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The Stark Effect on the Wave Function of Tritium in Relativistic Condition

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Abstract. Tritium Atom is one of the isotopes of Hydrogen that has two Neutrons in the nucleus and an electron that surrounds the nucleus. The Stark Effect is an effect of a shift or polarization of the atomic spectrum caused by the external electrostatic field. The interaction between the electrons and the external electric field can be reviewed using an approximation method of perturbation theory. The perturbation theory used is a time Independent non-degenerate perturbation and reviewed to second order to obtain correction of Tritium Atomic wave function. The condition that used in the system is a relativistic condition by reviewing the movement of electrons within the Atom. The effects of relativity also affect the correction of the wave function of Atom Tritium in the ground state. Tritium is radioactive material that is still relatively safe, and one of the applications of Tritium Atom is on the battery of betavoltaics (Nano Tritium Battery).

1. Introduction

Quantum physics has replaced the theory of classical physics for some cases and has grown faster science over the last 100 years. The theory of quantum has changed many components in the physics such as Quantum Mechanics, Quantum Electrodynamics, Quantum Thermodynamics and Astrophysics. All of the microscopic phenomena like an atomic case can be explained by using the theory of quantum mechanics and using the principle of wave-particle dualism. Calculations of the spectrum energy and wave functions of Hydrogen atoms use a second-order equation that known as the Schrodinger equation. Schrodinger equation is able to give a definition of the wave function of a particle [1]. This equation is formed by using the law of conservation of energy, obedient to the hypothesis of de Broglie so as to produce a complex analytical solution in the form of wave functions of a single value, continuous and finite. The Schrodinger equation can explain the problem of microscopic like atom until the macroscopic problems like Stars or universe [2]. The wave function must be normalized by using mathematical calculation. Based on the general characteristics of the wave function, the Schrodinger equation can be divided into two part, the first is time-dependent Schrodinger equations and time-independent Schrodinger equations or often referred to as steady state. The simplest form of Schrodinger equation is the time-independent schrodinger equation, where the wave function is only influenced by the potential (V) and position (r).

In this research will be studied about the effect of external electrostatic field (Stark Effect) on Tritium atom wave function in the ground state (*1s*). The approximation method is time-independent non-degenerate perturbation theory and reviewed until second order correction of the wave function in the ground state of Tritium. The motion of an electron in Tritium has a high velocity (2.1×10^6 m/s) and will be faster when the mass number (Z) is used is also large. So to get the real condition of the hydrogenic atom should to calculate the relativity effect of the movement of electrons. The relativistic correction used in this study is only in first order because for second order correction it gives very small effect in calculations.

Tritium is one of the isotopes of hydrogen that contains two neutrons in the nucleus and one of an electron that surrounds the nucleus. Tritium is a radioactive atom that have a half-life of 12.32 years[3]. Tritium is a radioactive material that is still relatively safe. The application of Tritium Atom is on the battery of betavoltaics (Nano Tritium Battery). Beta-voltaic battery is one type of radioactive isotope battery that has advantages such as a long service life, high energy density and free of maintenance [4].

The power of Tritium Beta-voltaic battery is about 0.5 – 1.5 μW and voltages between 500 – 1500 *V* [5]. In this research will be discussed the characteristics of Tritium due to the influence of external electric field on energy and wave function of Tritium. Then, It will examine the effect of the external electric field to the power of Tritium battery theoretically.

