Jurnal Pendidikan Fisika dan Keilmuan (JPFK)
Vol. 10, No. 1., March 2024, pp. 47-55
P-ISSN: 2442-8868, E-ISSN: 2442-904X, DOI: http://doi.org/10.25273/jpfk.v10i1.19715

Spectrum of kinetic energy of electrons of Helium ions in functions Radial Schrodinger waves on quantum numbers (n ≤ 3)

Dellya Natasha [1], Bambang Supriadi [2*], Kevin Cahya Andilla Unwaru[3], Rery Irmawati[4] Friscela Yona Nagifea[5] Naziroh Faiqohtul Herlia[6] Tiara Angelita[7]

[1,2*,3, 4,5,6,7]Department of Physics, Faculty of Education, University of Jember
Jl. Kalimantan Tegalboto No.37, Krajan Timur, Jember Regency 68121, Indonesia

E-mail: [1] natashadellya52@gmail.com, [2*] bambangsupriadi.fkip@unej.ac.id
*** Corresponding Author**

Abstract

The Schrodinger equation is an equation that describes the properties of a wave. The Schrodinger equation is solved using a variable separation method that produces a wave function. The wave function using the variable separation method is divided into 2 parts, namely the radial part and the angular part. The energy spectrum states the energy levels of electrons. Energy spectrum and wave function are related to each other. The energy level in the Schrodinger wave function in the form of kinetic energy is the energy for electrons to move from one point to another. The research aims to describe the kinetic energy spectrum of electrons in the radial wave function. The type of research used is basic research, namely the development of existing theories. The result obtained is a radial wave function with a certain quantum number n and an integrated Laplace constant that can produce electron kinetic energy, namely by integrating the wave function with each quantum number. The kinetic energy has its own value according to the quantum number. Kinetic energy in quantum numbers (n = 1,l = 0, Ek =171.18 eV ; n =2,l = 0, Ek =399.09 eV n =2,l = 1, Ek =152.16 eV n =3,l = 0, Ek =5096.81 eV n =3,l = 1, Ek =81142.43 eV n =3,l = 2, Ek =21.979 eV). The conclusion of this research is that the kinetic energy spectrum of electrons produces a directly proportional relationship to the quantum number n, where the greater the quantum number n, the greater the spectrum or kinetic energy level of the electron.

Keywords: wave function; spectrum; kinetic; electron

How to Cite: Natasha, D., Supriadi, B., Andilla Unwaru, K. C., Irmawati, R., Nagifea, F. Y., Herlia, N. F., & Angelita, T. (2024). Spectrum of kinetic energy of electrons of Helium ions in functions Radial Schrodinger waves on quantum numbers (n ≤ 3). Jurnal Pendidikan Fisika dan Keilmuan (JPFK), 10(1), 47-55. http://doi.org/10.25273/jpfk.v10i1.19715

INTRODUCTION

Quantum physics is a complement to the shortcomings of classical physics. This is evidenced by experiments that cannot be explained in classical physics, namely the photoelectric effect and the Compton effect. Sutarno et al (2017) stated that particles and waves are indistinguishable because they are fundamentally interconnected so that they cannot be explained by classical physical theory. While the photoelectric effect experiment and the Compton effect proved the nature of particle wave dualism which was also reinforced by de Broglie's hypothesis. De Broglie's hypothesis of particle wave dualism explains that particles can act as particles themselves and behave as waves (Yusrizal, 2022). Based on the nature of particle wave dualism, an equation is needed to explain wave behavior information on particles, namely the Schrodinger equation.

Schrödinger's equation is a second-order differential equation that describes quantum states and satisfies 3 principles, namely the law of conservation of energy, the de Broglie hypothesis and behaving well. Schrodinger equations are usually solved by reducing Schrodinger equations to second-order differential equations with special functions (Suparmi et al, 2021). The result of the solution of the Schrödinger equation is called the wave function. The wave function with the variable separation method is divided into 2 parts, namely the radial part and the angular part. The radial function depends on the distance of the electron to the nucleus and the angular function depends on the angle of the electron orbital (Hermanto, 2016). The Schrodinger wave function is commonly used on hydrogenic atoms. One of the Hydrogenic atoms is Helium which when ionized will become Helium ions. Karomah *et al* (2021) stated that in the ionization process there is a release of electrons which produces Helium ions that have single electrons and Hydrogenic properties so that hydrogenic atomic stages can be used to solve the Helium ion Schrodinger equation. In addition to the wave function, through the Schrodinger equation also obtained the relevant energies which are to describe atoms with a number of electrons (Men and Setianto, 2017). The radial wave function with quantum numbers n < 3 is as follows

