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Probability of Finding Tritium Atom Electrons in Momentum Space with Principal Quantum Number n ≤ 3

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Abstract: The tritium atom is an isotope of the hydrogen atom which only has one electron, so this research aims to determine the probability of finding a tritium atom electron ((_1^3)H) in momentum space with the principal quantum number n ≤ 3. This research is included in non-experimental research using literature study methods related to quantum mechanics. To determine the probability data for the electron momentum of the Tritium atom ((_1^3)H) numerical calculations were used using the Matlab R2021a program. The results obtained in this research are in the form of probability values for the electron momentum of the Tritium atom ((_1^3)H) which will provide an overview of the existence of electrons in the momentum space. Based on the research results, it can be shown that in momentum space, the probability of finding a Tritium atom electron increases as the principal quantum number (n) increases.

Keywords: Momentum probability; Momentum space; Tritium (_1^3)H

Introduction

In the 19th century, several phenomena were discovered that could not be explained by classical physics. This requires the development of even more fundamental physics concepts which are now called Modern Physics, usually associated with special reality and quantum theory (Aini, 2020). In 1925 a new theory was discovered which was known as "The New Quantum Mechanics Theory". This new theory emerged based on the theoretical descriptions of De Broglie, Heisenbergh and Schrodinger as well as the experimental experiments of Davision and Germer from G.R. Thomson. The theory was developed after observing microscopic objects such as atoms and molecules that have different behaviors from macroscopic objects in life (Halim & Herlina, 2020). The new quantum theory is based on the Schrodinger equation to determine the energy of particles or electrons (Festiana, 2018). The quantum mechanical theory of atomic structure is one of the fundamental concepts in quantum physics (Manik et al., 2022). Quantum physics is a branch of science that studies the relationship between waves and particles. According to Syahrial et al. (2022) quantum physics is the study of the behavior, characteristics, properties of matter and energy in molecules, atoms, sub-atoms, and even smaller than sub-atoms. The relationship between waves and particles can be explained by a single-electron atom (Makmum et al., 2020).

The hydrogen atom is a type of simple atom because it only has one proton and one electron (Suyanta, 2019). Hydrogenic atoms have one electron such as hydrogen atoms, deuterium, tritium atoms, helium ions, and lithium ions (Pratikha et al., 2022). Hydrogenic atoms themselves are atoms that have lost all but one of their electrons. Tritium atoms are similar to hydrogen atoms because there are two neutrons and one electron surrounding the nucleus of the tritium atom (Mardiana et al., 2019). Tritium atom is one of the hydrogenic atoms or a class of atoms with one electron moving around the atomic nucleus (Supriadi et al.,

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2023). Tritium atoms are useful for monitoring the environment from the impact of using nuclear installations in sea water. According to research conducted by Nurokhim (2014), the electrolysis process for the enrichment process using a tool, namely the LSC TRICARB 2910TR, was proven to be able to determine low tritium concentrations in seawater. Tritium is also useful as a material in making nuclear batteries, making military watches and pilots (Supriadi et al., 2018). Another benefit of the tritium atom is determining the age of groundwater, namely using the tritium isotope method (Hutasoit et al, 2021).

The use of tritium has been extensively studied in advanced countries. For instance, in the European DEMO project, effective isotope separation is crucial for managing tritium. Technologies such as the Thermal Cycle Absorption Process (TCAP) are required to handle low and radioactive tritium (Shere et al., 2024). In the DEMO project, tritium plays a significant role in fusion fuel breeding and processing to optimize reactor performance (Lawless et al., 2017). DEMO fusion power plants also need cryogenic distillation systems to separate tritium and deuterium isotopes from exhaust gases and to evaluate other separation technologies in terms of size, power, and safety (Shaw & Butler, 2019). Tritium is utilized in Disturbance Mitigation Systems (DMS) on tokamaks to reduce the risk of damage from plasma disturbances (Kruezi et al., 2015). Additionally, laser isotope separation methods can remove tritium from contaminants in heavy water reactors (Magnotta et al., 1982), and cryogenic distillation is effective for recovering tritium from tritiated water (Ana et al., 2016).

