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Expected Value of Helium Ion Electron Momentum in Momentum Space with Primary Quantum Numbers n≤3

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Abstract: The aim is the expected value of helium ions to determine its properties as a heat transmitter to reactors and chirogenic science. This research is non-experimental research using quantum mechanics literature study methods because there are many previous studies that are relevant to this research. Data on the expected value of electron momentum in helium ions is determined based on numerical calculations using the Matlab 2015a program to simplify calculations using ion expectation calculations in momentum. The results obtained are that the electron momentum value in the helium ion can provide an overview of the average momentum value of the helium ion electrons in momentum space. This research data also shows that in momentum space the expected value of electron momentum decreases as the principal quantum number (n) increases. This can be seen when n=1,l =0 then 3p0 = 1.3146, and when n=3,l =0 then 3p0 = 0.5098.

Keywords: Helium Ions ($24He^{+}$); Momentum Expectation; Momentum Space

Introduction

Atoms are objects that cannot be divided or cut (Kholilurrohman et al., 2022). In quantum theory, the Hydrogen atom is an atom that has only one electron in its shell with the Schrodinger equation obtained electron wave function (orbital) and associated energy (Men and Setianto, 2017). Hydrogenic atoms are a class of atoms that have a single electron that moves around the nucleus. One of the ions that have hydrogenic properties is Helium ion (Pratikha et al., 2022). Helium ions are ions derived from the ionization process of Helium atoms (Akhadi, 2011). The loss of one of the electrons from the Helium atom is caused by the Helium atom releasing electrons (Susdarwono, 2021). This ionization process occurs when helium moves at high speed in the solar atmosphere. This event causes the formation of single-electron ions that are hydrogenic (Makmum et al., 2020). The equation on the hydrogen atom also applies to the Helium ion because of its hydrogenic nature. In everyday life Helium is used as a cooling fluid to transmit heat to reactors with very high temperatures (Hafid, 2011). Helium has a low boiling point than other noble gases (Dewita et al., 2011). Therefore, helium is widely used in chirogenic science (Alimah et al., 2016). Where the boiling point is used to get the low temperature needed in lasers that are used to scan bar codes at supermarket checkouts (Chhandak et al., 2017). Helium in liquid form can be applied to chirogenic cooling and is produced commercially for use in semiconductor magnets, namely in Magnetic Resonance Imaging (MRI), Nuclear Magnet Resonance (NMR) (Rillo et al., 2015).

Helium ions have wave functions that can be obtained from solving the Schrodinger equation that applies to hydrogen atoms/ions (Hanafi et al., 2015). Hydrogenic atom/ion wave function in momentum space is divided into two functions (Damayanti et al., 2020), namely radial momentum function (F_(n,l) (p)) (Mehmood et al., 2021) and angular momentum function ($Y(\Theta,\Phi)$) (Sakimoto, 2010). The wave function of Hydrogenic atoms/ions in momentum space is obtained from the transformation of Helium ion wave function in position space using Fourier transform (Hage-Hassan,

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2008). The transformation equation of position space to momentum space in one-dimensional motion can be written as below:

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

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

equation (2) is the equation resulting from the inverse of equation (1). If we suppose as follows:

$$x = r\, sin\theta\, cos\phi \qquad p_x = p\, sin\Theta\, cos\Phi \quad (3)$$
$$y = r\, sin\theta\, sin\phi \qquad p_y = p\, sin\Theta\, sin\Phi \quad (4)$$
$$z = r\, cos\theta \qquad p_z = p\, cos\Theta \quad (5)$$

If it is known that the wave function in position space $\left(\psi_{n,l,m}(r,\theta,\phi)\right)$ that is:

$$\psi_{n,l,m}(r,\theta,\phi) = \frac{(2\gamma)^{l+1}}{(n+l)!} \sqrt{\frac{\gamma(n-l-1)!}{n(n+l)!}}\, e^{-(\gamma r)} r^l [\, L_{n+1}^{2l+1}\, (2\gamma r)] \sqrt{\frac{2l+1}{2} \left(\frac{(l-|m|)!}{(l+|m|)!}\right)} \sqrt{\frac{1}{2\pi}}\, e^{\pm im\phi}\, p_l^m\, cos\theta \quad (6)$$

so that the equation is obtained:

