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^{1}H, ^{2}H and ^{3}H nuclear magnetic dipole moment effects on the electron energy states

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Abstract. The effect of nuclear magnetic dipole moment of hydrogen, deuterium and tritium isotopes on the electron atomic energy has been studied and analysed in this work. The electromagnetic Hamiltonian was rewritten in terms of the orbital angular momentum L_e of the electron, the gyromagnetic ratio γ_N of the nucleus and its total angular momentum J_N. The first-order energy correction has been derived, and this correction splits each ℓ state into $2J_N + 1$ states. The energy corrections and the differences between the split states of the first two lowest energy states for each isotope were calculated and it is found that these two energy states are in the radiowave range.

Keywords. Nuclear magnetic dipole moment; gyromagnetic ratio; vector potential; hydrogen isotopes; radiowaves.

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1. Introduction

Hydrogen is the most abundant element in the Universe, and it represents the simplest atomic system [1]. Hydrogen is studied widely because of its importance. Different physical interactions between the electron and the atomic nucleus are exploited to describe the physical structure of this atom. The hydrogen atom was solved quantum mechanically using the predominant Coulomb potential between the electrically charged nucleus and the electron, Other interaction potentials have a small effect on the atomic energy and are considered as perturbations. Sommerfeld introduced the fine-structure correction [2]. He combined the relativistic correction with the spin–orbit coupling corrections. The fine structure kills the degeneracy in azimuthal quantum number ℓ. The hyperfine splitting represents the interaction between the magnetic moment of the nucleus and the electron spin in general [3,4]. The first-order energy correction due to the hyperfine splitting can be written as [3]

$$E_{hf} = \frac{2}{3}\mu_0\gamma_e\gamma_N\langle\vec{J}_N\cdot\vec{s}_e\rangle\,|\psi_{n\ell m}(0)|^2\,, \qquad (1)$$

where $\gamma_e(\gamma_N)$ is the electron(nucleus) gyromagnetic ratio, J_N is the total angular momentum of the nucleus and s_e is the electron spin. The wave unction of the atomic hydrogen, $\psi_{n\ell m}(0) = 0$ unless $\ell = 0$, and the $\langle\vec{J}_N\cdot\vec{s}_e\rangle$ interaction in eq. (1) reduces to $\langle\vec{s}_N\cdot\vec{s}_e\rangle$ spin–spin interaction and the hyperfine splitting affects essentially the atomic S-states.

In this work, the magnetic moment of the nucleus is rewritten in terms of the magnetic vector potential, and the interaction between this vector potential and the electron's angular momentum in the ^{1}H, ^{2}H and ^{3}H hydrogen isotopes was considered as a perturbation. The first-order energy corrections due to this interaction have been derived, and the energy corrections and differences between split states for the lowest energy states have been calculated in terms of the optical wavelength. As far as I know, this work has not been done before.

2. Energy correction analysis

The atomic nuclei in this work are characterised by the dominant magnetic dipole moment $\vec{\mu} = \gamma_N\vec{J}_N$. This magnetic dipole moment creates a magnetic vector potential $\vec{A}_N$ that interacts with the atomic electrons. The magnetic vector potential is presented in terms of nuclear gyromagnetic ratio γ_N and the total angular

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momentum $\vec{J}_N$ as

$$\vec{A}_N = \frac{\mu_0}{4\pi}\gamma_N \frac{\vec{J}_N \times \vec{r}}{r^3}. \tag{2}$$

The Hamiltonian operator in the presence of magnetic vector potential is

$$H = \frac{1}{2m_e}(\vec{p} + e\vec{A})^2 - eV(r). \tag{3}$$

The magnetic vector potential of the nucleus $\vec{A}_N$ has a small effect on the atomic energy states and it can be considered as a perturbation, where

$$H_0 = \frac{p_e^2}{2m_e} - eV(r)$$

and the perturbed Hamiltonian is

$$H' = \frac{e}{2m_e}(\vec{p}_e \cdot \vec{A}_N + \vec{A}_N \cdot \vec{p}_e) + \frac{e^2}{2m_e}A_N^2. \tag{4}$$

Substitute $\vec{A}_N$ into eq. (4), and the perturbed Hamiltonian becomes

$$H' = \frac{e}{m_e}\frac{\mu_0}{4\pi}\gamma_N \frac{1}{r^3}\, \vec{p}_e \cdot (\vec{J}_N \times \vec{r}) + \frac{e^2}{4m_e^2}A_N^2. \tag{5}$$

The vector product $\vec{p}_e \cdot (\vec{J}_N \times \vec{r})$ rewritten as $\vec{J}_N \cdot (\vec{r} \times \vec{p}_e)$, is simply the scalar product between the angular momentum of the atomic electron and the total angular momentum $(L_e \cdot J_N)$ of the nucleus. The interaction Hamiltonian becomes

$$H' = \frac{e}{m_e}\frac{\mu_0}{4\pi}\gamma_N \frac{1}{r^3}\vec{L}_e \cdot \vec{J}_N + \frac{e^2}{2m_e}\left(\frac{\mu_0}{4\pi}\gamma_N\right)^2 \left|\frac{\vec{J}_N \times \vec{r}}{r^3}\right|^2. \tag{6}$$

