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3-dimensional eksternal electric field effect (Stark effect) on the ground state energy of Tritium atom

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Abstract. Tritium Atom is a Radioisotope that has a half-life of 12.3 years. This atom produces beta decay with a maximum generated energy of 18.598 KeV and an average energy of 5.7 KeV. Tritium radiation is still relatively safe, so it is widely used in the field of electronics especially in the development of betavoltaics batteries. This research will delve into the effect of 3-dimensional external electric field on Tritium energy on the ground state. The method applied in this research is Rayleigh-Schrodinger Perturbation Theory, which also encompasses second order correction. In addition, by reviewing the movement of electrons fast enough to surround the nucleus, then the relativistic effect will also exert effect to the energy of Tritium atoms. The 3-dimensional electric field effect (in the x, y and z axis) will give different energy shifts with the 1-dimensional perturbation effect. This shift of energy will have an impact on the binding energy of nucleus and electron. The results of mathematical calculations have proven that a significant shift in energy only occurs in a strong external electric field, approximately higher than $1 \times 10^{11} \ V/m$.

1. Introduction

Tritium atoms are a family of Hydrogen atoms that have a nucleus of three times more than the mass of Hydrogen. Tritium has three neutrons and a proton inside a nucleus, called triton, while an electron travels around the nucleus. This atom is different from the other two families, namely Hydrogen and Deuterium. This is because Tritium is unstable and tends to emit beta radiation. Radiation beta is basically the event of electron emitted from the core. The events that occur within the Tritium nucleus are the change of neutrons into protons and electrons, so the effect of the atomic number of the Tritium atom will change, but the mass number remains 1. The process of beta radiation on Tritium atoms is shown in (1) and (2) [1],

$$^{3}H \rightarrow \ ^{3}He^{+} + e^{-}(\beta) + \bar{v}, \tag{1}$$

$$^{3}H \rightarrow \ ^{3}He^{+} + e^{-}(\beta) + e^{-} + \bar{v}, \tag{2}$$
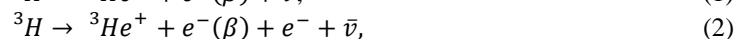
where $e^{-}(\beta)$ is fast β^{-} electron, $\bar{v}$ indicates the antineutrino of the electron and e^{-} represents the secondary (or slow) electron [2]. Tritium atoms decay with a half-life of 12.3 years, resulting in a maximum nuclear energy of 18.589 keV and an average electron energy of 5.7 keV [3]. As for making Tritium, using fusion reaction is generally at play, that is by firing neutron on Helium-3 shown in equation (3). The resultant energy of this reaction is $E_H = 0,573 \ MeV$ for Hydrogen and $E_T = 0,191 \ MeV$ MeV for Tritium.

$$n + \ _{2}^{3}He \rightarrow \ _{1}^{1}H + \ _{1}^{3}T + Q_1 \tag{3}$$

This decay reaction has tremendous benefits in the field of nuclear technology, especially in the application of betavoltaics battery. Betavoltaics battery is expected to become the battery of the future.

Betavoltaics is one type of non-thermal battery that utilizes semiconductor material sources to convert the energy of nuclear radiation into electricity [4]. Some types of atoms like Tritium ($^3_1 T$), Nikel (^{63}Ni) dan Promethium (^{147}Pm) is the most commonly used element as a betavoltaics battery. Tritium has a half-life of 12.3 years with an average beta beam emission of 5.7 keV. The sedans for Nickel have a half-life for 100 years with an average of 17.4 keV emitting energy as well as Promethium element has a half-life of 2.6 years with a beta energy emission of 224.1 keV [5]. Tritium atoms have properties susceptible to external electric fields. The external electric field will affect the electron binding energy to the nucleus. In a previous study, we have calculated the effect of static electric field on the direction of one dimension and effect on its binding energy and the function of Tritium atomic wave [6]. In this research, the authors discuss the influence of static electric field in 3 dimensional direction. In order to obtain more accurate results, the conditions operative are in relativistic conditions. This circumstance takes into account the condition of the electron velocity as it travels around the moving nucleus fast enough, thus affecting the energy value for each condition [7].

2. Method

2.1 Energy of Tririum with Relativistic Condition

In the Bohr atom model, the Hydrogen family's atomic energy is only influenced by the principal quantum number only. Whereas in relativistic state, atomic energy is not only influenced by the main quantum number only, but also influenced by the quantum number of orbits [8]. In Table 1, we can see Tritium atomic energy in some conditions.

