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The Expectation Value of Electron Position and Energy Spectrum of Lithium Ion (Li^{2+}) on Principal Quantum Number $n \leq 3$

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Abstract: The purpose of this study is to determine the electron's position expectation values and energy spectrum on the Li^{2+} ion on the principal quantum number $n \leq 3$. This research using literature study methods on quantum mechanics. The expectation values of the electron position and the energy spectrum of the Li^{2+} ion uses numerical calculations using the Matlab 2019a program. The steps in this research method include: preparation; theory development; simulation; validation of the results of theory development; results of theory development; discussion and conclusion. The results obtained in this study are the electron's position expectation values and energy of the Lithium ion. The electron's position expectation values indicate the presence of electrons that often appear around the x-axis by relying on the a_0 interval used. The larger the interval, the more constant the electron's position expectation values will be and towards an almost constant value. From the analysis results, the expectation value varies in positions from $0.0001a_0$ to $0.1637a_0$. The electron energy spectrum of the Li^{2+} ion is inversely proportional to the square of the principal quantum number (n), namely $E_1 = -122.4\ eV$; $E_2 = -30.6\ eV$; $E_3 = -13.6\ eV$

Keywords: Lithium Ion; Li^{2+}; Position Expectation; Energy

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Introduction

In the development of quantum physics in the 19th century, Max Planck put forward his ideas about the concept of quantum energy. After that, the concept was continued by Albert Einstein regarding the phenomenon of the photoelectric effect on electromagnetic waves. Niels Bohr developed the Max Planck concept and obtained results on the theory of phenomena on the Hydrogen atom (Zettili, 2009).

Lithium (Li) is a chemical element with the smallest atom of the alkali group. Lithium is the most reactive metal because Lithium's valence electrons are located in the K shell closest to the atomic nucleus. Lithium is the lightest metal with an average atomic weight of 7 and has the lowest density on the periodic table. Lithium atoms have three electrons orbiting around a charged nucleus which is $+3e$ (Krebs, 2006). Lithium can be utilized as one of the most needed resources in modern life. Lithium compounds can be used in ceramic products, pharmaceuticals, glass, aluminum, lubricating oils, battery technology and the nuclear industry (Krebs, 2006). Lithium is also the raw material for the cathode of rechargeable batteries (Wigayati and Purawiardi, 2018). One type of secondary battery that has been widely used is Lithium-ion (Li-ion) (Linden and Reddy., 2002).

A Hydrogenic Atom is an atom that has given up all but one of its electrons. In other words, this atom has one electron as in the Hydrogen atom. Although this system consists of one electron, in reality this system has two particles, namely an atomic nucleus and electrons (Sudiarta, 2019). An example of a hydrogenic atom is Helium which is single ionized ($He^{+}, Z = 2$), double ionized lithium ($Li^{2+}, Z = 3$), three times ionized Beryllium ($Be^{3+}, Z = 4$) and etc. These atoms behave

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like hydrogen in all aspects except the nucleus has a positive charge Ze, where Ze is the atomic number of an atom (Grautreau and Savin, 2005). The Hydrogenic atomic equation uses reduced mass $\mu = \frac{m_e m_p}{m_e + m_p}$.

In 1926, Erwin Schrodinger succeeded in formulating the wave equation to describe the motion of electrons in atoms. The energy and space structure of the orbitals are derived based on calculations using the Schrodinger wave equation (Syukri, 1999). The complete solution of the Schrodinger equation is a combination of the radial wave function and the angular wave function (Krane, 2012). With the radial equation written as:

$$R_{nl}(r) = \left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{(2n)\{(n+l)!\}^3}\right]^{\frac{1}{2}} \left[\frac{2Zr}{na_0}\right]^l e^{-\frac{r}{na_0}} L_{n+1}^{2L+1} \ldots\ldots (1)$$

(Singh, 2009).

