CHAPTER 12.

1. With a potential of the form

$$V(r) = \frac{1}{2} m\omega^2 r^2$$

the perturbation reduces to

$$H_1 = \frac{1}{2m^2c^2}\mathbf{S}\bullet\mathbf{L}\frac{1}{r}\frac{dV(r)}{dr} = \frac{\omega^2}{4mc^2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2)$$
$$= \frac{(\hbar\omega)^2}{4mc^2}\big(j(j+1) - l(l+1) - s(s+1)\big)$$

where l is the orbital angular momentum, s is the spin of the particle in the well (e.g. 1/2 for an electron or a nucleon) and j is the total angular momentum. The possible values of j are $l + s, l + s - 1, l + s - 2, \ldots |l - s|$.

The unperturbed energy spectrum is given by $E_{n_r l} = \hbar\omega(2n_r + l + \frac{3}{2})$. Each of the levels characterized by l is $(2l + 1)$-fold degenerate, but there is an additional degeneracy, not unlike that appearing in hydrogen. For example $n_r = 2$, $l = 0$. $n_r = 1$, $l = 2$, $n_r = 0$, $l = 4$ all have the same energy.
A picture of the levels and their spin-orbit splitting is given below.

2. The effects that enter into the energy levels corresponding to $n = 2$, are (I) the basic Coulomb interaction, (ii) relativistic and spin-orbit effects, and (iii) the hyperfine structure which we are instructed to ignore. Thus, in the absence of a magnetic field, the levels under the influence of the Coulomb potential consist of $2n^2 = 8$ degenerate levels. Two of the levels are associated with $l = 0$ (spin up and spin down) and six levels with l = 0, corresponding to m_l = 1,0,-1, spin up and spin down. The latter can be rearranged into states characterized by $\mathbf{J}^2$, $\mathbf{L}^2$ and J_z. There are two levels characterized by $j = l - 1/2 = 1/2$ and four levels with $j = l + 1/2 = 3/2$. These energies are split by relativistic effects and spin-orbit coupling, as given in Eq. (12-16). We ignore reduced mass effects (other than in the original Coulomb energies). We therefore have

$$\Delta E = -\frac{1}{2} m_e c^2 \alpha^4 \frac{1}{n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)$$
$$= -\frac{1}{2} m_e c^2 \alpha^4 \left(\frac{5}{64}\right) \qquad j = 1/2$$
$$= -\frac{1}{2} m_e c^2 \alpha^4 \left(\frac{1}{64}\right) \qquad j = 3/2$$

(b) The Zeeman splittings for a given j are

$$\Delta E_B = \frac{e\hbar B}{2m_e} m_j \left(\frac{2}{3}\right) \qquad j = 1/2$$
$$= \frac{e\hbar B}{2m_e} m_j \left(\frac{4}{3}\right) \qquad j = 3/2$$

Numerically $\frac{1}{128} m_e c^2 \alpha^4 \approx 1.132 \times 10^{-5} eV$, while for B = 2.5T $\frac{e\hbar B}{2m_e} = 14.47 \times 10^{-5} eV$, so under these circumstances the magnetic effects are a factor of 13 larger than the relativistic effects. Under these circumstances one could neglect these and use Eq. (12-26).

3. The unperturbed Hamiltonian is given by Eq. (12-34) and the magnetic field interacts both with the spin of the electron and the spin of the proton. This leads to

$$H = A\frac{\mathbf{S} \bullet \mathbf{I}}{\hbar^2} + a\frac{S_z}{\hbar} + b\frac{I_z}{\hbar}$$

Here

$$A = \frac{4}{3}\alpha^4 m_e c^2 g_P \left(\frac{m_e}{M_P}\right)\frac{\mathbf{I} \bullet \mathbf{S}}{\hbar^2}$$
$$a = 2\frac{e\hbar B}{2m_e}$$
$$b = -g_P \frac{e\hbar B}{2M_p}$$