Since the second part of eq. (6) is very small compared to the first one, it was ignored, and the first-order energy correction E^1 is rewritten as

$$\langle H' \rangle = \frac{e}{m_e}\frac{\mu_0}{4\pi}\gamma_N \left\langle \frac{1}{r^3} \right\rangle \left\langle \vec{L}_e \cdot \vec{J}_N \right\rangle. \tag{7}$$

This interaction depends on the expectation values of $\langle \vec{L}_e \cdot \vec{J}_N \rangle$ and $\langle 1/r^3 \rangle$. Assume that the sum of $\vec{L}_e$ and $\vec{J}_N$ is given by

$$\vec{I} = \vec{L}_e + \vec{J}_N. \tag{8}$$

Then the expected value of $\langle \vec{L}_e \cdot \vec{J}_N \rangle$ according to eq. (8) is given by

$$\langle \vec{L}_e \cdot \vec{J}_N \rangle = \frac{\hbar^2}{2}(i(i+1) - \ell_e(\ell_e + 1 - j_N(j_N + 1)). \tag{9}$$

The expectation value of $1/r^3$ was calculated using Kramer's relation [5] as

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\ell_e(\ell_e + 1/2)(\ell_e + 1)\, n^3\, a^3}. \tag{10}$$

The first-order energy correction due to the nuclear magnetic vector potential becomes

$$\langle H' \rangle = \left(\frac{e}{2m_e c^2}\frac{\mu_0}{4\pi}\frac{(\hbar c)^2}{a^3}\right) \times \frac{i(i+1) - j_N(j_N+1) - \ell_e(\ell_e+1)}{\ell_e(\ell_e + 1/2)(\ell_e + 1)\, n^3}\gamma_N, \tag{11}$$

where

$$\frac{e}{2m_e c^2}\frac{\mu_0}{4\pi}\frac{(\hbar c)^2}{a^3} = 4.118 \times 10^{-15}\ \text{eV T s}.$$

According to eq. (11), the first-order energy correction depends on the nuclear gyromagnetic ratio, energy state's principle number n, the nuclear total angular momentum, the electron's orbital angular momentum and its summation. This correction splits each atomic energy state into $2J_N + 1$ states.

3. Energy correction results

The interaction between the nuclear magnetic dipole moments of the hydrogen, deuterium and tritium isotopes and the orbital angular momentum of the atomic electron was derived in this work and the first-order energy correction is presented by eq. (11). The first-order energy correction equation for S-states ($\ell = 0$ and $i = j$) is reduced to

$$\langle H' \rangle = -2\,\gamma_N \left(\frac{4.118 \times 10^{-15}\ \text{eV T s}}{n^3}\right). \tag{12}$$

The first-order energy corrections for the first two lowest energy states have been calculated and listed in table 1. The energy differences between split energy states ($\ell = 1$) in terms of eV and the optical wavelengths are listed in table 1. As the energy correction for higher energy states ($n > 2$) becomes less significant, it was ignored.

The energy correction due to the interaction between the nuclear magnetic dipole moment and the orbital angular momentum of atomic electron is found to increase the S-state atomic potential depth for hydrogen and deuterium by 2.20×10^{-6} and 3.38×10^{-7} eV for $n = 1$ and by 2.75×10^{-7} and 4.23×10^{-8} eV for $n = 2$ respectively. Since the gyromagnetic ratio of tritium is negative [6], the energy correction decreases the S-state

Table 1. The atomic first-order energy corrections due to the nuclear magnetic dipole moment of ^{1}H, ^{2}H and ^{3}H in terms of eV and the optical wavelength units for the ground state and first excited state.

Isotope	γ_N ($s^{-1}T^{-1}$)	j_N	n	ℓ	i	E^1 (eV)	ΔE^1 (eV)	λ (m)
^{1}H	2.68×10^8 [6]	1/2	1	0	1/2	-2.20×10^{-6}	–	–
			2	0	1/2	-2.75×10^{-7}	–	–
			2	1	1/2	-9.18×10^{-8}	1.38×10^{-7}	9.0
			2	1	3/2	4.59×10^{-8}		
^{2}H	4.11×10^7 [6]	1	1	0	1	-3.38×10^{-7}	–	–
			2	0	1	-4.23×10^{-8}	–	–
			2	1	0	-2.82×10^{-8}	1.41×10^{-8}	87.9
			2	1	1	-1.41×10^{-8}	2.82×10^{-8}	43.9
			2	2	2	1.41×10^{-8}	4.23×10^{-8}	29.3
^{3}H	-2.04×10^8 [6]	1/2	1	0	1/2	1.68×10^{-6}	–	–
			2	0	1/2	2.10×10^{-7}	–	–
			2	1	1/2	6.99×10^{-8}	1.04×10^{-7}	11.8
			2	1	3/2	-3.50×10^{-8}		

potential depth by 1.68×10^{-6} and 2.10×10^{-7} eV for $n = 1$ and 2 respectively. The non-zero ℓ state splits into $2j_N + 1$ states under this correction, which kills the degeneracy in ℓ. The energy differences between the new split states were calculated in terms of the optical wavelength and they are found to be in the radiowave range. Radiowave lines such as 9.0 m can be emitted by the hydrogen atom, 29.3, 43.9, 87.9 m by deuterium, and 11.8 m by tritium. To the best of the author's knowledge, no recorded radiowave lines with these wavelengths were found in the literature.

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