Physics 4261: Lectures for week 3

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3.1 The spin-orbit interaction (Foot 2.3.2)

In addition to the other degrees of freedom, the electron posses a spin with coupling to an external magnetic field given by $H = -\boldsymbol{\mu} \cdot \mathbf{B} = g_s \mu_B \mathbf{s} \cdot \mathbf{B}$. Now μ_B is a constant equal to $e\hbar/2m_e$. What is the field that the electron experiences? We will make a boost to a reference frame comoving with the electron, and calculate the magnetic field given by the (now moving) proton. Let us consider the proton as moving with velocity $-\mathbf{v}$ and located a distance $\mathbf{r}$ away from the electron. Then, according to the Biot-Savart law,

$$\mathbf{B} = \frac{\mu_0}{4\pi} \frac{-e\mathbf{v} \times \mathbf{r}}{|\mathbf{r}|^3} = -\frac{1}{c^2} \mathbf{v} \times \mathbf{E} = \frac{1}{m_e c^2} \mathbf{E} \times \mathbf{p}.$$

Now the vector operator $\mathbf{E}$ points in the direction of r, and we can write it as

$$\mathbf{E} = \frac{1}{e} \frac{\partial V}{\partial r} \frac{\mathbf{r}}{r} = \frac{e/4\pi\epsilon_0}{r^3} \mathbf{r}.$$

Therefore we can express B in terms of the angular momentum $\mathbf{l}$ (adopting the books convention of pulling $\hbar$ out of $\mathbf{l}$),

$$\mathbf{B} = \frac{\hbar e/4\pi\epsilon_0}{m_e c^2} \frac{1}{r^3} \mathbf{l}.$$

Putting the entire interaction together, we ought to have

$$H = \frac{g_s \hbar^2 e^2/4\pi\epsilon_0}{2m_e^2 c^2} \frac{1}{r^3} \mathbf{s} \cdot \mathbf{l},$$
$$H = g_s \alpha^2 hc a_0^3 R_\infty \frac{1}{r^3} \mathbf{s} \cdot \mathbf{l},$$

where we introduced the fine structure constant $\alpha = e^2/4\pi\epsilon_0\hbar c$. Now, the factors of c showing up should convince us that this might be a relativistic effect, and indeed, the strength of the interaction depends on the velocity compared to c, in that the magnetic field strength can also be derived by. This should lead us to consider if there are other, relativistic effects which we missed, and of course there are. One, called the Thomas precession, predicts. These effects are sort of hard to work through, and the best way to get all relativistic atomic effects is to start from the Dirac equation (which we are not discussing), and derive them that way. But we are just going to quote the results. And that is, that g_s is replaced by $g_s - 1$, and that $g_s - 1$ is equal to 1.

The quantity $\mathbf{s} \cdot \mathbf{l}$ actually commutes with the Hamiltonian, whereas the factor $\frac{1}{r^3}$, does not. So we will use perturbation theory, which at this order is simply to replace $1/r^3$ by it's expectation value. This is something we can compute by various clever tricks, but this is all beside the point and we will just say, for now, that we have some number sitting in front of $\mathbf{s} \cdot \mathbf{l}$.

3.2 Angular momentum tricks

Now we want to compute the spectrum of $\mathbf{s} \cdot \mathbf{l}$. Let us consider the operator $\mathbf{j} = \mathbf{s} + \mathbf{l}$. Now, we want to prove a few things:

1. $[j_z, \mathbf{l}^2] = 0$
2. $[j_z, \mathbf{s}^2] = 0$
3. $[j_z, \mathbf{s} \cdot \mathbf{l}] = 0$.

A useful expansion is

$$\mathbf{j}^2 = l_z s_z + \frac{1}{2}\left(l_+ s_- + l_- s_+\right).$$

So we have a complete set of commuting observables $\mathbf{j}^2, j_z, \mathbf{s}^2, \mathbf{l}^2$. Now $\mathbf{s}^2 = 3/4$, $\mathbf{l}^2 = l(l+1)$. So we need to compute the spectrum of $\mathbf{j}^2$. Now, $\mathbf{j}^2$ will be $j(j+1)$ for some allowed values of j. The maximum possible value will be $l + s$, because this is the largest j_z can ever be! The next observation to make, is that the total number of states in the Hilbert space needs to be constant. In the l, s basis, we have $(2l+1)(2s+1)$ states. In the so-called "stretched" configuration, there are $(2l+2s+1)$ states. If we lower the total angular momentum j by 1, there would be a $(2l+2s-1)$ states. If we sum all the way down to zero (sort of, in the half integer case), we would get $(l+s+1)^2$ states. Some math now shows

$$(l+s+1)^2 = (2l+1)(2s+1) = l^2 + s^2 - 2sl = (l-s)^2.$$

So this suggests that the sum should run from $(2l+2s+1)$ down to $(2|l-s|+1)$. In fact it can be shown that this sum gets the required number of states.

