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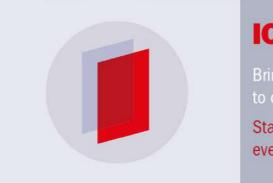
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## The stark effect on the spectrum energy of tritium in first excited state with relativistic condition

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### The stark effect on the spectrum energy of tritium in first excited state with relativistic condition

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Abstract. This research discussed about the correction of Stark Effect on Tritium atoms in the first excited state with relativistic conditions. The approach used to solve this Stark Effect correction was the perturbation theory which was from time independent degenerate perturbation theory to second-order correction. The Stark Effect on the excited state made the spectrum energy polarization of Tritium which was included in the isotope of hydrogen with an electron moving around the nucleus with high velocity. Hence, the relativistic correction affected the spectrum energy shift. Tritium was a radioactive material having half-time 12,3 years and relatively safe. The Tritium application was a material for the manufacture of nuclear battery. The most effective external electric field that should give to Tritium was  $10^8$  V/mith the total correction energy that was  $0.97398557 \times 10^{-21}$  Joule. Therefore, its effect reduced the binding energy between electron and nucleus, and increased the power of Tritium Betavoltaics Battery.

#### 1. Introduction

The microscopic phenomena can be explained by using quantum theory. For more than 100 years, the quantum theory has existed and influenced various aspects of physics such as in Mechanics, Electrodynamics and Thermodynamics[1]. Quantum mechanics can be explained the microscopic phenomena by using theory of particle wave dualism. In 1926, Erwin Schrodinger made a great equation that can give the definition of a particle wave function. The name of this equation was Schrodinger Equation [2,3] which was formed by using the energy conservation law. It was obedient to the hypothesis of de Broglie, so it produced a complex analytical solution in the form of wave functions of single value, continuous, and finite. The Schrodinger equation consisted of kinetic energy operators and potential energy V [4]. In the atomic case, the potential energy is caused by charges interaction between proton and electron.

The solution of Schrodinger equation for the real system is usually complicated. The exact solution is very difficult to find, or the solution does not exist; for example, Hydrogen atom on external field or in strong magnetic field. Therefore, to solve this problem, we need to rely on approximation method. The simple and powerful approximation method is perturbation theory. We usually call this method with Rayleigh-Schrodinger Perturbation Theory [5]. The research about external electric field on Atom was first noticed in 1913 by Stark who observed the separation (polarization) of Balmer lines by using external electric field 100.000 V/cm[6]. The Stark effect correction will be found until second order correction.

By using Bohr formula, we can find the velocity of electron, and the value is about  $2.6 \times 10^6 m/s$ . Hence, to get the real condition of the hydrogenic atom, we should calculate the relativity effect of the electrons movement. The relativistic correction used in this study was only in the first order because in the second order correction, it gives very small value and hardly any effect. The relativistic correction gives an energy shift that is depended by principal quantum number and orbital quantum number.

Tritium is one of unique types of atom which includes radioactive isotope of Hydrogen with 2 neutrons and a proton in nucleus [7]. Tritium emits Beta ray radiation energy with 0 - 18,6 keV (5,7

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keV in average) and 12,323 years of a half-life [8]. The kinetic energy of Beta radiation is used as a source of energy for Betavoltaic battery in semiconductors [9]. This battery has the advantages of being able to survive in a long time and in extreme conditions [10]. The problem of Tritium Betavoltaics Battery is the power of this battery is too small. The principle of the Betavoltaics battery is similar to the Photovoltaics[11]. The isotopes of Hydrogen atoms are likely to be easily disturbed like electric field or external magnetic field. In this research, The data were analyzed theoretically about the effect of perturbation caused by external electric field to reduce the binding energy between nucleus and electron. The effect was electron would be easier to release from its state and would increase the beta radiation of Tritium. The larger beta radiation could increase the power of Tritium Betavoltaics battery.

#### 2. Method

#### 2.1 Wave function and Energy Tritium in the first excitation condition.

Tritium has a lot of similar with Hydrogen, like an energy and wave function. The different between Tritium and Hydrogen is just in reduction mass. The mass used in Tritium is reduction mass  $(\mu_t)$  that occurs due to the interaction between the mass of electron  $(m_e)$  and the mass of nucleus  $(m_N)$ . The formula of reduction mass is shown in eq. (1),

$$\frac{1}{\mu_{t}} = \frac{1}{m_{a}} + \frac{1}{m_{N}}$$
(1)

The wave functions of Tritium in the first excited condition can be found by using Schrodinger equation (using spherical coordinates).

