Probability of Deuterium Atom Electrons in Momentum Space at Quantum Numbers n ≤ 3

Bambang Supriadi1*, Sinthia Lolita Lorensia1, Firda Shahira2, Audri Mely Prabandari3, Aurellya Abdillah Wijaya Putri4

1,2,3,4 Pendidikan Fisika, Universitas Jember, 23111, Indonesia

*Corresponding author: bambangsutiriadief@unej.ac.id

Abstract – Deuterium is one of the isotopes of the hydrogen atom, which consists of 1 proton, 1 neutron, and 1 electron, also called a hydrogenic atom. The position of electrons in the atom cannot be determined with certainty because it is probabilistic. The probability of finding a deuterium atom electron in momentum space at quantum number n ≤ 3. This research aims to find the probability value of deuterium atomic electrons in momentum space at n ≤ 3. This research uses the mathematical theory study method through several stages, namely collecting the latest and relevant literature sources, making a simulation program, and then validating the simulation program with existing theory. If it has been validated, continue taking data that will be analyzed and then discussed in the results and discussion stage, and the last step is drawing conclusions. The results of this study show that the probability value for finding atomic electrons in momentum space will be more excellent with increasing integration limit values and the value of the principal quantum number (n).

Keywords: Deuterium Atom, Momentum Space, Probability

Introduction

Quantum physics is the study of the relationship between waves and particles. According to Syahrial et al. (2022), quantum physics is the science of the behavior/characteristics/properties of matter and energy in molecules, atoms, sub-atomic, and even smaller than sub-atomic. The relationship between waves and particles can be explained by single-electron atoms (Makmun, Supriadi and Prihandono, 2020). The hydrogen atom is the simplest element containing one proton and one electron (Suyanta, 2019). There are also some atoms or ions that have properties like hydrogen atoms called hydrogenic atoms.

Hydrogenic atoms are atoms that have only one electron or atoms whose outer shell consists of only one electron (Makmun, Supriadi and Prihandono, 2020). In other words, hydrogenic atoms have one electron like hydrogen atoms, such as deuterium atoms, tritium atoms, helium ions, and lithium ions (Pratikha, Supriadi and Handayani, 2022). Deuterium atoms (\(^2\mathrm{H}\)) and tritium atoms (\(^3\mathrm{H}\)) which are isotopes of hydrogen atoms (Suyanta, 2019). Helium atoms are noble gases consisting of 2 protons, 2 neutrons, and 2 electrons in their orbitals and will behave like hydrogenic atoms if one of the two electrons is ionized (Makmun, Supriadi and Prihandono, 2020). Lithium atoms have 3 electrons in their shell (Men and Setianto, 2017).

The interaction between the two nuclei of hydrogen atoms in the formation of deuterium produces a mutual attraction force with the same force but in opposite directions, and the center of the mass coordinate of the interaction of the two nuclei of hydrogen atoms becomes the center of the deuterium atom so that the wave function of the deuterium atom can be represented in position space and momentum space (Karomah et al., 2021). In its solution, the wave function of the deuterium atom can be divided into two functions both in position space and in momentum space. The two functions are radial wave function and angular wave function which will provide fission information such as energy, position, momentum, probability density and other behavior of deuterium atoms (Suparmi et al., 2012). Research on hydrogenic atomic wave functions in position space has been conducted by Utami, Supriadi dan Lesmono (2019) on tritium atoms, Makmun, Supriadi and Prihandono (2020) on helium ions, and Saputra, Supriadi dan Prastowo (2019) deuterium atoms. Research on the wave function of deuterium at quantum number 4 has been conducted by deuterium atoms.
function of hydrogen atoms in momentum space was only conducted by Damayanti, Supriadi dan Nuraini (2019) on helium ions. In its application, deuterium atoms are utilized in the process of making heavy water (D$_2$O) for neutron moderators in uranium fission reactions. In this case, the neutron moderator according to Beiser (1990) is the process of slowing down the neutron rate by absorbing energy and colliding neutrons without absorbing their particles (Saputra dkk., 2019). In ultra-solid conditions, deuterium is used to observe particles with energies less than 10 MeV in the inductaster process. In addition, deuterium is used as a material for determining the genesis of groundwater sources (Fuadah dkk., 2018). Therefore, this study will further examine the wave function of the deuterium atom ($\frac{2}{3}H$) to obtain information on the electron probability of the atom in momentum space.

