Abstract

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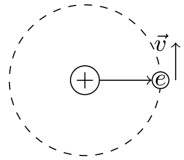
0.0.1 Relativistic Corrections to the Atom (Guest: Prof. Mike Zaletel)

Hydrogen atom hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_k + \hat{H}_{s.o.} + \hat{H}_D$$

where H_0 is the usual hamiltonian, H_k contains corrections gained by inclusion of $\hat{p}^4$, $\hat{H}_{s.o.}$ is $\vec{L} \cdot \vec{S}$, or the spin orbit coupling term, and $\hat{H}_D$ is the "Darwin" component.



If we switch to the frame of our electron, the proton should move with velocity $-\vec{v}$. Let the charge of the proton be Z, so we get, in CGS units that our magnetic field should be

$$\vec{B} = \frac{-Ze\vec{v} \times \vec{r}}{cr^3}$$

Since the electron carries a spin, we want

$$\hat{H}_{so} = -\vec{mu} \cdot \vec{B}$$

We're gonna be off by a factor of 2, but that's because we aren't using the dirac equation to find solutions here. Moving on with that in mind, we write that

$$\vec{\mu} = g\mu_B \vec{S}$$

so the spin orbit coupling becomes

$$\frac{Ze^2}{m_e^2 c^2 r^3} \vec{S} \cdot \vec{L}$$

Remember, we have the factor of two though, so the actual result should be

$$\frac{Ze^2}{2m_e^2 c^2 r^3} \vec{S} \cdot \vec{L}$$

Our base hamiltonian has eigenspectra $H_0 : |n, \ell, m\rangle$. When we go to spin, we get $|n, \ell, m\rangle \otimes \left|Z = \pm\frac{1}{2}\right\rangle$. This is gonna yeet our $SO(3)$ symmetry in ℓ, Z, which is sad! But if we want to make this easier, we should take

$$\vec{J} = \vec{L} + \vec{S}$$

We should note the following properties

$$[\vec{L}^2, \hat{H}_{so}] = 0 \qquad\qquad [\vec{S}^2, \hat{H}_{so}] = 0$$

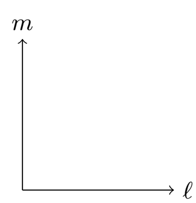
An easy way to show this is that

$$[J, J^2] = [J, (L+S)^2] = [L+S, L^2 + 2LS + S^2]$$

We have that $[L+S, L^2] = 0, [L+S, S^2] = 0$, o we have

$$2[J, LS] = 0$$

so $[J, LS] = 0$. Let's just yEET n into obliviou for a moment, and think about the level diagram of our basis for ℓ, m.



We now have this general set of states

$$|n, \ell, m\rangle |\uparrow\rangle , |n, \ell, m+1\rangle |\downarrow\rangle$$

that have the same ℓ, J^2. What we want to focus on is

$$H_{so} = \beta 2 L \cdot S$$

Let's break $L \sim L_+, L_-, L_z$, andsame for $S \sim S_-, S_+, S_z$. If we go through these relations, we should just get that

$$2L \cdot S = L_+ S_- + L_- S_+ + 2L_z S_z$$

WE can then try and write down the total contribution to the hamiltonian for each individual term

$$2L_z S_z = \hbar^2 \begin{bmatrix} m & 0 \\ 0 & -(m+1) \end{bmatrix}$$

We can try and make out the second component, which is tedious apprantly, so he just reports the result, which has all those cancer tier off diagonal elements

$$L_+S_- + L_-S_+ = \hbar^2 \begin{bmatrix} 0 & \sqrt{\ell(\ell+1) - m(m+1)} \\ \sqrt{\ell(\ell+1) - m(m+1)} & 0 \end{bmatrix}$$

We compute the characteristic polynomial to be

$$\lambda^\lambda - \ell(\ell+1) = 0$$

which gives

$$\ell_+ = \ell \qquad\qquad \ell_- = -(\ell+1)$$

We can use this to work out the new energy spectrum

$$\hbar j(j+1) = \vec{J}^2 = L^2 + 2LS + S^2 = \hbar^2 \left(\ell(\ell+1) + \frac{1}{2}\left(\frac{1}{2}+1\right) + 2LS \right)$$

or

$$\hbar^2 j(j+1) = \hbar^2 \left(\ell(\ell+1) + \frac{1}{2}\left(\frac{1}{2}+1\right) + \begin{cases} \ell \\ -\ell - 1 \end{cases} \right)$$

We can hybridize then, to get

$$|n, \ell, j, m_j\rangle \,; m_j = \hbar J_z$$

Now, all that's left to do is actually compute the correction. We know the basis is diagonal, so we just put it in

$$\frac{Ze^2}{4m_e^2c^2} \langle n, \ell, j, m_j| \, 2\vec{L} \cdot \vec{S} \frac{1}{\hat{r}^3} \, |n, \ell, j, m_j\rangle$$

We dont know the expectation value $\langle \frac{1}{r^3} \rangle_{n,\ell}$, which townsend leaves as an excercise, and comes out to be

$$\langle \frac{1}{r^3} \rangle = \frac{Z^3}{a_0^3 n^3 l \left(l + \frac{1}{2}\right)(l+1)}$$

Then,

$$\langle 2LS \rangle = \begin{cases} \ell \\ -(\ell+1) \end{cases}$$

Finally, in it's full glory, we should have

$$\frac{Ze^2}{4m_e^2c^2} \langle n, \ell, j, m_j| \, 2\vec{L} \cdot \vec{S} \frac{1}{\hat{r}^3} \, |n, \ell, j, m_j\rangle = \frac{Z^3}{a_0^3 n^3 l \left(l + \frac{1}{2}\right)(l+1)} \begin{cases} \ell \\ -(\ell+1) \end{cases}$$

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