Thirteenth quantum mechanics sheet

To be handed in on 07.07.

All points in this sheet are awarded as bonus points.

Q 34: *Hydrogen atom, fine structure* **(16 points)**

Remark: In this question $\vec{L}, \vec{S}$ and $\vec{J}$ are angular momentum operators. The notation ˆ is omitted for these operators.

We consider the Hamiltonian of the Hydrogen atom

$$\hat{H}_0 = \frac{\vec{\hat{P}}^2}{2m} - \frac{Ze^2}{\hat{R}} + \hat{W}, \qquad Z = 1$$

with the spin-orbit interaction (see the lectures)

$$\hat{W} = \frac{Ze^2}{2m_e^2c^2}\frac{1}{\hat{R}^3}\vec{S}\cdot\vec{L}$$

The aim of this exercise is to treat $\hat{W}$ as a perturbation from $\hat{H}_0$ and from this calculate the corrections to the energy levels $E_n^{(0)} = -\frac{m_e Z^2 e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{m_e c^2}{2}\alpha^2\frac{Z^2}{n^2}$ ($\alpha =$ finestructure constant) at first order in perturbation theory. The energy ${E_n}^0$ depends only on the main quantum number n and not on the angular momentum quantum numbers l and m. Therefore we must use the degenerate perturbation theory. We describe the joint Eigenstates $\hat{H}_0, \vec{L}^2$ and L_3 with $|n,l,m_l\rangle$. It follows:

$$\begin{aligned} \hat{H}_0|n,l,m_l\rangle &= E_n^{(0)}|n,l,m_l\rangle \\ \vec{L}^2|n,l,m_l\rangle &= \hbar^2 l(l+1)|n,l,m_l\rangle \\ L_3|n,l,m_l\rangle &= \hbar m_l|n,l,m_l\rangle \\ \psi_{nlm_l}(\vec{r}) &= \langle\vec{r}|n,l,m_l\rangle = R_{nl}(r)Y_{lm_l}(\Omega) \end{aligned}$$

The spin operator $\vec{S}$ is given by $\vec{S} = \frac{\hbar}{2}\vec{\tau}$ with the Pauli matrix τ_i. The state space of $\hat{H} = \hat{H}_0 + \hat{W}$ is spanned by the product of Eigenstates of $\hat{S}_3$ and the Eigenstates $|n,l,m_l\rangle$ of $\hat{H}_0, \vec{L}^2, L_3$:

$$|n,l,m_l,m_s\rangle := |n,l,m_l\rangle|m_s\rangle$$

a) Show that $\hat{W} \sim \vec{L}\cdot\vec{S}$ commutes with $\vec{L}^2$ and $\vec{S}^2$, but not with L_3 and S_3. **(4 points)**

This means that the product state $|n,l,m_l,m_s\rangle$ does not build an appropriate basis for the perturbed theory, because of the energy level degeneracy of l, m_l and m_s. One must build for a fixed l sub vector space, a new basis through linear combinations of $|n,l,m_l,m_s\rangle$, in which $\hat{W} \sim \vec{L}\cdot\vec{S}$ is diagonal (= angular momentum coupling). To do this one uses $\vec{L}$ and $\vec{S}$ to build a new operator $\vec{J}$ of the total angular momentum:

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

b) Show that the components J_i satisfy the angular momentum commutation relation, i.e. that

$$[J_i, J_j] = i\hbar\sum_k \epsilon_{ijk}J_k\,.$$

show furthermore that

$$\left[J_3, \vec{L}^2\right] = \left[J_3, \vec{S}^2\right] = \left[J_3, \vec{J}^2\right] = 0$$
$$\left[\vec{J}^2, \vec{L}^2\right] = \left[\vec{J}^2, \vec{S}^2\right] = \left[\vec{L}^2, \vec{S}^2\right] = 0$$

(5 points)

From b) it follows that it is possible to form joint Eigenvectors of $\vec{J}^2, J_3, \vec{L}^2$ and $\vec{S}^2$. We describe these Eigenvectors $|j, m_j; l, s\rangle$ with

$$\begin{aligned}
\vec{J}^2|j, m_j; l, s\rangle &= \hbar^2 j(j+1)|j, m_j; l, s\rangle \\
J_3|j, m_j; l, s\rangle &= \hbar m_j|j, m_j; l, s\rangle \\
\vec{L}^2|j, m_j; l, s\rangle &= \hbar^2 l(l+1)|j, m_j; l, s\rangle \\
\vec{S}^2|j, m_j; l, s\rangle &= \hbar^2 s(s+1)|j, m_j; l, s\rangle \quad .
\end{aligned} \tag{1}$$

Here $s = 1/2$.

c) Show that the states $|j, m_j; l, s\rangle$ are also Eigenstates of $\vec{L} \cdot \vec{S}$ and hence $\hat{W}$ is diagonal in this basis. Determine the corresponding Eigenvalues $\vec{L} \cdot \vec{S}$ (in terms of j, l and s). **(3 points)**

d) Calculate now the energy corrections at first order in perturbation theory

$$E_n^{(1)} = \langle n; j, m_j; l, s|\hat{W}|n; j, m_j; l, s\rangle \, .$$

For this use without proof that

$$\langle n; j, m_j; l, s|\frac{1}{\hat{R}^3}|n; j, m_j; l, s\rangle = \frac{Z^3}{a_0^3 n^3 l(l+1)(l+\frac{1}{2})}\,, \qquad a_0 = \frac{\hbar^2}{m_e e^2}$$

The degeneracy of the Energy Eigenvalues $E_n^{(0)}$ are broken by the energy corrections $E_n^{(1)}$. How large is the splitting ? Consider $\frac{E_n^{(1)}}{E_n^{(0)}}$. **(4 points)**