The polar equation is written as: (Krane, 2012:204).

$$\Theta_{\mathrm{lm}}(\theta) = \sqrt{\frac{(2l+1)(l-|m|)!}{2(l-|m|)!}} \left[\frac{1}{2^l l!} (1 - \cos^2\theta)^{\frac{|m|}{2}} \frac{d^{l+|m|}}{dcos^{l+|m|}\theta} (\cos^2\theta - 1)^l\right] \ldots\ldots\ldots (2)$$

The azimuth equation is written as: (Sugiyono, 2016).

$$\Phi_{\mathrm{m}}(\phi) = \sqrt{\frac{1}{2\pi}} e \pm^{imp} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots... (3)$$

(Sugiyono, 2016).

The complete solution of the wave function of the hydrogenic atom, especially the Lithium ion, can be written as follows: (Serway, 2005).

$$\psi_{\mathrm{n,l,m_l}}(r,\theta,\phi) = R_{n,l}(r) Y_l^{ml}(\theta,\phi)$$

Or it can be written as:

$$\psi_{\mathrm{n,l,m_l}}(r,\theta,\phi) = R_{n,l}(r)\Theta_{\mathrm{l,m_l}}(\theta)\Phi_{\mathrm{m_l}}(\phi) \ldots\ldots\ldots\ldots (4)$$

The complete solution to the Schrodinger equation is obtained by substituting equations (2.1), (2.2), and (2.3) into equation (2.4).

$$\psi_{\mathrm{n,l,m_l}}(r,\theta,\phi) = \left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{(2n)\{(n+l)!\}^3}\right]^{\frac{1}{2}} \mathrm{e}^{-\frac{\mathrm{Zr}}{\mathrm{na_0}}} \left(\frac{2Zr}{na_0}\right) L_{n+l}^{2l+1}(-1) \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(cos\theta) e^{im\phi} \ldots\ldots\ldots.. (5)$$

The position of electrons in an atom is uncertain (Yusron, et al., 2007). The position of the particle can be determined by finding the electron’s position expectation values using the wave function and assuming the electron is on the x-axis (Beiser, 1990). This average value is usually referred to as the expectation value of x or symbolized by $< \mathrm{x} >$ (Cresser, 2021). The expectation value of the electron motion for three dimensions can be written as:

$$\langle r \rangle = \int_{-\infty}^{\infty} r|\psi|^2 dV$$

with $dV = r^2 sin\theta dr d\theta d\phi$ and $\psi = R(r)\Theta(\theta)\Phi(\phi)$ so that the equation will form:

$$\langle r \rangle = \int_{-\infty}^{\infty} r|R(r)\Theta(\theta)\Phi(\phi)|^2 dV$$

$$= \int_{-\infty}^{\infty} r|R(r)\Theta(\theta)\Phi(\phi)|^2 r^2 sin\theta dr d\theta d\phi$$

$$= \int_{-\infty}^{\infty} r|R(r)^2|r^2 dr \int_0^{2\pi}\int_0^{\pi}|\Theta(\theta)\Phi(\phi)|\, r^2 sin\theta d\theta d\phi$$

$$\langle r \rangle = \int_{-\infty}^{\infty} |R(r)^2| r^3 dr \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (6)$$

(Sugiyono, 2016).

A collection of energy levels is called the energy spectrum of a system (Zettili, 2009). To determine the electron’s position expectation values, it depends on the principal quantum number (n) and the orbital quantum number (l) (Purwanto, 2016).

For hydrogen-like atoms, the electron energy levels are given by the formula:

$$E_n = \frac{(-13{,}6eV)(Z^2)}{n^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

with principal quantum number bilangan $(n) = 1, 2, 3, \ldots$ and $\Delta n = \pm 1$ (Mohammed, et al., 2009).

Method

This study uses a non-experimental method with a literature study. This research method has several steps, including:

Preparation

This stage is the initial stage used to prepare materials that will be used as information or references in supporting research to be studied by collecting books, articles and journals related to the electron’s position expectation values and energy spectrum of Hydrogenic atoms especially on Li^{2+} ion.

Theory Development

In the theory development stage, researchers developed theories from various reference sources regarding the application of the Schrodinger equation to the electron’s position expectation values and energy spectrum for single-electron atoms. The theory developed is a study of the wave function, the electron’s position expectation values shown in the formula (2.6) and the energy spectrum of ions Li^{2+} on principal quantum number $n \leq 3$ shown in the formula (2.7).