Table 1. Radial Wave Function Helium Ion quantum number n ≤ 3

n	ℓ	$R_{n\ell}$
1	0	$2\left(\frac{2}{a_0}\right)^{\frac{3}{2}} e^{-\frac{2r}{a_0}}$
2	0	$\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-\frac{r}{a_0}}\left(2-\frac{2r}{a_0}\right)$
	1	$\frac{1}{\sqrt{3}(a_0)^{\frac{3}{2}}} e^{-\left(\frac{r}{a_0}\right)} \left(\frac{2r}{a_0}\right)$
3	0	$\frac{8}{\sqrt{2}(3a_0)^{\frac{3}{2}}} e^{-\left(\frac{2r}{3a_0}\right)}\left(1-\frac{4r}{3a_0}+\frac{8r^2}{27{a_0}^2}\right)$
	1	$\frac{2\sqrt{2}}{9}\left(\frac{2}{3a_0}\right)^{3/2}\left(\frac{4r}{a_0}-\frac{4r^2}{3{a_0}^2}\right) e^{-\left(\frac{2r}{3a}\right)}$
	2	$\frac{4}{27\sqrt{10}}\left(\frac{2}{3a_0}\right)^{3/2} e^{-\frac{2r}{3a_0}}\left(\frac{4r^2}{{a_0}^2}\right)$

The energy in the Schrodinger wave function of the Helium ion is potential energy and kinetic energy. Klauder (2020) states the equation of observable kinetic energy operators is the dynamic variables of a system that can be measured experimentally (e.g., position, momentum and kinetic energy). In systems governed by classical mechanics these are real-valued functions (never complex), but in quantum physics, each observable is represented by an independent operator used to derive physical information about the observable from the wave function. It is a general principle of quantum mechanics that there is an operator for every observable physical. For the observable represented in classical physics by the function Q(x,p), the corresponding operator is Q $(\hat{x},\hat{p})$. Classical dynamic variables, such as x and p are represented in quantum mechanics by linear operators acting on wave functions. The operator for the position of a particle in three dimensions is simply the set of x, y, and z coordinates, written as vectors r

$$\overline{r} = (x, y, z) = \vec{x}i + \overrightarrow{yj} + \overrightarrow{zk} \tag{1}$$

The operator for the linear momentum component is

$$\hat{p}\mathrm{x} = -\,\mathrm{i}\hbar\frac{\partial}{\partial \mathrm{x}} \tag{2}$$

and the operators for kinetic energy in three dimensions are

$$\hat{p} = -i\hbar\nabla \tag{3}$$

$$\hat{T} = \left(-\frac{\hbar^2}{2m}\right)\nabla^2 \tag{4}$$

In the wave function, kinetic energy forms a level based on quantum numbers. This level of kinetic energy can be called the energy spectrum.

The energy spectrum expresses the level of energy in an electron. The energy spectrum and wave function are related to each other. Suparni (2019) states that electrons orbit the nucleus in a spherical shell, so that the wave function and energy spectrum of electrons can be determined where to get the spectrum or energy level it is necessary to determine the wave function. Every particle in motion has kinetic energy. Preskill (2022) states that the kinetic energy level in the Schrodinger wave function shows observable motion as the movement of a subatomic particle in the wave function. The level of kinetic energy itself depends on quantum numbers. Morisson (2010) states that the energy spectrum in a hydrogen atom can be determined by giving the quantum number n in the Schrodinger wave function. Quantum numbers are important in the wave function and energy spectrum. A quantum number is an integer that symbolizes the discrete value of an important quantity in an atom (Sani and Kadri, 2019). Based on research conducted by Syaifudin et al (2015) it can be seen that the relationship between kinetic energy and quantum numbers is directly proportional, which if the energy in the particle will increase along with the greater the quantum number.