Table 1. Atomic Tritium Energy in the Relativistic for Different Conditions

No.	States	Principal Quantum Number (n)	Orbital Quantum Number (l)	Energy (Joule)
1.	ER_{1s}	1	0	$-21{,}79331845 \times 10^{-19}$
2.	ER_{2s}	2	0	$-5{,}448456553 \times 10^{-19}$
3.	ER_{2p}	2	1	$-5{,}448649986 \times 10^{-19}$
4.	ER_{3s}	3	0	$-2{,}421565796 \times 10^{-19}$
5.	ER_{3p}	3	1	$-2{,}42162311 \times 10^{-19}$
6.	ER_{3d}	3	2	$-2{,}421634572 \times 10^{-19}$

2.2 Rayleigh-Schrodinger Perturbation Theory

In this study, the approach applied is the theory of time-independent perturbation theory. This perturbation theory is also called Rayleigh-Shrodinger Perturbation Theory [9]. A Hamiltonian initial condition without any perturbation is show in equation (4),

$$H\psi_n = E_n^{(0)}\psi_n \tag{4}$$

In perrurbation Theory, The Hamiltonian System is broken down into two main parts, the uperturbed Hamiltonian (H_0) and disturbed Hamiltonian (W). In equation (5), α means the expansion parameter for the perturbation correction order [10]. Hamiltonian system can be written as follow.

$$H = H_0 + \alpha W \tag{5}$$

Because the perturbation W is 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 is expressed as follow,

$$E = E^{(0)} + \alpha E^{(1)} + \alpha^2 E^{(2)} + ... \tag{6}$$

$$\psi = \psi^{(0)} + \alpha \psi^{(1)} + \alpha^2 \psi^{(2)} + ... \tag{7}$$

And then, eq. (6) is substituted by eq. (7), and eq. (5) is substituted by eq. (4).

$$(H_0 + \alpha W)(\psi^{(0)} + \alpha \psi^{(1)} + \alpha^2 \psi^{(2)} + ...) = (E^{(0)} + \alpha E^{(1)} + \alpha^2 E^{(2)} + ...)$$
$$(\psi^{(0)} + \alpha \psi^{(1)} + \alpha^2 \psi^{(2)} + ...) \tag{8}$$

By doing operation between two sides, the coefficients of successive power of α on both sides of this equation has to be equal. We obtain the following results.

$$(H_0 - E^{(0)})\psi^{(0)} = 0 \tag{9}$$

$$(H_0 - E^{(0)})\psi^{(1)} = (E^{(1)} - W)\psi^{(0)} \tag{10}$$

$$(H_0 - E^{(0)})\psi^{(2)} = (E^{(1)} - W)\psi^{(1)} + E^{(2)}\psi^{(0)} \tag{11}$$

Equation (9) is the zero-order correction solution, while equation (10) is the first –order correction solution and equation (11) is the second-order correction solution.

By using Equation (10), the energy and the wave function of the first order correction is as follows,

$$E_n^{(1)} = \left\langle \psi_n \left| W \right| \psi_n \right\rangle = \int_V \psi_n W \psi_n dV \tag{12}$$

$$\psi_n^{(1)} = \sum_{n \neq k} \frac{\left\langle \psi_k \left| W \right| \psi_n \right\rangle}{E_n^{(0)} - E_k^{(0)}} \psi_k^{(0)} \tag{13}$$

And if we use equation (12), we will get the result of second-order correction for energy and wave function as follows,

$$E_n^{(2)} = \sum_{n \neq k} \frac{\left| \left\langle \psi_k \left| W \right| \psi_n \right\rangle \right|^2}{E_n^{(0)} - E_k^{(0)}} \tag{14}$$

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

$$- \sum_{r \neq n} \frac{1}{2} \frac{\left| \left\langle \psi_r |W| \psi_n \right\rangle \right|^2}{\left(E_r^{(0)} - E_n^{(0)} \right)^2} \psi_n^{(0)} \tag{15}$$

3. Result and Discussion

3.1 The First-order correction of external electric field disturbance on Tritium atoms

Using equation (12), we can determine the magnitude of the electric field influence by using the interference theory approach. The first-order external electric field disturbance on the Tritium atom in the z direction at the ground state is expressed as follow,

$$W_z^{(1)} = \langle \psi_{1s} | e\xi z | \psi_{1s} \rangle$$
$$= \int_V \frac{1}{\pi a_0^3} e\xi \, r \cos\theta \, e^{-2r/a_0} \, dV$$
$$= \frac{e\xi}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} \, dr \int_0^\pi \sin\theta \cos\theta \, d\theta \int_0^{2\pi} d\phi$$
$$W_z^{(1)} = 0 \tag{16}$$