The wave functions are shown in table 1.

Table 1	. Wave Function of Tritium in the First Excitation State
States	Wave Functions
$ 2s\rangle$	$\frac{1}{4\sqrt{2\pi a_{1T}^3}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_{1T}}$
$ 2p_z\rangle$	$\frac{r}{4a_{1T}}\frac{1}{\sqrt{2\pi a_{1T}^3}}(\cos\theta)e^{-r/2a_{1T}}$
$\left 2p_{y}\right\rangle$	$\frac{r}{4a_{1T}}\frac{1}{\sqrt{2\pi a_{1T}^3}}(\sin\theta)(\sin\phi)e^{-r/2a_{1T}}$
$ 2p_x\rangle$	$\frac{r}{4a_{1T}}\frac{1}{\sqrt{2\pi a_{1T}^3}}(\sin\theta)(\cos\phi)e^{-r/2a_{1T}}$

The energy of Tritium can we found by using Bohr's formula [6],

$$E_n = -\left[\frac{\mu_T}{2\eta^2} \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right] \frac{1}{n^2}$$
(2)

#### 2.2 Perturbation Theory

This research used perturbation theory to solve the problem. Perturbation theory divides into two types: time-independent perturbation theory and time-dependent perturbation theory. In this research, we used time-independent perturbation theory because the Hamiltonian from Tritium was time-independent.

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The Hamiltonian H consists of two parts: imperturbation Hamiltonian  $H_0$  and perturbation Hamiltonian  $\alpha V \cdot \alpha$  means the expansion parameter for the perturbation correction order.

$$H = H_0 + \alpha V \tag{3}$$

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$$H_0 | l^0 \rangle = E_0 | l^0 \rangle \tag{4}$$

Because the perturbation V assumed to be very small, it should be possible to expand  $|l^n\rangle$  and  $E_n$  as a power series in V. The expansion of energy and wave function are,

$$E_{n} = E^{0} + \alpha E^{1} + \alpha^{2} E^{2} + \dots$$

$$\left| l^{n} \right\rangle = \left| l^{0} \right\rangle + \alpha \left| l^{1} \right\rangle + \alpha^{2} \left| l^{2} \right\rangle + \dots$$
(5)
(6)

The first order correction of stark effect is degenerate case because the unperturbed energy eigen kets are degenerate. The first order correction solves with matrix method like eq (5).

$$\begin{pmatrix} V_{11} & V_{12} & V_{13} & V_{14} \\ V_{21} & V_{22} & V_{23} & V_{24} \\ V_{31} & V_{32} & V_{33} & V_{34} \\ V_{41} & V_{42} & V_{43} & V_{44} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = E^{1} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$
(7)

The second order correction of stark effect on Tritium is non degenerate case. By using eq. (3) and eq. (4), we could find the second order correction of Energy.

$$E^{2} = \sum_{l \neq m} \frac{\left| \left\langle m^{0} | V | l^{0} \right\rangle \right|^{2}}{E_{l}^{(0)} - E_{m}^{(0)}}$$
(8)

#### 2.3 Relativistic Correction

The Hamiltonian of Tritium consists of two parts: potential energy and kinetic energy. The relativistic formula of kinetic energy is,

$$K = \frac{mc^2}{\sqrt{1 - (v/c)^2}} - mc^2$$
(9)

Momentum (*p*) expression on Tritium atom is,

$$K = \sqrt{p^2 c^2 + \mu_t^2 c^4} - \mu_t c^2 \tag{10}$$

The eq. (10) can solve to get easier expressions by using Taylor expansions.

$$\sqrt{p^2 c^2 + \mu_t^2 c^4} - \mu_t c^2 \cong \frac{p^2}{2\mu_T} - \frac{p^4}{8\mu_T^3 c^2} + \dots$$
(11)

The first order in eq.(11) is kinetic energy like classical theory and the second one is the perturbation Hamiltonian because of the relativistic condition. By using perturbation theory, we could find the energy correction.

$$ER_{nl}^{(1)} = \left\langle nlm \left| \frac{p^4}{8\mu_t^3 c^2} \right| nlm \right\rangle$$
(12)

By using Schrodinger equation, we could get the solution of quadratic momentum of electron to solve the eq. (12). Quadratic momentum is derived from Schrodinger equation given by eq (13).

$$p^2 = 2\mu_t \left( E_n - V(r) \right) \tag{13}$$

Then substitution of equation (13) into equation (12) functions to obtain the first order energy correction of relativity effect.