2. Tritium Atoms in Ground State

Tritium atom has nuclei containing a proton and two neutrons, and an electron that moving around the nucleus. The mass used in this research is the reduction mass (μ_T) that occurs due to the interaction between the mass of electrons (m_e) and the mass of the nucleus (m_N) and the equation is written as:

$$\frac{1}{\mu_T} = \frac{1}{m_e} + \frac{1}{m_N} \tag{1}$$

The general formula of schrodinger equation which describes the hamiltonian system in time-independent for the mass particles μ_T and moves in one dimension in the potential field $V_r(r)$ shown in equation (2). We used the schrodinger equation because this equation can describe the characteristic of wave in a particle on microscopics phenomena.

$$-\hbar^2 \nabla^2 (r)\psi + V_r(r)\psi = \xi\psi \tag{2}$$

the spherical coordinate given by,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\varphi}\frac{\partial}{\partial\varphi}\left(\sin\varphi \frac{\partial}{\partial\varphi}\right) + \frac{1}{r^2 \sin^2\phi}\frac{\partial^2}{\partial^2\phi} \tag{3}$$

By solving this schrodinger equation, we obtain a solution of radial wave function $(\Re_{nl}(r))$ and a spherical harmonic function symbolized by $\Theta_{lm}(\varphi,\phi)$, with *n*, *l* and *m* are a quantum number. The atomic energy of tritium, the solution of the radial function equation and the solution of the spherical harmonic equations are given by equations (4), (5) and (6),

$$\xi_n = -\frac{\mu_T e^4}{2(4\pi\varepsilon)^2 \hbar^2}\frac{1}{n^2} = -\frac{21.79477\times10^{-19}}{n^2}\, joule \tag{4}$$

$$\Re_{nl}(r) = -\left(\frac{2}{na_1}\right)^{3/2}\sqrt{\frac{(n-l-1)!}{2n[(n+l)!]^3}}\left(\frac{2r}{na_1}\right)^l e^{-r/na_1} L_{n-l-1}^{l+1}\left(\frac{2r}{na_1}\right) \tag{5}$$

$$\Theta_{lm}(\varphi,\phi) = (-1)^{(m+|m|)/2}\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\,\Omega_l^m(\cos\varphi)e^{im\phi} \tag{6}$$

where $L_{n-l-1}^{l+1}\left(\frac{2r}{na_1}\right)$ is the Associated Laguere Polynomial equation, a_1 is the first radius of Tritium atomic state and $\Omega_l^m(\cos\varphi)$ is an associated Legendre polynomial [6]. Using the equations (4), (5) and (6), the magnitude of the energy and the function of the Tritium wave in the ground state is,

$$\xi_1 = -21.79477\times10^{-19}\, joule = -13.6032255 eV \tag{7}$$

$$\psi_{1s} = \Re_{10}\Omega_{00} = \frac{1}{\sqrt{\pi a_1^3}} e^{-r/a_1} \tag{8}$$

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3. Time-Independent non Degenerate Perturbation theory

A Hamiltonian initial condition without any perturbation show in equation (9),

$$H\psi_n = E_n^{(0)}\psi_n \tag{9}$$

In perturbation theory, Hamiltonian system will divide by two part, part one is unperturbed Hamiltonian system (H_0) and the second part is Hamiltonian with small perturbances (*W*). In equation (10), α means the expansion parameter for the perturbation correction order[7].

$$H = H_0 + \alpha W \tag{10}$$

Because the perturbation *W* assumed to be small, it should be possible to expand ψ_n and E_n as a power series in *W*. The expansion of energy and wave function are,

$$E = E^{(0)} + \alpha E^{(1)} + \alpha^2 E^{(2)} + ... \tag{11}$$

$$\psi = \psi^{(0)} + \alpha\psi^{(1)} + \alpha^2\psi^{(2)} + ... \tag{12}$$

and then, subtitute eq. (10), eq. (11) and eq. (12) to eq. (9).

$$\begin{aligned}&(H_0 + \alpha W)(\psi^{(0)} + \alpha\psi^{(1)} + \alpha^2\psi^{(2)} + ...) = (E^{(0)} + \alpha E^{(1)} + \alpha^2 E^{(2)} + ...)\\&(\psi^{(0)} + \alpha\psi^{(1)} + \alpha^2\psi^{(2)} + ...)\end{aligned} \tag{13}$$

