EFFECT OF PARTICLE SIZE ON HYPERFINE STRUCTURE

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 hyperfine structure of the 2S energy level is calculated.

I. EFFECT OF PROTON SIZE ON THE HYPERFINE STRUCTURE

The vector potential $\mathbf{A}(\mathbf{r})$ at a point $\mathbf{r}$ in space, which is due to the magnetic moment $\mathbf{m}$ of a point proton at the origin is [1]

$$\mathbf{A}(\mathbf{r}) = \mathbf{m} \times \frac{\mathbf{r}}{|\mathbf{r}|^3} \tag{1}$$

in c.g.s. units where $\mathbf{m} = g_p \, e \, \mathbf{I}/(2M)$, g_P is the gyromagnetic ratio of the proton, $e > 0$ is the proton charge, $\mathbf{I}$ is the proton spin operator, and M is the proton mass. In naturalized units (used in this

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paper),

$$\mathbf{A}(\mathbf{r}) = \frac{g_p\, e}{2M}\mathbf{I} \times \frac{\mathbf{r}}{4\pi|\mathbf{r}|^3}. \tag{2}$$

If the proton magnetic moment is spread out in space, then

$$\mathbf{A}(\mathbf{r}) = \frac{g_p\, e}{2M}\int \rho_p(\mathbf{y})\mathbf{I} \times \frac{\mathbf{r}'}{4\pi|\mathbf{r}'|^3} d^3y \tag{3}$$

where $e\,\rho_p(\mathbf{y})$ is the proton charge density, $\mathbf{y}$ is the vector from the origin (center of the proton) to an element of the proton magnetic moment, $\mathbf{r}'$ is the vector from an element of the proton magnetic moment to a field point, and r is the vector from the origin to the field point. So $\mathbf{r} = \mathbf{y} + \mathbf{r}'$, and

$$\mathbf{A}(\mathbf{r}) = \frac{g_p\, e}{2M}\int \rho_p(\mathbf{y})\mathbf{I} \times \nabla_r\Big(\frac{-1}{4\pi|\mathbf{r}-\mathbf{y}|}\Big) d^3y \tag{4}$$

The magnetic field at a point $\mathbf{r}$ is [2]

$$\mathbf{B}(\mathbf{r}) = \nabla_r \times \mathbf{A}(\mathbf{r}) = \frac{g_p\, e}{2M}\int \rho_p(\mathbf{y})\nabla_r \times \Big(\mathbf{I} \times \nabla_r\Big(\frac{-1}{4\pi|\mathbf{r}-\mathbf{y}|}\Big)\Big) d^3y =$$
$$\frac{g_p\, e}{2M}\int \rho_p(\mathbf{y})\Big[-\nabla_r^2\Big(\frac{\mathbf{I}}{4\pi|\mathbf{r}-\mathbf{y}|}\Big) + \mathbf{I}\cdot\nabla_r\Big(\nabla_r\frac{1}{(4\pi|\mathbf{r}-\mathbf{y}|)}\Big)\Big] d^3y. \tag{5}$$

The electron magnetic moment $-e\vec{\sigma}/(2m)$ of a point electron interacts with the above magnetic field, yielding the hamiltonion $H' = e\vec{\sigma}\cdot\mathbf{B}/(2m)$ where m is the electron mass, and $\vec{\sigma}$ is the electron spin operator. The shift of the 2S energy level is given by $\Delta\, E_{20} = \int \psi^*_{200}\, H'\psi_{200}\, d^3r$ where $\psi_{200}(r,\theta,\phi) = R_{20}(r)Y_{00}(\theta,\phi)$, the normalized spherical harmonic $Y_{00}(\theta,\phi) = 1/(4\pi)^{1/2}$, and $R_{20}(r) = (2 - r/a_0)\exp\left(-r/(2a_0)\right)/(2a_0)^{3/2}$ where a_0 is the Bohr radius.[3] The term $\nabla_r(\nabla_r(1/(4\pi|\mathbf{r}-\mathbf{y}|)$ will contain linear terms of the components of $\mathbf{r}$ and the components of $\mathbf{y}$. These linear components integrate to zero leading to $\nabla_i\nabla_j \Rightarrow 1/3\,\delta_{ij}\nabla^2$ in the integral for ΔE_{20}. Note that $\nabla_r^2(1/(|\mathbf{r}-\mathbf{y}|) = -4\pi\delta^3(\mathbf{r}-\mathbf{y})$, so [2]

