EFFECT OF ELECTRON AND PROTON SIZE ON SPIN-ORBIT COUPLING

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 spin-orbit coupling of the $2P_{1/2}$ energy level is calculated.

I. SPIN-ORBIT COUPLING

For a proton of charge e at the origin and an electron at a distance r from the origin, the potential energy $V(r)$ is $-e^2/r$. For the hydrogen atom the unperturbed hamiltonian is $H_0 = -\hbar^2\nabla^2/(2m) + V(r)$ The hamiltonian due to spin-orbit coupling is [1]

$$H' = \frac{1}{2m^2c^2}\mathbf{S}\cdot\mathbf{L}\,\frac{1}{r}\frac{dV}{dr} \tag{1}$$

Since the operators $\mathbf{L}^2, \mathbf{S}^2, \mathbf{J}^2 = (\mathbf{L}+\mathbf{S})^2$, and $J_z = L_z + S_z$, all commute with $H_0 + H'$, the solution to the Schrödinger equation

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can be chosen to be eigenfunctions of $\mathbf{L}^2, \mathbf{S}^2, \mathbf{J}^2 = (\mathbf{L}+\mathbf{S})^2$, and $J_z = L_z + S_z$.[2] The spherical harmonics $Y_{lm}(\theta,\phi)$ are eigenfunctions of $\mathbf{L}^2$. The spin wave functions $\binom{1}{0}$ and $\binom{0}{1}$are eigenfunctions of $\mathbf{S}^2$. $Y_{lm}(\theta,\phi)\binom{1}{0}$ and $Y_{l,m+1}(\theta,\phi)\binom{0}{1}$ are both eigenfunctions of J_z with eigenvalue $m+1/2$. Form the linear combination [1]

$$\Upsilon^{\ell}_{j,m+1/2} = \alpha Y_{lm}(\theta,\phi)\begin{pmatrix}1\\0\end{pmatrix} + \beta Y_{l,m+1}(\theta,\phi)\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}\alpha Y_{lm}(\theta,\phi)\\ \beta Y_{l,m+1}(\theta,\phi)\end{pmatrix}, \tag{2}$$

which is an eigenfunction of j_z. Choose α and β so that $\Upsilon^{\ell}_{j,m+1/2}$ is normalized, and is an eigenfunction of $\mathbf{J}^2$. Application of the operator $\mathbf{S}\cdot\mathbf{L} = (\mathbf{J^2} - \mathbf{L^2} - \mathbf{S^2})/2$ to $\Upsilon^{\ell}_{j,m+1/2}$ yields

$$\mathbf{S}\cdot\mathbf{L}\,\Upsilon^{\ell}_{j,m+1/2} = \frac{1}{2}\big(j(j+1) - \ell(\ell+1) - s(s+1)\big)\hbar^2\,\Upsilon^{\ell}_{j,m+1/2}. \tag{3}$$

For the $2P^{1/2}$ energy level $j = 1/2$, $\ell = 1$, and $s = 1/2$, so $\mathbf{S}\cdot\mathbf{L}$ has eigenvalue $-\hbar^2$. Thus

$$H'\Upsilon^{1}_{1/2,1/2} = \frac{-\hbar^2}{2m^2c^2}\,\frac{1}{r}\frac{dV}{dr}\Upsilon^{1}_{1/2,1/2} \tag{4}$$

See reference 2 for for eigenvalues of $\mathbf{S}\cdot\mathbf{L}$ for arbitrary values of j, l, and j_z, and for α and β associated for each eigenvalue.

II. EFFECT OF PROTON SIZE ON SPIN-ORBIT COUPLING

In this section, the effect of proton size on the $2\,\mathrm{P}_{1/2}$ energy level is calculated. For the purpose of illustration, take the center of the proton to be at the origin, and take the proton charge to be distributed uniformly on a spherical shell of radius r_0. Then the potential of the proton is

$$\Phi(r) = \frac{e}{r_0} H(r_0 - r) + \frac{e}{r} H(r - r_0) \tag{5}$$

where H is the unit step function. The potential energy of the proton and a point electron is

$$V(r) = -\frac{e^2}{r_0} H(r_0 - r) - \frac{e^2}{r} H(r - r_0)\,. \tag{6}$$

H' with the above potential energy will be treated as a perturbation. Note that $dV/dr = +e^2 H(r - r_0)/r^2$.

