EFFECT OF PARTICLE SIZE ON H-ATOM

ABSTRACT

In the usual calculation of the H-atom energy levels, the potential energy of a point proton at rest and a point electron at rest is used in the Schrodinger equation. In this paper, the potential energy is modified by treating the electron and proton charges as extended in space. The effect of electron and proton size on the 1S energy level is calculated.

I. INTRODUCTION

Take the model of the H-atom to be a proton at rest with its center at the origin, and its charge distributed uniformly on a spherical shell of radius r_0. The electron will be treated as a point charge. The next section will calculate the potential energy of such a proton-electron system. The third section will calculate the shift of the 1S energy level for such a proton-electron system. Next take the proton charge to be uniformly distributed on a spherical shell of radius r_0, and take the electron charge to be uniformly distributed on a spherical shell of radius a. Both charges are at rest. The potential energy

Date: October 22, 2016.

of such a system is then calculated in the fourth section. The fifth section will calculate the energy shift of the 1S energy level for such a proton-electron system.

II. POTENTIAL ENERGY OF A PROTON SHELL OF CHARGE

Take the proton to be at rest with the proton center at the origin. Let $\mathbf{r}$ be the vector from the origin to the electron. Denote the distance from the origin to the electron by r. Let $\tilde{\mathbf{y}}$ be the vector from the origin to an element of proton charge. Denote the distance from the origin to an element of proton charge by $\tilde{y}$. Let $\mathbf{r}'$ be the vector from an element of proton charge to the electron. Denote the distance from the element of proton charge to the electron by r'. So $\mathbf{r} = \tilde{\mathbf{y}} + \mathbf{r}'$, and the vectors $\mathbf{r}, \mathbf{r}'$ and $\tilde{\mathbf{y}}$ form a triangle. By the law of cosines, $r' = \sqrt{r^2 + \tilde{y}^2 - 2r\tilde{y}\cos(\theta)}$.

For the proton charge to be uniformly distributed on a spherical shell of radius r_0, the charge density is $\rho = e\delta(\tilde{y} - r_0)/(4\pi r_0^2)$. An element of proton charge is $de = \rho\, d^3\tilde{y}$ where $d^3\tilde{y} = \tilde{y}^2 \sin(\theta)\, d\theta\, d\phi\, d\tilde{y}$, and θ is the angle between $\tilde{\mathbf{y}}$ and $\mathbf{r}$. The differential potential at r' due to an element of proton charge is

$$d\Phi = \frac{de}{r'} = \frac{e\delta(\tilde{y} - r_0)}{4\pi\, r_0^2} \frac{\tilde{y}^2 \sin(\theta)\, d\theta\, d\phi\, d\tilde{y}}{\sqrt{r^2 + \tilde{y}^2 - 2r\tilde{y}\cos(\theta)}}. \tag{1}$$

Upon integrating over $\tilde{y}$ and ϕ, and substituting $u = -\cos(\theta)$, the potential at r is given by

$$\Phi(r) = \int_{-1}^{+1} \frac{e\,du}{2\sqrt{r^2 + r_0^2 + 2rr_0u}} = \frac{e\sqrt{r^2 + r_0^2 + 2rr_0u}}{2rr_0}\Big|_{-1}^{+1} = \frac{e\sqrt{r^2 + r_0^2 + 2rr_0}}{2rr_0} - \frac{e\sqrt{r^2 + r_0^2 - 2rr_0}}{2rr_0}. \quad (2)$$

When $r > r_0$, $\Phi(r) = e/r$, and when $r < r_0$, $\Phi(r) = e/r_0$. So

$$\Phi(r) = \frac{e}{r_0}H(r_0 - r) + \frac{e}{r}H(r - r_0) \quad (3)$$

where the unit step function $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$. Then the potential energy of such a proton and a point electron is

$$V(r) = -e\Phi(r) = \frac{-e^2}{r_0}H(r_0 - r) + \frac{-e^2}{r}H(r - r_0). \quad (4)$$