By doing operation between two sides, and the coefficients of successive power of α on both sides of this equation must be equal. We obtain the results are,

$$(H_0 - E^{(0)})\psi^{(0)} = 0 \tag{14}$$

$$(H_0 - E^{(0)})\psi^{(1)} = (E^{(1)} - W)\psi^{(0)} \tag{15}$$

$$(H_0 - E^{(0)})\psi^{(2)} = (E^{(1)} - W)\psi^{(1)} + E^{(2)}\psi^{(0)} \tag{16}$$

Equation (14) is the zero-order correction solution, equation (15) is the first –order correction solution and equation (16) is the second-order correction solution.

From Equation (15), we can find the results of the first order correction of energy and wave function of Tritium,

$$E_n^{(1)} = \langle\psi_n|W|\psi_n\rangle = \int_V \psi_n W \psi_n dV \tag{17}$$

$$\psi_n^{(1)} = \sum_{n\neq k}\frac{\langle\psi_k|W|\psi_n\rangle}{E_n^{(0)} - E_k^{(0)}}\psi_k^{(0)} \tag{18}$$

From equation (16), we can get the result of second-order correction for energy and wave function of Tritium,

$$E_n^{(2)} = \sum_{n\neq k}\frac{\left|\langle\psi_k|W|\psi_n\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \tag{19}$$

$$\begin{aligned}\psi_n^{(2)} = &\sum_{r\neq n}\left[\sum_{m\neq n}\frac{\langle\psi_r|W|\psi_m\rangle\langle\psi_m|W|\psi_n\rangle}{\left(E_n^{(0)} - E_r^{(0)}\right)\left(E_n^{(0)} - E_m^{(0)}\right)} - \frac{\langle\psi_n|W|\psi_n\rangle\langle\psi_r|W|\psi_n\rangle}{\left(E_r^{(0)} - E_n^{(0)}\right)^2}\right]\psi_r^{(0)}\\&-\sum_{r\neq n}\frac{1}{2}\frac{\left|\langle\psi_r|W|\psi_n\rangle\right|^2}{\left(E_r^{(0)} - E_n^{(0)}\right)^2}\psi_n^{(0)}\end{aligned} \tag{20}$$

Where ψ_n mean the wave function of Tritium in the ground state that consist of ψ_{1s}. ψ_m is the wave function of Tritium in the first excited state, that consists of ψ_{2s}, ψ_{2pz}, ψ_{2px} and ψ_{2py}. And ψ_r is the wave function of Tritium in the second excited state, that consists of ψ_{3s}, ψ_{3pz}, ψ_{3pz}, ψ_{3pz}, ψ_{3dzz}, ψ_{3dyz}, ψ_{3dxz}, ψ_{3dxy}, and $\psi_{3dx^2-y^2}$.

4. Relativistic Correction

In principle, the relativistic effect for Tritium atoms will affect the magnitude of Energy for various circumstances. Relativistic kinetic energy of electrons

$$K = \sqrt{p^2c^2 + \mu_T^2 c^4} - \mu_T c^2 \tag{21}$$

With using Taylor expansions to get the simple solution of eq. (21), and the result is,

$$\sqrt{p^2c^2 + \mu_T^2 c^4} - \mu_T c^2 \cong \frac{p^2}{2\mu_T} - \frac{p^4}{8\mu_T^3 c^2} + ... \tag{22}$$

The next step is subtitute eq. (10) to total Hamiltonian system,

$$H = \left(\frac{p^2}{2\mu_T} - \frac{p^4}{8\mu_T^3 c^2} + ... \right) - \frac{e^2}{4\pi\varepsilon} \frac{1}{r} = H_0 + W \tag{23}$$

$$W = - \frac{p^4}{8\mu_T^3 c^2} \tag{24}$$

Equation (24) is perturbed Hamiltonian dan H_0 is unperturbed Hamiltonian of Atom. To find the Tritium first-order energy correction due to the effect of relativity is to use the theory of perturbation with using equation (17).