The solutions to the unperturbed H-atom, which are eigenfunctions of $\mathbf{L}^2, \mathbf{S}^2, \mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2$, and $J_z = L_z + S_z$, are

$$\Psi(r, \theta, \phi) = R_{n\ell}(r) \Upsilon^{\ell}_{j,m+1/2}(\theta, \phi). \tag{7}$$

The first order correction to an energy level is

$$\Delta E = \int \Psi^{\dagger}(r, \theta, \phi) H' \Psi(r, \theta, \phi) r^2\, dr\, d\Omega\,. \tag{8}$$

Since α and β have been chosen so that the $\Upsilon^{\ell}_{j,m+1/2}(\theta,\phi)$ are normalized, the first order correction to the $2\,\mathrm{P}_{1/2}$ energy level is

$$\Delta E(2\,P_{1/2}) = -\frac{\hbar^2}{2m^2c^2}\int_0^\infty R_{21}^2(r)\frac{1}{r}\frac{dV}{dr}r^2\,dr \tag{9}$$

where $R_{21}(r) = r\exp\left(-r/(2a_0)/\big((2a_0)^{3/2}\sqrt{3}a_0\big)\right.$, and a_0 is the Bohr radius. Then

$$\begin{aligned}\Delta E(2\,P_{1/2}) = -\frac{\hbar^2}{2m^2c^2}\frac{e^2}{(2a_0)^3 3a_0^2}\int_{r_0}^\infty r\exp\left(-r/a_0\right)dr = \\ -\frac{\hbar^2}{6m^2c^2}\frac{e^2}{(2a_0)^3}\frac{1}{a_0}^2\exp\left(-r/a_0\right)\Big(-ra_0-a_0^2\Big)\Big|_{r_0}^{\infty}.\end{aligned} \tag{10}$$

Expand the exponential in a Taylor series, and drop terms of the order $(r_0/a_0)^3$ and higher $(r_0/a_0 << 1)$. The result is

$$\Delta E(2\,P_{1/2}) = -\frac{\hbar^2e^2}{6m^2c^2(2a_0)^3}\left(1-\frac{1}{2}\left(\frac{r_0}{a_0}\right)^2\right). \tag{11}$$

Set $r_0 = 0$, and recover the energy shift for a point proton. [1]

III. EFFECT OF ELECTRON SIZE ON SPIN-ORBIT COUPLING

Take the electron charge to be uniformly distributed on a spherical shell of radius a. Again take the proton charge to be uniformly distributed on a spherical shell of radius r_0. Let $\tilde{\mathbf{y}}$ be the vector from the center of the proton to an element of proton charge, and let $\mathbf{r}'$ be the vector from an element of proton charge to an element of electron charge. Define $\mathbf{r}$ to be the vector from the center of the proton to the center of the electron, and define $\tilde{\mathbf{x}}$ to be the vector from the center of the electron to an element of electron charge. Then $\tilde{\mathbf{y}} + \mathbf{r}' = \mathbf{r} + \tilde{\mathbf{x}}$. When the electron is completely inside the proton($r < r_0 - a$), the potential energy is $-e^2/r_0$. When the electron is completely outside the proton($r > r_0 + a$), the potential energy is $-e^2/r$.

Next consider the case when the electron is partially inside and partially outside of the proton ($r_0 - a < r < r_0 + a$). The potential energy of the proton and an element of the electron inside the proton is

$$dV_i(r) = \frac{-e^2}{r_0} \frac{\delta(|\tilde{\mathbf{x}}| - a)}{4\pi a^2} \, d^3\tilde{x} \tag{12}$$

where in spherical coordinates $d^3\tilde{x} = |\tilde{\mathbf{x}}|^2 d|\tilde{\mathbf{x}}| \sin(\theta) \, d\theta \, d\phi$. The potential energy of the proton and that part of the electron inside of the proton is

$$V_i(r) = \int \frac{-e^2}{r_0} \frac{\delta(|\tilde{\mathbf{x}}| - a)}{4\pi a^2} \, |\tilde{\mathbf{x}}|^2 d|\tilde{\mathbf{x}}| \sin(\theta) \, d\theta \, d\phi = \frac{-e^2}{2r_0} \int_0^{\theta_c} \sin(\theta) \, d\theta \tag{13}$$

where θ is the angle between $\tilde{\mathbf{x}}$ and $-\mathbf{r}$, and θ_c is the angle between $\tilde{\mathbf{x}}$ and $-\mathbf{r}$ where the electron sphere intersects the proton sphere. Then θ_c is determined by $r^2 + a^2 - 2ra\cos(\theta_c) = r_0^2$. Set $u = \cos(\theta)$, and $du = -\sin(\theta)\,d\theta$. Then

$$V_i(r) = \frac{-e^2}{2r_0}\int_{\cos(0)}^{\cos(\theta_c)} -du = \frac{-e^2}{2r_0}\Big(1 + \frac{r_0^2 - r^2 - a^2}{2ra}\Big). \tag{14}$$

