Exercises to Advanced Quantum Mechanics — Sheet 9

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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,

$$\hat{H}_B = \frac{\mu_\mathrm{B}}{\hbar}\left(\vec{L} + g_\mathrm{e}\vec{S}\right)\cdot\vec{B}, \tag{1}$$

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

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

where $\hat{H}_\mathrm{FS}$ is the Hamiltonian responsible for the atomic fine structure. The unperturbed energy eigenstates $|nlsjm_j\rangle$ are eigenstates of the operators $\hat{H}$, $\vec{L}^2$, $\vec{S}^2$, $\vec{J}^2$, $\hat{J}_3$, with the usual parametrisation of their eigenvalues by the numbers $n \in \mathbb{N}_1$; $l = 0, 1, \ldots, n-1$; $s = \frac{1}{2}$; $j = l \pm \frac{1}{2}$; $m = -j, \ldots, j$. The unperturbed energy levels are

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

where α is the fine-structure constant and E_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

$$\begin{aligned}|j = l \pm \tfrac{1}{2}, m_j\rangle = {} & \pm\sqrt{\frac{l \pm m_j + \frac{1}{2}}{2l+1}}\;\left|l, s; m_l = m_j - \tfrac{1}{2}, m_s = \tfrac{1}{2}\right\rangle \\ & + \sqrt{\frac{l \mp m_j + \frac{1}{2}}{2l+1}}\;\left|l, s; m_l = m_j + \tfrac{1}{2}, m_s = -\tfrac{1}{2}\right\rangle\end{aligned} \tag{4}$$

between the eigenstates $|j, m_j\rangle$ of $\vec{L}^2$, $\vec{S}^2$, $\vec{J}^2$, $\hat{J}_3$ and the eigenstates $|l, s; m_l, m_s\rangle$ of $\vec{L}^2$, $\vec{S}^2$, L_3, S_3. *Hint:* $\hat{H}_B$ is diagonal in the basis $|j, m_j\rangle$.

b) To prepare an alternative derivation, first show that

$$\hbar^2 j(j+1)\langle j, m|\vec{V}|j, m'\rangle = \langle j, m|(\vec{V}\cdot\vec{J})\vec{J}|j, m'\rangle \tag{5}$$

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

$$[\vec{J}^2, [\vec{J}^2, \vec{V}]] = 2\hbar^2(\vec{J}^2\vec{V} + \vec{V}\vec{J}^2) - 4\hbar^2(\vec{V}\cdot\vec{J})\vec{J}. \tag{6}$$

c) Derive ΔE_B using relation (5).

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

Please turn over!

Exercise 9.2 *Linear and quadratic 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,

$$\hat{H}_E = e\mathcal{E}\hat{x}_3. \tag{7}$$

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

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m_\mathrm{e}} - \frac{Ze^2}{4\pi\varepsilon_0\hat{r}}. \tag{8}$$

The unperturbed energy eigenstates $|nlm\rangle$ are eigenstates of the operators $\hat{H}$, $\vec{L}^2$, and L_3, with the usual parametrisation of their eigenvalues by the numbers $n \in \mathbb{N}_1$, $l = 0, 1, \ldots, n-1$ and $m = -l, \ldots, l$, respectively.

a) Show that $\hat{H}_E$ is block diagonal in the degenerate subspace spanned by $|n, l, m\rangle$ for fixed n. How are the blocks characterised and which matrix elements can be non-zero?

   Hint: Use the Wigner–Eckart theorem, and show that the diagonal elements vanish.

b) Calculate the first-order energy shifts ΔE_{nlm} for the first excited states ($n = 2$).

   Hint: Energy eigenfunctions can be taken from the literature.

c) Calculate the second-order energy shift $\Delta E^{(2)}_{100}$ of the ground state approximately upon replacing $E_{n>1}$ by E_2 in the underlying formula.

   Hint: Using $\langle \hat{x}_j^2 \rangle_{100} = \langle \hat{r}^2 \rangle_{100}/3 = a_\mathrm{B}^2/Z^2$ 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 $\varepsilon > 0$. In the following we use $\phi_0(x) \propto \exp(-\alpha x^2)$ and $\phi_1(x) \propto x\exp(-\beta x^2)$ As normalised trial functions for variations, 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 minimising 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: Use symmetry arguments to constrain the ansatz for the trial functions.