$$\varphi_{(n,l,m)}(p,\Theta,\Phi) = h^{-\frac{3}{2}} \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-\left(i\frac{2\pi}{h} rp(sin\theta sin\Theta coscos\,(\Phi-\phi)\, + cos\theta cos\Theta)\right)} \sqrt{\frac{1}{2\pi}}\, e^{\pm im\phi}\, p_l^m\, cos\theta \sqrt{\frac{2l+1}{2} \left(\frac{(l-|m|)!}{(l+|m|)!}\right)} \frac{(2\gamma)^{l+1}}{(n+l)!} \sqrt{\frac{\gamma(n-l-1)!}{n(n+l)!}}\, e^{-(\gamma r)} r^l [\, L_{n+1}^{2l+1}\, (2\gamma r)]\, r^2 sin\theta\, dr d\theta d\phi \quad (7)$$

(Podolsky dan Pauling, 1929).

As a result of equation (7), the wave function of Hydrogenic atoms/ions in momentum space can be determined as follows:

$$\varphi(p,\Theta,\Phi) = \frac{1}{(2\pi)^{\frac{1}{2}}}\, e^{\pm im\Phi} \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}}\; p_l^m\, cos\, cos\, \Theta\, \frac{\pi\,(i)^l}{(\gamma h)^{\frac{3}{2}}}\, 2^{2l+4}\, l! \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \frac{\zeta^l}{(\zeta^2+1)^{l+2}}\, C_{n-l-1}^{l+1} \left(\frac{\zeta^2-1}{\zeta^2+1}\right) \quad (8)$$

Then substitute the value of $\zeta = \frac{2\pi h}{\gamma h} = \frac{np}{zp_0}$, and $\gamma = \frac{z}{na_0}$ it will be obtained that the radial momentum equation can be written:

$$\varphi(p,\Theta,\Phi) = \frac{1}{(2\pi)^{\frac{1}{2}}}\, e^{\pm im\Phi} \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}}\; p_l^m\, cos\, cos\, \Theta\, \frac{\pi(i)^l a_0^{\frac{3}{2}}}{z^{\frac{3}{2}} h^{\frac{3}{2}}}\, 2^{2l+4}\, l! \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \frac{\frac{n^l p^l}{z^l p_0^l}}{\left(\frac{n^2p^2+z^2p_0^2}{z^2p_0^2}\right)^{l+2}}\, C_{n-l-1}^{l+1} \left(\frac{n^2p^2-z^2p_0^2}{n^2p^2+z^2p_0^2}\right) \quad (9)$$

The equation is an equation that applies to determine the radial wave function in hydrogenic atoms/ions, while according to Bransden and Joachian (1983) it is known that in hydrogen atoms with z = 1, the equation to determine the radial momentum wave function can be written as follows:

$$F_{n,l}(p) = \left(\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} n^2 2^{2l+2}\, l!\; x\, \frac{n^l p^l}{[n^2p^2+1]^{l+2}}\, C_{n-l-1}^{l+1} \left[\frac{n^2p^2-1}{n^2p^2+1}\right] \quad (10)$$

(Bransden & Joachain, 1983).

The above equation is an equation that applies to Hydrogen atoms whose shape has been expressed in atomic units for momentum or has been divided by p_0 (Hey, 1993). Then for other hydrogenic atoms/ions with different z values, such as Helium ions which have a value of z = 2, the following equation is obtained:

$$\varphi(p,\Theta,\Phi) = \frac{1}{(2\pi)^{\frac{1}{2}}}\, e^{\pm im\Phi} \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}}\; p_l^m\, cos\, cos\, \Theta\, \frac{\pi(i)^l a_0^{\frac{3}{2}}}{2\sqrt{2} h^{\frac{3}{2}}}\, 2^{2l+4}\, l! \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \frac{\frac{n^l p^l}{2^l p_0^l}}{\left(\frac{n^2p^2+4p_0^2}{4p_0^2}\right)^{l+2}}\, C_{n-l-1}^{l+1} \left(\frac{n^2p^2-4p_0^2}{n^2p^2+4p_0^2}\right) \quad (11)$$

