Week 9 Worksheet
Fine Structure of Hydrogen

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Exercise 0. Warm up.

a) What are the physical effects that make up fine structure?

b) Write down H_r, the relativistic hamiltonian, and explain its physical origin.
   Hint: Expand the relativistic energy for $v \ll c$.

c) Starting with $H = -\boldsymbol{\mu} \cdot \mathbf{B}$, explain how you would determine H_{SO}, and explain its physical origin. You don't have to get an explicit expression.

d) ***Optional Challenge:*** Compute H_{SO}.

Exercise 1. Darwin Term. In class, you found that the spin-orbit coupling gave a first-order correction to the energy

$$E_{\text{SO}}^1 = \frac{E_n{}^2}{mc^2} \frac{n[j(j+1) - \ell(\ell+1) - 3/4]}{\ell(\ell+1/2)(\ell+1)}.$$

a) What is E_{SO}^1 for s-states, i.e. those with $\ell = 0$?
   Hint: If $\ell = 0$, then what values can $\mathbf{L} \cdot \mathbf{S}$ take?

b) There is an additional effect for s-states called the **Darwin term**:

$$H_D = \frac{\hbar^2}{8m^2c^2} e^2 \nabla^2 V_C,$$

where $V_C = -e/r$ is the Coulomb potential. This term can be derived from the Dirac equation, but we can get a handle on it using non-relativistic QM. To see where the term comes from, the Dirac equation (relativistic quantum mechanics) predicts that the electron does not have a constant position. Instead, it undergoes a frantic jittering motion due to the creation of virtual positron-electron pairs. The lifetime of these is given by the uncertainty principle $\Delta t \Delta E = \hbar$, so $\Delta t = \hbar/mc^2$. The position of the electron is smeared out due to this motion by the characteristic distance associated to this lifetime, the Compton wavelength: $\lambda_c \equiv c\Delta t = \hbar/mc \approx 4 \cdot 10^{-11}$ cm. So the potential energy is not at a particular position; rather, it is an average around that point. Suppose that r_0 is the average position, and expand the potential $V_C(r)$ as a Taylor expansion to second order about r_0.

c) Use symmetry to argue that the expectation value of the first term in the expansion is 0.

d) Use the same symmetry and dimensional analysis to argue that

$$\langle V_C(r) \rangle \approx V_C(r_0) + A\frac{\hbar^2}{m^2c^2}4\pi e^2 \delta^{(3)}(\mathbf{r}),$$

where A is a dimensionless constant. We call the second term the **Darwin term**. Calculate A, and show that this reproduces H_D exactly, *assuming that the characteristic length is actually $\lambda_c \sqrt{3/4}$.*

e) Argue that this term has an expectation value only for s-states.

f) Use the fact that $R_{n0}(0) = 2/(na_0)^{3/2}$, where $a_0 = \hbar^2/me^2$, and that

$$E_r^1 = -\frac{E_n{}^2}{2mc^2}(8n-3)$$

for s-states to calculate E_{fs}^1 for such states. Compare to the formula in Griffiths,

$$E_{\mathrm{fs}}^1 = -\frac{2E_n{}^2}{mc^2}\left(\frac{n}{j+1/2}-3/4\right).$$

Hints: Note that $E_n = -mc^2\alpha^2/2n^2$. You can determine α by combining the fundamental constants of the hydrogen atom ($\hbar$, e, c) into a dimensionless constant. By the way, why does m not appear in the fine structure constant?

Remark 1. This calculation agrees with the physical intuition that in s-states the spin-orbit coupling should be 0. It explains the fine structure energy correction derived in Griffiths. There, Griffiths makes the assumption that E_{SO}^1 is *not* zero for s-states in order to complete the derivation.

Remark 2. You may have noticed that we cheated by assuming that the characteristic length was $\lambda_c \sqrt{3/4}$ rather than just λ_c. Unfortunately, there isn't a good justification for this. The Darwin term and all of fine structure can be derived rigorously from the Dirac equation, and that's all there is to it. The Schrödinger theory just isn't a good theory for dealing with truly relativistic effects.