Simulation

The simulation stage is a numerical calculation stage to determine the electron’s position expectation values and the energy spectrum of the Lithium ion (Li^{2+}) using Matlab R2019a software.

Position Expectation

The data regarding the electron’s position expectation values of Li^{2+}ion is obtained by using the radial wave function only. The equation used to determine the electron’s position expectation values is shown in equation

The following is a flow chart for the electron's position expectation values

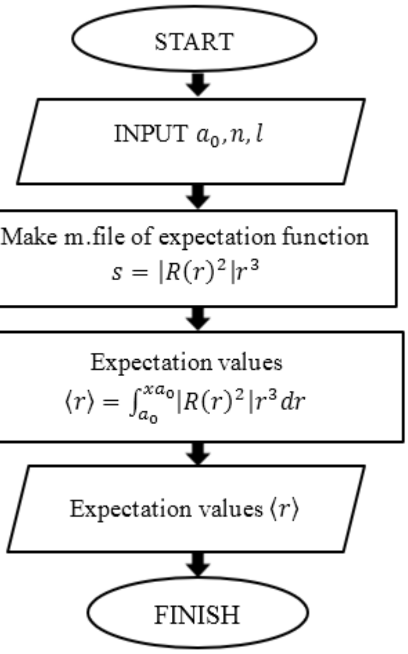

Figure 1: Flowchart for expectation values

Spectrum Energy

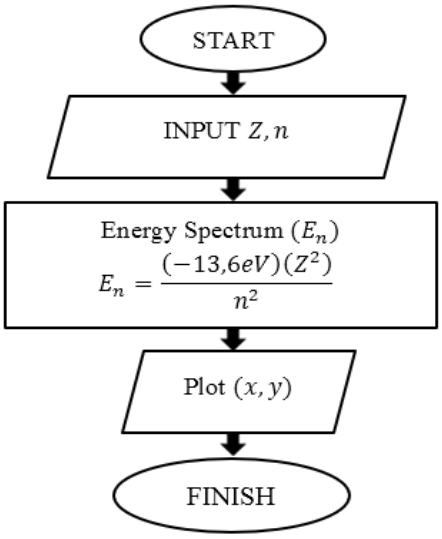

Figure 2: Flowchart for energy spectrum

Validation of Theory Development Results

Validation is done by matching the results of theory development with related research journals and books that are used as references. In this study, the validation material used is electron's position expectation values and energy spectrum. The literature used to validate this research is the electron's position expectation values on the Deuterium atom in the research conducted by Hermanto et al. (2006) and the energy spectrum of the Tritium atom in the research conducted by Wijayanto et al. (2016).

Result of Theory Development

At this stage the researchers obtained the results of the development, namely the electron's position expectation values and the energy spectrum of the Li^{2+}ion on $n \leq 3$ which is presented in the Table 1.

Discussion

At this stage, we will discuss in detail the results of data collection obtained and numerical simulations will be discussed in more depth physically accompanied by a theoretical discussion regarding the electron's position expectation values and the energy spectrum of the Li^{2+} ion on principal quantum number $n \leq 3$.

Summary

This stage is the final stage where the summary contains the answers or results of the discussion. Furthermore, it will be concluded to answer some of the problem formulations in the study.

Result and Discussion

The research conducted has gone through a validation process by validating the electron position expectations against previous studies. The validation results produce an average error value below 0.001 so that the simulation program used is valid.

Lithium ion is a particle that has one electron or single electron. The lithium ion is symbolized as(Li^{2+}) where this ion is formed from a Lithium atom that releases two electrons so that it is positively charged$2+$. The atomic number (Z) of $Li^{2+}$is 3 where Z represents the number of protons in the atomic nucleus. Lithium ion belongs to the hydrogenic atom because this ion has only one electron in the $n = 1$ shell. These electrons orbit the atomic nucleus which consists of the combined number of neutrons and protons. Hydrogenic atoms are similar to Hydrogen in that Hydrogen has one electron orbiting one proton as its atomic nucleus. In addition, Hydrogen is the simplest of atoms or ions with one electron. Wijayanto et al. (2016) stated that the atomic number is inversely proportional to the atomic radius because the greater the number of protons, the smaller the distance between the atomic nucleus and its valence electrons. These results are also in accordance with research by Prastowo et al. (2018) which states that the reduced mass can affect the atomic radius where the number of neutrons in the atomic nucleus and the binding force of the nucleus will be of greater value, followed by a smaller electron orbital radius.