$$\Delta E_{20} = \frac{g_p\, e^2}{(2M2m)}\vec{\sigma}\cdot\mathbf{I}\int \rho_p(\mathbf{y})R_{20}^2(r)\,Y_{00}^2\,\frac{2}{3}\,\delta^3(\mathbf{r}-\mathbf{y})d^3y\,d^3r. \qquad (6)$$

For the purpose of illustration, consider the magnetic moment of the proton distributed uniformly on a spherical shell of radius r_0. Then $\rho_p(\mathbf{y}) = \delta(|\mathbf{y}|-r_0)/(4\pi r_0^2)$. In spherical coordinates, $dr^3 = r^2 dr d\Omega$ where $d\Omega = \sin(\theta)d\theta d\phi$. Then

$$\Delta E_{20} = \frac{g_p\, e^2}{6Mm}\vec{\sigma}\cdot\mathbf{I}\int \frac{\delta(|\mathbf{r}|-r_0)}{4\pi r_0^2}R_{20}^2(r)\,r^2\,dr\,Y_{00}^2\,d\Omega = \frac{g_p\, e^2}{6Mm}\vec{\sigma}\cdot\mathbf{I}\frac{R_{20}^2(r_0)}{4\pi}. \qquad (7)$$

Expand the exponential in $R_{20}(r_0)$ in powers of $r_0/a_0 << 1$, and approximate $R_{20}^2(r)$ by $(4-8r_0/a_0)/(2a_0)^3$. Then find

$$\Delta\, E_{20} = \frac{2g_p\, e^2}{(3Mm)}\vec{\sigma}\cdot\mathbf{I}\frac{1}{4\pi(2a_0)^3}(1-\frac{2r_0}{a_0})\,. \qquad (8)$$

II. EFFECT OF ELECTRON SIZE ON THE HYPERFINE STRUCTURE

In this section, both the proton and electron magnetic moments will be assumed to be distributed in space. The magnetic field is again given by Eq. (5). Let $-e\rho_e(\mathbf{x})$ be the electron charge density where $\mathbf{x}$ is the vector from the center of the electron to an element of the electron magnetic moment. Then an element of the electron magnetic moment is given by$-e\rho_e(\mathbf{x})\,\vec{\sigma}\,d^3x/(2m)$ where m is the electron mass, and $\vec{\sigma}$ is the electron spin operator. Define $\mathbf{r}'$ to be the vector from an element of proton magnetic moment to an element of electron magnetic moment, $\mathbf{r}$ is the vector from the center of the proton to the center of the electron, again $\mathbf{y}$ is the vector from the center of the proton to an element of the proton magnetic moment, and $\mathbf{y}+\mathbf{r}'=\mathbf{r}+\mathbf{x}$. Then

$$\Delta E_{20} = \frac{g_p\, e^2\vec{\sigma}}{2M2m}\int \rho_e(\mathbf{x})\, d^3x\, \rho_p(\mathbf{y})\, d^3y$$
$$\Big[-\nabla_r^2\Big(\frac{\mathbf{I}}{4\pi|\mathbf{r}+\mathbf{x}-\mathbf{y}|}\Big) + \mathbf{I}\cdot\nabla_r\Big(\nabla_r\frac{1}{(4\pi|\mathbf{r}+\mathbf{x}-\mathbf{y}|)}\Big)\Big] R_{20}^2(r)\, r^2dr. \quad (9)$$

Proceed as in the previous section, and get

$$\Delta E_{20} = \frac{g_p\, e^2}{2M2m}\vec{\sigma}\cdot\mathbf{I}\int \rho_e(\mathbf{x})\, d^3x\, \rho_p(\mathbf{y})\, d^3y\, \frac{2}{3}\delta^3(\mathbf{r}+\mathbf{x}-\mathbf{y})R_{20}^2(r)\, r^2dr. \quad (10)$$