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

$$ER_{nl}^{(1)} = \frac{1}{8\mu_T c^2} \left( E_n^2 - \frac{2E_n e^2}{4\pi\varepsilon} \left\langle \frac{1}{r} \right\rangle + \frac{e^4}{(4\pi\varepsilon)^2} \left\langle \frac{1}{r^2} \right\rangle \right)$$
(14)

By using special theorem, we could describe the expectation of  $\frac{1}{r}$  and  $\frac{1}{r^2}$ ,

$$\left\langle \frac{1}{r} \right\rangle_{nl} = \frac{1}{a_0 n^2} \tag{15}$$

$$\left< \frac{1}{r^2} \right>_{nl} = \frac{1}{a_0^3 n^3 \left( l + \frac{1}{2} \right)}$$
 (16)

Then substitution of equation (15) and equation (16) to equation (14) resulted that a first-order tritium energy correction solution would be obtained,

$$ER_{nl}^{(1)} = -\frac{\beta^2 E_n}{4n^4} \left(\frac{8n}{2l+1} - 3\right)$$
(17)

 $\beta$  is fine structure constant, and  $ER_{nl}^{(1)}$  is the first-order relativistic correction of Energy Tritium in various state.

#### 3. Result and Discussion

#### 3.1 Energy Tritium in Relativistic Condition

By using equation (1), we could calculate the result of reduction mass of Tritium  $(\mu_T)$  and it would be compared with the reduction mass of Hydrogen  $(\mu_H)$  and mass of electron  $(m_e)$ .

$$\mu_{T} = \frac{m_{e}(m_{p} + 2m_{n})}{(m_{p} + 2m_{n}) + m_{e}} = 9,1067819 \times 10^{-31} Kg$$

$$\mu_{H} = \frac{m_{e}.m_{p}}{m_{p} + m_{e}} = 9,10443157 \times 10^{-31} Kg$$
(18)
(19)

$$m_e = 9,109390 \times 10^{-31} Kg$$
,  $m_p = 1,672623 \times 10^{-27} Kg$ , and  $m_n = 1,674929 \times 10^{-27} Kg$ . Jika

Now, we could compare among the reduction mass of Tritium, Hydrogen, and electron. When the nucleus mass was getting higher, the reduction mass was getting higher too. This reduction mass affected the radius of the electron's orbit. If the number of neutrons in the nucleus got larger, the binding force of the nucleus also got larger. This phenomenon caused the radius of the electron's orbit getting smaller. It could be proven from the equations of the radius of Bohr atoms in the ground state as below,

$$a_{1H} = \frac{4\pi\varepsilon_0 \eta^2}{\mu_H e^2} = 5,294541195 \times 10^{-11} m$$
(20)

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b.

e.

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$$a_{1T} = \frac{4\pi\varepsilon_0 \eta^2}{\mu_T e^2} = 5,29317475 \times 10^{-11} m$$
(21)

By using equation (2), we could find the energy of Tritium atom for the principal quantum number 1 to principal quantum number 3.

$$E_1^{(0)} = -21,7947692 \times 10^{-19} Joule$$
  

$$E_2^{(0)} = -5,4486923 \times 10^{-19} Joule$$
  

$$E_3^{(0)} = -2,42164102 \times 10^{-19} Joule$$

The relativistic correction was depended by principal quantum number (n) and orbital quantum number (l). It was very different from classical theory of energy. In classical theory, energy of atom was just depended by principal quantum number (n). Energy Tritium for every state in relativistic condition was,

a. 
$$n = 1$$
 and  $l = 0$  (1s)  
 $ER_{1s}^{(1)} = -\frac{5\beta^2 E_1^{(0)}}{4} = 1,45075 \times 10^{-22}$  Joule

The total energy in the state of *1s* under relativistic conditions is,

$$ER_{1s} = E_1^{(0)} + ER_{1s}^{(1)}$$

$$ER_{1s} = -21,79331845 \times 10^{-19} Joule$$

$$n = 2 \text{ and } l = 0.(2s)$$

$$ER_{2s}^{(1)} = -\frac{13\beta^2 E_2^{(0)}}{16} = 2,35747 \times 10^{-23} Joule$$