Now the task is to find the value of $\mathbf{s} \cdot \mathbf{l}$. But this can be seen form

$$2\mathbf{s} \cdot \mathbf{l} = \mathbf{j}^2 - \mathbf{l}^2 - \mathbf{s}^2.$$

For $s = 1/2$, the allowed values are $j + 1/2$ and $j - 1/2$, so the dot product takes the values $l/2$ and $-l/2 - 1/2$, which differ by $l + 1/2$. Quoting a result for the expectation of $1/r^3$, which is

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{(na_0)^3} \frac{1}{l(l+\frac{1}{2})(l+1)},$$

we arrive at the spin orbit splittings

$$E_+ = \frac{\alpha^2 hcR_\infty}{2n^3} \frac{l}{l(l+\frac{1}{2})(l+1)},$$
$$E_- = -\frac{\alpha^2 hcR_\infty}{2n^3} \frac{l+1}{l(l+\frac{1}{2})(l+1)}.$$

3.3 Full hydrogen atom picture

There are a few other relativistic effects which we have neglected. The first is the relativistic dispersion correction, which contributes and negative shift of $\alpha^2 hcR_\infty/2n^3(1/(l+1/2)-3/4n)$. The second is called the Darwin term, and only affects s states. When the dust settles, the most important factor is that only the total angular momentum j matters, not l or s. This means in particular that the Dirac equation predicts that the $2s$ and $2p_{1/2}$ states are degenerate. In fact, this is also not true, there is an effect called the Lamb shift, which is a QED calculation we won't discuss too much, but it predicts a small shift between these levels. So a full picture of the states is as follows. Schrödinger predicts a huge degeneracy, Dirac lifts the degeneracy but adds a new one based on j, and Lamb lifts all the degeneracies.

3.4 Lamb's experiment

Here we are going to talk briefly about the Lamb shift and how it's measured. In the late nineteen thirties, it was suspected that the $2s_{1/2}$ state was shifted up in energy relative to the $2p_{1/2}$ state, although the two should be the same. This was observed based on the splitting of the Balmer α line. Knowing about selection rules, let us count the sub-shell transitions which could possibly account for the Balmer α line. We start with principle quantum number 2, so we have the states $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$. The s state can transition to $3p_{1/2}$ or $3p_{3/2}$, and either of the $2p$ states can transition to $3s_{1/2}$, or to $3d_{3/2}$ or $3d_{5/2}$, for a total of 8 possible transitions. However, there is one which is forbidden, which is $2p_{1/2} \to 3d_{5/2}$, because total angular momentum cannot be conserved. The Dirac theory predicts the spacing for these transitions, and also predicts that $2s_{1/2} \to 3p_{1/2}$ and $2p_{1/2} \to 3s_{1/2}$ are coincident, as are $2s_{1/2} \to 3p_{3/2}$ and $2p_{1/2} \to 3d_{3/2}$. However, the observed spacings did not match the theory precisely, and it was suspected that $2s_{1/2}$ is shifted relative to $2p_{1/2}$. After the war, using microwave technology developed for radar, Lamb was able to shoot a beam of hydrogen in the metastable $2s_{1/2}$ state, and use microwaves to directly drive the $2s_{1/2} \to 2p_{3/2}$, and, importantly, the $2s_{1/2} \to 2p_{1/2}$ transition, the second of which was expected to occur at zero frequency, but which Lamb found to be shifted by about 1000 MHz. This was explained by Hans Bethe in an interesting way: perturbation theory by radiation and absorption of spontaneous photons predicts an (infinite) negative shift to the $2s$ level. However, for a free electron, there is a similar shift, such that if one subtracts the free electron shift from the $2s$ level shift, a finite positive shift of the $2s$ level results. This has major implications for the understanding of observed particle properties.