$$\xi R_{nl}^{(1)} = \left\langle \psi_{nlm} \middle| \frac{p^4}{8\mu_T^3 c^2} \middle| \psi_{nlm} \right\rangle \tag{25}$$

By using schrodinger equation, we can get the solution of quadratic momentum of electron to solve the equation (25). Quadratic momentum that derive from schrodinger equation given by eq. (26).

$$p^2 = 2\mu_T \left(\xi_n - V(r) \right) \tag{26}$$

Then substitute equation (26) into equation (25) to obtain the first order energy correction of relativity effect .

$$\xi R_{nl}^{(1)} = \frac{1}{8\mu_T c^2} \left\langle \psi_{nlm} \middle| \xi_n^2 - \frac{2\xi_n e^2}{4\pi\varepsilon} \frac{1}{r} + \frac{e^4}{(4\pi\varepsilon)^2} \frac{1}{r^2} \middle| \psi_{nlm} \right\rangle$$

$$\xi R_{nl}^{(1)} = \frac{1}{8\mu_T c^2} \left(\xi_n^2 - \frac{2\xi_n e^2}{4\pi\varepsilon} \left\langle \frac{1}{r} \right\rangle_{nl} + \frac{e^4}{(4\pi\varepsilon)^2} \left\langle \frac{1}{r^2} \right\rangle_{nl} \right) \tag{27}$$

To got the solution of $\left\langle \frac{1}{r} \right\rangle_{nl}$, we can use recursion method. From the radial equation of Tritium atom,

$$\left[-\frac{\hbar^2}{2\mu_T r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2\mu_T r^2} + V(r) \right] U_{nl}(r) = E U_{nl}(r)$$

$$\left[-\frac{\hbar^2}{2\mu_T r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2\mu_T r^2} - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{r} \right] U_{nl}(r) = \left(-\frac{\mu_T e^4}{2\hbar^2 (4\pi\varepsilon_0)^2} \frac{1}{n^2} \right) U_{nl}(r) \tag{28}$$

Where $U_{nl}(r)$ is the radial wave function that depended of r. And then do differential on equation (28) to e^2, and we could got the result in equation (29):

$$\left[\frac{1}{r}\right]U_{nl}(r)=\left[\frac{2\mu_T e^2}{2\hbar^2(4\pi\varepsilon_0)}\frac{1}{n^2}\right]U_{nl}(r) \tag{29}$$

The next step is to multiply in the both sides of equation (29) with the conjugate radial wave function and integrating to *r*.

$$\int_0^\infty U_{nl}^*\left[\frac{1}{r}\right]U_{nl}(r)dr=\int_0^\infty U_{nl}^*\left[\frac{2\mu_T e^2}{2\hbar^2(4\pi\varepsilon_0)}\frac{1}{n^2}\right]U_{nl}(r)dr$$

$$\left\langle\frac{1}{r}\right\rangle_{nl}=\left[\frac{2\mu_T e^2}{2\hbar^2(4\pi\varepsilon_0)}\frac{1}{n^2}\right]$$

With the radius of Tritium atom in ground state is $a_1=\frac{4\pi\varepsilon_0\hbar^2}{\mu_T e^2}$, so the result is:

$$\left\langle\frac{1}{r}\right\rangle_{nl}=\frac{1}{a_1 n^2} \tag{30}$$

Whereas to find the value of $\left\langle\frac{1}{r^2}\right\rangle_{nl}$, we would to differentize the equation (28) to the quantum number *l* on each segment.

$$\frac{d}{dl}\left[-\frac{\hbar^2}{2\mu_T r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{l(l+1)\hbar^2}{2\mu_T r^2}-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right]U_{nl}(r)=\frac{d}{dl}\left(-\frac{\mu_T e^4}{2\hbar^2(4\pi\varepsilon_0)^2}\frac{1}{n^2}\right)U_{nl}(r) \tag{31}$$

