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## Problem 4.1: The relativistic hydrogen atom

[**Written** | 6 (+1 bonus) pt(s)]

ID: ex_relativistic_hydrogen_atom:qft23

> **Learning objective**
>
> From your quantum mechanics course, you know how to solve the non-relativistic Schrödinger equation for the hydrogen atom. Here we describe the electron of the hydrogen atom by the relativistic Dirac equation instead. That is, we interpret the bispinor field $\psi(x)$ as a single-particle wave function (not an operator!) and the Dirac equation as the relativistic analogue of the non-relativistic Schrödinger equation. For the hydrogen atom, we will see that corrections that had to be put in by hand in the non-relativistic description now emerge naturally (notably, the fine structure).

To describe the electron in the hydrogen atom by the Dirac equation, we incorporate the coupling to an external (classical) electromagnetic field—described by the gauge field $A_\mu$—via *minimal coupling*

$$\partial_\mu \mapsto D_\mu = \partial_\mu + ieA_\mu \,, \tag{1}$$

where $e < 0$ is the electric charge of the electron. The Dirac equation now reads

$$(i\not{D} - m)\psi = (i\not{\partial} - e\not{A} - m)\psi = 0 \,, \tag{2}$$

where $\not{A} = \gamma^\mu A_\mu$ as usual.

The elementary charge $|e|$ is dimensionless in natural units ($\varepsilon_0 = c = \hbar = 1$); it is the *coupling constant* of quantum electrodynamics and describes the strength of the coupling between charged particles and the electromagnetic field. It is related to the fine-structure constant by $\alpha = \frac{e^2}{4\pi} \approx \frac{1}{137}$.

a) Show that Eq. (2) is invariant under the gauge transformation **1**pt(s)

$$A_\mu(x) \;\mapsto\; A_\mu(x) - \partial_\mu\lambda(x) \tag{3a}$$
$$\psi(x) \;\mapsto\; e^{ie\lambda(x)}\psi(x) \tag{3b}$$

for arbitrary $\lambda(x)$.

b) Multiply the Dirac equation (2) by $(i\not{\partial} - e\not{A} + m)$ and bring your result into the form **1**pt(s)

$$\left[(i\partial_\mu - eA_\mu)^2 - eS^{\mu\nu}F_{\mu\nu} - m^2\right]\psi = 0 \,, \tag{4}$$

with the generators of the Lorentz algebra

$$S^{\mu\nu} = \frac{i}{4}\left[\gamma^\mu, \gamma^\nu\right] \tag{5}$$

and the electric field tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

Using the gauge invariance of the Dirac equation, we choose for the four-potential

$$A_0 = -\frac{Ze}{4\pi r} \quad \text{and} \quad A_i = 0 \tag{6}$$

to describe the Coulomb potential of a nucleus with $Z$ protons.

Use this to show that

$$eS^{\mu\nu}F_{\mu\nu} = i\frac{Z\alpha}{r^2}\begin{pmatrix} \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} \end{pmatrix} \tag{7}$$

with $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$.

**Note:** Use the Weyl representation of the gamma matrices from Peskin & Schroeder.

Thus, (4) is block-diagonal, and we can make the ansatz $\psi(x) = e^{-iEt}\,(\phi_+(\boldsymbol{r}), \phi_-(\boldsymbol{r}))^T$ with two-component spinors $\phi_\pm$ to derive the spectrum $E$.

Show that Eq. (4) reduces to

$$\left[-\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\boldsymbol{L}^2 - Z^2\alpha^2 \pm iZ\alpha\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}}{r^2} - \frac{2Z\alpha E}{r} - (E^2 - m^2)\right]\phi_\pm = 0\,, \tag{8}$$

where $\boldsymbol{L}$ is the (orbital) angular momentum operator.

**Hint:** Recall that

$$\Delta = -\partial_i\partial^i = \partial_r^2 + \frac{2}{r}\partial_r - \frac{\boldsymbol{L}^2}{r^2} \tag{9}$$

in spherical coordinates.

c) To solve the differential equation (8), we introduce the total angular momentum operator $\boldsymbol{J} = \boldsymbol{L} + \frac{1}{2}\boldsymbol{\sigma}$. **1pt(s)**

Explain why $\boldsymbol{J}$ commutes with the differential operator in (8) and with $\boldsymbol{L}^2$.

d) Consider now the subspace where $\boldsymbol{J}^2 = j(j+1)$, $J_z = m_j$ (for $j = \frac{1}{2}, \frac{3}{2}, \ldots$ and $-j \le m_j \le j$) and $\boldsymbol{L}^2 = l(l+1)$. For given $j$ and $m_j$, only two values $l_\pm = j \pm \frac{1}{2}$ for $l$ are possible. Thus, an arbitrary state $|j, m_j\rangle = a_+\left|j, m_j, l_+, s = \frac{1}{2}\right\rangle + a_-\left|j, m_j, l_-, s = \frac{1}{2}\right\rangle$ can be decomposed into the orthogonal states $|l_\pm\rangle \equiv \left|j, m_j, l_\pm, s = \frac{1}{2}\right\rangle$. **1pt(s)**