For the purpose of illustration, choose $\rho_p(\mathbf{y}) = \delta(|\mathbf{y}|-r_0)/(4\pi r_0^2)$, and choose $\rho_e(\mathbf{x}) = \delta(|\mathbf{x}|-a)/(4\pi a^2)$. Then

$$\Delta E_{20} = \frac{g_p\, e^2}{2M2m}\vec{\sigma}\cdot\mathbf{I}\int \frac{\delta(|\mathbf{x}|-a)}{4\pi a^2}\, d^3x\, \frac{\delta(|\mathbf{y}|-r_0)}{4\pi r_0^2}\, d^3y$$
$$\frac{2}{3}\delta^3(\mathbf{r}+\mathbf{x}-\mathbf{y})R_{20}^2(r)\, r^2dr. \quad (11)$$

Use $\int \delta(|\mathbf{y}| - r_0)\, \delta^3(\mathbf{r} + \mathbf{x} - \mathbf{y})\, d^3y = \delta(|\mathbf{r} + \mathbf{x}| - r_0)$, and get

$$\Delta E_{20} = \frac{2}{3}\frac{g_p\, e^2}{(2M2m)}\vec{\sigma}\cdot\mathbf{I}\int \frac{\delta(|\mathbf{x}| - a)}{4\pi a^2}\, d^3x$$

$$\frac{\delta(\sqrt{r^2 + x^2 - 2rx\cos(\theta)} - r_0)}{4\pi r_0^2}\, R_{20}^2(r)\, r^2dr =$$

$$\frac{2}{3}\frac{g_p\, e^2}{(2M2m)}\vec{\sigma}\cdot\mathbf{I}\int \frac{\sin(\theta)\, d\theta}{2}\frac{\delta(\sqrt{r^2 + a^2 - 2ra\cos(\theta)} - r_0)}{4\pi r_0^2}\, R_{20}^2(r)\, r^2dr. \tag{12}$$

Set $u = -\cos(\theta)$, so $du = \sin(\theta)\, d\theta$. Since $-1 \le u \le +1$, it follows that $r_0 - a \le r \le r_0 + a$. Use the property of the delta function that $\int du\, \delta(\sqrt{r^2 + a^2 + 2rau} - r_0) = \int \delta(u - \bar{u}) du/(f'(u))$ where $\bar{u}$ is determined by $r^2 + a^2 + 2ra\bar{u} = r_0^2$, and $f(u) = \sqrt{r^2 + a^2 + 2rau} - r_0$. So

$$\Delta E_{20} = \frac{g_p\, e^2}{6Mm}\vec{\sigma}\cdot\mathbf{I}\int \frac{du\, \delta(u - \bar{u})}{2ra}\frac{\sqrt{r^2 + a^2 - 2rau}}{4\pi r_0^2}\, R_{20}^2(r)\, r^2dr$$

$$\frac{g_p\, e^2}{6Mm}\int_{r_0 - a}^{r_0 + a}\frac{\vec{\sigma}\cdot\mathbf{I}}{2ra}\frac{r_0}{4\pi r_0^2} R_{20}^2(r)\, r^2dr. \tag{13}$$

Approximate $R_{20}^2(r)$ by $(4 - 8r/a_0)/(2a_0)^3$, and get

$$\Delta E_{20} = \frac{2g_p\, e^2}{(3Mm)}\frac{\vec{\sigma}\cdot\mathbf{I}}{4\pi(2a_0)^3}\Big(1 - \frac{2r_0}{a_0} - \frac{2a^2}{3a_0^2}\Big). \tag{14}$$

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References

[1] John D. Jackson, *Classical Electrodynamics*(John Wiley and Sons, New York, 1962), p 58.

[2] J.D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw-Hill, New York, 1964), p 58.

[3] Leonard Schiff, *Quantum Mechanics* (McGraw-Hill, New York, NY, 1955), pp. 80-85.