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January 29th, 2024
WS 2023/24

Problem 14.1: Relativistic corrections for the hydrogen atom [**Oral** | 8 pt(s)]

ID: ex_relativistic_corrections_hydrogen:aqt2324

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 **2pt(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

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

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. **2pt(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. **2**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. **2**pt(s)

Problem 14.2: Relativistic free electrons in a magnetic field

[**Written** | 6 pt(s)]

ID: ex_relativistic_electrons_in_magnetic_field:aqt2324

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. **2**pt(s)

b) Use the result from a) to calculate the spectrum E of the Dirac Hamiltonian. **2**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. **2**pt(s)

Problem 14.3: Klein Paradox

[**Written** | 0 (+8 bonus) pt(s)]

ID: ex_Klein_Paradox:aqt2324

Learning objective

Here, you study the scattering of an electron off a step potential using Dirac theory. In this problem, you will encounter the paradox that the flux reflected from the potential is larger than the incident one. This is called the Klein paradox and can be resolved by the introduction of antiparticles showing that the single-particle picture breaks down in Dirac theory.

We consider the scattering of an electron having energy E and momentum $\boldsymbol{p} = p\boldsymbol{e_z}$ with $p_z > 0$ at a potential step in the relativistic theory of the Dirac equation. The 1D step potential is described by

$$V(z) = e \cdot \phi(z) = e \cdot \phi_0 \, \theta(z) \qquad \text{with } \theta(z) = \begin{cases} 0 & z \leq 0 \\ 1 & z > 0 \end{cases}, \tag{6}$$

where e is the elementary charge and $\phi_0 > 0$ is the potential for $z > 0$. Using the minimal coupling principle, we obtain the Dirac equation for an electron in the electromagnetic potential $A_\mu = (\phi(z)/c, 0, 0, 0)^t$ of the form

$$i\hbar\partial_t \Psi = \big(V(z) + mc^2\beta + c\boldsymbol{\alpha}\boldsymbol{p}\big)\, \Psi. \tag{7}$$

*a) Find a stationary solution of the Dirac equation of the form **+2pt(s)**

$$\Psi(z,t) = \mathrm{e}^{-iEt/\hbar}\, \Psi(z) \qquad \text{with } \Psi(z) = \begin{cases} \Psi_\mathrm{i}(z) + \Psi_\mathrm{r}(z) & z \leq 0 \\ \Psi_\mathrm{t}(z) & z > 0 \end{cases}, \tag{8}$$

where the time-independent spinors denote the incident, reflected and transmitted wave. Use the individual contributions to derive the solutions for free particles:

$$\Psi_\mathrm{i}(z) = c_\mathrm{i}\, \tilde{u}(\boldsymbol{p}, \uparrow)\, \mathrm{e}^{ipz/\hbar} \tag{9}$$
$$\Psi_\mathrm{r}(z) = c_\mathrm{r}\, \tilde{u}(-\boldsymbol{p}, \uparrow)\, \mathrm{e}^{-ipz/\hbar} \tag{10}$$
$$\Psi_\mathrm{t}(z) = c_\mathrm{t}\, \tilde{u}(\boldsymbol{p}', \uparrow)\, \mathrm{e}^{ip'z/\hbar} \tag{11}$$

where

$$\tilde{u}(\boldsymbol{p}, s) = \begin{pmatrix} \chi^{(s)} \\ \frac{c\boldsymbol{\sigma}\boldsymbol{p}}{E_p + mc^2}\chi^{(s)} \end{pmatrix} \qquad \chi^{(\uparrow)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \chi^{(\downarrow)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{12}$$

and coefficients $c_i \in \mathbb{C}$.

*b) Determine the momentum p' depending on p. At the point $z = 0$, the spinor $\Psi(z)$ has to be continuous (Why do we not demand continuity relations for the derivative?). Derive relations between the coefficients $c_\mathrm{i}, c_\mathrm{r}$ and c_t. **+2pt(s)**

*c) Now calculate the incident (j_i), reflected (j_r) and transmitted (j_t) current density. The current density operator in the Dirac formalism is given by $j^\mu = c\,\overline{\Psi}\gamma^\mu\Psi$. Discuss the three cases: **+2pt(s)**

(1) $E - e\phi_0 > mc^2$

(2) $-mc^2 < E - e\phi_0 < mc^2$

(3) $E - e\phi_0 < -mc^2$

*d) Consider case (3) where $E - e\phi_0 < -mc^2$. Show that the total current is conserved but that the reflected flux is larger than the incident one. Interpret and discuss this result. **+2pt(s)**