To distinguish energy levels and determine the size of an atom, the principal quantum number (n) is used. This quantum number is equivalent to a certain energy level, the value of this main quantum number is an integer n= 1,2,3,... and not zero. Quantum numbers themselves are the basis for determining the wave function (Krane, 2012). The wave function is used to represent the dynamics of moving particles obtained from solving the Schrodinger Equation of these particles (Festiana, 2018). The wave function itself can provide information about the condition of a system at any time, but does not have physical meaning. However, the absolute value of the wave function which is squared and integrated over certain variables can provide information about the physical meaning in the form of probability values (Makmum et al., 2020).

The wave function in hydrogenic atoms is a complex quantity which can be divided into two, namely the radial function and the angular function. According to Singh (2009) the formula for the wave function in position on an atom can be mathematically expressed as follows:

$$\psi_{n,l,m}(r,\theta,\phi) = \frac{(2\gamma)^{l+1}}{n(n+l)}\sqrt{\frac{\gamma(n-l-1)!}{n(n+1)!}}\, e^{-(\gamma r)} r^l [L_{n+1}^{2l+1}(2\gamma r)] \sqrt{\frac{2l+1}{2}\left(\frac{(l-|m|)!}{(l+|m|)!}\right)}\sqrt{\frac{1}{2\pi}}\, e^{\pm im\phi} p_l^m \cos\theta \quad (1)$$

So, to determine the wave function in momentum space, it can be obtained by transforming the wave function in position space using the Fourier transformation which is expressed in the formula equation 2 and 3 (Damayanti et al., 2019):

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int \varphi(p)^{\frac{ipx}{\hbar}}\, dp$$
$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \varphi(x)^{-\frac{ipx}{\hbar}}\, dx \quad (2)$$

Therefore, we get the wave function in momentum space as follows:

$$\varphi = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{\pm im\Phi}\sqrt{\frac{2l+1}{2}\frac{(l-|m|!)}{(l-|m|!)}}\, p_l^m \cos\Theta \frac{\pi(i)^l}{(\gamma h)^{\frac{3}{2}}} 2^{2l+4} l! \left(\frac{n(n-l-1)!}{(n+1)!}\right)^{\frac{1}{2}} \frac{\zeta^l}{(\zeta^2+1)^{l+2}} C_{n-l-1}^{l+1}\left(\frac{\zeta^2-1}{\zeta^2+1}\right) \quad (3)$$

Below is the radial function for the (_1^3)H atom in momentum space (Hey, 1993):

$$F_{(n,l)}(p) = -(-i)^i\left[\frac{2(n-i-1)!}{\pi(n+i)!}\right]^{\frac{1}{2}}. \; n^2 2^{2(l+1)} l!\, n^l p^l (n^2p^2+1)^{-(l+2)} C_{n-l-1}^{l+1}\left(\frac{n^2p^2-1}{n^2p^2+1}\right) \quad (4)$$

In accordance with Max Born's interpretation where the particle wave function is related to the probability of finding a particle in a space, the particle wave function must fulfill several important criteria, one of which is probability (Supriadi et al., 2022). Probability comes from the word "probably" which means possibility. Therefore, probability can be interpreted as the possibility of an event occurring (Chamdani, 2022). Probability is the square modulus of a wave function. Electron probability is a description of the electron found in space (Kharismawati & Supriadi, 2021). Probability can also be interpreted as a possibility that occurs in the position or momentum of a particle. Where to find particles in a room can be determined by:

$$P = \int_0^\infty P\, dx = \int_0^\infty P\, |\psi|^2\, dx \quad (5)$$

From the equation above, the probability of a particle being between r and r+ dr at a certain time is high (Supriadi et al., 2022). Therefore, the probability of finding an electron in momentum space can be formulated:

$$P = \int_0^\infty p^2 |F_{nl}(p)^2| dp \quad (6)$$

(Podolsky & Pauling, 1929)

Based on the research that has been carried out, it only examines the probability of finding electrons in position space. As has been done by Utami et al. (2019), the radial probability in the tritium atom shows that the chance of finding an electron is smaller if the position of the electron is far from the atomic nucleus. Therefore, this research aims to determine the existence or possibility of electrons in the tritium atom in momentum space using radial function calculations

