EFFECT OF PARTICLE SIZE ON THE 2P LEVEL OF H-ATOM (DIRAC EQ.)

ABSTRACT

The charge of the electron and the proton is assumed to be distributed in space. The potential energy of a specific charge distribution is determined. Perturbation theory is used to calculate the shift in the $2P_{3/2}$ energy level of the hydrogen atom due to the proton and electron size.

I. SOLUTION TO THE DIRAC EQUATION

The potential energy of a point proton and a point electron at rest is $V(r) = -e^2/r$. When this potential energy is put into the Dirac equation, the wave function for the $2P_{3/2}$ energy level is [1]

$$\psi_{n,\ell,j}(\rho,\theta,\phi) = \psi_{2,1,3/2}(\rho,\theta,\phi) = \begin{pmatrix} g(\rho)Y_{11}(\theta,\phi) \\ 0 \\ -if(\rho)\sqrt{\frac{1}{5}}\,Y_{21}(\theta,\phi) \\ -if(\rho)\sqrt{\frac{4}{5}}\,Y_{22}(\theta,\phi) \end{pmatrix} \tag{1}$$

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where $Y_{\ell m}$ is a spherical harmonic [2],

$$g(\rho) = \Big(\frac{1}{a_0}\Big)^{3/2}\sqrt{\frac{1+\epsilon}{2\Gamma(2\gamma_2+1)}}\,\exp\left(-\rho/2\right)\rho^{\gamma_2-1}\,, \tag{2}$$

$f(\rho) = -\sqrt{1-\epsilon}\,g(\rho)/\sqrt{1+\epsilon}$, $\rho = 2r/\big(a_0\sqrt{2(1+\gamma_1)}\,\big)$, a_0 is the Bohr radius, $\gamma_2 = \sqrt{4-\alpha^2}$, $\gamma_1 = \sqrt{1-\alpha^2}$, the fine structure constant $\alpha = e^2/\hbar\,c$, $\epsilon = E/mc^2$, and Γ refers to the gamma function.

II. THE POTENTIAL ENERGY

Take the proton charge to be uniformly distributed on a spherical shell of radius r_0 in its rest frame. The potential energy of this proton and a point electron is

$$V(r) = \frac{-e^2}{r_0}H(r_0-r) + \frac{-e^2}{r}H(r-r_0) \tag{3}$$

where $H()$ is the unit step function. Subtract $-e^2/r$ from $V(r)$ to get the perturbing potential energy, $\delta V(r)$, due to the proton size. The result is

$$\delta V(r) = \frac{-e^2}{r_0}H(r_0-r) + \frac{+e^2}{r}H(r_0-r)\,, \tag{4}$$

and in terms of ρ

$$\delta V(\rho) = \frac{2}{a_0\sqrt{2(1+\gamma_1)}}\Big[\frac{-e^2}{\rho_0}H(\rho_0-\rho) + \frac{+e^2}{\rho}H(\rho_0-\rho)\Big] \tag{5}$$

where $\rho_0 = 2r_0/\big(a_0\sqrt{2(1+\gamma_1)}\,\big)$.

III. SHIFT OF THE $2P_{3/2}$ ENERGY LEVEL DUE TO PROTON SIZE

The energy shift of the $2P_{3/2}$ energy level due to proton size is

$$\delta E(2P_{3/2}) = \int \psi^{\dagger}_{2,1,3/2}(r,\theta,\phi)\delta V(r)\psi_{2,1,3/2}(r,\theta,\phi)\, d^3r\,. \tag{6}$$

