# EFFECT OF PARTICLE SIZE ON H-ATOM SPECTRUM (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 1S 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 1S energy level is [1]

$$\psi_{n,\ell,j}(\rho,\theta,\phi) = \psi_{1,0,1/2}(\rho,\theta,\phi) = \begin{pmatrix} g(\rho)Y_{00}(\theta,\phi) \\ 0 \\ -if(\rho)\sqrt{\frac{1}{3}}\,Y_{10}(\theta,\phi) \\ -if(\rho)\sqrt{\frac{2}{3}}\,Y_{11}(\theta,\phi) \end{pmatrix} \tag{1}$$

*Date*: December 10, 2015.

where $Y_{\ell,m}$ is a spherical harmonic [2], $\rho = 2r/a_0$, $a_0$ is the Bohr radius,

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

$f(\rho) = -\sqrt{1-\epsilon}\, g(\rho)/\sqrt{1+\epsilon}$, $\gamma = \sqrt{1-\alpha^2}$, the fine structure constant $\alpha = e^2/\hbar\, c$, $\epsilon = E/mc^2$, and $\Gamma$ 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

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

## III. SHIFT OF THE 1S ENERGY LEVEL DUE TO PROTON SIZE

The energy shift of the 1S energy level due to proton size is

$$\delta E_1 = \int \psi^\dagger_{1,0,1/2}(r,\theta,\phi)\delta V(r)\psi_{1,0,1/2}(r,\theta,\phi)\, d^3r\,. \tag{5}$$

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

$$\delta E_1 = \int \psi^{\dagger}_{1,0,1/2}(\rho,\theta,\phi)\delta V(\rho)\psi_{1,0,1/2}(\rho,\theta,\phi)\Big(\frac{a_0}{2}\Big)^3 d^3\rho \tag{6}$$

where $d^3\rho = \rho^2 \sin(\theta) d\theta\, d\phi\, d\rho = \rho^2\, d\rho\, d\Omega$, $\rho_0 = 2r_0/a_0$ and

$$\delta V(\rho) = \frac{2e^2}{a_0}\Big(\frac{-1}{\rho_0} + \frac{1}{\rho}\Big) H(\rho_0 - \rho)\,. \tag{7}$$

Note that

$$\int \psi^{\dagger}_{1,0,1/2}(\rho,\theta,\phi)\psi_{1,0,1/2}(\rho,\theta,\phi)\sin(\theta) d\theta\, d\phi =$$
$$\int [\,g(\rho)^2 Y^2_{00}(\theta,\phi) + f^2(\rho)\Big(\frac{1}{3}Y^2_{10}(\theta,\phi) + \frac{2}{3}Y^*_{11}(\theta,\phi)Y_{11}(\theta,\phi)\Big)]d\Omega =$$
$$g(\rho)^2\frac{2}{1-\epsilon} \tag{8}$$

since the spherical harmonics are normalized. So

$$\delta E_1 = \frac{2e^2}{a_0\Gamma(2\gamma+1)}\int_0^{\rho_0} \exp(-\rho)\rho^{2\gamma}\Big(\frac{-1}{\rho_0} + \frac{1}{\rho}\Big)d\rho\,. \tag{9}$$

Taylor expand the exponential dropping terms of the order $\rho$ squared and higher. Note $\rho_0 = 2r_0/a_0 << 1$. Then

$$\delta E_1 = \frac{2e^2}{a_0\Gamma(2\gamma+1)}\Big[-\int_0^{\rho_0}(\rho^{2\gamma} - \rho^{2\gamma+1})\frac{d\rho}{\rho_0} + \int_0^{\rho_0}\rho^{2\gamma-1} - \rho^{2\gamma})d\rho\Big]. \tag{10}$$

After integration and a little algebra

$$\delta E_1 = \frac{2e^2}{a_0\Gamma(2\gamma+1)}\Big[+\frac{\rho^{2\gamma}}{2\gamma(2\gamma+1)} - \frac{\rho_0^{2\gamma+1}}{(2\gamma+1)(2\gamma+2)}\Big]. \tag{11}$$

Substitute $\rho_0 = 2r_0/a_0$, and get

$$\delta E_1 = \frac{2e^2}{a_0\Gamma(2\gamma+1)}\Big(\frac{2r_0}{a_0}\Big)^{2\gamma}\frac{1}{2\gamma(2\gamma+1)}\Big[1-\frac{2r_0}{a_0}\frac{\gamma}{\gamma+1}\Big], \tag{12}$$

where $\gamma = \sqrt{1-\alpha^2} \approx 1$ since $\alpha \approx \frac{1}{137}$. Set $\gamma = 1$, and find

$$\delta E_1 \approx \frac{e^2}{a_0}\frac{2r_0^2}{3a_0^2}\Big(1-\frac{r_0}{a_0}\Big). \tag{13}$$