Method

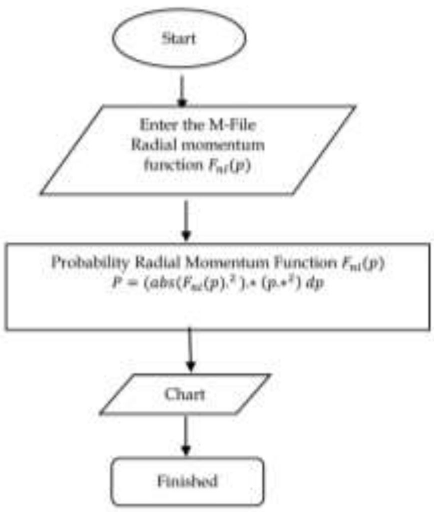


Figure 1. Flow chart

This research uses non-experimental research with a literature study approach. In this study, to obtain probability values, equations (4) and (6) were used. The results of solving the probability of the radial momentum function are plotted into a 2D graph using Matlab R2021a. The 2D graph presents the probability distribution of finding a tritium atom electron in momentum space. Figure 1 shows the input parameters for the Matlab simulation program, namely the radial momentum function F_((n,l)) (p). In the ground state, the solution to the radial momentum function is obtained. From this function, the probability of the radial momentum function is obtained so that the probability of finding a tritium atom electron in the momentum space is obtained which is presented in the form of a 2D graph.

Result and Discussion

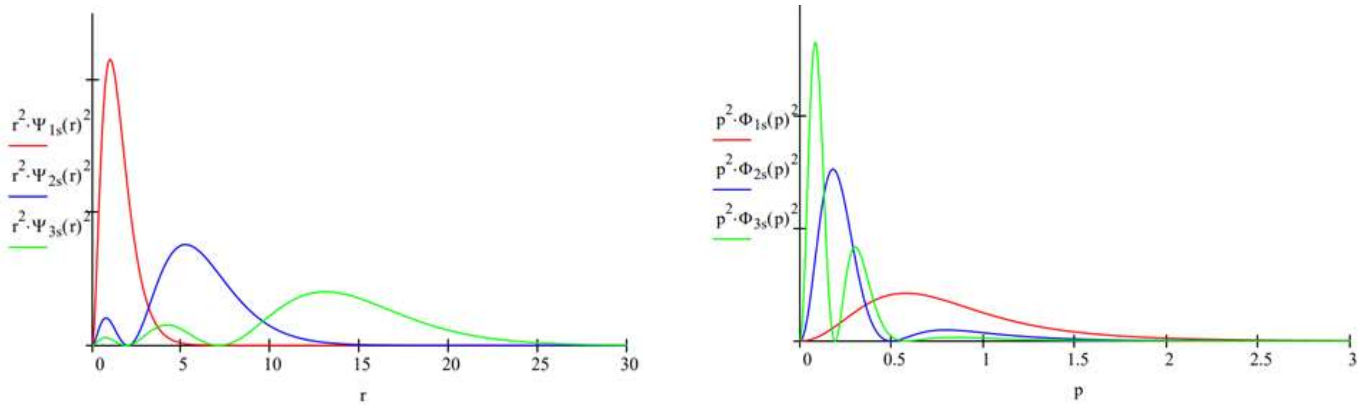
Research related to the probability of finding an electron in a tritium atom in the momentum space with a quantum number n ≤ 3 obtained results in the form of a large value of the probability of finding an electron in a tritium atom. The following table shows a recapitulation of the results of the probability of electron momentum in a tritium atom at a quantum number n ≤ 3.

Table 1. Recapitulation of the Results of the Probability of Finding an Electron in a Tritium Atom at Quantum Number n ≤ 3

P	n = 1	n = 2		n = 3		
	l = 0	l = 0	l = 1	l = 0	l = 1	l = 2
p_0	0.71	0.92	0.97	0.97	0.99	0.99
$2p_0$	0.96	0.99	0.99	0.99	0.99	0.99
$3p_0$	0.99	0.99	0.99	0.99	0.99	0.99
$4p_0$	0.99	0.99	0.99	0.99	0.99	0.99
$5p_0$	0.99	0.99	0.99	0.99	0.99	0.99
$6p_0$	0.99	0.99	0.99	0.99	0.99	0.99
$7p_0$	0.99	0.99	0.99	0.99	0.99	0.99
$8p_0$	0.99	0.99	0.99	0.99	0.99	1.00
$9p_0$	0.99	0.99	0.99	0.99	1.00	1.00

