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Problem 1: Relativistic corrections for the hydrogen atom (Written)

Learning objective

In this problem, you examine the relativistic corrections to the hydrogen atom and derive the energy levels including relativistic effects like spin-orbit coupling and quantum fluctuations in the electron's position. These effects give rise to the fine structure of the hydrogen energy levels and can also be derived directly from the Dirac equation.

We examine the corrections after an expansion of the relativistic theory in powers of v/c for a single hydrogen atom. The expansion reads

$$H = mc^2 + \underbrace{\frac{\mathbf{p}^2}{2m} + V(r)}_{H_0} \underbrace{- \frac{\mathbf{p}^4}{8m^3c^2}}_{H_\text{kin}} + \underbrace{\frac{1}{2m^2c^2}\frac{1}{r}\frac{\mathrm{d}V(r)}{\mathrm{d}r}\mathbf{L}\cdot\mathbf{S}}_{H_\text{SO}} + \underbrace{\frac{\hbar^2}{8m^2c^2}\Delta V(r)}_{H_\text{D}} + \dots, \tag{1}$$

where $V(r) = -e^2/r$. The first term is given by the rest mass of the electron and plays no role in the dynamics. The Hamiltonian H_0, known from the non-relativistic theory of the hydrogen atom, has the well-known eigenstates $|n, l, m\rangle$ which we use in the following as a starting point for perturbation theory.

a) First, show that the term H_kin is obtained from the expansion of the (classical) expression for the kinetic energy $E = \sqrt{p^2c^2 + m^2c^4}$.

   Now consider first order perturbation theory. The states $|n, l, m\rangle$ are degenerate with respect to H_0 because energy depends only on the principal quantum number n. Write the matrix elements of H_kin in the form

$$\langle H_\text{kin}\rangle = -\frac{1}{2mc^2}\left[\left\langle H_0^2\right\rangle + e^2\left\langle H_0\frac{1}{r}\right\rangle + e^2\left\langle\frac{1}{r}H_0\right\rangle + e^4\left\langle\frac{1}{r^2}\right\rangle\right] \tag{2}$$

   and argue that one can actually use *non-degenerate* perturbation theory for this problem. Show that the occurring matrix elements $\langle r^{-s}\rangle$, $s = 1, 2$, can be written in the form

$$\left\langle r^{-s}\right\rangle = \int_0^\infty \mathrm{d}r\, r^{2-s}\left|R_{nl}(r)\right|^2. \tag{3}$$

   Calculate the energy corrections for $1s$, $2s$ and $2p$ orbitals explicitly.

b) The term H_SO is kown as *spin-orbit coupling* and was discussed on Problem Set 3 (Problem 3) and on Problem Set 4 (Problem 2). What are the good quantum numbers for this Hamiltonian? Write down the energy corrections for the $1s$, $2s$ and $2p$ orbitals explicitly. Comment on the degeneracy of the $2p$ orbital.

c) The term H_D is called *Darwin term*. Calculate the energy corrections to the $n = 1$ and $n = 2$ orbitals due to this term. Read about the origin of the name and its relation to *the* Charles Darwin.

d) After having taken into account all the corrections to lowest order, write down the energy $E = E_0 + E_{\text{kin}} + E_{\text{SO}} + E_{\text{D}}$ as a function of $\alpha = e^2/\hbar c$ and the rest energy mc^2 for the considered energy levels. What is the degeneracy in the relativistic theory and which quantum numbers does the energy depend on? Compare your results to the non-relativistic case.

Problem 2: Relativistic free electrons in a magnetic field (Oral)

Learning objective

In this problem, you study relativistic free electrons in an external magnetic field by solving the Dirac equation. This problem has applications in condensed matter physics where it describes the (anomalous) integer quantum Hall effect in graphene.

Consider the Dirac Hamiltonian of an electron in an external field (we set $\hbar = c = 1$ in this problem)

$$H = \sum_{i=1}^{3} \alpha_i \pi_i + m\beta, \tag{4}$$

where $\pi_i = p_i - eA_i$ is the canonical momentum of a particle with charge e in a magnetic field with vector potential $\mathbf{A}$.

a) Calculate H^2 and derive an equation for the eigenvalues of the Dirac equation $H\Psi = E\Psi$.

b) Use the result from a) to calculate the spectrum and the wave functions of the Dirac equation.

Hints: Consider the magnetic field $\mathbf{B} = B\mathbf{e}_z$ and use Landau gauge $\mathbf{A} = -By\mathbf{e}_x$. Split the four-component spinor Ψ into two two-component parts $\chi^{1,2}$, i.e., $\Psi = (\chi^1, \chi^2)$, and derive an eigenvalue equation for their components $\chi_\sigma^{1,2}$ with $\sigma \in \{\uparrow, \downarrow\}$. Use the ansatz $e^{ik_x x}e^{ik_z z}\phi(y)$ and show that it simplifies to the eigenvalue problem of a shifted harmonic oscillator. You are not required to write down the eigenfunctions explicitly.

c) Show that in the massless case, $m = 0$, there is a Landau level with zero energy. This peculiarity leads to the (anomalous) integer quantum Hall effect that can be observed in graphene.