## 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

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

Express $\delta V_e(r)$ in terms of $\rho = 2r/a_0$, $\rho_0 = 2r_0/a_0$, and $\bar{a} = 2a/a_0$, and find

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

where

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

and

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

Substitute $\delta V_e(\rho)$ into Eq. (6). The resulting energy shift of the 1S energy level is $\delta E_1' = \delta E_{11}' + \delta E_{12}' + \delta E_{13}'$ where

$$\delta E_{11}' = \frac{-2e^2}{a_0 \Gamma(2\gamma + 1)\rho_0} \int_0^{\rho_0 - \bar{a}} \exp(-\rho)\rho^{2\gamma} d\rho\,, \tag{21}$$

$$\delta E_{12}' = \frac{2e^2}{a_0 \Gamma(2\gamma + 1)} \int_0^{\rho_0 + \bar{a}} \exp(-\rho)\rho^{2\gamma - 1} d\rho\,, \tag{22}$$

and

$$\delta E_{13}' = \frac{1}{\Gamma(2\gamma + 1)} \int_{\rho_0 - \bar{a}}^{\rho_0 + \bar{a}} \exp(-\rho)\rho^{2\gamma}[V_i(\rho) + V_o(\rho)] d\rho\,. \tag{23}$$

Taylor expand the exponential, and drop higher order terms in $\rho$. Then

$$\delta E_{11}' = \frac{-2e^2}{a_0 \Gamma(2\gamma + 1)\rho_0} \int_0^{\rho_0 - \bar{a}} (\rho^{2\gamma} - \rho^{2\gamma + 1}) d\rho\,, \tag{24}$$

$$\delta E_{12}' = \frac{2e^2}{a_0 \Gamma(2\gamma + 1)} \int_0^{\rho_0 + \bar{a}} (\rho^{2\gamma - 1} - \rho^{2\gamma}) d\rho\,, \tag{25}$$

and

$$\delta E'_{13} = \frac{1}{\Gamma(2\gamma+1)} \int_{\rho_0-\bar{a}}^{\rho_0+\bar{a}} (\rho^{2\gamma} - \rho^{2\gamma+1})[V_i(\rho) + V_o(\rho)]d\rho\,. \tag{26}$$

After integration, $\delta E'_{11}$ can be put in the form

$$\delta E'_{11} = \frac{-2e^2}{a_0\Gamma(2\gamma+1)\rho_0}\Big[\frac{\rho_0^{2\gamma+1}}{2\gamma+1}\Big(1-\frac{\bar{a}}{\rho_0}\Big)^{2\gamma+1} - \frac{\rho_0^{2\gamma+2}}{2\gamma+2}\Big(1-\frac{\bar{a}}{\rho_0}\Big)^{2\gamma+2}\Big]\,. \tag{27}$$

Taylor expand the two terms in parentheses dropping higher order terms in $\bar{a}/\rho_0$, and find

$$\delta E'_{11} = \frac{-2e^2}{a_0\Gamma(2\gamma+1)}\big[\rho_0^{2\gamma}\Big(\frac{1}{2\gamma+1} - \frac{\bar{a}}{\rho_0} + \frac{2\gamma\bar{a}^2}{2\rho_0^2}\Big)$$
$$- \rho_0^{2\gamma+1}\Big(\frac{1}{2\gamma+2} - \frac{\bar{a}}{\rho_0} + (2\gamma+1)\frac{\bar{a}2}{2\rho_0^2}\Big)\big]\,. \tag{28}$$

Similarly after integration,

$$\delta E'_{12} = \frac{-2e^2}{a_0\Gamma(2\gamma+1)}\Big[\frac{\rho_0^{2\gamma}}{2\gamma}\Big(1-\frac{\bar{a}}{\rho_0}\Big)^{2\gamma} - \frac{\rho_0^{2\gamma+1}}{2\gamma+1}\Big(1-\frac{\bar{a}}{\rho_0}\Big)^{2\gamma+1}\,. \tag{29}$$