Based on the table above, the results of numerical calculations using Matlab can be shown with a limit of p0 to a limit of 9p0. Because this research only examines the quantum number n<3, the greatest possibility of obtaining an electron is n. The table shows that when the quantum number n=1, l=0, the p0 value is 0.71and the 9p0 value is 0.99. Therefore, it can be said that the greater p0, the greater the probability of finding an electron in a tritium atom. This is in accordance with the probability formula which states that p is directly proportional to p_0. Likewise, when viewed based on quantum numbers in the same orbital number, namely l=0, the result for n=1 is 0.71, for n=2 it is 0.92 and then for n=3 it is 0.97. And in the case of orbital numbers l=1 and l=2, it also shows the same results, namely that the larger the quantum number, the greater the probability of finding an electron in a tritium atom or the easier it is to find an electron at the largest quantum number.

This is due to the difference in orbitals in each quantum number because the more elliptical the orbital shape, the easier it is to find electrons (Krane, 2012). The probability distribution graph of radial momentum in a tritium atom shows the graph of the function P(p) which is the radial probability as a function of momentum. The momentum probability distribution graph in the tritium atom was obtained using Matlab R2021a software. The following is a graph of the probability distribution of momentum in a tritium atom (_1^3)H at quantum number n ≤ 3.



(a) (b)

Figure 2. (a). Probability distribution graph of finding hydrogen atom electrons in position space by Frank Rioux (b). Probability distribution graph of finding hydrogen atom electrons in momentum space by Frank Rioux

Based on graphs a and graph b above, it can be seen that the probability of finding an electron in position space is opposite to the probability of finding an electron in momentum space. This is because position and momentum are conjugate variables where the momentum space wave function is obtained from the inverse of the position space wave function and also according to the Heisen uncertainty principle, if two variables such as position and momentum are measured simultaneously it is impossible to obtain accurate results for both of them as regulated by the formula $\Delta x \Delta p \geq \hbar/2$ (Jesi, 2020). In line with the results of the graph of the probability of finding a tritium atom electron inthe momentum space as follows.

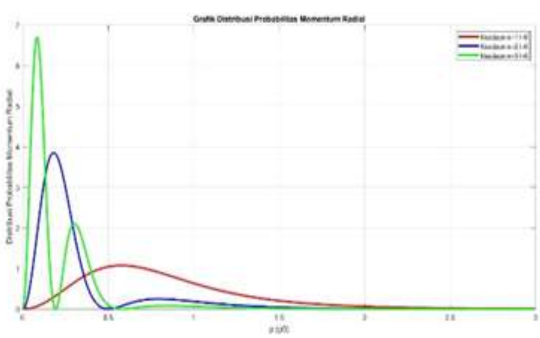


Figure 3. Probability distribution graph of finding tritium atom electrons in momentum space

Based on the resulting graph, it can be seen that for the quantum number n=1 there is 1 peak, then for the quantum number n=2 there are 2 and for the quantum number n=3 there are 3 peaks. This can be interpreted as that for n=1 there is 1 point that has the possibility of finding an electron, for n=2 there are 2 points that have the possibility of finding an electron and for n=3 there are 3 points that have the possibility of finding an electron. Therefore, the greater the quantum number, the easier it is to find electrons or it could be said that the greater the quantum number, the probability value of finding an electron in a tritium atom in momentum space increases.

Conclusion

Based on the results of research that has been carried out by solving the Schrodinger equation on the tritium atom, the probability distribution results for finding tritium atom electrons (_1^3)H in momentum space are obtained. For the quantum number n=1 there is 1 peak, then for the quantum number n=2 there are 2 and for the quantum number n=3 there are 3 peaks. So the probability value of finding a tritium atom electron in the momentum space depends on the principal quantum number n and the orbital quantum number l. The larger the quantum number, the probability value of finding an electron in a tritium atom in momentum space will also increase. This data shows the opposite outcome with probabilities in position space because position and momentum are conjugate.

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Author Contributions
Conceptualization; B.S., H.Z., S.Z.A., A.S., E.D. C.: methodology; B. S., validation; H.Z.: formal analysis; S.Z.A.: investigation; A. Sresources; E.D.C: data curation: B.S: writing—original; H.Z: draft preparation; S.Z.A: writing—review and editing: A.S.; visualization: E.D.C. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest
The authors declare no conflict of interest.

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