The first-order external electric field disturbance on Tritium atoms in the y- axis of the ground state is expressed as follow,

$$W_y^{(1)} = \langle \psi_{1s} | e\xi y | \psi_{1s} \rangle$$
$$= \int_V \frac{1}{\pi a_0^3} e\xi \, r \sin\theta \sin\phi \, e^{-2r/a_0} \, dV$$
$$= \frac{e\xi}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} \, dr \int_0^\pi \sin^2\theta \, d\theta \int_0^{2\pi} \sin\phi \, d\phi$$
$$W_y^{(1)} = 0 \tag{17}$$

The first-order external electric field disturbance on Tritium atoms in the *x*-axis of the ground state is,

$$
\begin{aligned}
W_x^{(1)} &= \langle \psi_{1s} | e\xi x | \psi_{1s} \rangle \\
&= \int_V \frac{1}{\pi a_0^3} e\xi \, r \sin\theta \cos\phi \, e^{-2r/a_0} \, dV \\
&= \frac{e\xi}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} \, dr \int_0^\pi \sin^2\theta \, d\theta \int_0^{2\pi} \cos\phi \, d\phi \\
W_x^{(1)} &= 0
\end{aligned}
\tag{18}
$$

The whole calculation of first order correction for each coordinate produced the same value, that is zero. The first-order correction does not contribute to the energy change of the Tritium atoms in the ground state.

3.2 The second order correction of external electric field to Tritium atom

Using equation (14), we can look for the influence of external electric field at second order by using the interference theory method. The second-order external electric field disturbance on the Tritium atom in the z direction at the ground state is expressed as follow,

$$
\begin{aligned}
W_z^{(2)} &= \sum_{n \neq k} \frac{|\langle \psi_k | e\xi z | \psi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \\
&= \frac{\left| \langle \psi_{2pz} | e\xi z | \psi_{1s} \rangle \right|^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}} \\
&= \frac{\left(\frac{e\xi}{4\sqrt{2}\,\pi a_0^3} \int_0^\infty r^4 e^{-3r/2a_0} \, dr \int_0^\pi \sin\theta \cos^2\theta \, d\theta \int_0^{2\pi} d\phi \right)^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}} \\
W_z^{(2)} &= \frac{\left(\frac{256\,a_0 e\xi}{243\sqrt{2}} \right)^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}}
\end{aligned}
\tag{19}
$$

The second-order external electric field disturbance on the Tritium atom in the y direction at the ground state is expressed as follow,

$$
\begin{aligned}
W_y^{(2)} &= \sum_{n \neq k} \frac{|\langle \psi_k | e\xi y | \psi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \\
&= \frac{\left| \langle \psi_{2py} | e\xi \, r \sin\theta \sin\phi | \psi_{1s} \rangle \right|^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}} \\
&= \frac{\left(\frac{e\xi}{4\sqrt{2}\,\pi a_0^3} \int_0^\infty r^4 e^{-3r/2a_0} \, dr \int_0^\pi \sin^3\theta \, d\theta \int_0^{2\pi} \sin^2\phi \, d\phi \right)^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}} \\
W_y^{(2)} &= \frac{\left(\frac{256\,a_0 e\xi}{243\sqrt{2}} \right)^2}{E_{1s}^{(0)} - E_{2py}^{(0)}}
\end{aligned}
\tag{20}
$$

The second-order external electric field disturbance on the Tritium atom in the x direction at the ground state is expressed as follow,

$$
\begin{aligned}
W_x^{(2)} &= \sum_{n \neq k} \frac{|\langle \psi_k | e\xi x | \psi_n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \\
&= \frac{\left| \langle \psi_{2px} | e\xi \, r \sin\theta \cos\phi | \psi_{1s} \rangle \right|^2}{E_{1s}^{(0)} - E_{2px}^{(0)}} \\
&= \frac{\left(\frac{e\xi}{4\sqrt{2}\,\pi a_0^3} \int_0^\infty r^4 e^{-3r/2a_0} \, dr \int_0^\pi \sin^3\theta \, d\theta \int_0^{2\pi} \cos^2\phi \, d\phi \right)^2}{E_{1s}^{(0)} - E_{2px}^{(0)}} \\
W_x^{(2)} &= \frac{\left(\frac{256\,a_0 e\xi}{243\sqrt{2}} \right)^2}{E_{1s}^{(0)} - E_{2px}^{(0)}}
\end{aligned}
\tag{21}
$$