The total energy in the state 2s in relativistic conditions is,

$$ER_{2s} = E_2^{(0)} + ER_{2s}^{(1)}$$
$$ER_{2s} = -5,448456553 \times 10^{-19} Jouole$$

c. 
$$n = 2$$
 and  $l = 1(2p)$ 

$$ER_{2p}^{(1)} = -\frac{7\beta^2 E_2^{(0)}}{48} = 4,231357 \times 10^{-24} Joule$$

The total energy in the state 2p in relativistic conditions is,

$$ER_{2p} = E_2^{(0)} + ER_{2p}^{(1)}$$
$$ER_{2p} = -5,448649986 \times 10^{-19} Joul$$

d. 
$$n = 3$$
 and  $l = 0(3s)$   
 $ER_{3s}^{(1)} = -\frac{21\beta^2 E_3^{(0)}}{36} = 7,5224 \times 10^{-24}$  Joule

The total energy in the state 3s in relativistic conditions is,

$$ER_{3s} = E_3^{(0)} + ER_{3s}^{(1)}$$
  

$$ER_{3s} = -2,421565796 \times 10^{-19} Joule$$

$$n = 3$$
 and  $l = 1(3p)$   
 $ER_{3p}^{(1)} = -\frac{5\beta^2 E_3^{(0)}}{36} = 1,79105 \times 10^{-24}$  Joule

The total energy in the state 3p in relativistic conditions is,

$$ER_{3p} = E_3^{(0)} + ER_{3p}^{(1)}$$

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 $ER_{3p} = -2,42162311 \times 10^{-19}$  Joule

f. 
$$n = 3$$
 and  $l = 2(3d)$   
 $ER_{3d}^{(1)} = -\frac{9\beta^2 E_3^{(0)}}{180} = 6,44778 \times 10^{-25}$  Joule

The total energy in the state 3d in relativistic conditions is,

$$ER_{3d} = E_3^{(0)} + ER_{3d}^{(1)}$$
$$ER_{3d} = -2,421634572 \times 10^{-19} Joule$$

The correction of relativity gave a shift in the energy value of Tritium at every level[13,14]. The higher of the atomic state, the smaller shift of energy would be. It happened because the speed of electron orbit would also be reduced. The principal quantum numbers described the atoms' energy levels, whereas the azimuth quantum numbers described the shape of the electrons' movement around the nucleus. At the same principal quantum number, the energy correction would decrease as the quantum azimuth number increased.

#### 3.2 The Stark Effect on Energy of Tritium in the First Excitation State with Relativistic Condition

The correction result of external electric field affected on Tritium atom for first order was shown in equation (25),

 $E_2^1 = \pm \langle 2s | V | 2p_z \rangle$ 

$$\frac{-E_2^1}{\langle 2s|V|2p_z\rangle} = \left(E_2^1\right)^2 - \left|\langle 2s|V|2p_z\rangle\right|^2 = 0$$

$$(22)$$

Where,

$$\frac{2s|V|2p_z}{e\xi\langle 2s|z|2p_z\rangle} = -3e\xi a_{1T}$$
(24)

So, the first order correction was.

While the calculation result of external electric field correction on Tritium atom for second order correction was shown in equation (26),

$$E_{2}^{2} = \sum_{l \neq m} \frac{\left| \left\langle m^{0} | V | l^{0} \right\rangle \right|^{2}}{E_{l}^{(0)} - E_{m}^{(0)}}$$
(26)

 $|m^{0}\rangle$  was the wave function of the second excitations state of Tritium, and  $|l^{0}\rangle$  was the wave function of first excitations state of Tritium. Therefore, the value of second order correction became,

$$E_{2}^{2} = \frac{\left(25,36243 e \xi a_{1T}\right)^{2}}{\left(ER_{2s} - ER_{3pz}\right)} + \frac{\left(0,54178 e \xi a_{1T}\right)^{2}}{\left(ER_{2pz} - ER_{3s}\right)} + \frac{\left(2,45185 e \xi a_{1T}\right)^{2}}{\left(ER_{2pz} - ER_{3dzz}\right)} + \frac{\left(1,06168 e \xi a_{1T}\right)^{2}}{\left(ER_{2pz} - ER_{3dzy}\right)}$$

$$+\frac{\left(1,06168e\xi a_{1T}\right)^{2}}{\left(ER_{2pz}-ER_{3dx^{2}-y^{2}}\right)}+\frac{\left(2,12336e\xi a_{1T}\right)^{2}}{\left(ER_{2py}-ER_{3dyz}\right)}+\frac{\left(2,12336e\xi a_{1T}\right)^{2}}{\left(ER_{2px}-ER_{3dxz}\right)}$$
(27)

$$E_{2}^{2} = -2,183233874 \times 10^{21} e^{2} a_{1T}^{2} \xi^{2}$$

$$E_{2}^{2} = -1,57019459 \times 10^{-37} \xi^{2}$$
(28)

