eigenvalues and eigenfunctions:

$$\mathrm{H}\psi_n = E_n\psi_n \tag{2}$$

We want to solve this Schrodinger equation for the new eigenvalues E_n and eigenfunctions ψ_n. The purpose of perturbation theory is to find approximate expressions for the new eigenvalues E_n and eigenfunctions ψ_n in terms of the eigenvalues and eigenfunctions of the unperturbed problem, and the perturbing Hamiltonian.