3.3 External electric field in 3 Dimensional Tritium Atom

The electric field acting on the Tritium atom is directed at 3 axes, i.e. the x, y and z axes. The form of the equation of the 3-dimensional interference in the first order ground state is given by equation (16) and the second order of equation (19).

$$W_{3D}^{(1)} = \langle \psi_{1s} | \sum_N e\xi N |\psi_{1s}\rangle \quad \text{dengan } N = x, y \text{ dan } z \tag{22}$$

$$W_{3D}^{(1)} = \langle \psi_{1s} | e\xi z + e\xi y + e\xi x |\psi_{1s}\rangle$$

$$W_{3D}^{(1)} = W_z^{(1)} + W_y^{(1)} + W_x^{(1)}$$

$$W_{3D}^{(1)} = 0 \tag{23}$$

In equation (23), it can be seen that the tritium atomic energy interference at ground state in 3-dimensional cartesian coordinates is zero, meaning that there is no contribution to the shifting energy of Tritium atoms. While the correction for the second order is shown in equation (24).

$$W_{3D}^{(2)} = \sum_{n \neq k} \frac{\left|\langle \psi_k | \sum_N e\xi N |\psi_n\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}} \quad \text{dengan } N = x, y \text{ dan } z \tag{24}$$

$$W_{3D}^{(2)} = \sum_{n \neq k} \frac{\left|\langle \psi_k | (e\xi z + e\xi y + e\xi x) |\psi_n\rangle\right|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$W_{3D}^{(2)} = \frac{\left|\langle \psi_{2pz} | e\xi z |\psi_{1s}\rangle\right|^2}{E_{1s}^{(0)} - E_{2pz}^{(0)}} + \frac{\left|\langle \psi_{2py} | e\xi y |\psi_{1s}\rangle\right|^2}{E_{1s}^{(0)} - E_{2py}^{(0)}} + \frac{\left|\langle \psi_{2px} | e\xi x |\psi_{1s}\rangle\right|^2}{E_{1s}^{(0)} - E_{2px}^{(0)}}$$

$$W_{3D}^{(2)} = \left(\frac{256\, a_0 e\xi}{243\sqrt{2}}\right)^2 \left(\frac{1}{E_{1s}^{(0)} - E_{2pz}^{(0)}} + \frac{1}{E_{1s}^{(0)} - E_{2py}^{(0)}} + \frac{1}{E_{1s}^{(0)} - E_{2px}^{(0)}}\right) \tag{26}$$

Tritium atomic energy in the ground state when exposed to external electric field interference 3 dimension in relativistic frame is expressed as follow,

$$E_{Tritium} = ER_{1s} + W_{3D}^{(1)} + W_{3D}^{(2)}$$

$$E_{Tritium} = ER_{1s} + 0 + \left(\frac{256\, a_0 e\xi}{243\sqrt{2}}\right)^2 \left(\frac{1}{ER_{1s}^{(0)} - ER_{2pz}^{(0)}} + \frac{1}{ER_{1s}^{(0)} - ER_{2py}^{(0)}} + \frac{1}{ER_{1s}^{(0)} - ER_{2px}^{(0)}}\right) \tag{27}$$

Table 2. Tritium atomic energy shifts in external electric field variations

No.	Exrernal Electric Field ξ ($Volt/m$)	Energy (Joule)
E0	0	$-21{,}79331845 \times 10^{-19}$
E1.	1×10^9	$-21{,}79331845 \times 10^{-19} - 7{,}3236066 \times 10^{-23}$
E2.	1×10^{10}	$-21{,}79331845 \times 10^{-19} - 7{,}3236066 \times 10^{-21}$
E3.	1×10^{11}	$-21{,}79331845 \times 10^{-19} - 7{,}3236066 \times 10^{-19}$
E4.	1×10^{12}	$-21{,}79331845 \times 10^{-19} - 7{,}3236066 \times 10^{-17}$
E5.	1×10^{13}	$-21{,}79331845 \times 10^{-19} - 7{,}3236066 \times 10^{-15}$