The mass of the nucleus in Lithium ion uses reduced mass where the reduced mass is the combination of the proton mass and the mass of the neuron. In the study of Lithium ions, the approach is used that the atomic nucleus only rotates in its center of mass without any influence by external electrons. By approaching the concept of the central force concept of the electron and nucleus system, the formula for reduced mass is obtained which is written as $= \frac{m_e m_p}{m_e+m_p}$. The result of the calculation of the reduced mass of the Lithium ion is $9{,}1070 \times 10^{-31}$ kg. The value of μ is close to the electron mass, which is $9{,}1095 \times 10^{-31}$ kg or it can be written as $m_{electron} \approx \mu$. The determination of the radius of Lithium ion using Bohr's theoretical approach. The radius of Lithium ion is close to $a_0 = 0{,}01763\, nm$ or $0{,}1763 \times 10^{-10} m$. The Lithium-ion radius indicates the distance between the atomic nucleus and its outermost electrons. When compared with the radius of the Hydrogen atom in the literature, the Hydrogen atomic radius is close to the value of $a_0 = 0{,}0529\, nm$ or $0{,}529 \times 10^{-10}\, m$. The difference between the radius of the Lithium ion and the Hydrogen atom lies in the Z value they have. The Lithium ion has an atomic number of 3 while the Hydrogen atom has an atomic number of 1. This affects the Z value which is owned where $Z\ Li^{2+}$ is 3 times larger than the Hydrogen atom so that the Lithium ion has a smaller radius than the Hydrogen atom. From these results it is concluded that the atomic radius is inversely proportional to the value of the principal quantum number (n).

The following shows the electron's position expectation values of Lithium ion Li^{2+}

Table 1. Result of Electron's Expectation Value of Li^{2+}

r	$n = 1$	$n = 2$		$n = 3$		
	$l = 0$	$l = 0$	$l = 1$	$l = 0$	$l = 1$	$l = 2$
a_0	$0.0157a_0$	$0.0012a_0$	$0.0052a_0$	$0.0004a_0$	$0.0014a_0$	$0.0001a_0$
$2a_0$	$0.0184a_0$	$0.0282a_0$	$0.0342a_0$	$0.0052a_0$	$0.0042a_0$	$0.0066a_0$
$3a_0$	$0.0184a_0$	$0.0599a_0$	$0.0546a_0$	$0.0076a_0$	$0.0112a_0$	$0.0332a_0$
$4a_0$	$0.0186a_0$	$0.0714a_0$	$0.0605a_0$	$0.0346a_0$	$0.0457a_0$	$0.0709a_0$
$5a_0$	$0.0193a_0$	$0.0742a_0$	$0.0617a_0$	$0.0838a_0$	$0.0915a_0$	$0.1010a_0$
$6a_0$	$0.0203a_0$	$0.0749a_0$	$0.0617a_0$	$0.1259a_0$	$0.1250a_0$	$0.1179a_0$
$7a_0$	$0.0213a_0$	$0.0750a_0$	$0.0614a_0$	$0.1496a_0$	$0.1423a_0$	$0.1255a_0$
$8a_0$	$0.0220a_0$	$0.0747a_0$	$0.0610a_0$	$0.1598a_0$	$0.1495a_0$	$0.1285a_0$
$9a_0$	$0.0222a_0$	$0.0740a_0$	$0.0604a_0$	$0.1637a_0$	$0.1525a_0$	$0.1297a_0$

The electron's position expectation values of the electron position indicate the presence of electrons that appear frequently around the x-axis. In this study, the solution of the function uses the time-independent Schrodinger equation. The solution to the radial function depends on the value of the principal quantum number (n) and the angular quantum number (l). In the quantum number $n \leq 3$, this study uses a combination of quantum numbers (n, l) by (1,0), (2,0), (2,1), (3,0), (3,1), and (3,2). Determination of electron's position expectation values using an interval starting from a_0 to $9a_0$.