Show that in the two-dimensional subspace spanned by $|l_\pm\rangle$, we can write

$$\boldsymbol{L}^2 - Z^2\alpha^2 \pm iZ\alpha\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} = \begin{pmatrix} (j+\frac{1}{2})(j+\frac{3}{2}) - Z^2\alpha^2 & \pm iZ\alpha \\ \pm iZ\alpha & (j-\frac{1}{2})(j+\frac{1}{2}) - Z^2\alpha^2 \end{pmatrix}. \tag{10}$$

**Hint:** Use the matrix elements $\langle l_\pm|\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}\,|l_\pm\rangle = 0$ and $\langle l_\mp|\,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}\,|l_\pm\rangle = 1$.

Write the two eigenvalues of (10) in the form $\lambda_k(\lambda_k + 1)$ and show that

$$\lambda_1 = \left(j + \frac{1}{2}\right) - \delta_j \quad \text{and} \quad \lambda_2 = \left(j - \frac{1}{2}\right) - \delta_j \tag{11}$$

with

$$\delta_j = j + \frac{1}{2} - \sqrt{\left(j + \frac{1}{2}\right)^2 - Z^2\alpha^2}\,. \tag{12}$$

*e) Prove the previous hint. **+1**pt(s)

That is, show that $\langle l_\pm | \boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}} | l_\pm \rangle = 0$ and $\langle l_\mp | \boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}} | l_\pm \rangle = 1$.

f) In the corresponding eigenbasis, Eq. (8) takes the form **1**pt(s)

$$\left[-\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\lambda_k(\lambda_k+1)}{r^2} - \frac{2Z\alpha E}{r} - (E^2 - m^2)\right]\varphi = 0 \tag{13}$$

where $\varphi = \varphi(r)$ describes only the radial part of $\phi_\pm(\boldsymbol{r})$.

**Note:** $\varphi(r)$ is a *scalar* function without angular dependence of its argument whereas $\phi_\pm(\boldsymbol{r})$ is a (two-component) *spinor* field with angular dependence of its argument.

Make the substitutions

$$\tilde{\alpha} = \frac{\alpha E}{m} \quad \text{and} \quad \tilde{E} = \frac{E^2 - m^2}{2m} \tag{14}$$

and show that Eq. (13) takes the form of the Hamiltonian for the non-relativistic hydrogen atom:

$$\left[-\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\lambda_k(\lambda_k+1)}{r^2} - \frac{2Zm\tilde{\alpha}}{r} - 2m\tilde{E}\right]\varphi = 0\,. \tag{15}$$

Use your knowledge from your quantum mechanics course to derive the eigenenergies $E = E_{nj}$ and show that the spectrum is given by

$$E_{nj} = \frac{m}{\sqrt{1 + \frac{Z^2\alpha^2}{(n-\delta_j)^2}}}\,, \tag{16}$$

where $n = 1, 2, \ldots$ and $j = \frac{1}{2}, \frac{3}{2}, \ldots, n - \frac{1}{2}$.

**Hint:** To determine the spectrum $\tilde{E}$ in Eq. (15), use the substitution $\varphi(r) = \frac{u(r)}{r}$ and that the spectrum $\epsilon^2$ of the differential equation

$$\left[\partial_\rho^2 - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} - \epsilon^2\right]u(\rho) = 0 \tag{17}$$

is given by $\epsilon^2 = (l + 1 + \nu)^{-2}$ with $\nu = 0, 1, 2, \ldots$ .

What is the difference between $l$ and $\lambda_k$?

g) Expand the energy $E_{nj}$ up to fourth order in $\alpha$. **1**pt(s)

What are the differences to the non-relativistic spectrum?

How is the $j$-dependence of $E_{nj}$ called?

## Problem 4.2: Parity transformation of Dirac spinors [**Oral** | 4 pt(s)]

ID: ex_parity_transformation_dirac_spinors:qft23

> **Learning objective**
>
> The Dirac equation is Lorentz-covariant under proper, orthochronous Lorentz transformations (which continuously connect to the identity). Spatial inversion (*parity*) is a discrete generator of the complete Lorentz group that allows for "improper" Lorentz transformations. Here we study the representation of this symmetry on the spinor fields of the Dirac theory. We will find that the Dirac Hamiltonian commutes with parity transformations.

In addition to the continuous (proper and orthochronous) Lorentz transformations (that is, rotations and boosts), there are three *discrete* symmetries acting on the spinor fields: Parity ($P$), time reversal ($T$) and charge conjugation ($C$).

