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The Expectation Value of Electron Momentum of Li^{2+} ion on Principal Quantum Number n ≤ 3 in Momentum Space

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Abstract

Information on electron behavior in a hydrogen atom, such as electron expectation, electron probability, electron position, electron energy spectrum, etc. can be obtained through Schrodinger equation. Li^{2+}ions are Li atoms that lose $2\mathrm{e}$ so that they become hydrogenic atoms. This research aims to determine the expectation value of electron momentum of Li^{2+} ion in momentum space at the main quantum number $\mathrm{n} \leq 3$ using Schrodinger equation approach. The method used in this research is literature study with non-experimental research type. The results obtained expectation value depends on the interval p_0 and the value of the quantum number. The larger the interval, the expectation value of electron momentum increases. While the greater the value of quantum numbers, the expectation value of electron momentum is getting smaller. Based on the analysis, the expectation value of electron momentum is quite varied from $0{,}0713\mathrm{p}_0$ to $2{,}4703\mathrm{p}_0$. From this research, it is found that the expectation value of electron momentum is the same as the expectation value of electron position.

Keywords: Expected value; Lithium ion; Scrodinger equation

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Introduction

By the end of the 19th century, theories of classical physics (theories of mechanics, electromagnetics, and thermodynamics) could not explain physical observations on a microscopic scale (Vilmala, 2020). So that quantum theory was developed by a physicist, Erwin Schrodinger and Werner Heisenberg after observing microscopic objects such as atoms and molecules that have very different behavior from the behavior of macroscopic objects in everyday life (Halim & Herlina, 2020).

Lithium is a chemical element that has atomic number 3. Lithium is a metal element with the smallest atomic size. Lithium has only 3 electrons, meaning that a lithium atom has only two orbital shells with one electron in the outer shell (Sumarno et al., 2012). Lithium can be used as an electronic component (Krebs, 2006). Lithium can be utilized as a raw material for rechargeable battery cathodes (Wigayati & Purawiardi, 2018).

Lithium ions (Li^{2+}) are lithium atoms that are missing two electrons and are therefore positively charged with two. Lithium ions ($\boldsymbol{Li^{2+}}$) are Lithium atoms that have lost 2 electrons, meaning they are particles that have one electron. Lithium ($\boldsymbol{Li^{2+}}$) ions are similar to Hydrogen atoms, but there are differences in their properties and characteristics. Lithium ion ($\boldsymbol{Li^{2+}}$) has 3 number of protons in the ion ($\boldsymbol{Z=3}$). Lithium ions can be utilized as rechargeable batteries that are rechargeable, environmentally friendly, and do not contain hazardous materials (Perdana, 2020). Lithium-ion batteries have several advantages, namely good energy storage stability with power that can last up to 10 years more, have high energy density, no memory effect, and have a relatively lighter mass than other types of batteries (Mossali dkk, 2020).

The electron function in the atom is the solution of the Schrodinger equation in spherical coordinates. The electron wave function in position space is formulated as:

$$\psi_{n,l,m}(r,\theta,\phi) = \left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{(2n)\{(n+1)\}^3}\right]^{\frac{1}{2}} \left[\frac{2Zr}{na_0}\right]^l e^{-\left(\frac{zr}{na_0}\right)} L_{n+1}^{2l+1}\left[\frac{2Zr}{na_0}\right] \sqrt{\frac{2l+1}{2}\left(\frac{l-|m|!}{l+|m|!}\right)} \sqrt{\frac{1}{2\pi}} e^{\pm im\phi} p_l^m cos\theta \quad (1)$$

(Singh, 2009)

If from the above equation, γ=Z/na_0 is given, then equation (1) can be written as:

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

(Podolsky & Pauling, 1929)

The electron wave function in hydrogenic atoms can be expressed in position space as well as in momentum space. The wave function in momentum space can be obtained by performing mathematical calculations using the help of the fourier transform, as follows:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \varphi(p)^{\frac{ipx}{\hbar}} dp \quad (3)$$

