

# PROBLEM SHEET 10

## FYS3110

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### PROBLEM 10.1

The Zeeman correction, when choosing the external field  $\mathbf{B}_{ext}$  to lie along the  $z$ -axis, can be expressed by the following condensed formula.

$$(1) \quad E_Z^1 = \mu_B g_J B_{ext} j_z,$$

where

$$(2) \quad \mu_B = \frac{e\hbar}{2m} = 5.788 \times 10^{-5} eV/T$$

is the Bohr magneton, and

$$(3) \quad g_J = 1 + \frac{j(j+1) + \frac{3}{4} - l(l+1)}{2j(j+1)}$$

is the Landé g-factor. Adding the fine structure equation

$$(4) \quad E_{nj} = -\frac{13.6eV}{n^2} \left[ 1 + \frac{\alpha^2}{n^2} \left( \frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right]$$

to the Zeeman correction (equation 1) yields an equation for total energy in presence of weak-field Zeeman effect

$$(5) \quad E_{nljj_z} = -\frac{13.6eV}{n^2} \left[ 1 + \frac{\alpha}{n^2} \left( \frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right] + \mu_B g_J B_{ext} j_z.$$

The weak-field Zeeman splitting for the first excited state of the hydrogen atom ( $n = 2$ ) is shown in figure 1. The energy  $E_2$  is plotted against  $\mu_B B_{ext}$  and we, evidently, get straight lines with slope  $g_J j_z$ , for every possible value of  $j_z$ . The energy splitting is very clear.

### PROBLEM 10.2

Assume that the proton of the hydrogen atom has finite size, in the shape of a sphere with radius  $b = 1 \times 10^{-15} m$ . This would give it the proton an electric potential of

$$(6) \quad V(r) = \begin{cases} \frac{e}{4\pi\epsilon_0 b} \left( \frac{3}{2} - \frac{r^2}{2b^2} \right), & r \leq b \\ \frac{e}{4\pi\epsilon_0 r}, & r > b \end{cases}$$

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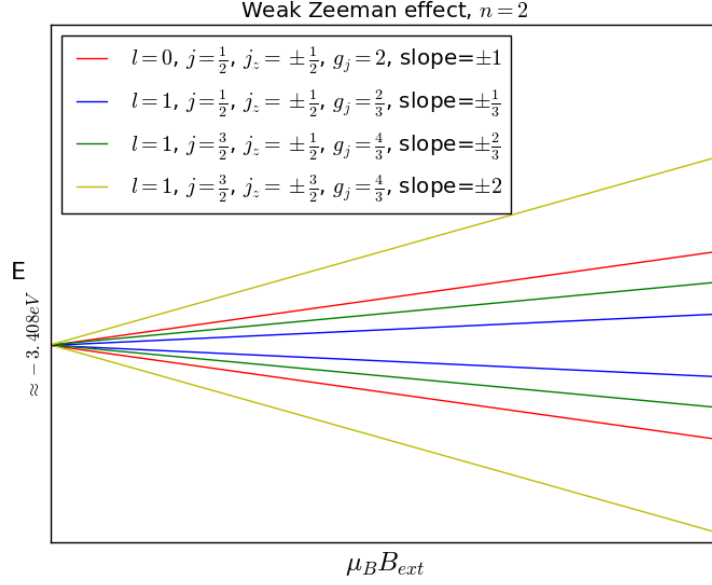


FIGURE 1. Weak-field Zeeman splitting of the first excited state of hydrogen

and the electrostatic potential of an electron present in this potential would be  $-eV(r)$ . Unperturbed potential is  $-\frac{e^2}{4\pi\epsilon_0 r}$  which gives a perturbation of

$$(7) \quad \Delta V(r) = \begin{cases} -\frac{e^2}{4\pi\epsilon_0 b} \left( \frac{3}{2} - \frac{r^2}{2b^2} \right) + \frac{e^2}{4\pi\epsilon_0 r}, & r \leq b \\ 0, & r > b. \end{cases}$$

