Zentralübung zur Quantenmechanik II

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12. Übungsblatt

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Aufgabe 15: Spin-orbit eigenstates

Consider an electron with spin $s = \frac{1}{2}$ and orbital angular momentum l in a hydrogen-like atom. When discussing relativistic (or 'fine structure') corrections to atomic orbitals, it is convenient to construct simultaneous eigenstates of the operators $\vec{l}^{\,2}$, $\vec{s}^{\,2}$, $\vec{j}^{\,2}$, and j_z, as will become clear in Aufgabe 16. Such states are constructed as follows

$$\Omega_{ljm}(\hat{\vec{r}}) := \sum_{m_l,\, m_s} \langle l\ m_l\ \frac{1}{2}\ m_s | j\ m\rangle\ Y_{l\, m_l}(\hat{\vec{r}})\ \chi_{m_s} \quad , \quad \hat{\vec{r}} := \frac{\vec{r}}{r}$$

where

$$\begin{aligned} Y_{l\, m_l} &: \quad \text{Spherical harmonics,} \\ \chi_{m_s} &: \quad \text{Pauli spinors with } m_s = \pm\frac{1}{2}\ , \\ \langle l\ m_l\ \frac{1}{2}\ m_s | j\ m\rangle &: \quad \text{Clebsch-Gordan coefficients.} \end{aligned}$$

a) With $\vec{l} = \vec{r} \times \vec{p}$ and $\kappa = \pm(j + \frac{1}{2})$ for $l = j \pm \frac{1}{2}$, show that

$$\vec{l} \cdot \vec{\sigma}\ \Omega_{ljm} = -(1 + \kappa)\Omega_{ljm} \quad .$$

b) Why can one equivalently label the eigenstates as $\Omega_{\kappa m}$? Show that

$$\vec{\sigma} \cdot \hat{\vec{r}}\, \Omega_{-\kappa m} = (\text{phasefactor}) \times \Omega_{\kappa m} \quad .$$

Tipp: Convince yourself that the operator $\vec{\sigma} \cdot \hat{\vec{r}}$ conserves the total angular momentum $\vec{j}$ but not the parity.

c) Verify the following properties of the function $\Phi_{ljm}(\vec{r}) = f(r)\Omega_{ljm}(\hat{\vec{r}})$:

i)

$$(\vec{\sigma} \cdot \vec{p})\ \Phi_{ljm}(\vec{r}) = -\mathrm{i} \left[\frac{\mathrm{d}f(r)}{\mathrm{d}r} + \frac{1+\kappa}{r}\ f(r) \right] (\vec{\sigma} \cdot \hat{\vec{r}})\ \Omega_{ljm}(\hat{\vec{r}})$$

ii)

$$(\vec{\sigma} \cdot \vec{l})(\vec{\sigma} \cdot \hat{\vec{r}})\ \Omega_{ljm} = (\kappa - 1)\ (\vec{\sigma} \cdot \hat{\vec{r}})\ \Omega_{ljm}.$$

Aufgabe Z16: Fine-structure of hydrogen-like atoms

In the Hamiltonian for an electron in a hydrogenic atom (with charge Ze), a spin-orbit term arises from the interaction between the electron spin magnetic moment and the magnetic field the electron sees as a result of its motion through the electric field of the nucleus:

$$H_{SO} = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\,\vec{l}\cdot\vec{s},$$

where V is the electrostatic potential energy. Assuming that H_{SO} can be treated as small, we will derive the spin-orbit splitting of energy levels in perturbation theory.

a) Show that the first-order energy shift for the state $|nlsjm_j\rangle$, with $l \neq 0$, is given by

$$\Delta E_{SO}^{(1)} = \frac{1}{2m^2c^2}\left[\frac{j(j+1) - l(l+1) - s(s+1)}{2}\right]\left\langle \frac{1}{r}\frac{dV}{dr}\right\rangle,$$

where

$$\left\langle \frac{1}{r}\frac{dV}{dr}\right\rangle = \frac{Z^4\,e^2}{a_0^3\,n^3\,l\,(l+\frac{1}{2})\,(l+1)}.$$

Therefore, show that the energy shift can be written

$$\Delta E_{SO}^{(1)} = -E_n\frac{(Z\alpha)^2}{2nl(l+\frac{1}{2})(l+1)}\cdot\begin{cases} l & \text{for } j = l+\frac{1}{2} \\ -(l+1) & \text{for } j = l-\frac{1}{2}\end{cases}.$$

Note that this relativistic effect would therefore be much more important for heavy nuclei than light nuclei.

b) Calculate the spin-orbit spectral splitting of hydrogen (in units of cm^{-1}) between the previously-degenerate $n = 2$ states.