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \varphi(x)^{-\frac{ipx}{\hbar}} dx \quad (4)$$

(Yousif et al., 2015)

so, we get the wave function for atoms in momentum space as follows:

$$\varphi = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{\pm im\Phi} \sqrt{\frac{2l+1}{2} \frac{(l-|m|!)}{(l-|m|!)}} p_l^m cos\Theta \frac{\pi(i)^l}{(\gamma h)^{\frac{3}{2}}} 2^{2l+4} l! \left(\frac{n(n-l-1)!}{(n+1)!}\right)^{\frac{1}{2}} \frac{\zeta^l}{(\zeta^2+1)^{l+2}} C_{n-l-1}^{l+1} \left(\frac{\zeta^2-1}{\zeta^2+1}\right) \quad (5)$$

(Podolsky & Pauling, 1929)

The variable separation method is often used in solving the hydrogenic atom Schrodinger equation so that 2 functions are obtained, namely the radial function and the angular function (Supriadi, 2022). The radial function will provide information on the behavior of electrons in a hydrogenic atom, including electron probability, electron expectation, electron energy spectrum, and others. In momentum space, the radial function for hydrogenic atoms is expressed as follows:

$$F_{nl}(p) = \left[\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!}\right]^{\frac{1}{2}} n^2 2^{2l+2} l! \times \frac{n^l p^l}{(n^l p^l+1)^{l+2}} C_{n-l-1}^{l+1} \left(\frac{n^2p^2-1}{n^2p^2+1}\right) \quad (6)$$

(Hey, 1993)

The radial function above cannot provide physical meaning, so there is still no information on electron behavior. Through the help of operators, various information on electron behavior can be obtained, including electron expectation, electron probability, electron position, electron energy spectrum, and others. Furthermore, if the value of $\zeta = \frac{2\pi p}{\gamma h} = \frac{np}{zp_0}$ is known, where p_0 is the momentum of the Bohr orbit electron which has a value of $p_0 = \frac{2\pi\mu e^2}{h}$. Based on this value, the radial function that has been expressed in atomic units for momentum will apply to each hydrogenic atom, so that the wave function can be expressed as follows :

$$F_{n,l} = \frac{2^{2l+4} l! \pi}{\left(\frac{z}{na_0}\right)(h)^{\frac{3}{2}}} \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \frac{\left(\frac{np}{zp_0}\right)^2}{\left[\left(\frac{np}{zp_0}\right)^2+1\right]^{l+2}} \; C_{n-l-1}^{l+1}\left(\frac{\frac{n^2p^2}{z^2p_0^2}-1}{\frac{n^2p^2}{z^2p_0^2}+1}\right) \tag{7}$$

Based on equation (7) for the radial wave function of hydrogenic atoms above, the radial wave function of $\boldsymbol{Li^{2+}}$ ions with $\boldsymbol{Z = 3}$ can be obtained as follows :

$$F_{n,l}(p) = \frac{2^{2l+\frac{5}{2}} 3^{l+\frac{5}{2}}}{\sqrt{\pi}} \; n^2 l! \left(\frac{(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} n^l p^l \times \frac{p_0^{l+\frac{5}{2}}}{[n^2p^2+9p_0^2]^{l+2}} \; C_{n-l-1}^{l+1}\left(\frac{n^2p^2-9p_0^2}{n^2p^2+9p_0^2}\right) \tag{8}$$

Physical quantities in quantum physics are obtained through a probabilistic measurement process (Saputra et al., 2019). Because it is probabilistic, measurements are taken repeatedly. Furthermore, the final value can be obtained through the calculation of the average value of repeated measurements. In the language of quantum physics, the average value is referred to as the expectation value.