Let us now introduce the total spin **F = S + I.** It follows that

$$\frac{\mathbf{S}\bullet\mathbf{I}}{\hbar^2} = \frac{1}{2\hbar^2}\left(\hbar^2 F(F+1) - \frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2\right)$$
$$= \frac{1}{4} \qquad for \quad F = 1$$
$$= -\frac{3}{4} \qquad for \quad F = 0$$

We next need to calculate the matrix elements of $aS_z + bI_z$ for eigenstates of $\mathbf{F}^2$ and F_z . These will be exactly like the spin triplet and spin singlet eigenstates. These are

$$\langle 1,1 |\, aS_z + bI_z \,| 1,1\rangle = \langle \chi_+\xi_+ \,|\, aS_z + bI_z \,|\, \chi_+\xi_+\rangle = \frac{1}{2}(a+b)$$
$$\langle 1,0 |\, aS_z + bI_z \,| 1,0\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \langle \chi_+\xi_- + \chi_-\xi_+ \,|\, aS_z + bI_z \,|\, \chi_+\xi_- + \chi_+\xi_-\rangle = 0$$
$$\langle 1,-1 |\, aS_z + bI_z \,| 1,-1\rangle = \langle \chi_-\xi_- \,|\, aS_z + bI_z \,|\, \chi_-\xi_-\rangle = -\frac{1}{2}(a+b)$$

And for the singlet state (F = 0)

$$\langle 1,0 |\, aS_z + bI_z \,| 0,0\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \langle \chi_+\xi_- + \chi_-\xi_+ \,|\, aS_z + bI_z \,|\, \chi_+\xi_- - \chi_+\xi_-\rangle = \frac{1}{2}(a-b)$$
$$\langle 0,0 |\, aS_z + bI_z \,| 0,0\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \langle \chi_+\xi_- - \chi_-\xi_+ \,|\, aS_z + bI_z \,|\, \chi_+\xi_- - \chi_+\xi_-\rangle = 0$$

Thus the magnetic field introduces mixing between the |1,0> state and the |0.0> state. We must therefore diagonalize the submatrix

$$\begin{pmatrix} A/4 & (a-b)/2 \\ (a-b)/2 & -3A/4 \end{pmatrix} = \begin{pmatrix} -A/4 & 0 \\ 0 & -A/4 \end{pmatrix} + \begin{pmatrix} A/2 & (a-b)/2 \\ (a-b)/2 & -A/2 \end{pmatrix}$$

The second submatrix commutes with the first one. Its eigenvalues are easily determined to be $\pm\sqrt{A^2/4 + (a-b)^2/4}$ so that the overall eigenvalues are

$$-A/4 \pm \sqrt{A^2/4 + (a-b)^2/4}$$

Thus the spectrum consists of the following states:

F = 1, F_z = 1 $\qquad E = A/4 + (a+b)/2$

F =1, F_z = -1 $\qquad E = A/4 - (a+b)/2$

F = 1,0; F_z = 0 $\qquad E = -A/4 \pm \sqrt{(A^2/4 + (a-b)^2/4}$

We can now put in numbers.
For $B = 10^{-4}$ T, the values, in units of 10^{-6} eV are 1.451, 1.439, 0(10^{-10}), -2.89
For B = 1 T, the values in units of 10^{-6} eV are 57.21,-54.32, 54.29 and 7 x 10^{-6}.