The potential energy of the proton and an element of the electron outside the proton is

$$dV_o(r) = \frac{-e^2\delta(|\tilde{\mathbf{x}}| - a)}{4\pi a^2}\,\frac{d^3\tilde{x}}{|\mathbf{r} + \tilde{\mathbf{x}}|}. \tag{15}$$

The potential energy of the proton and that part of the electron outside of the proton is

$$V_o(r) = \int \frac{\delta(|\tilde{\mathbf{x}}^{\mathbf{2}}| - a)}{4\pi a^2}\,\frac{-e^2|\tilde{\mathbf{x}}|^2 d|\tilde{\mathbf{x}}|\sin(\theta)\,d\theta\,d\phi}{\sqrt{r^2 + |\tilde{\mathbf{x}}^2| - 2r|\tilde{\mathbf{x}}|\cos(\theta)}}\,. \tag{16}$$

Again set $u = cos(\theta)$, and find

$$V_o = \frac{-e^2}{2}\int_{\cos(\theta_c)}^{\cos(\pi)} \frac{-du}{\sqrt{r^2 + |\tilde{\mathbf{x}}^2| - 2r|\tilde{\mathbf{x}}|\cos(\theta)}} = \frac{-e^2}{2ra}(r + a - r_0)\,. \tag{17}$$

Put these results together , and get for the potential energy

$$V(r) = \frac{-e^2}{r_0}H(r_0 - a - r) + \frac{-e^2}{r}H(r - r_0 - a)$$
$$+[H(r+a-r_0)-H(r-r_0-a)]\Big[\frac{-e^2}{2r_0}\Big(1+\frac{r_0^2 - a^2}{2ra} - \frac{r}{2a}\Big) - \frac{e^2}{2a}\Big(1+\frac{(a - r_0)}{r}\Big)\Big]. \tag{18}$$

Then

$$\frac{dV(r)}{dr} = +\frac{+e^2}{r^2}H(r-r_0-a) + [H(r+a-r_0) - H(r-r_0-a)]\times \left[\frac{e^2}{2r_0}\Big(\frac{r_0^2-a^2}{2r^2a}+\frac{1}{2a}\Big)+\frac{e^2}{2a}\Big(\frac{a-r_0}{r^2}\Big)\right]. \quad (19)$$

Since $V(r)$ is continuous, no delta functions appear in dV/dr. Substitute the above dV/dr in Eq. (9). and find for the first order correction to the $2P^{1/2}$ energy level due to spin-orbit coupling

$$\Delta E(2\,P_{1/2}) = \frac{-\hbar^2 e^2}{2m^2c^2(2a_0)^3\,3\,a_0^2}\left[I_1+I_2\Big(\frac{r_0^2-a^2}{4r_0a}\Big)+I_2\Big(\frac{a-r_0}{2a}\Big)+\frac{I_3}{4r_0a}\right] \quad (20)$$

where

$$I_1 = \int_{r_0+a}^{\infty} r\exp(-r/a_0)dr = \exp[-(r_0+a)/a_0]\big((r_0+a)a_0+a_0^2\big)\,, \quad (21)$$

$$I_2 = \int_{r_0-a}^{r_0+a} r\exp(-r/a_0)dr = \exp[-(r_0+a)/a_0]\big(-(r_0+a)a_0-a_0^2\big)+ \exp[-(r_0-a)/a_0]\big(+(r_0-a)a_0+a_0^2\big)\,, \quad (22)$$

and

$$I_3 = \int_{r_0-a}^{r_0+a} r^3\exp(-r/a_0)dr = \exp(-r/a_0)\left[-r^3a_0-3r^2a_0^2-6ra_0^3-6a_0^4\right]\Big|_{r_0-a}^{r_0+a} \quad (23)$$

Taylor expand the exponentials dropping higher order terms in r_0/a_0 and a/a_0. Then $I_1 \approx a_0^2 - (r_0 + a)^2/2$, $I_2 \approx 2r_0 a$, and $I_3 \approx 2ar_0^3 + 2a^3 r_0$. Finally

$$\Delta E(2\,P_{1/2}) = \frac{-\hbar^2 e^2}{6\,m^2 c^2 (2a_0)^3}\left[1 - \left(\frac{r_0^2 + a^2}{2a_0^2}\right)\right]. \qquad (24)$$

Set $r_0 = 0$ and $a = 0$, and recover the energy shift for a point proton and point electron.[1]

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References

[1] Stephen Gasiorowicz, *Quantum Physics*(John Wiley and Sons, New York, 1974), pp 272-275.

[2] Stephen Gasiorowicz, *Quantum Physics*(John Wiley and Sons, New York, 1974), pp 246-248.