Solutions Atomic Physics for FYSC11 190826.

1a. $f = \frac{1}{\sqrt{20}}(2\mathrm{Y}_{1,-1} + 4\mathrm{Y}_{1,1})$.

$$\hat{L}_z f = \frac{1}{\sqrt{20}}(2\hat{L}_z \mathrm{Y}_{1,-1} + 4\hat{L}_z \mathrm{Y}_{1,1}) = \frac{1}{\sqrt{20}}(-2\hbar \mathrm{Y}_{1,-1} + 4\hbar \mathrm{Y}_{1,1}) =$$

$\frac{\hbar}{\sqrt{20}}(-2\mathrm{Y}_{1,-1} + 4\mathrm{Y}_{1,1}) \neq a \cdot f$. Thus no eigenfunction.

1b. $$\left\langle \hat{L}_z \right\rangle = \left\langle f \middle| \hat{L}_z f \right\rangle = \frac{\hbar}{20}\left\langle 2\mathrm{Y}_{1,-1} + 4\mathrm{Y}_{1,1} \middle| -2\mathrm{Y}_{1,-1} + 4\mathrm{Y}_{1,1} \right\rangle =$$

$$\frac{\hbar}{20}(-4\left\langle \mathrm{Y}_{1,-1} \middle| \mathrm{Y}_{1,-1} \right\rangle + 16\left\langle \mathrm{Y}_{1,1} \middle| \mathrm{Y}_{1,1} \right\rangle) = \frac{3}{5}\hbar$$

2. Expectation value of radius:

$$\left\langle r \right\rangle = \iiint Y_{0,0}^* R_{1,0}^* \, r \, Y_{0,0} R_{1,0} \, r^2 \sin\theta dr d\theta d\varphi = \text{ (Y normalized)} \int_0^\infty r^3 R_{1,0}^2(r) dr = (\frac{4}{a_0})^3 \cdot 2^2 \cdot \int_0^\infty r^3 e^{-2\cdot 4r/a_0} dr$$

Let $b = \frac{8}{a_0}$ and $B = (\frac{4}{a_0})^3 \cdot 2^2$

$$\left\langle r \right\rangle / B = \text{(partial integration)} \left[-\frac{1}{b} r^3 e^{-br} \right]_0^\infty + \frac{3}{b}\int_0^\infty r^2 e^{-br} dr = \frac{3}{b}\left\{ \left[-\frac{1}{b} r^2 e^{-br} \right]_0^\infty + \frac{2}{b}\int_0^\infty r e^{-br} dr \right\} =$$

$$\frac{6}{b^2}\left\{ \left[-\frac{1}{b} r e^{-br} \right]_0^\infty + \frac{1}{b}\int_0^\infty e^{-br} dr \right\} = \frac{6}{b^4} \Rightarrow \left\langle r \right\rangle = B \cdot \frac{6}{b^4} = (\frac{4}{a_0})^3 \cdot 2^2 \cdot \frac{6}{8^4} a_0^4 = \frac{3}{8} a_0$$

This can be compared to the Bohr radius of $\frac{1}{4} a_0$

3. $R(C)$=109732 cm^{-1}, $\zeta(\text{C V}) = 5$.

$$E_{\text{ion}} = E(3\text{s}) + T(3\text{s}) = E(4\text{s}) + T(4\text{s}) \Rightarrow T(3\text{s}) - T(4\text{s}) = E(4\text{s}) - E(3\text{s}) \Leftrightarrow$$

$$R\zeta^2 \cdot (\frac{1}{(3-\delta)^2} - \frac{1}{(4-\delta)^2}) = E(4\text{s}) - E(3\text{s}) \Leftrightarrow \frac{1}{(3-\delta)^2} - \frac{1}{(4-\delta)^2} = 0,04996$$

We iterate by trial and error

With $\delta = 0,03$ we get $T(3\text{s}) = 311000 \Rightarrow$

$E_{\text{ion}} = 3162180 \text{ cm}^{-1}$

and $T(4\text{s}) = 174060 \Rightarrow$

$E_{\text{ion}} = 3162303 \text{ cm}^{-1}$

NIST value is 1362423 cm^{-1}.

δ	HL
0	0,0486
0,1	0,0532
0,05	0,0508
0,03	0,04992

4a. The central field approximation:

- Each electron moves <u>independently</u> of the other in the electrostatic field from the nucleus and the other N - 1 electrons.
- This field is assumed to be <u>spherically symmetric.</u>

4b. $E = \varepsilon_1 + \varepsilon_2$ and $\Psi = \varphi_1 \cdot \varphi_1$. $\varphi_i = R_{n_i \ell_i}(r_i) \cdot Y_{\ell_i, m_{\ell_i}}(\theta_i, \varphi_i) \cdot \chi_{m_{s_i}}(s_{z_i})$

The first two relations follow from the assumption of independent electrons and the form of the individual wavefunctions follows from the assumption of a spin-independent spherically symmetric potential. Note that in the wavefunction only the radial part is unknown and determined numerically in this model.

5. Magnetic interactions. See literature and lecture notes (summary lecture in particular)

6. A_{6p} = (.041/5+.042/5)/2 = 0.0083 cm^{-1}.
A_{5s} = (Δ_{34}/4 + Δ_{45}/5 +Δ_{56}/6)/3 = (.483/4 + .665/5 + .770/6)/3 = 0.127 cm^{-1}.