Prof. Dr. Hans-Peter Büchler
Institute for Theoretical Physics III, University of Stuttgart

January 19th, 2023
WS 2022/23

Problem 12.1: Relativistic corrections for the hydrogen atom

[**Written** | 4 pt(s)]

ID: ex_relativistic_corrections_hydrogen:aqt2223

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

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

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. The non-perturbed eigenenergies are given by $E_n^0 = -\frac{mc^2\alpha^2}{2n^2}$, which are n^2-fold degenerate for a fixed n.

a) First, show that the term H_{kin} is obtained from the expansion of the (classical) expression for the kinetic energy $E = \sqrt{p^2c^2 + m^2c^4}$. Furthermore, rewrite the kinetic energy in the form **1**pt(s)

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

Now consider first order perturbation theory. The states $|n, l, m\rangle$ are n^2-fold degenerate with respect to H_0. Argue with equation (2), that the perturbation H_{kin}, nevertheless, can be treated by *non-degenerate* perturbation theory.

To calculate the energy corrections, first show that the occurring matrix elements $\langle r^{-s}\rangle$ can be written in the form

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

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

b) The term H_{SO} is known as *spin-orbit coupling*. 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. **1**pt(s)

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. **1**pt(s)

d) After having taken into account all the corrections to the lowest order, write down the energy $E = E_0 + E_\mathrm{kin} + E_\mathrm{SO} + E_\mathrm{D}$ 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. **1**pt(s)

Problem 12.2: Relativistic free electrons in a magnetic field [**Oral** | 3 pt(s)]

ID: ex_relativistic_electrons_in_magnetic_field:aqt2223

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 kinetic momentum of a particle with charge $e = -|e|$ in a magnetic field with vector potential $\boldsymbol{A}$.

a) Calculate H^2 and write down an equation for the eigenvalues E of the Dirac Hamiltonian. **1**pt(s)

b) Use the result from a) to calculate the spectrum E of the Dirac Hamiltonian. **1**pt(s)

Hints: Consider the magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ and use Landau gauge $\boldsymbol{A} = -By\boldsymbol{e}_x$.

Since H^2 is block-diagonal, the spectrum can be solved for the parts χ^+ and χ^- of the eigenfunction

$$\Psi = \left(\chi^+, \chi^-\right)^T = \left(\chi^+_\uparrow, \chi^+_\downarrow, \chi^-_\uparrow, \chi^-_\downarrow\right)^T \tag{5}$$

separately. Show that the problem simplifies to the eigenvalue problem of a shifted harmonic oscillator by using the ansatz $e^{ik_x x} e^{ik_z z} \phi(y)$.

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. **1**pt(s)