Materials and Methods

Schrodinger's equation is a second-order differential equation that is widely used in hydrogenic atoms. The characteristics of Schrodinger equation are divided into time-dependent Schrodinger equation and time-free (steady-state) Schrodinger equation. Given the spherical symmetry of the hydrogen atom, solving the Schrodinger equation of the hydrogen atom uses the time-free Schrodinger equation in three dimensions (Beiser, 1990):

$$\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) + (E - V(x)) \psi(x, y, z) = 0$$  (1)

The steady-state Schrodinger equation in spherical coordinates is

$$-\frac{\hbar^2}{2m} \left( \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial \theta^2} \sin \theta + \frac{\partial^2}{\partial \phi^2} \right) \psi(r, \theta, \phi) + \left[ V(r) - E \right] \psi(r, \theta, \phi) = 0$$  (2)

The method used to solve the Schrodinger equation uses the variable separation method by assuming:

$$\psi(r, \theta, \phi) = R(r) Y(\theta, \phi).$$  (3)

With $R(r)$ is the radial part of the Schrodinger function, also known as the radial wave function, obtained by solving the radial part of the Schrodinger equation,

$$\frac{1}{R(r)} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} + \frac{2m \gamma^2}{\hbar^2} \right) \left[ E - V(r) \right] = \beta$$  (4)

and $Y(\theta, \phi)$ is the angular part of Schrodinger function obtained by solving the angular part of Schrodinger equation (Saputra, Supriadi and Prastowo, 2019).

$$\frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} = -\beta$$  (5)

The above wave function is the wave function of hydrogenic atoms in position space. The wave function of hydrogenic atoms in momentum space is obtained by transforming the above function using the fourier transform (Damayanti, Supriadi and Nuraini, 201).

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \varphi(p) \frac{e^{ipx}}{\hbar} dp$$  (6)

$$\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) \frac{e^{ipx}}{\pi} dx$$  (7)

So that equation (3) above can be expressed as:

$$\varphi(p, \theta, \phi) = \tilde{F}(p) Y(\theta, \phi)$$  (8)

With $F(p)$ is the radial wave function of hydrogenic atoms in momentum space. According to Singh (2009), the solution of the Schrodinger equation of hydrogenic atoms in position space or called the wave function of hydrogenic atoms in position space is written as:

$$\psi_{n\ell m}(r, \theta, \phi) = \left[ \frac{2z}{n a_0} \right]^3 \frac{1}{(2\pi)^{1/2}} \left[ \frac{2\pi}{2m} \right]^{1/2} \frac{r^{2\ell + 1}}{n_{\ell m}^0} e^{-\frac{2r}{n a_0}} \sum_{l=0}^{2\ell + 1} \frac{2\ell + 1}{2\ell + 1} \sqrt{\frac{2\ell + 1}{(2\ell + 1)!}} \frac{1}{2\pi} e^{\pm im\phi} \left[ \psi_{l\ell m}^n \right] (9)

Podolsky and Pauling (1929) generalized $\gamma = \frac{Z}{n a_0}$ so that the wave function of hydrogenic atoms can be simplified to:

$$\psi_{n\ell m}(r, \theta, \phi) = \frac{2\gamma}{n a_0} \left[ \frac{2\gamma}{n a_0} \right]^l \frac{1}{(2\pi)^{1/2}} \frac{1}{2\ell + 1} \sqrt{\frac{2\ell + 1}{(2\ell + 1)!}} \frac{1}{2\pi} e^{\pm im\phi} \left[ \psi_{l\ell m}^n \right]$$  (10)