If we use some value of certain external electric field, then the calculation result of electric field effect is shown in table 2. From Table 2 we can see that the greater the external electric field given to Tritium atoms, the greater the energy shift. For more details we can see the magnitude of the shift in Figure 1.
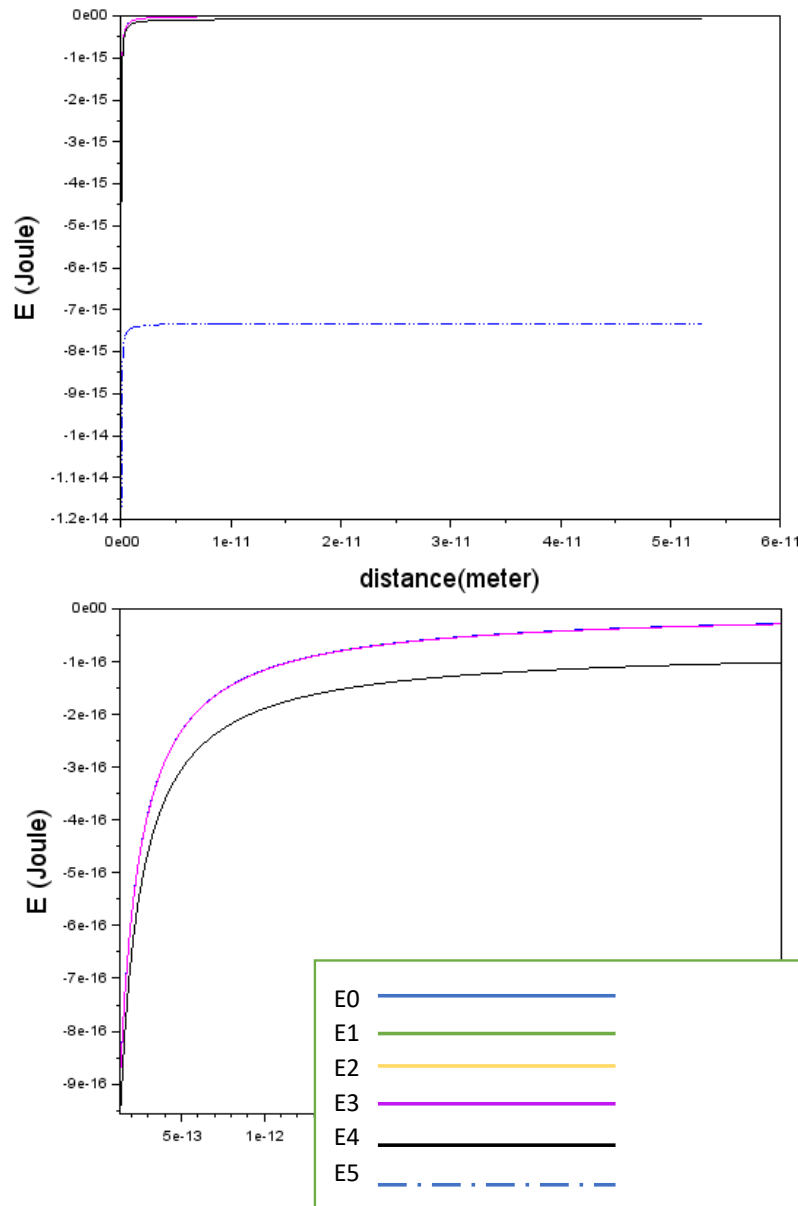
Figure 1. Tritium atomic energy shifts in external electric field variations

The figure above shows that an electric field of 1×10^9 volt/m until 1×10^{11} does not give a clear effect on the Tritium energy shift. By contrast, at the time of electric field given above, 1×10^{12} will be apparent magnitude of energy shift from Tritium. This means only the state of a strong magnetic field is capable of affecting Tritium atoms. In other studies, external electric fields also affect the condition of materials [11].

The polarizability is found in the second order correction in 3 dimensional perturbation as follows:

$$\alpha = 2 \left(\frac{256\, a_0 e}{243\sqrt{2}} \right)^2 \left(\frac{1}{E_{1s}^{(0)} - E_{2pz}^{(0)}} + \frac{1}{E_{1s}^{(0)} - E_{2py}^{(0)}} + \frac{1}{E_{1s}^{(0)} - E_{2px}^{(0)}} \right) \tag{28}$$

This equation (29) is related to classical theory is written as follows,

$$E = E_0 + \frac{1}{2}\alpha\xi^2 \tag{29}$$

Tritium atoms belong to the family of Hydrogen atoms which are also included as alkaline atoms, which are very easily disturbed by external electric fields. This stark effect has resulted in electrons experiencing polarization phenomena [12].

4. Conclusion

3-dimensional electric field disturbances generate different results with 1 dimensional disturbance on Tritium at the ground state atoms. The greater the magnitude or strength of the external electric field given to Tritium atoms, the greater energy shifts will emerge. The external electric field (Stark Effect) causes the electron to experience a polarization phenomenon. This phenomenon corresponds to the classical theory of electrodynamics.

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