There have been several studies on the energy spectrum of the Schrodiner wave function with quantum number n, especially on the total energy or basic energy of the wave function. One of them is previous research conducted by Makmun et al (2020) regarding solving the hydrogenic atom problem with the Schrodinger equation. The study said that the solution in the form of a wave function can be obtained using the Scrhodinger equation in coordinates using the variable separation method in the steady state. The result of this study is to find radial wave functions and radial probability simulations. Sunarmi (2022) states that the solution of the Schrodinger equation of a particle system can provide information on the characteristics of the particle. The solution of the Schrödinger equation can give the wave equation and the energy equation of the particle. The energy equation of particles is obtained on the basis of the Schrodinger equation of the radial section. Based on this previous research, this research was made to develop a theory about the wave function that already exists. The purpose of this study was to determine the kinetic energy spectrum of Helium ion Schrodinger wave function electrons with quantum numbers $n \leq 3$.

METHODS

This research is an analytical descriptive quantitative research to obtain the energy level or energy spectrum of the Helium ion radial wave function with quantum numbers n $\leq$ 3. The kinetic energy expectation equation can be written as follows,

$$< K > = \int R_{nl} \left(\frac{p^2}{2m}\right) R_{nl}\, dV \quad (5)$$

By turning into a ball coordinate and giving definitions $p = -i\hbar\nabla$ then equation (1.1) becomes

$$< K > = \frac{1}{2m} \int R_{nl} (-i\hbar\nabla)^2 R_{nl}\, 4\pi r^2 dr \quad (6)$$

In determining a kinetic energy value of electrons expressed by an integral equation, a limit is given where the limit used is 0 to ∞ So that the kinetic energy expectation equation can be written

$$< K > = \frac{1}{2m} \int_0^\infty R_{nl} (-i\hbar\nabla)^2 R_{nl}\ \ 4\pi r^2 dr \quad (7)$$

∇^2 is a Laplace operator, because the wave function used is radial part, the Laplace operator is taken radial part only, namely

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}\right) \quad (8)$$

With the Laplace operator the equation (1.3) can be written

$$< K > = -\frac{\pi\hbar^2}{2m} \int_0^\infty R_{nl} \left(\frac{d^2}{dr^2} + \frac{2}{R}\frac{d}{dr}\right) R_{nl}\, r^2 dr \quad (9)$$

The radial wave function contains an exponential part so that the solution of the exponential integral then uses the equation

$$\int_0^\infty x e^{ax} dx = \frac{e^{ax}}{a^2}(ax - 1) \quad (10)$$

And for degree two

$$\int_0^\infty x^2 e^{ax} dx = \frac{1}{a} x^n e^{ax} - \frac{n}{a}\left(\frac{e^{ax}}{a^2}(ax - 1)\right) \quad (11)$$

Likewise for the next degree.

After solving the integral, to obtain the value of kinetic energy operate the values of variables such as

$m = 9{,}1 \times 10^{-31}\ \ kg; \propto = 2{,}307 \times 10^{-28}; \hbar = 1{,}054 \times 10^{-34}\ J.s; \pi = 3{,}14$.

In addition, this study also used the method of studying literature from several articles. The main article used is two articles where the article Supriadi et al (2023) which corresponds to the wave function of the radial part with n $\leq$ 3, then uses the article Klauder (2020) which corresponds to the kinetic electron energy equation of the radial wave function. In addition, to validate using quantum physics books written by Supriadi et al and Krane et al (2013).

RESULTS AND DISCUSSION

The spectrum is the collection of all possible waves and frequencies of electromagnetic radiation. The spectrum and allowable energy level of a particle in the three-dimensional region depend on the price of the main quantum number of the particle, so the energy value E for the particle has certain values and must be discrete (Kharismawati et al, 2017). The Energy Level and the principal quantum number "n" indicate the energy level or electron shell in an atom. Electrons at the same energy level have the same average distance from the nucleus, and electrons at higher energy levels have a greater distance from the nucleus. The energy spectrum can be said by the energy level of a particle. The form of energy is various such as electron kinetic energy and electron potential energy.