Since the wave function was given in terms of ρ and not r, rewrite the above equation as

$$\delta E(2P_{3/2}) = \int \psi^{\dagger}_{2,1,3/2}(\rho,\theta,\phi)\delta V(\rho)\psi_{2,1,3/2}(\rho,\theta,\phi)\, \frac{[2(1+\gamma_1)]^{3/2}}{2^3} a_0^3\, d^3\rho \tag{7}$$

where $d^3\rho = \rho^2\,\sin(\theta)d\theta\, d\phi\, d\rho = \rho^2\, d\rho\, d\Omega$. Note that

$$\int \psi^{\dagger}_{2,1,3/2}(\rho,\theta,\phi)\psi_{2,1,3/2}(\rho,\theta,\phi)\,\sin(\theta)d\theta\, d\phi = \int [\, g^2(\rho)\, Y^*_{11}(\theta,\phi)Y_{11}(\theta,\phi) + f^2(\rho)\Big(\frac{1}{5}Y^*_{21}(\theta,\phi)Y_{21}(\theta,\phi) + \frac{4}{5}Y^*_{22}(\theta,\phi)Y_{22}(\theta,\phi)\Big)]d\Omega = g^2(\rho)\frac{2}{1+\epsilon} \tag{8}$$

since the spherical harmonics are normalized. So

$$\delta E(2P_{3/2}) = \int_0^{\infty} \frac{2g^2(\rho)}{1+\epsilon}\delta V(\rho)\Big)\frac{[2(1+\gamma_1)]^{3/2}}{2^3}\, a_0^3\,\rho^2\, d\rho = \frac{e^2}{a_0\Gamma(2\gamma_2+1)}\frac{[2(1+\gamma_1)]}{2^2}\int_0^{\rho_0} \exp(-\rho)\rho^{2\gamma_2}\Big(\frac{-1}{\rho_0}+\frac{1}{\rho}\Big)\, d\rho\,. \tag{9}$$

Since $\alpha \approx 1/137$, $\gamma_1 = \sqrt{1-\alpha^2} \approx 1$, $\gamma_2 = \sqrt{4-\alpha^2} \approx 2$, and $\rho_0 \approx r_0/a_0$. These approximations in the above equation yield

$$\delta E(2P_{3/2}) = \frac{e^2}{a_0\Gamma(5)}\int_0^{\rho_0} \exp(-\rho)\rho^4\Big(\frac{-1}{\rho_0}+\frac{1}{\rho}\Big)\, d\rho\,. \tag{10}$$

Taylor expand the exponential dropping terms of the order ρ squared and higher. Note $\rho_0 = r_0/a_0 << 1$. Then

$$\delta E(2P_{3/2}) = \frac{e^2}{a_0 \Gamma(5)} \Big[- \int_0^{\rho_0} (\rho^4 - \rho^5) \frac{d\rho}{\rho_0} + \int_0^{\rho_0} (\rho^3 - \rho^4) d\rho \Big] . \tag{11}$$

After integration and a little algebra

$$\delta E(2P_{3/2}) \approx \frac{e^2}{a_0\, 4!} \Big[\frac{\rho_0^4}{20} - \frac{\rho_0^5}{30} \Big], \tag{12}$$

Substitute $\rho_0 = r_0/a_0$, and get

$$\delta E(2P_{3/2}) \approx \frac{e^2}{a_0} \frac{1}{480} \frac{r_0^4}{a_0^4} \Big(1 - \frac{2r_0}{3a_0} \Big) . \tag{13}$$

IV. ELECTRON SIZE INCLUDED IN THE POTENTIAL ENERGY

Again take the proton charge to be uniformly distributed on a spherical shell of radius r_0 in the proton rest frame, and take the electron charge to be uniformly distributed on a spherical shell of radius a in the electron rest frame. The potential energy of the proton and electron is [3]

$$V_e(r) = \frac{-e^2}{r_0} H(r_0 - a - r) - \frac{-e^2}{r} H(r - r_0 - a) + [V_i(r) + V_o(r)][H(r + a - r_0) - H(r - r_0 - a)] \tag{14}$$

where

$$V_i(r) = \frac{-e^2}{2r_0} \Big(1 + \frac{r_0^2 - a^2 - r^2}{2ra} \Big) , \tag{15}$$

and

$$V_o(r) = \frac{-e^2}{2ra} (r + a - r_0) . \tag{16}$$

Subtract $-e^2/r$ from $V_e(r)$ to get the perturbing potential energy

$$\delta V_e(r) = \frac{-e^2}{r_0} H(r_0-a-r) + \frac{+e^2}{r} H(r_0+a-r) + [V_i(r)+V_o(r)][H(r+a-r_0)-H(r-r_0-a)]\,. \tag{17}$$