4. According to Eq. (12-17) the energies of hydrogen-like states, including relativistic + spin-orbit contributions is given by

$$E_{n,j} = -\frac{1}{2}\frac{m_e c^2 (Z\alpha)^2}{(1+m_e/M_p)}\frac{1}{n^2} - \frac{1}{2}m_e c^2 (Z\alpha)^4 \frac{1}{n^3}\left(\frac{1}{j+1/2} - \frac{3}{4n}\right)$$

The wavelength in a transition between two states is given by

$$\lambda = \frac{2\pi\hbar c}{\Delta E}$$

where ΔE is the change in energy in the transition. We now consider the transitions n =3, j = 3/2 → n = 1, j = 1/2 and n = 3 , j = 1/2 → n = 1, j = 1/2.. The corresponding energy differences (neglecting the reduced mass effect) is

(3,3/2→1,1/2) $\qquad \Delta E = \frac{1}{2}m_e c^2 (Z\alpha)^2 (1-\frac{1}{9}) + \frac{1}{2}m_e c^2 (Z\alpha)^4 \frac{1}{4}(1-\frac{1}{27})$

(3,1/2→1,1/2) $\qquad \frac{1}{2}m_e c^2 (Z\alpha)^2 (1-\frac{1}{9}) + \frac{1}{2}m_e c^2 (Z\alpha)^4 \frac{1}{4}(1-\frac{3}{27})$

We can write these in the form

(3,3/2→1,1/2) $\qquad \Delta E_0 (1 + \frac{13}{48}(Z\alpha)^2)$

(3,1/2→1,1/2) $\qquad \Delta E_0 (1 + \frac{1}{18}(Z\alpha)^2)$

where

$$\Delta E_0 = \frac{1}{2}m_e c^2 (Z\alpha)^2 \frac{8}{9}$$

The corresponding wavelengths are

(3,3/2→1,1/2) $\lambda_0(1-\frac{13}{48}(Z\alpha)^2) = 588.995\times 10^{-9}m$

(3,1/2→1,1/2) $\lambda_0(1-\frac{1}{18}(Z\alpha)^2) = 589.592\times 10^{-9}m$

We may use the two equations to calculate λ_0 and Z. Dividing one equation by the other we get, after a little arithmetic Z = 11.5, which fits with the Z = 11 for Sodium. (Note that if we take for λ_0 the average of the two wavelengths, then , using $\lambda_0 = 2\pi\hbar c / \Delta E_0 = 9\pi\hbar / 2mc(Z\alpha)^2$, we get a seemingly unreasonably small value of Z = 0.4! This is not surprising. The ionization potential for sodium is 5.1 eV instead of Z^2(13.6 eV), for reasons that will be discussed in Chapter 14)

4. The relativistic correction to the kinetic energy term is $-\frac{1}{2mc^2}\left(\frac{\mathbf{p}^2}{2m}\right)^2$. The energy shift in the ground state is therefore

$$\Delta E = -\frac{1}{2mc^2}\langle 0|\left(\frac{\mathbf{p}^2}{2m}\right)^2|0\rangle = -\frac{1}{2mc^2}\langle 0|(H-\frac{1}{2}m\omega^2 r^2)^2|0\rangle$$

To calculate $< 0 | r^2 | 0 >$ and $< 0 | r^4 | 0 >$ we need the ground state wave function. We know that for the one-dimensional oscillator it is

$$u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

so that for the three dimensional oscillator it is

$$u_0(r) = u_0(x)u_0(y)u_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar}$$

It follows that

$$\langle 0|r^2|0\rangle = \int_0^\infty 4\pi r^2 dr \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} r^2 e^{-m\omega r^2/\hbar} =$$

$$= 4\pi\left(\frac{m\omega}{\pi\hbar}\right)^{3/2}\left(\frac{\hbar}{m\omega}\right)^{5/2}\int_0^\infty dy y^4 e^{-y^2}$$

$$= \frac{3\hbar}{2m\omega}$$

We can also calculate

$$
\begin{aligned}
\langle 0 | r^4 \, | 0 \rangle &= \int_0^\infty 4\pi r^2 dr \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} r^4 e^{-m\omega r^2/\hbar} = \\
&= 4\pi \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} \left(\frac{\hbar}{m\omega} \right)^{7/2} \int_0^\infty dy y^6 e^{-y^2} \\
&= \frac{15}{4} \left(\frac{\hbar}{m\omega} \right)^2
\end{aligned}
$$