Because the value of $n=N+l+1$, so $dn/dl=1$ or $dn=dl$, the eq. (31) become

$$\frac{d}{dl}\left[-\frac{\hbar^2}{2\mu_T r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{l(l+1)\hbar^2}{2\mu_T r^2}-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right]U_{nl}(r)=\frac{d}{dn}\left(-\frac{\mu_T e^4}{2\hbar^2(4\pi\varepsilon_0)^2}\frac{1}{n^2}\right)U_{nl}(r)$$

$$\left[\frac{(2l+1)\hbar^2}{2\mu_T r^2}\right]U_{nl}(r)=\left(\frac{\mu_T e^4}{\hbar^2(4\pi\varepsilon_0)^2}\frac{1}{n^3}\right)U_{nl}(r)$$

$$\left[\frac{1}{r^2}\right]U_{nl}(r)=\left(\frac{2\mu_T{}^2 e^4}{\hbar^4(2l+1)(4\pi\varepsilon_0)^2}\frac{1}{n^3}\right)U_{nl}(r) \tag{32}$$

The next step is to multiply in the both sides of equation (32) with the conjugate radial wave function and integrating to *r*.

$$\int_0^\infty U_{nl}^*\left[\frac{1}{r^2}\right]U_{nl}(r)dr=\int_0^\infty U_{nl}^*\left[\frac{2m^2 e^4}{\hbar^4(2l+1)(4\pi\varepsilon_0)^2}\frac{1}{n^3}\right]U_{nl}(r)dr$$

$$\left\langle\frac{1}{r^2}\right\rangle_{nl}=\frac{1}{a_1^2 n^3} \tag{33}$$

Then substitute equation (30) and equation (33) to equation (27), so that a first-order tritium energy correction solution will be obtained,

$$\xi R_{nl}^{(1)}=-\frac{\beta^2\xi_n}{4n^4}\left(\frac{8n}{2l+1}-3\right) \tag{34}$$

Where β is a fine structure constant and $\xi R_{nl}^{(1)}$ is the first-order relativistic correction of Energy Tritium in various state.

5. Result and Discussion

5.1. Result of Relativistic Correction in the Various of State

Relativistic correction of Tritium depend of the primary quantum number (*n*) and the orbital quantum number (*l*). The total momentum angular of Tritium given by $j = l \pm \frac{1}{2}$, so by using the equation (30) we could to find the correction of energy Tritium atom for the ground state , the first excitted state and the second excited state such as $1s, 2s, 2p_z, 2p_x, 2p_y, 3s, 3p_z, 3p_x, 3p_y, 3d_{zz}, 3d_{xz}, 3d_{yz}, 3d_{xy}, 3d_{x^2-y^2}$ and the result of correction shown in table 1.

Table 1. The result of relativistic correction until state $n \leq 3$

State	Initial Energy (Joule)	Correction Energy (Joule)
1s	$-21.7947692 \times 10^{-19}$	$1.45075116 \times 10^{-22}$
2s	$-5.4486923 \times 10^{-19}$	$2.357470986 \times 10^{-23}$
$2p_z$, $2p_x$, $2p_y$	$-5.4486923 \times 10^{-19}$	$4.231357811 \times 10^{-24}$
3s	$-2.42164102 \times 10^{-19}$	$7.52241373 \times 10^{-24}$
$3p_z$, $3p_x$, $3p_y$, $3d_{xz}$, $3d_{yz}$	$-2.42164102 \times 10^{-19}$	$1.79105103 \times 10^{-24}$
$3d_{zz}$, $3d_{xy}$, $3d_{x^2-y^2}$	$-2.42164102 \times 10^{-19}$	$6.44778389 \times 10^{-25}$

