

Lecture 5 Highlights

Phys 402

We considered the spin-orbit interaction in Hydrogen. The objective is to calculate the “fine-structure” energy splitting due to the spin-orbit effect. The magnetic moment of the electron interacts with the magnetic field created by the proton to produce a small energy difference between the \vec{L} parallel to \vec{S} and \vec{L} anti-parallel to \vec{S} situations for the atom. This difference is due to “spin-orbit coupling.”

We first did a series of classical calculations for a current loop in a magnetic field. A planar current loop has associated with it a magnetic moment $\vec{\mu} = I\vec{A}$, where I is the current flowing in the loop of area A . The vector direction of the area is perpendicular to the plane of the loop (see Griffiths *Introduction to Electrodynamics*, 3rd Edition, Eq. [5.84]). An external magnetic field \vec{B} will create a torque on the current loop given by $\vec{\tau} = \vec{\mu} \times \vec{B}$ which will try to align the magnetic moment with the magnetic field. This can be summarized by a Hamiltonian of the form $H = -\vec{\mu} \cdot \vec{B}$. The Hamiltonian favors the parallel alignment of $\vec{\mu}$ and \vec{B} (i.e. this configuration has the lowest energy). A nice [demo](#) shows the torque exerted on the current loop by a magnetic field.

As discussed in Griffiths QM page 300 the magnetic field experienced by the electron in the Hydrogen atom is given (classically) by:

$$\vec{B} = \frac{e\vec{L}}{8\pi\epsilon_0 mc^2 r^3},$$

where e is the electronic charge, m is the electron mass, c is the speed of light in vacuum, r is the proton-electron distance, and \vec{L} is the orbital angular momentum of the electron in the Hydrogen atom bound state. Note that the magnetic field is parallel to the electron orbital angular momentum vector. To see why, consider things from the proton’s rest frame as the electron moves with velocity \vec{v} through the static electric field \vec{E} produced by the proton. The electron will experience an effective magnetic field given by $\vec{B} = -\frac{\vec{v}}{c} \times \vec{E}$ (from relativity). By comparing the direction of this field with the direction of the orbital angular momentum of the electron in its orbit about the proton, this argument shows that \vec{B} is parallel to \vec{L} .

The magnetic moment of a charged “spinning” particle is given by:

$$\vec{\mu} = \gamma \vec{S},$$

where γ is called the **gyromagnetic ratio**. It relates the gyration (or rotation) of the particle (as embodied in \vec{S}) to the magnetic moment developed ($\vec{\mu}$). A moving charge creates a magnetic field. A charge moving in a “small” current loop can be treated as a magnetic moment, or magnetic dipole, at least for distances large compared to the diameter of the current loop. For the electron the gyromagnetic ratio is found to be $\gamma_e = -\frac{e}{m_e}$ to very good

approximation (there are corrections due to vacuum fluctuations of the electromagnetic field, worked out by Feynman using Quantum Electrodynamics - QED). {As a side note, our treatment of the hydrogen atom is quantum mechanical as far as the electron and proton are concerned, but it is entirely classical as far as the electromagnetic fields are concerned.

This situation is corrected in QED.} See Griffiths page 301 for a “derivation” of this result. For heavier particles like the proton the gyromagnetic ratio is much smaller due to the larger mass in the denominator and the fact that angular momentum is quantized and of order \hbar for *all* particles. This fact allows us to ignore the interaction of the proton’s magnetic moment with the magnetic field created by the electron, at least for now. It will be treated in a higher order correction (‘hyperfine’ splitting) in perturbation theory.

The electron’s magnetic moment experiences a torque due to its motion around the proton. There is a perturbing interaction energy given by;

$$H_{so} = -\vec{\mu} \cdot \vec{B}$$

which becomes;

$$H_{so} = -\left(-\frac{e}{m}\vec{S}\right) \cdot \left(\frac{e\vec{L}}{8\pi\epsilon_0 mc^2 r^3}\right) \sim \vec{S} \cdot \vec{L}$$

This new operator $\vec{S} \cdot \vec{L}$ has some interesting properties. It commutes with L^2 and S^2 , but does not commute with \vec{S} or \vec{L} (Homework 3). This means that \vec{S} and \vec{L} are no longer “constants of the motion” under the perturbed Hamiltonian $H^0 + H_{so}$ (this follows from Griffiths [3.73] with $Q = \vec{L}$ or \vec{S}). This means that ℓ and s are still “good quantum numbers”, but m_ℓ and m_s are not. The perturbation mixes together states with different values of m_ℓ and m_s .