III. ENERGY SHIFT DUE TO PROTON SIZE

The potential energy of a point proton at rest and a point electron at rest is $-e^2/r$. The energy levels and associated wave functions are found using this potential energy.[1] To find the first order correction to the energy levels, we start with Eq. (4), and subtract $-e^2/r$ to get the perturbing potential energy

$$\delta V(r) = \frac{-e^2 H(r_0 - r)}{r_0} + \frac{e^2 H(r_0 - r)}{r}. \quad (5)$$

The first order correction to the H-atom energy levels due to proton size is [2]

$$\delta E_{nlm} = \int R_{nl}(r) Y^*_{lm}(\theta, \phi) \delta V(r) R_{nl}(r) Y_{lm}(\theta, \phi) r^2 \sin(\theta) d\theta d\phi dr \qquad (6)$$

The correction to the 1S energy level will now be calculated. The Y_{lm} are normalized to one, so

$$\delta E(1S) = \delta E_{100} = \int R^2_{10}(r) \delta V(r) r^2 dr \qquad (7)$$

where $R_{10}(r) = 2\exp(-r/a_0)/(a_0)^{3/2}$ and a_0 is the Bohr radius. [1]

$$\delta E(1S) = \frac{4e^2}{a_0^3}\left\{\frac{-1}{r_0}\int_0^{r_0} \exp(-2r/a_0) r^2 dr + \int_0^{r_0} \exp(-2r/a_0) r dr\right\}. \qquad (8)$$

Taylor expand the exponential, $\exp(-2r/a_0) = 1 - 2r/a_0 + ...$ Since $r \leq r_0$ in the integral, and $r_0 << a_0$, approximate the exponential by 1. Integration yields

$$\delta E_{10} \approx \frac{e^2}{a_0}\frac{2r_0^2}{3a_0^2}. \qquad (9)$$

There is a considerable amount of theoretical and experimental literature on the effect of proton size on the H-atom spectra. At present experiments have led to two different values for the proton radius [3,4]

IV. POTENTIAL ENERGY WHEN BOTH PARTICLES HAVE SIZE

Take the proton charge to be uniformly distributed on a spherical shell of radius r_0, and take the electron charge to be uniformly distributed on a spherical shell of radius a. Both particles are at rest. The potential of the proton is given by Eq. (3) where r is the distance from the center of the proton to the point electron. In this section, change the definition of $\mathbf{r}$ to be the vector from the center of the proton to the center of the electron, so r is the distance form the center of the proton to the center of the electron. Change the definition of $\mathbf{r}'$ to be the vector from the center of the proton to an element of electron charge, so r' is the distance fron the center of the proton to an element of the electron charge Define the vector $\tilde{\mathbf{x}}$ to be the vector from the center of the electron to an element of electon charge, so $\tilde{x}$ is the distance from the center of the electron to an element of electron charge. So $\mathbf{r}' = \tilde{\mathbf{x}} + \mathbf{r}$, and the vectors $\mathbf{r}, \mathbf{r}'$ and $\tilde{\mathbf{x}}$ form a triangle. Thus $r' = \sqrt{r^2 + \tilde{x}^2 - 2r\tilde{x}\cos(\theta)}$ where θ is the angle between $\tilde{\mathbf{x}}$ and $\mathbf{r}$. The potential of the proton at the point $\mathbf{r}'$ is

$$\Phi(r') = \frac{e}{r_0} H(r_0 - r') + \frac{e}{r'} H(r' - r_0) \,. \tag{10}$$

For the electron charge to be uniformly distributed on a spherical shell of radius a, the charge density $\rho_e = -e\delta(\tilde{x} - a)/(4\pi a^2)$. An element of electron charge $de_e = \rho_e \, d^3\tilde{x}$ where $d^3\tilde{x} = \tilde{x}^2 \, \sin(\theta) \, d\theta \, d\phi \, d\tilde{x}$. Then the differential potential energy is

$$dV(r') = \Phi(r') de_e = \left(\frac{e}{r_0} H(r_0' - r) + \frac{e}{r'} H(r' - r_0) \right) \frac{-e\delta(\tilde{x} - a)}{(4\pi a^2)} d^3\tilde{x} \,. \tag{11}$$