The unperturbed ground state wave function for hydrogen is

$$(8) \quad |100\rangle = \frac{1}{\sqrt{\pi a^3}} e^{-r/a},$$

and the first order energy correction is

$$\begin{aligned} \Delta E &= \langle 100 | \Delta V(r) | 100 \rangle = \frac{1}{\pi a^3} \int_0^\pi \int_0^{2\pi} \int_0^b \Delta V e^{-2r/a} r^2 \sin \phi dr d\theta d\phi \\ &= \frac{4\pi}{\pi a^3} \int_0^b \Delta V(r) e^{-2r/a} r^2 dr \end{aligned}$$

if  $b \ll a$  then  $e^{-2r/a}$ , and we are left with

$$\begin{aligned}\Delta E &= \frac{4}{a^3} \int_0^b \Delta V(r) r^2 dr = \frac{4}{a^3} \int_0^b -\frac{e^2 r^2}{4\pi\epsilon b} \left( \frac{3}{2} - \frac{r^2}{2b^2} \right) + \frac{e^2 r^2}{4\pi\epsilon_0 r} dr \\ &= \frac{4}{a^3} \frac{e^2}{4\pi\epsilon_0} \int_0^b -\frac{3r^2}{2b} + \frac{r^4}{2b^3} + r dr = \frac{4}{a^3} \frac{e^2}{4\pi\epsilon_0} \left( -\left[ \frac{1}{2b} r^3 \right]_0^b + \left[ \frac{1}{10b^3} r^5 \right]_0^b + \left[ \frac{1}{2} r^2 \right]_0^b \right) \\ &= \frac{4}{a^3} \frac{e^2}{4\pi\epsilon_0} \left( -\frac{1}{2} b^2 + \frac{1}{10} b^2 + \frac{1}{2} b^2 \right) = \frac{4}{5} \left( \frac{b}{a} \right)^2 \frac{e^2}{2(4\pi\epsilon_0)a}.\end{aligned}$$

Inserting for the Bohr radius,  $a$ , in the last fraction yields

(9)

$$\Delta E = \frac{4}{5} \left( \frac{b}{a} \right)^2 \frac{m_e e^4}{2(4\pi\epsilon_0)^2 \hbar^2} = \frac{4}{5} \left( \frac{b}{a} \right)^2 Ry \approx 2.85 \times 10^{-10} Ry \approx 3.87 \times 10^{-9} eV$$

For comparison, the fine structure shift is (for  $n = 1$  and  $j = \frac{1}{2}$ )

$$\Delta E_{fs} = 1.8088 \times 10^{-4} eV$$

and the hyperfine structure shift is

$$\Delta E_{hs} = 5.88 \times 10^{-6} eV$$

One can see that the shift due to the perturbation of a finite-size proton is smaller than both the fine structure and hyperfine structure shift.

### PROBLEM 10.3

The wave function for helium is the product of two hydrogen-like electron wave functions in 1s orbitals

$$(10) \quad \psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_{100}(\mathbf{r}_1) \psi_{100}(\mathbf{r}_2) = \frac{Z^3}{\pi a^3} e^{-Z(r_1+r_2)/a},$$

and the helium Hamiltonian is

(11)

$$H = \frac{\hbar^2}{2m_e} (-\nabla_1^2 - \nabla_2^2) \psi(\mathbf{r}_1, \mathbf{r}_2) - \frac{2e^2}{4\pi\epsilon_0} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_2 - \mathbf{r}_1|} = H^0 + H'$$

The first order perturbative correction to the energy level is, as always

$$(12) \quad E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

which, by inserting

$$H' = \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_2 - \mathbf{r}_1|},$$

gives

$$(13) \quad E_n^1 = \frac{e^2}{4\pi\epsilon_0} \left( \frac{Z^3}{\pi a^3} \right)^2 \int \frac{e^{-2Z(r_1+r_2)}}{|\mathbf{r}_2 - \mathbf{r}_1|} d^3\mathbf{r}_1 d^3\mathbf{r}_2 = \frac{5Z}{8a} \left( \frac{e^2}{4\pi\epsilon_0} \right) = -\frac{5Z}{4} E_h$$

Thus the ground state with first order perturbation correction is

$$(14) \quad E_0 = E_0^0 + E_0^1 = -4E_h + \frac{5}{8} Z E_h = -\frac{11}{4} E_h = -74.8 eV$$

when inserting  $Z = 2$ . Variational theory gives the same result.