Note that the proton exerts a torque on the electron spin. This means that the force of interaction between the two particles is non-central, although this effect is a “small perturbation.” This means that \vec{S} will precess in its motion about the proton. As a consequence \vec{L} will also precess, since the net external torque on the atom is zero, and the total angular momentum of the atom, $\vec{J} = \vec{L} + \vec{S}$, must therefore remain fixed.

This new total angular momentum quantum mechanical operator \vec{J} has properties analogous to \vec{S} and \vec{L} . It has a ladder of states symmetric about zero. The ladder has a top rung and a bottom rung. There is a J^2 operator with eigenvalues $j(j+1)\hbar^2$, and a J_z operator with eigenvalues $m_j\hbar$. (The eigenfunctions $|j m_j\rangle$ of J^2 and J_z will be found in the next lecture) There are raising and lowering operators $J_\pm = J_x \pm iJ_y$ that move one up and down the ladder of states, and commutators such as $[J_x, J_y] = i\hbar J_z$, etc.

One nice feature of \vec{J} is the fact that it is a “constant of the motion” for the perturbed Hamiltonian $H^0 + H_{so}$. This is because $[\vec{J}, \vec{L} \cdot \vec{S}] = 0$, and therefore $[\vec{J}, \mathcal{H} + \mathcal{H}_{so}] = 0$, and so $\langle \vec{J} \rangle$ is a constant of the motion according to Griffiths Eq. [3.73]. Hence although we lose m_ℓ and m_s as good quantum numbers, we gain j and m_j . This allows us to write the spin-orbit perturbation operator $\vec{S} \cdot \vec{L}$ in terms of “constants of the motion” as (using the definition of $\vec{J} = \vec{L} + \vec{S}$, squaring it, and solving for $\vec{S} \cdot \vec{L}$, and using the fact that $[\vec{L}, \vec{S}] = 0$);

$$\vec{S} \cdot \vec{L} = \frac{1}{2}(J^2 - L^2 - S^2),$$

so the eigenvalues of $\vec{S} \cdot \vec{L}$ are $\frac{\hbar^2}{2}(j(j+1) - \ell(\ell+1) - s(s+1))$, where $s = 1/2$ for the electron (this assumes we have found the simultaneous eigenfunctions of J^2 , L^2 , and S^2 , which we will do in the next lecture).

Finally we can calculate the first-order correction to the energy of the Hydrogen atom due to the spin-orbit perturbation. Perturbation theory is valid because $\langle \mathcal{H}_{so} \rangle \sim 10^{-4} \text{ eV} \ll |E_n^0| \sim 10 \text{ eV}$. By the standard expression for first order energy correction:

$$E_{n,\ell,s,j}^1 = \iiint \psi_n^{0*} \mathcal{H}_{so} \psi_n^0 d^3r$$

After substituting the appropriate Hydrogen atom wavefunctions (that we shall derive later) and spin-orbit Hamiltonian one arrives at;

$$E_{n,\ell,s,j}^1 = \frac{|E_n^0| \alpha^2}{n} \frac{j(j+1) - \ell(\ell+1) - 3/4}{2\ell(\ell + \frac{1}{2})(\ell+1)}$$

(here we are using the fact that $s = 1/2$ for the electron.) Note that this energy shift is on the order of the fine structure constant squared times the unperturbed eigen-energy, exactly the same form as the relativistic correction. When the two results are combined (Homework 3) the result is the fine structure formula:

$$\Delta E = E_n^{1Relativity} + E_n^{1SpinOrbit} = \frac{|E_n^0| \alpha^2}{n^2} \left[\frac{3}{4} - \frac{n}{j + \frac{1}{2}} \right]$$

This correction is always negative and partially lifts the degeneracy of the unperturbed eigen-energies. See the schematic plot of the fine structure corrections to the energy levels of the Hydrogen atom elsewhere on the [class web site](#). Note that the hydrogen atom states are now labeled by the code " $n\ell_j$ ", where n is the principal quantum number, ℓ is a code letter (s, p, d, f, ...) standing for the value of the orbital angular momentum quantum number (see this [site](#) for the origin of these code letters), and j is the new total angular momentum quantum number. We will figure out the values of j , and the associated eigenfunctions, in the next lecture.

What is the connection between the total angular momentum \vec{J} and our old friends \vec{L}, \vec{S} ? If $\vec{J} = \vec{L} + \vec{S}$ and J^2 has eigenvalue $j(j+1)\hbar^2$, L^2 has eigenvalue $\ell(\ell+1)\hbar^2$, and S^2 has eigenvalue $s(s+1)\hbar^2$, then one might naively think that $j = \ell + s$. However this is not the whole story.