Exercise 9.1 Anomalous Zeeman effect (4 points)

We consider a one-electron atom (relative nucleus charge Z) in a weak homogeneous magnetic field of the strength $\vec{B} = B\vec{e}_3$ and consider the interaction Hamiltonian \hat{H}_B of the atom with the magnetic field as perturbation,

$$\hat{H}_B = \frac{\mu_{\rm B}}{\hbar} \left(\hat{\vec{L}} + g_{\rm e} \vec{S} \right) \cdot \vec{B},$$

where $\mu_{\rm B} = \frac{e\hbar}{2m_{\rm e}}$ is Bohr's magneton and $g_{\rm e} = 2.0023...$ the gyromagnetic ratio of the electron. The unperturbed Hamiltonian reads

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m_{\rm e}} - \frac{Ze^2}{4\pi\varepsilon_0\hat{r}} + \hat{H}_{\rm FS},$$

where $\hat{H}_{\rm FS}$ is the Hamiltonian responsible for the atomic fine structure (as discussed in the lecture). The unperturbed energy eigenstates $|nljm\rangle$ are eigenstates of the operators $\hat{\vec{L}}^2$, \vec{S}^2 , \vec{J}^2 , \hat{J}_3 , with the usual parametrization of their eigenvalues by the numbers $l = 0, 1, \ldots$; $s = \frac{1}{2}$; $j = l \pm \frac{1}{2}$; $m = -j, \ldots, j$, respectively. The unperturbed energy levels are

$$E_{nj} = E_n \left[1 + \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) \right], \qquad E_n = -\frac{Z^2}{n^2} E_{\rm R}, \quad n = 1, 2, \dots,$$

where α is the fine-structure constant and $E_{\rm R}$ Rydberg's energy.

a) Derive the energy shift ΔE_B of the energy levels induced by \hat{H}_B , using 1st-order perturbation theory and the relation

$$\begin{aligned} |j = l \pm \frac{1}{2}, m \rangle &= \pm \sqrt{\frac{l \pm m + \frac{1}{2}}{2l + 1}} \Big| m_l = m - \frac{1}{2}, m_s = \frac{1}{2} \rangle \\ &+ \sqrt{\frac{l \mp m + \frac{1}{2}}{2l + 1}} \Big| m_l = m + \frac{1}{2}, m_s = -\frac{1}{2} \rangle \end{aligned}$$

between the eigenstates $|j,m\rangle$ of \vec{J}^2 , \hat{J}_3 and the eigenstates $|m_l,m_s\rangle$ of \hat{L}_3 and S_3 . b) To prepare an alternative derivation, first show that

$$\hbar^2 j(j+1)\langle j,m|\vec{V}|j,m\rangle = \langle j,m|(\vec{V}\cdot\vec{J})\vec{J}|j,m\rangle$$
(1)

for any vector operator \vec{V} , upon exploiting the identity

$$[\vec{J}^2, [\vec{J}^2, \vec{V}]] = 2\hbar^2 (\vec{J}^2 \vec{V} + \vec{V} \vec{J}^2) - 4\hbar^2 (\vec{V} \cdot \vec{J}) \vec{J}.$$

- c) Derive ΔE_B using relation (1).
- d) Sketch the energy levels $E_{nj} + \Delta E_B$ as functions of B for all states emerging from the unperturbed states $nl_j = 1s_{1/2}, 2s_{1/2}, 2p_{1/2}, 2p_{3/2}$.

Exercise 9.2 Linear Stark effect (3 points)

We consider a one-electron atom (relative nucleus charge Z) in a homogeneous electric field of the strength $\vec{\mathcal{E}} = \mathcal{E}\vec{e}_3$ and consider the interaction Hamiltonian \hat{H}_E of the atom with the electric field as perturbation,

$$\hat{H}_E = e\mathcal{E}\hat{x}_3.$$

For sufficiently strong electric fields, spin effects, atomic fine structure, and other corrections can be neglected in a first approximation, so that the unperturbed Hamiltonian reads

$$\hat{H} = \frac{\vec{p}^2}{2m_{\rm e}} - \frac{Ze^2}{4\pi\varepsilon_0\hat{r}}$$

The unperturbed energy eigenstates $|nlm_l\rangle$ are eigenstates of the operators $\hat{\vec{L}}^2$ and \hat{L}_3 , with the usual parametrization of their eigenvalues by the numbers $l = 0, 1, \ldots$ and $m_l = -l, \ldots, l$, respectively.

- a) Calculate the first-order energy shift ΔE_{nlm_l} of a general s state (l=0).
- b) Calculate the first-order energy shifts ΔE_{nlm_l} for the first excited states (n = 2).
- c) Calculate the second-order energy shift $\Delta E_{100}^{(2)}$ of the ground state approximately upon replacing $E_{n>1}$ by E_2 in the underlying formula.

[Hint: Using $\langle \hat{x}_j^2 \rangle_{100} = \langle \hat{r}^2 \rangle_{100}/3 = a_{\rm B}^2/Z^2$ saves you the radial integral.]

Exercise 9.3 Linear potential and variational method (2 points)

As in Exercise 8.3, consider a particle with mass m in a one-dimensional potential $V(x) = \varepsilon |x|$ with $\varepsilon > 0$. As trial function for variations we use $\phi_0(x) = \exp(-\alpha x^2)$ and $\phi_1(x) = x \exp(-\beta x^2)$ in the following, where α and β are independent free real parameters and $\alpha, \beta > 0$.

- a) Determine an approximation for the ground state energy E_0 upon minimizing the energy expectation value for a wave function $\psi(x)$ formed by an optimal linear combination of the trial functions. Compare the result with the one obtained in Exercise 8.3.
- b) Determine an approximation for the energy E_1 of the first excited state similar to the procedure for the ground state. Again, compare the result with the one obtained in Exercise 8.3.

Hint: Symmetry arguments simplify the actual calculations.