Electron potential energy is an electron's energy to move from one point to another. While kinetic energy is the energy of electrons to move from one point to another. The kinetic energy of an electron can be determined by the integral of the wave function with a certain principal quantum number shown in equation 1.5 with a limit of 0 to ∞ For example in the wave function n = 1 then,

(i) Wave function $R_{10} = 2\left(\frac{2}{a_0}\right)^{\frac{3}{2}} e^{-\left(\frac{2r}{a_0}\right)}$

(ii) Kinetic energy $< K > = -\frac{\pi\hbar^2}{2m}\int_0^\infty R_{nl}\left(\frac{d^2}{dr^2}+\frac{2}{R}\frac{d}{dr}\right)R_{nl}\, r^2\, dr$

(iii) The substitution of the wave function in kinetic energy is

$$< K > = -\frac{\pi\hbar^2}{2m}\int_0^\infty 2\left(\frac{2}{a_0}\right)^{\frac{3}{2}} e^{-\left(\frac{2r}{a_0}\right)}\left(\frac{d^2}{dr^2}+\frac{2}{R}\frac{d}{dr}\right)2\left(\frac{2}{a_0}\right)^{\frac{3}{2}} e^{-\left(\frac{2r}{a_0}\right)} r^2 dr$$

$$< K > = -\frac{2^8\pi\hbar^2}{m{a_0}^5}\int_0^\infty e^{-\left(\frac{4r}{a_0}\right)} r^2 dr + \frac{2^6\pi\hbar^2}{m{a_0}^4}\int_0^\infty e^{-\left(\frac{4r}{a_0}\right)} r\, dr$$

(iv) Taking into account the integral properties of equations (1.6) and (1.7), then,

$$\int_0^\infty e^{-\left(\frac{4r}{a_0}\right)} r\, dr = \left[\frac{e^{-\left(\frac{4r}{a_0}\right)}}{\left(-\frac{4r}{a_0}\right)^2}\left(-\frac{4r}{a_0}-1\right)\right]_0^\infty = \frac{{a_0}^2}{16}$$

$$\int_0^\infty e^{-\left(\frac{4r}{a_0}\right)} r^2 dr = \left[-\frac{a_0}{4} r^2 e^{-\left(\frac{4r}{a_0}\right)} - \frac{2}{-\frac{4r}{a_0}}\left(\frac{e^{-\left(\frac{4r}{a_0}\right)}}{\left(-\frac{4r}{a_0}\right)^2}\left(-\frac{4r}{a_0}-1\right)\right)\right]_0^\infty = \frac{{a_0}^3}{32}$$

(v) Substitution of the result of step (iv) in the equation ()

$$< K > = -\frac{2^8\pi\hbar^2}{m{a_0}^5}\left(\frac{{a_0}^3}{32}\right) + \frac{2^6\pi\hbar^2}{m{a_0}^4}\left(\frac{{a_0}^2}{16}\right)$$

$$< K > = -\frac{2\pi\hbar^2}{m{a_0}^2}$$

(vi) By providing the value of the permanence contained in the integral result, namely:
$m = 9{,}1 \times 10^{-31}, \propto = 2{,}307 \times 10^{-28}, \hbar = 1{,}054 \times 10^{-34}\, Js, \pi = 3{,}14$
then the kinetic energy of an electron with the quantum number n = 1 is
$< K > = -171{,}18\ eV$.

The negative sign (-) in the expectation of kinetic energy does not indicate in the physical sense. Kinetic energy expectation is a mathematical quantity that provides information about the average measurement result of a particular observation in a given quantum state. The expectation value of an observation in quantum mechanics can be positive, negative, or zero, depending on the quantum state and the particular observation under consideration (Julian et al, 2020).

The quantum number n = 2 and so on is determined in the same steps, then kinetic energy is obtained with quantum numbers n ≤ 3 in the radial wave function of the Helium ion as follows.

Table 2. Kinetic Energy Radial wave function

n	*l*	E_k
1	0	171.18 eV
2	0	399.09 eV
	1	152.16 eV
3	0	5096.81 eV
	1	81142.43 eV
	2	21.979 eV