In terms of position space, the position of a particle can be determined by finding the electron position expectation value using the wave function by assuming the electron is on the x-axis (Beiser, 1990). Particle wave functions can be used to determine the expected value of a measurement process that contains electron information (Supriadi & Anggraeni, 2022). In addition to position space, expectation values can be viewed in momentum space.

The expectation value of electron momentum in an atom can be interpreted as the average value or how often electrons appear in a momentum space p and p+dp. The expectation value is only found in radial functions because the expectation value does not depend on angular functions. The expectation value of electron momentum in momentum space review can be formulated using the following equation:

$$\langle p \rangle = \int_{a_0}^{xa_0} p^3 \left|F_{(n,l)}\right|^2 dr \tag{9}$$

(Bransden & Joachain, 1983)

Based on the description above, there have been many studies that review the expectation value of electrons for various atoms but in position space. So that in this study aims to determine the expectation value of electron momentum of Li^{2+} ions in the review of momentum space at the main quantum number $n \leq 3$.

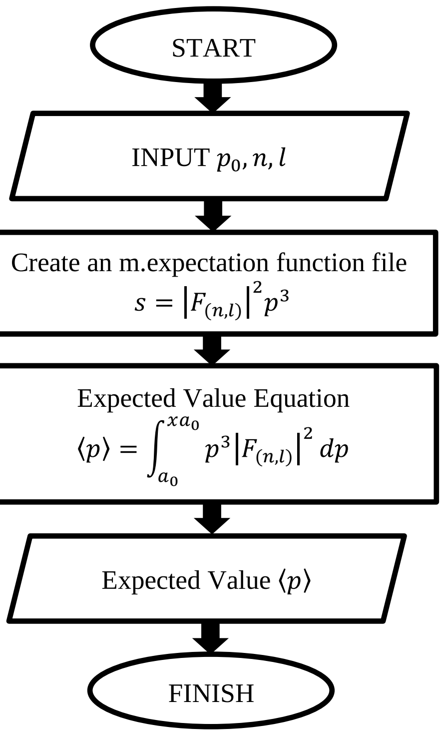
METHODS

This research uses non-experimental research with a literature study approach. The research method consists of the following steps.

1. Preparation

   The preparation stage is used to prepare materials that will be used as supporting references for research. This stage is done by reviewing quantum physics, modern physics, and mathematical physics books as well as articles from national and international journals related to the Schrodinger equation, electron position, expectation value, hydrogenic atoms, and Lithium ions.

2. Theory Development
   At this stage, theory development is carried out from various relevant reference sources related to the application of the Schrodinger equation to determine the expected value of electron momentum of Li^{2+} ions. The theory is developed by examining the wave function, namely the electron function and the expected value of electron momentum of Li^{2+} ions at quantum numbers $n \leq 3$.
3. Simulation
   The simulation stage is a numerical calculation stage to determine the expected value of electron momentum in Li^{2+} ions using Matlab 2021a *software*.
4. Momentum Expectation
   The expected value of electron momentum of Li^{2+} ions is obtained from the wave function.
   The following is a diagram to determine the expectation value of electron momentum.



Gambar 1. *Flowchart* untuk nilai ekspektasi

5. Validation of Theory Development Results
   The validation stage is carried out by comparing the results of the calculation of the expected value of the momentum of Li^{2+} ions in momentum space manually with the results of the calculation of the expected value of the momentum of Li^{2+} ions in momentum space numerically using Matlab 2021a.
6. Results of Theory Development
   At this stage the development results obtained in the form of the expected value of electron momentum of Li^{2+} ions at quantum numbers $n \leq 3$ are presented in table 1.
7. Discussion
   At this stage the development results are discussed in detail, and the numerical simulations that have been carried out will be discussed physically

accompanied by theoretical discussions regarding the expectation value of the electron momentum of Li^{2+} ions at the main quantum number $n \leq 3$.

8. Summary
This stage is the final stage in the form of a summary of the results of the discussion, then conclusions can be drawn to answer the formulation of research problems.