By applying the Fourier transform to equation (8), the particle wave function in momentum space is obtained as follows:
\[\varphi(p, \Theta, \Phi) = h^{-\frac{3}{2}} \int_0^\infty \int_0^{2\pi} \int_0^{\pi} e^{-(\frac{2m}{\hbar}) r^2 p (\sin\Theta \cos\Phi \sin\Theta \cos\Phi + \sin\Theta \sin\Theta \sin\Phi \cos\Theta)} \left(2\gamma \right) (\frac{m}{\hbar}) d\Theta d\Phi \]

\[
\int_{-\infty}^{1} \left[ L_{n+l}^{(+)} \right] (2\gamma r) \sqrt{\frac{2l+1}{2l+2}} \left( \frac{l!}{(l+m)!} \right) \sqrt{\frac{1}{2\pi}} e^{-\frac{\lambda \sin\phi \rho}{2 \gamma r}} \cos\theta dr d\phi d\gamma
\]

(Damayanti, Supriadi and Nuraini, 2019)

With the radial wave function of a hydrogenic atom in its momentum space (Podolsky and Pauling, 1929) is:

\[F_{nl} = \frac{\pi 2^{l+4} \left( n - l - 1 \right)! \left( \frac{n}{\hbar} \right)^{3/2}}{(n+l)!} \frac{l!}{(l+1)!} C_{n-l-1}^{l+1} \left( \frac{2 - \gamma^2}{\gamma^2 + 1} \right)
\]

By introducing \( z = \frac{np}{\hbar} \) the above radial wave function can be written as

\[F_{nl} = \frac{\pi 2^{l+4} \left( n - l - 1 \right)! \left( \frac{n}{\hbar} \right)^{3/2}}{(n+l)!} \frac{l! \left( \frac{n}{\hbar} \right)^{2}}{\left( \frac{n}{\hbar} \right)^{2} + 1} C_{n-l-1}^{l+1} \left( \frac{\gamma^2}{\gamma^2 + 1} \right)
\]

For deuterium atoms, the z value is equal to 1, so the radial wave function of deuterium atoms in momentum space is,

\[F_{nl} = \frac{\pi 2^{l+4} \left( n - l - 1 \right)! \left( \frac{n}{\hbar} \right)^{3/2}}{(n+l)!} \frac{l! \left( \frac{n}{\hbar} \right)^{2}}{\left( \frac{n}{\hbar} \right)^{2} + 1} C_{n-l-1}^{l+1} \left( \frac{\gamma^2}{\gamma^2 + 1} \right)
\]

Deuterium \((^2H)\) as a nucleus called deuterium. Deuterium is a stable isotope consisting of 1 electron, 1 proton, and 1 neutron. Deuterium is formed due to the fusion reaction between the two nuclei of the hydrogen atom so that there is a merger of the two nuclei of the hydrogen atom with mutual attraction (Saputra, Supriadi and Prastowo, 2019). In the process of merging, two hydrogen atomic nuclei involve converting one proton into one proton followed by positron emission (Fuadah, Prastowo and Nuraini, 2018; Karomah et al., 2021). So that the atomic weight of deuterium is twice as heavy as a hydrogen atom (Santoso, 2015).

From equation (14), the behavior of deuterium atomic electrons such as position, energy and probability and others can be known with the help of operators. Probability is the chance of finding an electron in an atom or ion (Utami, Supriadi and Lesmono, 2019). The probability of finding an electron in a deuterium atom Bransden and Joachain (1987) is written as follows:

\[P = \int_0^\infty P^2 |F_{nl}(P)|^2 dP
\]

This research is included in the type of non-experimental research, because this research is done by developing pre-existing physics theories. The method in this research uses a mathematical theory study with several stages, namely collecting literature sources obtained from several recent and relevant research articles, as well as books that discuss the theories of hydrogenic atoms. make a simulation program, then the simulation program will be validated with existing theory. If it has been validated, continued data collection will be analyzed and discussed at the results and discussion stage, and the last stage is drawing conclusions. As for the simulation program, it is presented in the following flow chart diagram.