A wave function is a quantity that contains some information related to particle behavior (Handayani, 2013). However, this information cannot be directly known from the existing wave function, so it requires additional mathematical operations on the wave function. Multiplication between the wave function and its conjugate can obtain information about the probability of particle position in an atom/ion (Kharismawati et al., 2012). From the results of the probability calculation, the average value can be taken to obtain an accurate final value, or in quantum terms is the expectation value. The expectation value can be used to determine the presence of an electron using its wave function (Setianingsih et al., 2017). The expectation value is determined to obtain an average of the results of repeated probability measurements, due to the quantum nature based on the interpretation of possibilities. The expectation value of momentum used for electron motion in three-dimensional space in terms of momentum space can be written with the equation:

$$\langle p \rangle = \int_{-\infty}^{\infty} p^3 |F_{nl}(p)|^2 \, dp \quad (12)$$

The expectation value of momentum can be used in knowing the average momentum value for helium ion electrons in momentum space (Sudiarta, 2019). Calculation of the expected value of electron momentum in helium ions plays an important role in knowing the properties of helium ions. The properties of the helium ion obtained from calculating the expectation value are probability, momentum, and position of the helium ion in momentum space. This property of helium ions functions as a cooling fluid to channel heat to the reactor and is used in chirogenic science which studies materials at very low temperatures (Alimah et al., 2016; Hafid, 2011).

Method

The aim is the expected value of helium ions to determine its properties as a heat transmitter to reactors and chirogenic science. This research is included in non-experimental research by using the literature study method on quantum mechanics because many previous studies have been conducted on quantum mechanics. The initial step that can be done in this research is to prepare the things needed, for example journals and books as reference sources that are in accordance with the research topic, as well as Matlab software to perform numerical calculations. If the initial preparation has been completed, then after that it can develop a simulation tool by utilizing Matlab 2015a software as a second step because to simplify the calculation by using the ion expectation formula in momentum The simulation is prepared by applying Simpson's rule to numerically calculate the expected value of momentum. Simpson's rule is a numerical integration method in the almost numerical form of a definite integral. After the simulation is completed, the simulation results can be compared with the relevant literature. The simulation is able to be used if the results obtained show the validity of the simulation. The flowchart of numerical calculation using Matlab 2015a simulation includes the following:

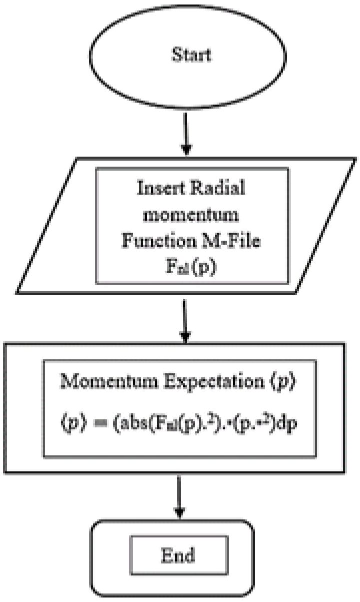

Figure 1. Flowchart of momentum expectation value simulation

Data is taken when the simulation has been validated. In this study, the data obtained is the expected value of Helium ion electron momentum in momentum space with momentum number n≤3. The data obtained is presented in the form of tables and graphs in order to obtain a more detailed picture. Then after the data is taken, the data will be validated with the results of previous studies that are in accordance with this research. This is done to find out whether the data obtained is in accordance with the existing theory or not. Then data analysis and discussion will be carried out in detail if the data is in accordance with the literature. Furthermore, conclusions are drawn from the research data, data analysis, and discussion to answer the problem formulation. In this study there are several studies that are used as references for validation, among others: Supriadi et al (2019) and Pratikha et al (2022).

Result and Discussion

Based on the results of the research, several data were obtained including data on the expected value of the momentum of Helium ion electrons in momentum space with the main quantum number n≤3. The data is expressed in tabular form to facilitate data analysis, as follows:

Tabel 1. Momentum Expectation Research Data

p	n=1	n=2		n=3		(in p0)
	l=0	l=0	l=1	l=0	l=1	l=2
p0	0.1766	0.3395	0.4527	0.3212	0.3151	0.5354
2p0	0.8488	0.4808	0.8546	0.3622	0.4899	0.6217
3p0	1.3146	0.5948	0.8996	0.5098	0.4649	0.6169
4p0	1.5222	0.6374	0.8970	0.4684	0.5766	0.5640
5p0	1.6100	0.7022	0.8737	0.2752	0.7441	0.5461
6p0	1.6468	0.7980	0.8492	0.1857	0.7670	0.6246
7p0	1.6609	0.8716	0.8521	0.2953	0.6128	0.7693
8p0	1.6642	0.8822	0.8952	0.5075	0.3862	0.9102
9p0	1.6629	0.8222	0.9725	0.6729	0.2084	0.9922

