Review, Jan 27, 2012

We showed,

$$\boldsymbol{\sigma} \cdot \mathbf{p}\psi_A = \frac{1}{c}(E - V(r) + mc^2)\psi_B.$$
$$\boldsymbol{\sigma} \cdot \mathbf{p}\psi_B = \frac{1}{c}(E - V(r) - mc^2)\psi_A$$

and used

$$\boldsymbol{\sigma} \cdot \mathbf{p} = \frac{1}{r}(\boldsymbol{\sigma} \cdot \hat{r})\left(-i\hbar r\frac{\partial}{\partial r} + i\boldsymbol{\sigma} \cdot \mathbf{L}\right)$$
$$\psi_{A,B} = \frac{1}{r}\phi_{A,B}(r)\mathcal{Y}_{j,m,\ell_{A,B}}$$
$$\boldsymbol{\sigma} \cdot \hat{r}\mathcal{Y}_{j,m,\ell=j\pm 1/2} = -\mathcal{Y}_{j,m,\ell=j\mp 1/2}$$
$$\boldsymbol{\sigma} \cdot \mathbf{L}\mathcal{Y}_{j,m,\ell} = \frac{2}{\hbar}\mathbf{S} \cdot \mathbf{L}\mathcal{Y}_{j,m,\ell} = \frac{2}{\hbar}(j(j+1) - \ell(\ell+1) - 3/4)\mathcal{Y}_{j,m,\ell}$$

to obtain

$$\hbar c\left(\frac{dF}{dr} + \frac{\kappa}{r}F\right) = (E - V(r) + mc^2)G$$

$$\hbar c\left(\frac{dG}{dr} - \frac{\kappa}{r}G\right) = -(E - V(r) - mc^2)F$$

Our task is to solve these coupled first order differential equations.

Solution

Use atomic units and rationalize variables

$\varepsilon = E/mc^2 \quad e^2/\hbar c = \alpha = \text{fine structure constant}, \ c = \frac{1}{\alpha},$

$\lambda = \frac{1}{\alpha\sqrt{1-\varepsilon^2}}, \ \rho = 2\lambda r,$

$$\frac{dG}{d\rho} - \frac{\kappa}{\rho} G = \left(\frac{1}{2}\sqrt{\frac{1-\varepsilon}{1+\varepsilon}} - \frac{Z\alpha}{\rho} \right) F$$

$$\frac{dF}{d\rho} + \frac{\kappa}{\rho} F = \left(\frac{1}{2}\sqrt{\frac{1+\varepsilon}{1-\varepsilon}} + \frac{Z\alpha}{\rho} \right) G$$

$F = \sqrt{1+\varepsilon} e^{-\rho/2}(\phi_1 + \phi_2), \ G = \sqrt{1-\varepsilon} e^{-\rho/2}(\phi_1 - \phi_2)$

to get

$$\frac{d\phi_1}{d\rho} = \left(1 - \frac{\alpha\varepsilon}{\sqrt{1-\varepsilon^2}\frac{Z}{\rho}} \right) \phi_1 + \left(-\frac{\kappa}{\rho} - \frac{Z\alpha}{\sqrt{1-\varepsilon^2}} \right) \phi_2 \qquad (1)$$

$$\frac{d\phi_2}{d\rho} = \left(-\frac{\kappa}{\rho} + \frac{\alpha}{\sqrt{1-\varepsilon^2}} \frac{Z}{\rho} \right) \phi_1 + \frac{\alpha\varepsilon}{\sqrt{1-\varepsilon^2}\frac{Z}{\rho}} \phi_2 \qquad (2)$$

Solution continued

Solve Eq.(2) for ϕ_2 and substitute into Eq.(1). This gives a second order differential equation for ϕ_1 whose solution can be recognized as

$$\phi_1 = \frac{n'}{\sqrt{-\kappa+\alpha Z/\sqrt{1-\varepsilon^2}}} \; \rho^\gamma F(-n'+1, 2\gamma+1, \rho)$$

$$\phi_2 = \sqrt{-\kappa+\alpha Z/\sqrt{1-\varepsilon^2}}\rho^\gamma F(-n', 2\gamma+1, \rho)$$

where

$$n' = \frac{Z\alpha\varepsilon}{\sqrt{1-\varepsilon^2}} - \gamma$$

$$\gamma = \sqrt{\kappa^2 - Z^2\alpha^2}$$

and $F(a, b, z)$ is the confluent hypergeometric function of Eq.(A.59) in Appendix A.5. As for the Schrödinger equation, bound states occur when the series for $F(a, b, z)$ terminates. This requires that n' is an integer greater than or equal to 1. Solve for ε in terms of n':

$$\varepsilon = \frac{1}{\sqrt{1+\frac{Z^2\alpha^2}{(n'+\gamma)^2}}} = \frac{1}{\sqrt{1+\frac{Z^2\alpha^2}{(n-\delta_j)^2}}}$$

With $\kappa^2 = (j+1/2)^2$, $n' = n - |\kappa|$ and $\delta_j = |\kappa| - \gamma$ we see that the equation for the eigenenergy agrees with Eq. (2.35) of the text.