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Exercise 1: Relativistic corrections for the hydrogen atom (Oral)

We examine the corrections after an expansion of the relativistic theory in powers of $\frac{v}{c}$ for a single hydrogen atom. The expansion reads

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

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 eigenstates $|nlm\rangle$ which we use in the following as a starting point for the perturbation theory.

a) Show that you get the term H_{kin} from the expansion of the (classical) expression for the kinetic energy $E = \sqrt{p^2c^2 + m^2c^4}$. Next, we consider only the first order perturbation theory. The states $|nlm\rangle$ are degenerate with regard to H_0 because energy depends only on n. Show that we can still apply the non-degenerate perturbation theory by writing the matrix element in the form

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

Why we do not need the degenerate perturbation theory? Show that the occurring matrix elements $\langle r^{-p}\rangle$ can be written in the form

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

Calculate the energy corrections for *1s*, *2s* and *2p* orbitals explicitly (possibly using a CAS).

b) With the term H_{SO}, we have already dealt in detail in Assignment 3 (Note that for simplicity we use here the CGS system with $4\pi\epsilon_0 = 1$). Give the corrections for the considered orbitals explicitly. Bear in mind the splitting of the *2p* orbital into the degenerate manifolds. Give the *good quantum numbers* for the angular momentum coupling.

c) The term H_{D} is called Darwin-term. Calculate also for this term the corrections for the $n = 1$ and $n = 2$ orbitals.

d) We have therefore taken into account all the corrections in the lowest order. Show all considered energy corrections $E = E_0 + E_{\text{kin}} + E_{\text{SO}} + E_{\text{D}}$ together. Write the energy as a function of $\alpha = e^2/\hbar c$ and the rest energy mc^2. In the non-relativistic theory is the $n = 1$ state twofold-degenerate and the $n = 2$ state eightfold-degenerate. What is the degeneracy in the relativistic theory? On which quantum numbers does the energy depend?

Exercise 2: Klein Paradox (Written, 4pts)

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

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

where e he 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

$$i\hbar\partial_t\Psi = \left(V(z) + mc^2\beta + c\boldsymbol{\alpha}\mathbf{p}\right)\Psi.$$

a) Find a stationary solution of the Dirac equation of the form

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

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

$$\begin{aligned} \Psi_\mathrm{i}(z) &= c_\mathrm{i}\,\tilde{u}(\mathbf{p},\uparrow)\,\mathrm{e}^{ipz/\hbar} \\ \Psi_\mathrm{r}(z) &= c_\mathrm{r}\,\tilde{u}(-\mathbf{p},\uparrow)\,\mathrm{e}^{-ipz/\hbar} \\ \Psi_\mathrm{t}(z) &= c_\mathrm{t}\,\tilde{u}(\mathbf{p}',\uparrow)\,\mathrm{e}^{ip'z/\hbar} \end{aligned}$$

where

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

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 we demand no continuity relations for the derivative?). Derive relations between the coefficients $c_\mathrm{i}, c_\mathrm{r}$ and c_t.

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

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

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

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

d) Show that in the case (3) the reflection coefficient $R \equiv |j_\mathrm{r}/j_\mathrm{i}|$ is greater than one, i.e., more particles are reflected than are incoming.

This phenomena is called Klein paradox and is an example of the fact that in the relativistic quantum mechanics the particles/antiparticles pairs can be generated. In single particle picture of the Dirac formalism this generation of particles does not cost energy. From the theory of relativity, we expect that for such a process the energy $2mc^2$ is needed. This inconsistency is a sign that in the relativistic quantum mechanics the single-particle approach breaks down. This issue is solved by using the relativistic quantum field theory.