**Results**

The results of research on the probability of electron momentum of deuterium at \( n \leq 3 \) obtained the probability value of electron momentum and the distribution graph of radial momentum probability on deuterium atom \((^2H)\). Based on the results of the literature study, several provisions are obtained to find the value of electron momentum \((p)\) which will be used to determine the probability value of the electron momentum of the deuterium atom. The constants include the Planck constant \((\hbar = 1.054571800 \times 10^{-34} \text{Js})\), proton mass \((m_p = 1.6726219 \times 10^{-27} \text{kg})\), deuterium mass \((m_{^2H} = 3.34449439655 \times 10^{-27} \text{kg})\), the fine structure constant \((\alpha = \frac{1}{4\pi\epsilon_0 \hbar c} = 2.31027932 \times 10^{-28})\). From the above provisions, the value of the reduced mass of the deuterium atom is obtained as \(\mu = 9.10690170787562 \times 10^{-31} \text{kg} \) and the radius of the deuterium atom is \(r = 5.28589301188439 \times 10^{-11} \text{m} \). The value of electron momentum can be seen in Table 1.
**Figure 1.** Research Methods

**Table 1.** Results of Probability Value of Deuterium Atom Electron ($\frac{2}{3}H$) in Momentum Space at $n \leq 3$

<table>
<thead>
<tr>
<th>$p$</th>
<th>$n = 1$</th>
<th></th>
<th>$n = 2$</th>
<th></th>
<th>$n = 3$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$l = 0$</td>
<td>$l = 0$</td>
<td>$l = 1$</td>
<td></td>
<td>$l = 0$</td>
<td>$l = 1$</td>
</tr>
<tr>
<td>$p_0$</td>
<td>0.7122</td>
<td>0.9298</td>
<td>0.9784</td>
<td></td>
<td>0.9759</td>
<td>0.9907</td>
</tr>
<tr>
<td>2$p_0$</td>
<td>0.9663</td>
<td>0.9944</td>
<td>0.9998</td>
<td></td>
<td>0.9982</td>
<td>0.9999</td>
</tr>
<tr>
<td>3$p_0$</td>
<td>0.9938</td>
<td>0.9991</td>
<td>1.0000</td>
<td></td>
<td>0.9997</td>
<td>1.0000</td>
</tr>
<tr>
<td>4$p_0$</td>
<td>0.9983</td>
<td>0.9998</td>
<td>1.0001</td>
<td></td>
<td>0.9999</td>
<td>1.0000</td>
</tr>
<tr>
<td>5$p_0$</td>
<td>0.9994</td>
<td>0.9999</td>
<td>1.0000</td>
<td></td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>6$p_0$</td>
<td>0.9998</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>7$p_0$</td>
<td>0.9999</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>8$p_0$</td>
<td>0.9999</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>9$p_0$</td>
<td>1.0000</td>
<td>1.0000</td>
<td>1.0000</td>
<td></td>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

Based on Table 1, it can be seen that the greater the momentum interval ($p$) the greater the probability. The radial momentum probability distribution describes the radius length of atomic orbitals in a space. The radial momentum probability distribution graph shows the graph of the function $p(p_0)$ as the probability of electron momentum in various orbits. The radial momentum probability distribution graph is presented in the Figure 2. Figure 2 shows a graph of the deviation function $p(p_0)$, which gets higher as the main quantum number increases.
The wave function obtained is the radial wave function where this wave function depends on $n$ (main quantum number) and $l$ (orbital quantum number). The radial wave function states that the existence of an electron is found along the orbital distance of the electron. In order to determine the spatial distribution of electrons, the utilization of the radial wave function and probability value is essential. Based on table 1, the greater the momentum interval ($p$) the greater the probability. The same thing happens to the quantum number ($n$) where the greater the main quantum number, the greater the probability value.

In terms of the state of the azimuth quantum number $l = 0$ at $n = 1$, the value of $p_0$ obtained 0.7122 and a value of $9p_0$ obtained 1.000, at $n = 2$ the value of $p_0$ obtained 0.9298 and a value of $9p_0$ obtained 1.000, at $n = 3$ the value of $p_0$ obtained 0.9759 and a value of $9p_0$ obtained 1.000. In the state of $l = 1$ at $n = 2$ the $p_0$ value is obtained at 0.9784, and the $9p_0$ value is obtained 1.000, at $n = 3$, the $p_0$ value is obtained 0.9907. In the state of $l = 2$ at $n = 3$ the $p_0$ value is obtained at 0.9993, and the $9p_0$ value is obtained as 1.000. From these data, it is evident that the probability value increases as the momentum interval increases. This happens because the momentum interval $p$ is directly proportional to the probability value.