Results And Discussion

Lithium ions are particles that are referred to as single electrons because they have one electron so they are included in hydrogenic atoms. Lithium ions ($\boldsymbol{Li^{2+}}$) are Lithium atoms that have lost 2 electrons, meaning they are particles that have one electron. Lithium ions ($\boldsymbol{Li^{2+}}$) are similar to Hydrogen atoms, but have different properties and characteristics. Lithium atoms are isotopes of Hydrogen atoms and therefore have Hydrogenic properties. Lithium ions ($\boldsymbol{Li^{2+}}$) have 3 number of protons in the ion ($\boldsymbol{Z = 3}$).

The expected value of electron momentum in an atom is the average value of electrons appearing somewhere in momentum space. Based on the results of numerical calculations using the Matlab 2021a program and the equations that have been developed, the results of the expected value of electron momentum of $\boldsymbol{Li^{2+}}$ ions at quantum numbers $\boldsymbol{n \leq 3}$ are shown in table 1 below.

Table 1 Expected value of electron momentum of $\boldsymbol{Li^{2+}}$ ions using Matlab 2021 a simulation

p	$n = 1$	$n = 2$		$n = 3$		
	$l = 0$	$l = 0$	$l = 1$	$l = 0$	$l = 1$	$l = 2$
p_0	0.0713 p_0	0.4432 p_0	0.2355 p_0	0.3288 p_0	0.3873 p_0	0.4657 p_0
$2p_0$	0.5749 p_0	0.5375 p_0	1.0168 p_0	0.4878 p_0	0.6174 p_0	0.9020 p_0
$3p_0$	1.2732 p_0	0.7211 p_0	1.2818 p_0	0.5433 p_0	0.7348 p_0	0.9326 p_0
$4p_0$	1.7940 p_0	0.8537 p_0	1.3414 p_0	0.6898 p_0	0.7085 p_0	0.9347 p_0
$5p_0$	2.1064 p_0	0.9177 p_0	1.3519 p_0	0.7933 p_0	0.7210 p_0	0.9042 p_0
$6p_0$	2.2833 p_0	0.9561 p_0	1.3455 p_0	0.7026 p_0	0.8649 p_0	0.8460 p_0
$7p_0$	2.3829 p_0	1.0131 p_0	1.3246 p_0	0.5082 p_0	1.0460 p_0	0.8133 p_0
$8p_0$	2.4390 p_0	1.0995 p_0	1.2961 p_0	0.3369 p_0	1.1598 p_0	0.8423 p_0
$9p_0$	2.4703 p_0	1.1970 p_0	1.2737 p_0	0.2785 p_0	1.1505 p_0	0.9370 p_0

This study uses quantum numbers $\boldsymbol{n \leq 3}$, so there are 6 combinations of quantum numbers ($\boldsymbol{n, l}$), namely (1,0); (2,0); (2,1); (3,0); (3,1); (3,2) and the limit to find the presence of electrons in momentum space at the interval $\boldsymbol{p_0}$ to $\boldsymbol{9p_0}$. Table 1 above shows the expected value of the electron momentum of $\boldsymbol{Li^{2+}}$ ions at the main quantum number $\boldsymbol{n \leq 3}$ in terms of momentum space expressed in $\boldsymbol{p_0}$ with a value of $\boldsymbol{p_0 = 1.99285 \times 10^{-24} Js/m}$. Based on the table, each large increase in the main quantum number $\boldsymbol{n}$ followed by the addition of azimuth quantum number $\boldsymbol{l}$. The azimuth quantum number $\boldsymbol{l}$ shows the quantum number of an atomic orbital that affects the angular momentum of the orbital and describes the shape of the orbital.

