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Problem 1: Klein-Gordon theory for the hydrogen atom (Written)

Learning objective

In this problem, you will derive the spectrum of the relativistic hydrogen atom within the Klein-Gordon theory and compare it to that obtained from the Dirac equation for relativistic particles.

The radial part of the *non*-relativistic (stationary) Schrödinger equation for the hydrogen atom can be written as

$$\left[-\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{l(l+1)}{r^2} - \frac{2mcZ\alpha}{\hbar r} - E\frac{2m}{\hbar^2}\right]\psi(r) = 0 \tag{1}$$

with the fine-structure constant $\alpha = e^2/\hbar c$. On the other hand, the (stationary) Klein-Gordon equation takes the following form:

$$\left[c^2\hbar^2\Delta + \left(E + \frac{Ze^2}{r}\right)^2 - m^2c^4\right]\psi(r) = 0 \tag{2}$$

Show that (1) can be transformed into (2) by using the following substitutions:

$$l(l+1) \quad\longrightarrow\quad l(l+1) - Z^2\alpha^2 = \lambda(\lambda+1), \tag{3}$$

$$E \quad\longrightarrow\quad \frac{E^2 - m^2c^4}{2mc^2}, \tag{4}$$

$$\alpha \quad\longrightarrow\quad \alpha\frac{E}{mc^2}. \tag{5}$$

Here, we have defined $\lambda = l - \delta_l$ and the quantum defect

$$\delta_l = l + 1/2 - \sqrt{(l+1/2)^2 - Z^2\alpha^2}. \tag{6}$$

Consequently, we can find the energies of the Klein-Gordon problem by using the analogy to the non-relativistic case. Show that the energies are given by

$$E_{n,l} = mc^2\left[1 + \left(\frac{Z\alpha}{n-\delta_l}\right)^2\right]^{-1/2}. \tag{7}$$

Note: Use the hydrogen atom energies which include the quantum defect δ_l. Compare the solution to the energies that one gets from the Dirac equation:

$$E_{n,j} = mc^2\left[1 + \left(\frac{Z\alpha}{n - (j+1/2) + \sqrt{(j+1/2)^2 - (Z\alpha)^2}}\right)^2\right]^{-1/2}. \tag{8}$$

What is missing in the Klein-Gordon description of the hydrogen atom?

Problem 2: Klein Paradox (Oral)

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 $\mathbf{p} = p\mathbf{e_z}$ with $p_z > 0$ at a potential step in the relativistic theory of the Dirac equation. The 1D step potential is described by

$$V(z) = e \cdot \phi(z) = e \cdot \phi_0 \, \theta(z) \qquad \text{with } \theta(z) = \begin{cases} 0 & z \leq 0 \\ 1 & z > 0 \end{cases}, \tag{9}$$

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

$$i\hbar\partial_t \Psi = \big(V(z) + mc^2\beta + c\boldsymbol{\alpha}\mathbf{p}\big)\, \Psi. \tag{10}$$

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

$$\Psi(z,t) = \mathrm{e}^{-iEt/\hbar}\, \Psi(z) \qquad \text{with } \Psi(z) = \begin{cases} \Psi_\mathrm{i}(z) + \Psi_\mathrm{r}(z) & z \leq 0 \\ \Psi_\mathrm{t}(z) & z > 0 \end{cases}, \tag{11}$$

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

$$\Psi_\mathrm{i}(z) = c_\mathrm{i}\, \tilde{u}(\mathbf{p}, \uparrow)\, \mathrm{e}^{ipz/\hbar} \tag{12}$$

$$\Psi_\mathrm{r}(z) = c_\mathrm{r}\, \tilde{u}(-\mathbf{p}, \uparrow)\, \mathrm{e}^{-ipz/\hbar} \tag{13}$$

$$\Psi_\mathrm{t}(z) = c_\mathrm{t}\, \tilde{u}(\mathbf{p}', \uparrow)\, \mathrm{e}^{ip'z/\hbar} \tag{14}$$

where

$$\tilde{u}(\mathbf{p}, s) = \begin{pmatrix} \chi^{(s)} \\ \frac{c\,\boldsymbol{\sigma}\mathbf{p}}{E_p + mc^2}\chi^{(s)} \end{pmatrix} \qquad \chi^{(\uparrow)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \chi^{(\downarrow)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{15}$$

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.

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:

(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.