We made use of $\int_0^\infty dz z^n e^{-z} = \Gamma(n+1) = n\Gamma(n) \quad and \quad \Gamma(\frac{1}{2}) = \sqrt{\pi}$

Thus

$$
\begin{aligned}
\Delta E &= -\frac{1}{2mc^2} \left(\left(\frac{3}{2} \hbar\omega \right)^2 - \left(\frac{3}{2} \hbar\omega \right) \left(m\omega^2 \frac{3\hbar}{2m\omega} \right) + \frac{1}{4} m^2 \omega^4 \left(\frac{15}{4} \right) \left(\frac{\hbar}{m\omega} \right)^2 \right) \\
&= -\frac{15}{32} \frac{(\hbar\omega)^2}{mc^2}
\end{aligned}
$$

6. (a) With $J = 1$ and $S = 1$, the possible values of the orbital angular momentum, such that $j = L + S, L + S - 1 \ldots |L - S|$ can only be $L = 0,1,2$. Thus the possible states are ${}^3S_1, {}^3P_1, {}^3D_1$. The parity of the deuteron is $(-1)^L$ assuming that the intrinsic parities of the proton and neutron are taken to be +1. Thus the S and D states have positive parity and the P state has opposite parity. Given parity conservation, the only possible admixture can be the ${}^3D_1$ state.

(b)The interaction with a magnetic field consists of three contributions: the interaction of the spins of the proton and neutron with the magnetic field, and the **L.B** term, if L is not zero. We write

$$
H = -\mathbf{M}_p \bullet \mathbf{B} - \mathbf{M}_n \bullet \mathbf{B} - \mathbf{M}_L \bullet \mathbf{B}
$$

$$
\mathbf{M}_p = \frac{eg_p}{2M} \mathbf{S}_p = (5.5792) \frac{e\hbar}{2M} \left(\frac{\mathbf{S}_p}{\hbar} \right)
$$

where $\mathbf{M}_n = \frac{eg_n}{2M} \mathbf{S}_n = (-3.8206) \frac{e\hbar}{2M} \left(\frac{\mathbf{S}_n}{\hbar} \right)$

$$
\mathbf{M}_L = \frac{e}{2M_{red}} \mathbf{L}
$$

We take the neutron and proton masses equal (= M) and the reduced mass of the two-particle system for equal masses is $M/2$. For the ${}^3S_1$ stgate, the last term does not contribute.

If we choose **B** to define the *z* axis, then the energy shift is

$$-\frac{eB\hbar}{2M}\langle {}^3S_1 \,|\, g_p\left(\frac{S_{pz}}{\hbar}\right) + g_n\left(\frac{S_{nz}}{\hbar}\right)|{}^3S_1\rangle$$

We write

$$g_p\left(\frac{S_{pz}}{\hbar}\right) + g_n\left(\frac{S_{nz}}{\hbar}\right) = \frac{g_p + g_n}{2}\frac{S_{pz} + S_{nz}}{\hbar} + \frac{g_p - g_n}{2}\frac{S_{pz} - S_{nz}}{\hbar}$$

It is easy to check that the last term has zero matrix elements in the triplet states, so that we are left with $\frac{1}{2}(g_p + g_n)\frac{S_z}{\hbar}$, where S_z is the z-component of the total spin.. Hence

$$\langle {}^3S_1 \,|\, H_1|{}^3S_1\rangle = -\frac{3B\hbar}{2M}\frac{g_p + g_n}{2}m_s$$

where m_s is the magnetic quantum number (m_s = 1,0,-1) for the total spin. We may therefore write the magnetic moment of the deuteron as

$$\mu_{eff} = -\frac{e}{2M}\frac{g_p + g_n}{2}\mathbf{S} = -(0.8793)\frac{e}{2M}\mathbf{S}$$

The experimental measurements correspond to g_d = 0.8574 which suggests a small admixture of the ${}^3D_1$ to the deuteron wave function.