The approximations $\gamma_1 \approx 1$, $\gamma_2 \approx 2$, $\rho \approx r/a_0$, $\rho_0 \approx r_0/a_0$, and $\bar{a} \approx a/a_0$, will now be made.

$$\delta V_e(\rho) \approx \frac{-e^2}{a_0\rho_0} H(\rho_0-\bar{a}-\rho) + \frac{e^2}{a_0\rho} H(\rho_0+\bar{a}-\rho) + [V_i(\rho)+V_o(\rho)][H(\rho+\bar{a}-\rho_0)-H(\rho-\rho_0-\bar{a})] \tag{18}$$

where

$$V_i(\rho) = \frac{-e^2}{2\rho_0 a_0}\Big(1 + \frac{\rho_0^2 - \bar{a}^2 - \rho^2}{2\rho a}\Big)\,, \tag{19}$$

and

$$V_o(\rho) = \frac{-e^2}{2\rho a_0 \bar{a}}(\rho + \bar{a} - \rho_0)\,. \tag{20}$$

Substitute $\delta V_e(\rho)$ into Eq. (7). The resulting energy shift of the $2P_{3/2}$ energy level is $\delta E'(2P_{3/2}) = \delta E'_1 + \delta E'_2 + \delta E'_3$ where

$$\delta E'_1 = \frac{-e^2}{a_0 \Gamma(5) \rho_0} \int_0^{\rho_0-\bar{a}} \exp(-\rho)\rho^4 d\rho\,, \tag{21}$$

$$\delta E'_2 = \frac{e^2}{a_0 \Gamma(5)} \int_0^{\rho_0+\bar{a}} \exp(-\rho)\rho^3 d\rho\,, \tag{22}$$

and

$$\delta E'_3 = \frac{1}{\Gamma(5)} \int_{\rho_0-\bar{a}}^{\rho_0+\bar{a}} \exp(-\rho)\rho^4 [V_i(\rho) + V_o(\rho)] d\rho\,. \tag{23}$$

Taylor expand the exponential, and drop higher order terms in ρ. Then

$$\delta E'_1 = \frac{-e^2}{a_0\, 4!\, \rho_0} \int_0^{\rho_0-\bar{a}} (\rho^4 - \rho^{5)} d\rho\,, \tag{24}$$

$$\delta E_2' = \frac{e^2}{a_0\,4!}\int_0^{\rho_0+\bar{a}} (\rho^3 - \rho^4 d\rho\,, \tag{25}$$

and

$$\delta E_3' = \frac{1}{4!}\int_{\rho_0-\bar{a}}^{\rho_0+\bar{a}} (\rho^4-\rho^5)[V_i(\rho)+V_o(\rho)]d\rho\,. \tag{26}$$

After integration, $\delta E_1'$ can be put in the form

$$\delta E_1' = \frac{-e^2}{a_0\,4!\,\rho_0}\Big[\frac{(\rho_0-\bar{a})^5}{5} - \frac{(\rho_0-\bar{a})^6}{6}\Big]\,. \tag{27}$$

Drop higher order terms in $\bar{a}$, and find

$$\delta E_1' \approx \frac{e^2}{a_0\,4!}\Big[\frac{-\rho_0^4+5\rho_0^3\bar{a}-10\rho^2\bar{a}^2}{5} + \frac{+\rho_0^5-6\rho_0^4\bar{a}+15\rho^3\bar{a}^2}{6}\Big]\,. \tag{28}$$