When viewed from the increase in the main quantum number, in the state $l = 0$, the probability value of $p_0$ on $n = 1$ obtained 0.7122, on $n = 2$ obtained 0.9298, and on $n = 3$ obtained 0.9759. Similarly, in the state $l = 1$, the probability value of $p_0$ at $n = 2$ is 0.9784, at $n = 3$ is 0.9907. The data shows an increasing probability value as the quantum number gets bigger. This is due to the difference in orbital shape at each quantum number.

The azimuth quantum number ($l$) delineates the geometric characteristics of multiple orbitals. Large $l$ values have a circular shape and small $l$ values have an elliptical shape. In the deuterium atom, $n = 1$ has 1 orbital with $l = 0$ in the shape of an ellipse, $n = 2$ has 2 orbitals with $l = 0$ in the shape of an ellipse, and $l = 1$ in the shape of a circle, $n = 3$ has 3 orbitals with $l = 0$ in the shape of a flat ellipse, $l = 2$ in the shape of an ellipse, and $l = 3$ in the shape of a circle. So that when combined, $n = 1$ with $l = 0$ is circular, $n = 2$ with $l = 0$ is elliptical, and $n = 3$ with $l = 0$ is flat elliptical (Sugiyono, 2016; Sudiarta, 2019). According to Krane (2012), the more elliptical the orbital shape, the easier the electrons will be found. Because the orbital shape at $n = 3$ is flat elliptical, the probability value has the highest value or it can be stated that electrons will be easily found at more significant quantum numbers.

Based on the simulation results, the probability distribution graph of the radial momentum of the deuterium atom ($\frac{1}{4}H$) shows agreement with the literature. In Figure 2, the deviation graph of the $p(p_0)$ function is shown which is getting higher as the main quantum number increases. As the principal quantum number increases, the probability of locating electrons in momentum space also increases. This result shows the opposite result to the probability in position space as in the research of Saputra, Supriadi, and Prastowo (2019), Utami, Supriadi, and

![Graph of Radial Momentum Probability Distribution](image-url)
Lesmono (2019), and Makmun, Supriadi, and Prihandono (2020), which shows that the greater the main quantum number (n), the smaller the probability value in the position space.

This data is in line with Rioux (2023) who explained that the coordinates of the hydrogen atom illustrate the uncertainty relationship in position and momentum space. Rioux (2023) describes the position-momentum uncertainty relationship on the hydrogen atom as in the following graph.

The graph above shows the opposite form. In position space the greater the main quantum number (n), the probability distribution decreases, while in momentum space the greater the main quantum number (n), the probability distribution increases. The above relationship occurs because position and momentum are two variables that are conjugate (opposite), where the wave function in momentum space is obtained from the inverse of the wave function in position space using the Fourier transform. Thus, the outcomes exhibit a tendency toward being opposite.

In quantum theory, it is also explained that if two variables, such as position and momentum, if measured simultaneously, it is impossible to produce accurate results on both variables. As explained in the Heisenberg uncertainty principle, which states that if measuring particle momentum in the x-axis direction can be done with uncertainty $\Delta p_x$, then to measure the position in the x-axis direction at the same time cannot have an accuracy greater than $\Delta x = \frac{\hbar}{2p_x}$, this accuracy is expressed in Pebralia (2020), that the uncertainty value between the position and momentum operators is defined $\Delta x \Delta p \geq \frac{\hbar}{2}$. So that with increasing momentum, a smaller position uncertainty will be obtained.
Conclusion

Based on the results of this study, it can be concluded that the radial wave function of the deuterium atom ($\psi_d^2$) is influenced by the main quantum number and orbital quantum number. By knowing the radial wave function, it will be easier to find the probability value of electron momentum with electron momentum interval limit $p_0$. The probability value obtained from this study is getting bigger as the electron momentum interval and the main quantum number increase. Similarly, the probability distribution of radial momentum of the deuterium atom ($\psi_d^2$), with the main quantum number getting bigger, the deviation of the probability function of electron momentum in various orbits $p(p_0)$ is getting higher. This data shows the opposite relationship with the probability value in position space. The relationship occurs because the position variables and momentum variables are conjugate.

References