When the electron shell is completely outside of the proton shell, $r > r_0 + a$ and $r' > r_0$. Then the potential energy is

$$V_o(r) = \int \frac{-e^2 \delta(\tilde{x} - a)\tilde{x}^2 \sin(\theta)\, d\theta\, d\phi\, d\tilde{x}}{\sqrt{r^2 + \tilde{x}^2 - 2r\tilde{x}\cos(\theta)}4\pi\, a^2} = -\frac{e^2}{r}\,. \tag{12}$$

When the electron shell is completely inside the proton shell, $r < r_0 - a$, $r' < r_0$, and the the potential energy is

$$V_i(r) = \int \frac{-e^2 \delta(\tilde{x} - a)\tilde{x}^2 \sin(\theta)\, d\theta\, d\phi\, d\tilde{x}}{r_0 4\pi\, a^2} = \frac{-e^2}{r_0}. \tag{13}$$

When only part of the electron shell is inside of the proton shell, $r_0 - a < r < r_0 + a$. Then set $V_b(r) = V_{bi}(r) + V_{bo}(r)$ where $V_{bi}(r)$ is that part of the potential energy associated with the electron shell inside of the proton shell, and $V_{bo}(r)$ is that part of the potential energy associated with the electron shell outside of the proton shell. Recall θ is the angle between $\mathbf{r}$ and $\tilde{\mathbf{x}}$. For that part of the electron, which is inside the proton, the angle θ varies between 0 and θ_c where θ_c is the angle where the two shells intersect, i.e. when $r' = r_0$. So

$$r_0^2 = r^2 + a^2 - 2ra\cos(\theta_c)\,. \tag{14}$$

Make the substitution $u = -\cos(\theta)$. Then

$$V_{bi}(r) = \int \frac{-e^2}{r_0} \frac{\delta(\tilde{x} - a)}{4\pi a^2}\, d^3\tilde{x} = \frac{-e^2}{r_0} \int_{-cos(0)}^{-\cos(\theta_c)} \frac{du}{2} = \frac{-e^2}{2r_0}(1 - \cos(\theta_c)) = \frac{-e^2}{2r_0}\Big(1 - \frac{(r^2 + a^2 - r_0^2)}{2ra}\Big)\,. \tag{15}$$

For that part of the electron , which is outside of the proton shell, θ varies from θ_c to π. So

$$V_{bo}(r) = \int \frac{-e^2}{r'}\frac{\delta(\tilde{x}-a)}{4\pi a^2}\,d^3\tilde{x} = \frac{-e^2}{2}\int_{-cos(\theta_c)}^{-cos(\pi)} \frac{du}{\sqrt{r^2+a^2+2rau}} =$$

$$-e^2\frac{\sqrt{r^2+a^2+2rau}}{2ra}\Big|_{-cos(\theta_c)}^{+1} = -e^2\Big(\frac{r+a}{2ra} - \frac{r_0}{2ra}\Big). \quad (16)$$

Thus for $r_0 - a < r < r_0 + a$,

$$V_b(r) = \frac{-e^2}{2r_0}\Big(1 - \frac{(r^2+a^2-r_0^2)}{2ra}\Big) + -e^2\Big(\frac{r+a}{2ra} - \frac{r_0}{2ra}\Big). \quad (17)$$

Finally,

$$V(r) = -\frac{e^2}{r_0}H(r_0-a-r) - \frac{e^2}{r}H(r-r_0-a) + \Big[\frac{-e^2}{2r_0}\Big(\frac{2ra-(r^2+a^2-r_0^2)}{2ra}\Big) +$$

$$-e^2\Big(\frac{r+a-r_0}{2ra}\Big)\Big]\big(H(r_0-a-r) - H(r-r_0-a)\big). \quad (18)$$