From table 1, we can know that in every state have a different correction of relativistic. It's because of relationalistic correction depend of electron's motion.We can compare the relativistic correction in the ground state (*n=1*), the first excited state (*n=2*) and in the second excited state (*n=3*). If the principal quantum number (*n*) became larger, the correction relativistic in the first order will get smaller. The correction relativistic energy between *2s (l=0)* and *2p (l=1)* have a different, It prove that orbital quantum number (*l*) affect to the relativistic energy of atom. If the orbital quantum number get higher in each state, the relativistic correction energy will get smaller. The relativistic correction of Tritium atoms leads to a reduction in the value of classical energy proposed by Bohr models[8]. In the classical atomic theory, the energy of an atom is only influenced by the principal quantum number, whereas in relativistic atomic theory the energy level of the atom is also influenced by the orbital quantum number. In Relativistic condition, It will give more accurate calculations about energy and wave functions of atom[9].

5.2. Result of Stark Effect on Wave Function of Tritium in Relativistic Condition

The solution from the problem of stark effects on Tritium in a relativistic condition is to combine these two corrections between external electric field and relativistic correction. By using equation (17) we could to find the first-order correction of energy from the influence of the external electric field and will give a zero value. while in second order correction we use equation (19) to found the solution and it gives the effect on the energy shift for the ground state [10,11]. The effect of electric field will influenced to the energy atoms or crystals[12]. The solution of the resulting equation is shown as follows,

$$\xi_{1s} = \xi R_{1s}^{(0)} - \frac{(e\mathrm{E})^2}{(\xi R_{1s} - \xi R_{2pz})}\left(\frac{256 a_1}{243\sqrt{2}}\right)^2 \tag{35}$$

In equation (35), the result of the difference of energy is negative value, so that the disturbance given by the external electric field will increase the binding energy of electron and nucleus. If the binding energy get higher, the radiation of beta will get smaller and the power of Tritium Battery will get smaller too.

By using the equations (18) and (20), we could find the correction of wave function Tritium until second-order correction. And the result of wave function of Tritium in the ground state with the correction in the first order is,

$$\psi_{1s}^{(1)} = \frac{\frac{256 a_1 e \mathrm{E}}{243\sqrt{2}}}{\xi R_{1s} - \xi R_{2pz}} \psi_{2pz}^{(0)} \tag{36}$$

And the second order correction of the wave function Tritium is,

$$\begin{aligned}\psi_{1s}^{(2)} = \frac{0.7443554 a_1^2 e^2 E^2}{(-16.3446682 \times 10^{-19})} \Bigg(&\frac{25.36243}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3pz}^{(0)} + \frac{0.54178767}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3s}^{(0)} \\ &+ \frac{2.45185216}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3dzz}^{(0)} + \frac{1.06168313}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3dxy}^{(0)} + \frac{1.06168313}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3dx^2-y^2}^{(0)} \\ &+ \frac{2.12336625}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3dyz}^{(0)} + \frac{2.12336625}{\left(-19.37169511 \times 10^{-19}\right)} \psi_{3dxz}^{(0)} \Bigg) \\ &- \frac{0.088989255 a_1^2 e^2 E^2}{2(3.752625714 \times 10^{-36})} \psi_{1s}^{(0)}\end{aligned} \tag{37}$$

The wave function of Tritium atom with correction until second-order perturbation in relativistic condisition is,

$$\psi_{1s} = \psi_{1s}^{(0)} + \psi_{1s}^{(1)} + \psi_{1s}^{(2)} \tag{38}$$

6. Conclusion

The effect of the external electrostatic field on Tritium atom with the relativistic condition will cause a shift in energy and wave function at the ground state. The magnitude of the shift from energy correction and wave function is influenced by the principal quantum number (n), the orbital quantum number (l) and the magnitude of the given external electric field. The stark effect on the ground state of Tritium will increase the binding energy of electron and nucleus. It will decrease the power of Tritium battery because the radiation beta decay got smaller when the binding energy got higher.

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