Again Taylor expand dropping higher powers of $\bar{a}/\rho_0$, and find

$$\delta E'_{12} = \frac{+2e^2}{a_0\Gamma(2\gamma+1)}\big[\rho_0^{2\gamma}\Big(\frac{1}{2\gamma} + \frac{\bar{a}}{\rho_0} + \frac{(2\gamma-1)\bar{a}^2}{2\rho_0^2}\Big)$$
$$- \rho_0^{2\gamma+1}\Big(\frac{1}{2\gamma+1} + \frac{\bar{a}}{\rho_0} + \frac{2\gamma\bar{a}^2}{2\rho_0^2}\Big)\big]\,. \tag{30}$$

Note that $\delta E'_{11}$ and $\delta E'_{12}$ can be added to yield

$$\delta E'_{11} + \delta E'_{12} = \frac{+2e^2}{a_0\Gamma(2\gamma+1)}\big[\rho_0^{2\gamma}\Big(\frac{1}{(2\gamma+1)2\gamma} + \frac{2\bar{a}}{\rho_0} - \frac{\hat{a}^2}{2\rho_0^2}\Big)$$
$$\rho_0^{2\gamma+1}\Big(\frac{-1}{(2\gamma+2)(2\gamma+1)} - \frac{2\hat{a}}{\rho_0} + \frac{\bar{a}^2}{2\rho_0^2}\Big)\big]\,. \tag{31}$$

It is convenient to set $\gamma = 1$ now. Then

$$\delta E'_{11} + \delta E'_{12} = \frac{+2e^2}{a_0 2}\left[\rho_0^2\Big(\frac{1}{6} + \frac{2\bar{a}}{\rho_0} - \frac{\hat{a}^2}{2\rho_0^2}\Big) + \rho_0^3\Big(\frac{-1}{12} - \frac{2\hat{a}}{\rho_0} + \frac{\bar{a}^2}{2\rho_0^2}\Big)\right]. \quad (32)$$

Next substitute $\rho_0 = 2r_0/a_0$ and $\bar{a} = 2a/a_0$ in Eq. (32), and get

$$\delta E'_{11} + \delta E'_{12} = \frac{+e^2}{a_0}\left[\frac{2r_0^2}{3a_0^2}\Big(1 - \frac{r_0}{a_0}\Big) + \frac{8r_0 a}{a_0^2}\Big(1 - \frac{2r_0}{a_0}\Big) - \frac{2a^2}{a_0^2}\Big(1 - \frac{2r_0}{a_0}\Big)\right]. \quad (33)$$

Finally substitute $V_i(\rho)$ and $V_o(\rho)$ in Eq. (26), and get

$$\delta E'_{13} = \frac{-2e^2}{a_0\Gamma(2\gamma+1)}\int_{\rho_0-\bar{a}}^{\rho_0+\bar{a}}\Big[\rho^{2\gamma} - \rho^{2\gamma+1}\Big]\Big[\frac{1}{2\rho_0}\Big(1 + \frac{\rho^2 - \bar{a}^2 - \rho_0^2}{2\rho\bar{a}}\Big) + \frac{\rho + \bar{a} - \rho_0}{2\rho\bar{a}}\Big]d\rho\,. \quad (34)$$

To avoid a lot of algebra, $\delta E'_{13}$ will be approximated using the mean value theorem for integrals. Since $\rho_0$ is in the middle of the limits of integration, set $\rho = \rho_0$ in the integrand. Then

$$\delta E'_{13} = \frac{-2e^2 2\bar{a}}{a_0\Gamma(2\gamma+1)}(\rho_0^{2\gamma} - \rho_0^{2\gamma+1})\Big(\frac{1}{2\rho_0}\Big)\Big[2 - \frac{\bar{a}}{2\rho_0}\Big]. \quad (35)$$

Again set $\gamma = 1$, and find

$$\delta E'_{13} = \frac{-2e^2 2\bar{a}}{a_0 2!}\Big[\rho_0(1-\rho_0) - \frac{\bar{a}}{4}(1-\rho_0)\Big]. \quad (36)$$

Substitute $\rho_0 = 2r_0/a_0$ and $\bar{a} = 2a/a_0$ in Eq. (36), and get

$$\delta E'_{13} = \frac{-e^2}{a_0}\left[\frac{8ar_0}{a_0^2}\Big(1 - \frac{2r_0}{a_0}\Big) - \frac{8a^2}{4a_0^2}\Big(1 - \frac{2r_0}{a_0}\Big)\right]. \quad (37)$$

Add the results, and find

$$\delta E'_1 = \delta E'_{11} + \delta E'_{12} + \delta E'_{13} = \frac{e^2}{a_0}\frac{2r_0^2}{3a_0^2}\Big(1 - \frac{r_0}{a_0}\Big). \quad (38)$$

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.

## ACKNOWLEDGEMENTS

I thank Ben for his many improvements to the paper.

## 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