V. ENERGY SHIFT DUE TO ELECTRON AND PROTON SIZE

Start with Eq. (18), and subtract $-e^2/r$ to get the perturbing potential energy $\delta V(r)$. So

$$\delta V(r) = -\frac{e^2}{r_0}H(r_0-a-r) + \frac{e^2}{r}H(r_0+a-r) + \Big[\frac{-e^2}{2r_0}\Big(\frac{2ra-(r^2+a^2-r_0^2)}{2ra}\Big) +$$

$$-e^2\Big(\frac{r+a-r_0}{2ra}\Big)\Big]\big(H(r_0-a-r) - H(r-r_0-a)\big). \quad (19)$$

Use Eq. (7) to calculate $\delta E(1S)$, but use Eq. (19) as the perturbing potential energy. Again approximate the exponential by 1. Write

$\delta E(1S) = \delta E_i + \delta E_o + \delta E_{bi} + \delta E_{bo}$ where

$$\delta E_i = \frac{-4e^2}{a_0^3\, r_0} \int_0^{r_0-a} r^2\, dr = \frac{+e^2}{a_0}\Big(\frac{-4r_0^2}{3a_0^2} + \frac{4r_0 a}{a_0^2} - \frac{4a^2}{a_0^2}\Big)\,, \tag{20}$$

$$\delta E_o = \frac{+4e^2}{a_0^3} \int_0^{r_0+a} r\, dr = \frac{+e^2}{a_0}\Big(\frac{2r_0^2}{a_0^2} + \frac{4r_0 a}{a_0^2} + \frac{2a^2}{a_0^2}\Big)\,, \tag{21}$$

$$\begin{aligned}\delta E_{bi} = \frac{-4\, e^2}{2a_0^3\, r_0} \int_{r_0-a}^{r_0 * a} \Big(\frac{2ra - r^2 - a^2 + r_0^2)}{2ra}\Big) r^2\, dr = \\ \frac{-4\, e^2}{a_0^3} \int_{r_0-a}^{r_0 * a} \Big(\frac{2r^2 a - r^3 - a^2 r + r_0^2 r}{4r_0\, a}\Big) dr = \\ \frac{-e^2}{a_0^3 r_0 a}\Big(\frac{2r^3 a}{3} - \frac{r^4}{4} - \frac{a^2 r^2}{2} + \frac{r_0^2 r^2}{2}\Big)\Big|_{r_0-a}^{r_0 * a} = \frac{e^2}{a_0^3}\big(-4r_0 a + 4a^2\big)\,,\end{aligned} \tag{22}$$

and

$$\begin{aligned}\delta E_{bo} = -4\frac{e^2}{a_0^3}\frac{1}{2} \int_{r_0-a}^{r_0+a} \Big(\frac{r + a - r_0}{2ra}\Big) r^2\, dr = \\ -4\frac{e^2}{a_0^3\, 2a}\Big(\frac{r^3}{3} + \frac{ar^2}{2} - \frac{r_0 r^2}{2}\Big)\Big|_{r_0-a}^{r_0+a} = \frac{e^2}{a_0^3}\Big(-\frac{4}{3}a^2 - 4r_0 a\Big)\,.\end{aligned} \tag{23}$$

Thus

$$\delta E_{bi} + \delta E_{bo} = \frac{e^2}{a_0}\Big(-\frac{4r_0 a}{a_0^2} + \frac{4a^2}{a_0^2}\Big) + \frac{e^2}{a_0}\big(-\frac{4r_0 a}{a_0^2} - \frac{4a^2}{3a_0^2}\Big) \tag{24}$$

and

$$\delta E(1S) \approx \frac{e^2}{a_0}\Big(\frac{2r_0^2}{3a_0^2} + \frac{2a^2}{3a_0^2}\Big)\,. \tag{25}$$

ACKNOWLEDGEMENTS

References

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