Table 1 is the average momentum value for helium ion electrons in momentum space expressed in p_0 where the value of $p_0 = 1.99285\,x\,10^{-24}\,J.s/m$. The momentum interval used ranges between p_0 up to $9p_0$. Based on the results of the above calculations, it is known that in quantum numbers $l = 0$, average momentum value for helium ion electrons in momentum space at quantum number $n = 1$ has the smallest value of $0.1766\,p_0$ which lies in the interval p_0 and its largest expected value is in the interval $9p_0$ which is equal to $1.6629\,p_0$. Meanwhile, in $n = 2$ the smallest expected value lies on the interval p_0 with a value of $0.3395\,p_0$, and $0.8222\,p_0$ is the largest average momentum value for electron ions helium in momentum space at $n = 2$ which is in the interval $9p_0$.

Then, for $n = 3$ has the smallest average value of $0.3212\,p_0$ which is in the interval p_0 and on the interval $9p_0$ is its largest expected value which is equal to $0.6729p_0$. The data shows that the average momentum value for helium ion electrons in momentum space (expectation value) increases as the momentum interval increases. The same is true for the $l = 1$for $n = 2$ as well as on $n = 3$, the expected value will increase when the momentum interval used is larger.

Then, if viewed based on the main quantum number (n) for the same orbital quantum number as in $l = 0$ by reviewing on the interval $9p_0$ electrons have the largest average (expected) value is $1.6629\,p_0$ that are on $n = 1$by $0.8222\,p_0$ for $n = 2$, and the smallest average momentum value that is at$n = 3$ worth$0.6729\,p_0$. As well as for $l = 1$ with the same review on the interval $9p_0$, the largest average value is located at $n = 2$ that is $0.9725\,p_0$ and its smallest expected value is $0.2084\,p_0$ which is located at $n = 3$.

This information shows that the greater the main quantum number (n), the value of the average momentum for helium ion electrons in momentum space will decrease, in other words, the average electron in Helium ions with a review of momentum space will rarely be found at large quantum numbers, and most are found in the position p_0. The momentum expectation value data in the momentum space that has been obtained shows results that are in accordance with the expectation value in the position space. Where in the position space the expectation value will decrease as the main quantum number increases. This is because if the electron is at a large quantum number, the average distance between the electron and the core will be farther (large), and the farther the electron distance to the core, the average momentum value for helium ion electrons in momentum space will be smaller.The expected value of electron momentum depends on the number of intervals ($\boldsymbol{p0}$) and the value of the main quantum number ($\boldsymbol{n}$). The greater the interval, the expectation value of electron momentum increases. While the greater the value of the main quantum number ($\boldsymbol{n}$), the smaller the expected value of electron momentum. The expected value of electron momentum depends on the number of intervals ($\boldsymbol{p0}$) and the value of the main quantum number ($\boldsymbol{n}$). The greater the interval, the expectation value of electron momentum increases. While the greater the value of the main quantum number ($\boldsymbol{n}$), the smaller the expected value of electron momentum (Al Bawani et al., 2023).

Conclusion

Based on the research results that have been obtained, it can be concluded that the expectation of Helium ion electron momentum in momentum space will decrease with increasing main quantum number(n) and will increase with increasing electron momentum interval limit (p_0) which is used. This can be seen when n=1,l =0 then 3p0 = 1.3146, and when n=3,l =0 then 3p0 = 0.5098. This research can be developed by other researchers to find the momentum expectation value for different ions or different principal quantum numbers. Other researchers can also develop this research in the form of looking for the implementation of the expected value of helium ion electron momentum in the development of scientific technology.

Author Contributions

The author's contribution to this research is: Bambang Supriadi played a role in guiding the work on the article. Hana Mardiana and Wendy Indra Kristiawan played a role in creating the method and abstract sections. Diana Kamalia and Ike Kumala Sari played a role in working on the introduction and conclusion. The results and discussion sections were carried out together.

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Conflicts of Interest

The author declares there is no conflict of interest.

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