Here we focus on the parity transformation $P$ which acts on Minkowski space and inverts all spatial coordinates:

$$P\,:\,\mathbb{R}^{1,3}\to\mathbb{R}^{1,3}\,,\quad (t,\boldsymbol{x})\mapsto(t,-\boldsymbol{x})\,. \tag{18}$$

Thus, parity flips the three-momentum of a particle without flipping its spin:
$\boldsymbol{p}\mapsto-\boldsymbol{p}$ and $s\mapsto s$ (motivate this!).

We are now interested in the representation of parity on the *Hilbert space* of the Dirac theory. The parity transformation should be represented by a unitary operator $U(P)$ which transforms a single particle with momentum $\boldsymbol{p}$ into a particle with momentum $-\boldsymbol{p}$ with the same spin. Therefore we make the ansatz

$$U(P)a^s_{\mathbf{p}}U^{-1}(P)=\eta_a a^s_{-\mathbf{p}}\,,\qquad U(P)b^s_{\mathbf{p}}U^{-1}(P)=\eta_b b^s_{-\mathbf{p}}\,, \tag{19}$$

where we allow for yet undetermined phases $\eta_a,\eta_b\in\mathbb{C}$.

a) We make two observations: **1**pt(s)
   - *Physically allowed observables* should not change if we apply the parity operator twice.
   - Physically allowed observables are built from an *even* number of fermion operators (this is known as a *superselection rule*).

   What are the allowed values for $\eta_a$ and $\eta_b$?

b) Next, we want to determine the representation $P_{\frac{1}{2}}$ of parity acting on *bispinors* in $\mathbb{C}^2\oplus\mathbb{C}^2$. To this end, we use the quantized Dirac fields **1**pt(s)

$$\psi(x)=\int\frac{\mathrm{d}^3p}{(2\pi)^3}\frac{1}{\sqrt{2E_{\mathbf{p}}}}\sum_s\left(a^s_{\mathbf{p}}u^s(p)e^{-ipx}+b^{s\dagger}_{\mathbf{p}}v^s(p)e^{ipx}\right), \tag{20a}$$

$$\bar\psi(x)=\int\frac{\mathrm{d}^3p}{(2\pi)^3}\frac{1}{\sqrt{2E_{\mathbf{p}}}}\sum_s\left(b^s_{\mathbf{p}}\bar v^s(p)e^{-ipx}+a^{s\dagger}_{\mathbf{p}}\bar u^s(p)e^{ipx}\right) \tag{20b}$$

   and require that the transformation $U(P)$ acting on the Hilbert space can be rewritten as a transformation $P_{\frac{1}{2}}$ acting on the bispinors and $P$ acting on Minkowski space:

$$U(P)\Psi(x)U^{-1}(P)=P_{\frac{1}{2}}^{-1}\Psi(Px)\,. \tag{21}$$

   Which additional condition does this impose on $\eta_a$ and $\eta_b$? Determine $P_{\frac{1}{2}}^{-1}$.

c) Using the results for the transformation of the fields, **1**pt(s)

$$U(P)\psi(t,\boldsymbol{x})U^{-1}(P)=\eta_a\gamma^0\psi(t,-\boldsymbol{x}) \quad \text{and} \quad U(P)\bar{\psi}(t,\boldsymbol{x})U^{-1}(P)=\eta_a^*\bar{\psi}(t,-\boldsymbol{x})\gamma^0\,, \tag{22}$$

evaluate the fermion bilinears

$$\begin{aligned}&\text{(i) } U(P)\bar{\psi}\psi U^{-1}(P)\,, \quad \text{(ii) } U(P)\bar{\psi}\gamma^\mu\psi U^{-1}(P)\,, \quad \text{(iii) } U(P)\bar{\psi}[\gamma^\mu,\gamma^\nu]\psi U^{-1}(P)\\ &\text{(iv) } U(P)\bar{\psi}\gamma^5\psi U^{-1}(P) \quad \text{and} \quad \text{(v) } U(P)\bar{\psi}\gamma^\mu\gamma^5\psi U^{-1}(P)\,.\end{aligned} \tag{23}$$

d) Finally, show that the quantized Dirac Hamiltonian **1**pt(s)

$$H=\int \mathrm{d}^3x\,\bar{\psi}(x)\left(-i\gamma_i\nabla_i+m\right)\psi(x) \tag{24}$$

commutes with the parity operator $U(P)$ by using your results from subtask c).

**Note:** This is equivalent to the fact that the Dirac Hamiltonian in the diagonalized form

$$H=\sum_s\int\frac{\mathrm{d}^3p}{(2\pi)^3}E_{\boldsymbol{p}}\left(a_{\mathbf{p}}^{s\dagger}a_{\mathbf{p}}^s+b_{\mathbf{p}}^{s\dagger}b_{\mathbf{p}}^s\right)\,, \tag{25}$$

commutes with $U(P)$.