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So the total Energy of Tritium in the first excitated state with l=0 was,

$$E_{2s} = ER_{2s} + E_2^1 + E_2^2$$

$$E_{2s} = \left(-5,448456553 \times 10^{-19} + 2,54418016 \times 10^{-29} \xi - 1,57019459 \times 10^{-37} \xi^2\right) joule$$
(29)

And the total Energy of Tritium in the first excitated state with l=1 was,

$$E_{2p} = ER_{2p} + E_2^1 + E_2^2$$

$$E_{2p} = \left(-5,448649986 \times 10^{-19} + 2,54418016 \times 10^{-29} \xi - 1,57019459 \times 10^{-37} \xi^2\right) Joule$$
(30)

Table 2. The results of correction energy with various external electric field						
External	The first order	The second order	Total Energy			
Electric	correction of Energy	Correction of Energy	Correction (Joule)			
Field	(Joule)	(Joule)				
$\xi(V/m)$						
10 <sup>5</sup>	2,54418016 ×10 <sup>-24</sup>	$-1,57019459 \times 10^{-27}$	2,54260997 ×10 <sup>-24</sup>			
10 <sup>6</sup>	2,54418016 ×10 <sup>-23</sup>	$-1,57019459 \times 10^{-25}$	2,52847821 × 10 <sup>-23</sup>			
10 <sup>7</sup>	2,54418016 ×10 <sup>-22</sup>	$-1,57019459 \times 10^{-23}$	$2,3871607 \times 10^{-22}$			
10 <sup>8</sup>	2,54418016 ×10 <sup>-21</sup>	$-1,57019459 \times 10^{-21}$	0,97398557 ×10 <sup>-21</sup>			
10 <sup>9</sup>	$2,54418016 \times 10^{-20}$	$-1,57019459 \times 10^{-19}$	$-1,31577657 \times 10^{-19}$			
10 <sup>10</sup>	$2,54418016 \times 10^{-19}$	$-1,57019459 \times 10^{-17}$	$-1,54475279 \times 10^{-17}$			

In this research, the disturbance was the external electric field ( $\xi$ ) that imposed on Tritium atom in the *z*-axis. The external electric field given to Tritium atom would affect to the level of Hamiltonian energy of Tritium[15]. In the first order correction, the perturbation theory was degenerate case because the energy value in the first excited state was identical. On the other hand, in the second order correction, the perturbation theory was non-degeneration case because the energy value in the first excited state was identical. On the other hand, in the second order correction, the perturbation theory was non-degeneration case because the energy value in the first excited state energy was different from the second excited state. From equation (25), the first order correction would reduce the binding energy between electron and nucleus, but it would increase the Beta radiation from Tritium Atom. However, in equation (28), the second order correction would reduce. From Table 2, the binding energy would reduce when the external electric field given to Tritium was  $10^5 V/m - 10^8 V/m$ . It was because the first order correction was bigger than the second order correction. The binding energy between electron and nucleus increased when the external electric field given to Tritium was higher than  $10^9 V/m$ . The effective external electric field that should give to Tritium atom to increase the Beta radiation and the power of Betavoltaic Battery was  $10^8 V/m$  with the total correction energy that was  $0.97398557 \times 10^{-21}$  Joule.

#### 4. Conclusion

The results of energy correction of Tritium until the second order caused by external electric field in relativistic condition indicated that in the relativistic conditions, the energy value of the Tritium atom depended on the principal quantum number (n) and the quantum azimuth number (l). The energy value correction caused by relativity would decrease as the value of n got higher. At the same n value, the energy correction value caused by relativity would decrease as well as the greater of the l value. Tritium Energy correction at the first order caused by external electric field used degenerate case, while in second order correction used non-degenerate case. The effective external electric field that

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should give to Tritium atom was  $10^8 V / m$ . For the future research, it is expected to use other forms of perturbation such as external magnetic field, the influence of spin coupling, and the others.

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