Similarly after integration and dropping higher order terms in $\bar{a}$

$$\delta E_2' \approx \frac{e^2}{a_0\,4!}\Big[\frac{+\rho_0^4+4\rho_0^3\bar{a}+6\rho^2\bar{a}^2}{4} + \frac{-\rho_0^5-5\rho_0^4\bar{a}-10\rho^3\bar{a}^2}{5}\Big] \tag{29}$$

Note that

$$\delta E_1' + \delta E_2' \approx \frac{+e^2}{a_0 4!}\big[\rho_0^4\Big(\frac{1}{20}+\frac{2\bar{a}}{\rho_0}-\frac{\hat{a}^2}{2\rho_0^2}\Big)+\rho_0^5\Big(\frac{-1}{30}-\frac{2\hat{a}}{\rho_0}+\frac{\bar{a}^2}{2\rho_0^2}\Big)\big]\,. \tag{30}$$

Substitute $\rho_0 \approx r_0/a_0$ and $\bar{a} \approx a/a_0$ in Eq. (30), and find

$$\delta E_1' + \delta E_2' \approx \frac{+e^2}{a_0 4!}\Big[\frac{r_0^4}{20\,a_0^4}\Big(1-\frac{2r_0}{3a_0}\Big)+\frac{2r_0^3 a}{a_0^4}\Big(1-\frac{r_0}{a_0}\Big)-\frac{a^2r_0^2}{a_0^4}\Big(1-\frac{r_0}{a_0}\Big)\Big]\,. \tag{31}$$

Continue by substituting $V_i(\rho)$ and $V_o(\rho)$ in Eq. (26), and get

$$\delta E_3' \approx \frac{-e^2}{a_0\,4!}\int_{\rho_0-\bar{a}}^{\rho_0+\bar{a}}\Big[\rho^4-\rho^5\Big]\Big[\frac{1}{2\rho_0}\Big(1+\frac{\rho^2-\bar{a}^2-\rho_0^2}{2\rho\bar{a}}\Big)+\frac{\rho+\bar{a}-\rho_0}{2\rho\bar{a}}\Big]d\rho\,. \tag{32}$$

To avoid a lot of algebra, $\delta E_3'$ will be approximated using the mean value theorem for integrals. Since ρ_0 is in the middle of the limits of integration, set $\rho = \rho_0$ in the integrand. Then

$$\delta E_3' \approx \frac{-e^2 \bar{a}}{a_0\, 4!}\Big[2\rho_0^3(1-\rho_0) - \frac{\rho_0^2 \bar{a}}{2}(1-\rho_0)\Big]\,. \tag{33}$$

Next substitute $\rho_0 = r_0/a_0$ and $\bar{a} = a/a_0$ in Eq. (33), and get

$$\delta E_3' \approx \frac{-e^2}{a_0\, 4!}\Big[\frac{2ar_0^3}{a_0^4}\Big(1-\frac{r_0}{a_0}\Big) - \frac{a^2 r_0^2}{2a_0^4}\Big(1-\frac{r_0}{a_0}\Big)\Big]\,. \tag{34}$$

Add the results, and find

$$\delta E'(2P_{3/2}) \approx \frac{e^2}{480\, a_0}\frac{r_0^4}{a_0^4}\Big(1-\frac{2r_0}{3a_0}\Big)\,. \tag{35}$$

Terms like $r_0 a/a_0^2$ and a^2/a_0^2 do not appear. Presumably the electron radius will appear as a^3/a_0^3 when more terms are kept in the Taylor expansion of the exponential. However a^3/a_0^3 is quite small.

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References

[1] Hans A. Bethe and Edwin E. Salpeter, *Quantum Mechanics of One and Two-Electron Atoms*(Springer-Verlag, Berlin, 1957), p 69.

[2] Hans A. Bethe and Edwin E. Salpeter, *Quantum Mechanics of One and Two-Electron Atoms*(Springer-Verlag, Berlin, 1957), p 5.

[3] http://www.electronformfactor.com/ Effect of Electron and Proton Size On Spin-Orbit Coupling