Exercise 1. Spin-orbit coupling and Zeeman effect

Goal: In this exercise we study how the atomic levels of the hydrogen atom change due to spin-orbit (SO) coupling and an external magnetic field. Specifically we want to see how the degenerate atomic levels split as a function of external magnetic field.

The energy levels of the hydrogen atom $E_n = -E_{\rm R}/n^2$ ($E_{\rm R} = e^4 m/2\hbar^2 \approx 13.6\,\text{eV}$) of the state $|n, l, m_l, m_s\rangle$ for a non-relativistic electron are independent of the quantum numbers l, m_l and m_s. We want to see how this degeneracy is lifted in the presence of a homogeneous external magnetic field $\boldsymbol{B} = B_z \hat{\boldsymbol{z}}$ and by the SO coupling, which is a relativistic effect following from the Dirac equation. The Hamiltonian operator H', which can be treated as a perturbation on top of the Coulomb Hamiltonian, acts on the $2(2l+1)$ dimensional Hilbert space $\mathcal{H} = \text{span}\{|l, m_l, m_s\rangle, m_l = -l, ..., l, m_s = \pm 1/2\}$ and is given by

$$H' = H_{\rm SO} + H_{\rm Z} = \kappa \boldsymbol{L} \cdot \boldsymbol{S} + \frac{eB_z}{2mc}(L_z + 2S_z). \tag{1}$$

For the hydrogen atom $\kappa = \frac{1}{2m^2c^2}\langle \frac{1}{r}\frac{dV}{dr}\rangle_{n,l} = \frac{e^2}{2m^2c^2}\langle \frac{1}{r^3}\rangle_{n,l}$ and $e > 0$. The first term of H' describes the SO coupling, and the second term is the Zeeman term.

Calculate the splitting of the hydrogen levels in first-order perturbation theory, when

(a) the external magnetic field is so weak, that the SO term dominates and the small Zeeman term can be treated as perturbation to the SO term.

Hint: Note that $\boldsymbol{L}\cdot\boldsymbol{S} = \frac{1}{2}(J^2 - L^2 - S^2)$ and the states $|j = l \pm 1/2, m_j, l\rangle$ are eigenstates of the operator $\boldsymbol{L}\cdot\boldsymbol{S}$.

(b) the external magnetic field is so strong, that the Zeeman term dominates and the SO term is small (*Paschen-Back effect*). How strong should the magnetic field be in order for this approximation to be valid?

Hint: Use that $\boldsymbol{L}\cdot\boldsymbol{S} = \frac{1}{2}(L_- S_+ + L_+ S_-) + L_z S_z$.

(c) the external magnetic field is such, that the two terms in H' are comparable. Plot the splitting of the energy levels $^2\text{P}_{1/2}$ and $^2\text{P}_{3/2}$ as a function of $x := \mu_{\rm B} B_z/\kappa\hbar^2$, $\mu_{\rm B} = e\hbar/2mc$.

Hint: Using the fact that $[J_z, H'] = 0$ show that H' acts on the Hilbert space $\mathcal{H}$ as a block-diagonal matrix, and each block corresponding to one m_j is a 2×2 matrix.

For the parts (a) and (b) count the degeneracy degrees before and after applying the small term and sketch the splitting of energy levels.

Exercise 2. The reduced matrix element of $\boldsymbol{J}$

Goal: In this exercise we want to evaluate the reduced matrix element appearing in the Wigner-Eckart theorem for a simple example.

The Wigner-Eckart theorem (see section 14.5) is a powerful tool for calculating matrix elements $\langle \alpha' j' m' | T^k_q | \alpha j m\rangle$ of tensor operators T^k_q, $q = -k, -k+1, ..., k$, (for tensor operators see section 4.6)

$$\langle \alpha' j' m' | T^k_q | \alpha j m\rangle = \frac{\langle \alpha' j' || T^k || \alpha j\rangle}{\sqrt{2j'+1}} \langle kjqm | kjj'm'\rangle. \tag{2}$$

Here $\langle kjqm|kjj'm'\rangle$ is the Clebsch-Gordan coefficient of $|k, q\rangle \otimes |j, m\rangle \to |k, j, j', m'\rangle$, and $\langle \alpha' j' || T^k || \alpha j\rangle$ is the reduced matrix element. The fact the reduced matrix element is independent of q and m, allows to calculate the matrix elements of all $2k+1$ tensor operators T^k_q by only knowing one of them.

From the total angular momentum operator $\boldsymbol{J}$ define a first order tensor operator J^1 and calculate its reduced matrix element $\langle \alpha' j' || J^1 || \alpha j\rangle$.