Based on the calculation results in table 1 above, it is known that at the main quantum number $\boldsymbol{n = 1}$ and the azimuth quantum number $\boldsymbol{l = 0}$, the smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum is in the interval $\boldsymbol{p_0}$ with a value of $\boldsymbol{0.0713 p_0}$ and the largest value is in the interval $\boldsymbol{9p_0}$ with a value of $\boldsymbol{2.4703 p_0}$. Then the main quantum number $\boldsymbol{n = 2}$ has two azimuth quantum numbers, namely $\boldsymbol{l = 0}$ and $\boldsymbol{l = 1}$. At $\boldsymbol{l = 0}$ the smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum is in the $\boldsymbol{p_0}$ interval with a value of $\boldsymbol{0.4432\, p_0}$ and the largest value is in the $\boldsymbol{9p_0}$ interval with a value of $\boldsymbol{1.1970\, p_0}$ as well as at $\boldsymbol{l = 1}$, the smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum is in the $\boldsymbol{p_0}$ interval with a value of $\boldsymbol{0.2355\, p_0}$ and the largest value is in the $\mathbf{9\,p_0}$ interval of $\mathbf{1.2737\,p_0}$. Furthermore, for $\boldsymbol{n=3}$ there are three azimuth quantum numbers namely $\boldsymbol{l=0}$, $\boldsymbol{l=1}$, and $\boldsymbol{l=2}$. The smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum obtained at $\boldsymbol{l=0}$ of $\mathbf{0.2785\,p_0}$is in the interval $\mathbf{9p_0}$ and the largest expected value with a value of $\mathbf{0.7933\,p_0}$ in the interval $\mathbf{5p_0}$. For azimuth number $\boldsymbol{l=1}$, the smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum obtained is $\mathbf{0.3873\,p_0}$ at interval $\mathbf{p_0}$ and the largest expected value is $\mathbf{1.1505\,p_0}$ at interval $\mathbf{9p_0}$. Likewise, at $\boldsymbol{l=2}$, the smallest expected value of $\boldsymbol{Li^{2+}}$ ion momentum is in the $\mathbf{p_0}$ interval with a value of $\mathbf{0.4567\,p_0}$ and the largest value is in the $\mathbf{9\,p_0}$ interval of $\mathbf{0.9370p_0}$.

Furthermore, if viewed from the main quantum number $\boldsymbol{n}$ and the same azimuth number $\boldsymbol{l}$ ($\boldsymbol{l=0}$).. At the main quantum number $\boldsymbol{n=1}$, the largest expected value is $\mathbf{2.4703\,p_0}$. Then, at the main quantum number $\boldsymbol{n=2}$, the largest expected value is $\mathbf{1.1970\,p_0}$. At the main quantum number $\boldsymbol{n=3}$, the largest expected value is $\mathbf{0.2785\,p_0}$.

Based on the calculation and analysis results above, it is found that the main quantum number ($\boldsymbol{n}$) affects the expected value of average momentum for lithium ion electrons. the expected value of average momentum for lithium ion electrons will decrease along with the increasing quantum value ($\boldsymbol{n}$), and vice versa. So that it shows if the average electron in lithium ion will rarely be found along with the greater the main quantum number and vice versa, at position $\mathbf{p_0}$ many average electrons in lithium ion are found. This is also in accordance with research conducted by (Pratikha et al., 2022) with a review of lithium ions in position space which shows that the greater the main quantum value, the smaller the expectation value and vice versa. The inverse relationship between the main quantum value and the expectation value is because if the electron is at a large main quantum value, the average distance of the electron to the atomic nucleus will be further away. So that the average momentum value for lihtium ion electrons in momentum space will be smaller.

Conclusion

Based on the results of the above research, the wave function of $\boldsymbol{Li^{2+}}$ ions is obtained through the Schrodinger equation approach. The wave function consists of radial function and angular function. To determine the behavior of electrons in momentum space can be reviewed through radial functions. The expected value of electron momentum depends on the number of intervals ($\mathbf{p_0}$) 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.

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