Lesson 5 - Relativistic Wave Equations
Unit 5.3 Energy spectrum of the relativistic hydrogen atom

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Dirac equation with a central potential (I)

We now consider the stationary Dirac equation with the confining spherically-symmetric potential $V(r) = V(|\mathbf{r}|)$, namely

$$\left(-i\hbar c\,\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{\nabla} + \hat{\beta}\,mc^2 + V(r)\right)\Phi(\mathbf{r}) = E\,\Phi(\mathbf{r})\ . \tag{1}$$

This equation is easily derived from the Dirac equation with electromagnetic field setting $\mathbf{A} = \mathbf{0}$, $q\phi = V(r)$, and

$$\Psi(\mathbf{r},t) = e^{-iEt/\hbar}\,\Phi(\mathbf{r})\ . \tag{2}$$

In this way we find

$$\left(-i\hbar c\,\hat{\boldsymbol{\alpha}}\cdot\boldsymbol{\nabla} + \hat{\beta}\,mc^2 + V(r)\right)\Phi(\mathbf{r}) = E\,\Phi(\mathbf{r}) \tag{3}$$

Dirac equation with a central potential (II)

The relativistic Hamiltonian

$$\hat{H} = -i\hbar c\, \hat{\boldsymbol{\alpha}} \cdot \boldsymbol{\nabla} + \hat{\beta}\, mc^2 + V(r) \tag{4}$$

commutes with the total angular momentum operator

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} = \mathbf{r} \wedge \hat{\mathbf{p}} + \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \tag{5}$$

because the external potential is spherically symmetric. Consequently one has

$$[\hat{H}, \hat{\mathbf{J}}] = \mathbf{0}\ , \tag{6}$$

and also

$$[\hat{H}, \hat{J}^2] = 0\ , \qquad [\hat{J}^2, \hat{J}_x] = [\hat{J}^2, \hat{J}_y] = [\hat{J}^2, \hat{J}_z] = 0\ , \tag{7}$$

where the three components $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$ of the total angular momentum $\hat{\mathbf{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$ satisfy the familiar commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hbar\ \epsilon_{ijk}\ \hat{J}_k \tag{8}$$

with ϵ_{ijk} the Levi-Civita symbol.

Dirac equation with a central potential (III)

These commutation relations can be symbolically synthesized as

$$\hat{\mathbf{J}} \wedge \hat{\mathbf{J}} = i\hbar \, \hat{\mathbf{J}} \, . \tag{9}$$

Indicating the states which are simultaneous eigenstates of $\hat{H}$, $\hat{J}^2$ and $\hat{J}_z$ as $|njm_j\rangle$, one has

$$\hat{H}|njm_j\rangle = E_{nj}\,|njm_j\rangle \, , \tag{10}$$

$$\hat{J}^2|njm_j\rangle = \hbar^2 j(j+1)\,|njm_j\rangle \, , \tag{11}$$

$$\hat{J}_z|njm_j\rangle = \hbar m_j\,|njm_j\rangle \, , \tag{12}$$

where j is the quantum number of the total angular momentum and $m_j = -j, -j+1, -j+2, ..., j-2, j-1, j$ the quantum number of the third component of the total angular momentum.
It it important to stress that, in the relativistic case, contrary to the total angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$, the orbital angular momentum $\hat{\mathbf{L}}$ and the spin $\hat{\mathbf{S}}$ are not constants of motion of a particle in a central potential.

Relativistic hydrogen atom (I)

Let us consider now the electron of the hydrogen atom. We set $q = -e$, $m = m_e$ and

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 |\mathbf{r}|} = -\frac{e^2}{4\pi\varepsilon_0\, r}\ . \tag{13}$$

Then it is possible to prove that the eigenvalues E_{nj} of $\hat{H}$ are given by

$$E_{nj} = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-\alpha^2}\right)^2}}} - mc^2\ , \tag{14}$$

with $\alpha = e^2/(4\pi\epsilon_0 \hbar c) \simeq 1/137$ the fine-structure constant. We do not prove this remarkable quantization formula, obtained independently in 1928 by Charles Galton Darwin and Walter Gordon.

Relativistic hydrogen atom (II)

Expanding the formula

$$E_{nj} = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{\left(n - j - \frac{1}{2} + \sqrt{(j+\frac{1}{2})^2 - \alpha^2}\right)^2}}} - mc^2 \,, \tag{15}$$

in powers of the fine-structure constant α to order α^4 one gets

$$E_{nj} = E_n^{(0)} \left[1 + \frac{\alpha^2}{n} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \right] \,, \tag{16}$$

where

$$E_n^{(0)} = -\frac{1}{2} mc^2 \frac{\alpha^2}{n^2} = -\frac{13.6 \ eV}{n^2} \tag{17}$$

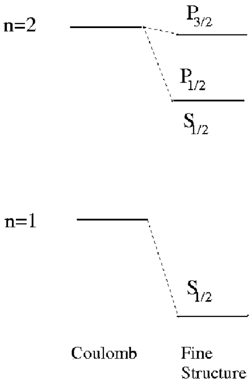
is the familiar Bohr quantization formula of the non relativistic hydrogen atom. The term which corrects the Bohr formula, given by

$$\Delta E = E_n^{(0)} \frac{\alpha^2}{n} \left(\frac{1}{j + \frac{1}{2}} - \frac{3}{4n} \right) \,, \tag{18}$$

is called fine splitting correction.

Relativistic hydrogen atom (III)

The fine splitting removes the non-relativistic degeneracy of energy levels, but not completely: double-degenerate levels remain with the same quantum numbers n and j but different orbital quantum number $l = j \pm 1/2$.



In the figure, on the left there are the non-relativistic energy levels with a Coulomb potential (Coulomb) while on the right there are the relativistic energy levels (Fine Structure).