The kinetic energy of electrons in radial wave functions in quantum numbers (n ≤ 3) with quantum numbers n = 1 at *l* = 0 has a kinetic energy of 171.18 eV, quantum numbers n = 2 have a kinetic energy of 399.09 eV and quantum numbers n = 3 have a kinetic energy of 5095.3 eV. While at *l* = 1 has a kinetic energy of 152.16 eV at quantum number 2 and has a kinetic energy of 811402.43 eV at quantum number 3 and at *l* = 2 has a kinetic energy of 21.979 eV. In the results of the data there are different quantum orbital (*l*) numbers. At the time n = 1 only *l* = 0 is used. If n = 2 exists *l* = 0 and *l* = 1. Meanwhile, the result obtained on the kinetic energy graph of the following wave function is only I = 0, because *l* acts as a control variable. However, when viewed from the value of *l* = 1 on each value of n, it can be seen that the results obtained are also directly proportional. At the time n = 2, *l* = 1 obtained a kinetic energy result of 152.16 eV and at the time n = 2, *l* = 1 obtained a kinetic energy result of 81142.43 eV. The kinetic energy of the electron wave function can be illustrated with the following graph,

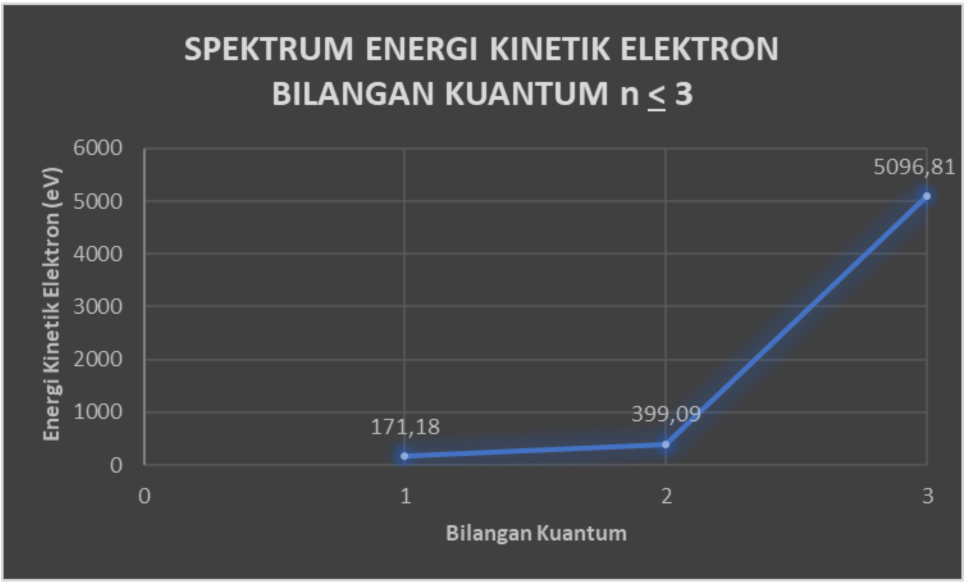

Figure 1. Electron Kinetic Energy Spectrum Helium ion wave function

The graph shows that the kinetic energy spectrum of electrons in radial wave functions with quantum say n ≤ 3. In the graph, the vertical part is kinetic energy and the horizontal part is a quantum number. The quantum number used in this graph is the principal quantum number (n) with the orbital quantum number (*l*). The quantum number (n) and the orbital quantum number (*l*) are used because the wave function used is the radial Schrodinger wave function. The graph shows that the principal quantum number (n) is directly proportional to the kinetic energy of the electron where the greater the quantum number n, the greater the kinetic energy of the electron. This is in accordance with the theory where energy increases with "n": As the principal quantum number "n" increases, the energy level of electrons also increases. Electrons at higher energy levels have higher energy states and are located farther from the nucleus. This means they are less tightly bound to the nucleus of an atom. These results are in accordance with the results contained in Klauder's article (2020) and Krane's book (2013) that energy spectra have a relationship that is directly proportional to quantum numbers.

CONCLUSION

The radial wave function is obtained by substituting the quantum numbers n and l so that a wave function with a certain quantum number n is obtained. A radial wave function with a specific quantum number n and an integral Laplace constant can produce the kinetic energy of an electron with a wave function integral with each quantum number. Kinetic energy at quantum numbers (n = 1.l = 0, Ek = 171.18 eV ; n =2.l = 0, Ek =399.09 eV n =2.l = 1, Ek = 152.16 eV n =3.l = 0, Ek =5096.81 eV n =3.l = 1, Ek =81142.43 eV n =3.l = 2, Ek = 21.979 eV). The kinetic energy spectrum of electrons produces a relationship directly proportional to the quantum number n where the greater the quantum number n, the greater the spectrum or level of kinetic energy of the electron.

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