The electron expectation value shows a more stable value at an increasing a_0 interval. This indicates that more and more electrons will be found at that position. The smaller the electron's position expectation values will be more difficult to find at the larger the quantum number. The electron's position expectation values vary according to its respective n, l states. This value is in accordance with the radial probability density of the Li^{2+} ion in the previous study.

Table 2: Result of energy Spectrum of Li^{2+} ion

Energy Level	n	Energy of Li^{2+} ion	
		eV unit	Joule unit
E_1	1	-122.4	$-195.84\, e \times 10^{-19}$
E_2	2	-30.6	$-48.960\, e \times 10^{-19}$
E_3	3	-13.6	$-21.760\, e \times 10^{-19}$

Hydrogenic atomic energy spectrum is a state of electrons or energy levels possessed by one-electron atoms. Since the (Li^{2+}) ion is a Hydrogenic ion, the electron energy spectrum of the ion (Li^{2+}) uses Bohr's spectrum theory. The negative sign of the energy indicates that there is binding energy due to the attraction in the atomic nucleus. From the table, it is found that the value of the energy spectrum will decrease as the main quantum number increases. The value in the first excited state (E_2) is 4 times the value in the ground state (E_1). While the value of the second excited state (E_3) has a value 9 times greater than the ground state. Previous research has discussed the energy in Hydrogenic atoms. Wijayanto et al. (2016) has researched regarding the wave function and ion energy of Li^{2+} at state $n = 1$ is $122.4\, eV$ which has the same value as table 2 in this research. Supriadi (2019) stated that the higher the excitation level (the longer the particle moves), the less energy it has. In this case, a recombination process occurs, which is the return of the particles to their initial state after experiencing excitation for a while.

To make it easier to understand this electron energy spectrum, a visualization in the form of an energy spectrum graph is needed as Figure 3.

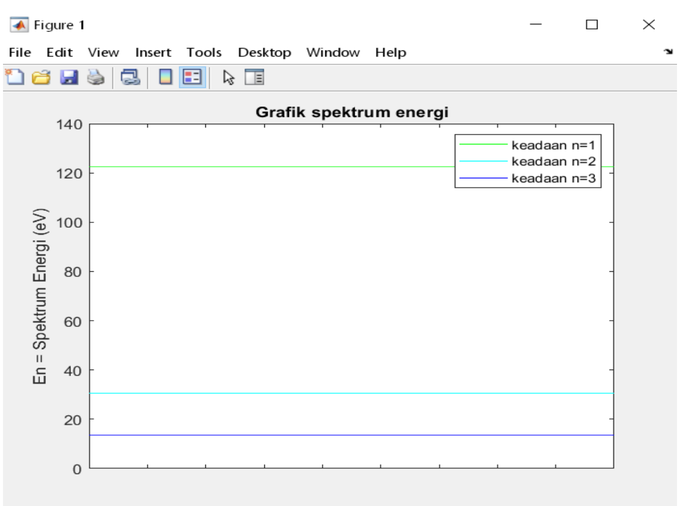

Figure 3: Lithium-ion electron energy spectrum graph

The graph of the electron energy spectrum of the Lithium ion (Li^{2+}) displayed by the program shows the line spectrum so that it is a straight line. Each graph represents the energy in each state. The green line shows the energy of the electron in the ground state ($n = 1$), the light blue line shows the energy of the electron in the first excited state ($n = 2$), and the dark blue line shows the energy of the electron in the second excited state ($n = 3$). The energy spectrum data is displayed in graphical form so that it can be seen that the shape of the spectrum is a line spectrum that expresses the energy levels in each orbital. Energy is plotted vertically with the lowest or bottom state at the bottom and the excited state above it. These energies are discrete. From these results, the value of electron energy at the main quantum number level is getting bigger, the energy is getting smaller.

Conclusion

Based on and discussion, some conclusions are obtained as follows; the electron's position expectation values of the Li^{2+}ion depends on the principal quantum number (n) and its azimuth (l). The larger the interval a_0, it will show a pattern that is close to a constant value in each situation. The electron energy spectrum of the Li^{2+} ion is based on the spectrum of the Hydrogen atom. The value of the energy spectrum is inversely proportional to the square of the principal quantum number where the larger the principal quantum number, the smaller the electron energy.

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