The function of the radial wave of a hydrogen atom in the principal quantum numbers \((n)\) 4 and 5

B Supriadi, A Harijanto, M Maulana, Z R Ridlo, W D Wisesa and A Nurdiniaya
1Departement Physics Education, University of Jember, Jember, Indonesia

Email: bambangsscmsgc@gmail.com

Abstract. The simplest atom consisting of a proton and an electron is a hydrogen atom. The energy level and the probability of finding an electron in a hydrogen atom can be determined based on the function of radial wave. The function of radial wave of a hydrogen atom is influenced by the principal quantum number \((n)\) and the orbital quantum number \((\ell)\). Completion of the function of radial wave of a hydrogen atom in the principal quantum numbers \((n)\) 4 and 5 uses the time-independent Schrödinger equation approach in spherical coordinates, variable separation method and uses the associated Laguerre function. The normalized of the function of radial wave of hydrogen atom \(R_n(\rho)\) at \(n = 4\) produces four wave functions: \(R_{40}(\rho)\); \(R_{41}(\rho)\); \(R_{42}(\rho)\); \(R_{43}(\rho)\), whereas at \(n = 5\) produces five wave functions: \(R_{50}(\rho)\); \(R_{51}(\rho)\); \(R_{52}(\rho)\); \(R_{53}(\rho)\); \(R_{54}(\rho)\). The results of this research in the form of the functions of radial wave of hydrogen atom can be used to determine the behavior of electron in a hydrogen atom.

1. Introduction
In 1924 by considering the nature of symmetry from nature, de Broglie hypothesized that if a wave could be particle, then the particle should also be a wave. Each particle having mass \((m)\) and moving at the rate \((v)\) can behave as a wave with a de Broglie wave length \(\lambda = \frac{\hbar}{mv} = \frac{\hbar}{p}\) [1]. De Broglie’s hypothesis of the dualism of particle waves is the basis for the emergence of quantum mechanics [2].

The wave properties of particles in quantum mechanics can be explained by the Schrödinger equation [3]. Schrödinger’s equation is a second-order differential equation that adheres to de Broglie’s hypothesis and energy conservation law [4]. Based on the characteristics of the Schrödinger equation, it is divided into time-dependent Schrödinger equations and time-free Schrödinger equations (steady). The Schrödinger equation which is only influenced by potential \((V)\) and position \((r)\) is a steady Schrödinger equation [5]. Schrödinger’s equation is very useful in solving problem in microscopic systems such as atoms [6]. The solution to the Schrödinger equation is called the Schrödinger function which has a linear, single and finity property [7].

According to Bohr, electron charged negatively \((-e)\) in a hydrogen atom orbit in certain orbital and circulate positively charged proton \((+e)\). Electron orbits are circular with certain radius [8]. Often atoms are considered symmetry with spheres, so the Schrödinger equation for hydrogen atoms is expressed in spherical coordinates \((r, \theta, \phi)\) and can be separated into radial equations that only depend on distance \((r)\) and angular equation which depend on angle \((\theta, \phi)\) using variable separation method [9,10]. Variable separation method can make it easier to solve differential equations that depend on two or more variables such as the Schrödinger equation for hydrogen atom.

The radial equation of a hydrogen atom is a wave equation that propagates spread from the centre of the atom to all directions and depends on the distance \((r)\). The solution of the radial equation of
hydrogen atom is a normalized wave function and containing a quantum number which states a three-
dimensional region with the greatest chance of finding an electron in a hydrogen atom [11]. Then to
obtain the function of radial wave of a hydrogen atom is to use a special function in the form of
associated Laguerre polynomials [12]. The complete solution of the function of radial wave of the
hydrogen atom obtained can be useful for determining the energy level and the probability of finding
electron in a hydrogen atom [13,14,15].

2. Method
In this research, the steady Schrödinger equation approach is used in spherical coordinates because the
potential energy of particles in many situations does not depend on time but only depends on the
position of electrons in the atom. The steady Schrödinger equations in spherical coordinates are given by:

$$-\frac{\hbar^2}{2m} \frac{1}{r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \psi(r, \theta, \phi) + [V(r) - E] \psi(r, \theta, \phi) = 0 \quad (1)$$

The effective technique used in solving the types of differential equations above are variable
separation method[16]. In using variable separation method, we assume the solution of the wave
function $\psi(r, \theta, \phi)$ as a linear combination of functions that depend on radius $(r)$ and function that
depend on angle $(\theta, \phi)$ as follows

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \quad (2)$$

Substituting equation (2) into equation (1) will be obtained

$$\frac{1}{R(r)} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2m r^2}{\hbar^2} [E - V(r)] \frac{1}{Y(\theta, \phi)} \sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} = 0 \quad (3)$$

The equation (3) is divided into two terms, namely the first term depends only the radius $(r)$ and
the second term depends on the angle $(\theta, \phi)$. If the separating constant is chosen $\ell(\ell + 1)$, then equation
(3) can be divided into terms which only depend on radius $(r)$

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

And the term that depends on angle $(\theta, \phi)$

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

We can name a tribe that only depend on radius $(r)$ in equation (4) as radial equation. Then by defining the following new variable

$$U(r) = r R(r) \quad (6)$$

We will get the radial equation in the form

$$-\frac{\hbar^2}{2m} \frac{d^2 U(r)}{d r^2} + \left[ V(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] U(r) = E U(r) \quad (7)$$

Looking at equation (7), we can write the radial equation of the hydrogen atom as follows

$$-\frac{\hbar^2}{2\mu} \frac{d^2 U(r)}{d r^2} + \left[ -\frac{1}{4\pi \varepsilon_0 \varepsilon r^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu} \right] U(r) = E U(r) \quad (8)$$

We can also see that the radial equation of the hydrogen atom is identical to the Schrodinger equation
in one dimension, where $(\mu)$ is the reduced mass of the proton $(m_p)$ and an electron $(m_e)$ in the
hydrogen atom is given by

$$\mu = \frac{m_p m_e}{m_p + m_e} \quad (9)$$

Whereas its potential energy is called effective potential energy is given by

$$V_{eff} = -\frac{1}{4\pi \varepsilon_0 \varepsilon r^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu} \quad (10)$$
The first term is the potential energy for the force of interaction between proton and electron where electron in orbit tend to be attracted to near proton, while the second term can be termed as a centrifugal part which causes electron in orbit to tend to be thrown out away from proton [8]. So that physically, the potential energy effectively presents the movement of electron orbiting proton to remain balance don the trajectory.

The function of radial wave of a hydrogen atom as a solution to the radial equation of a hydrogen atom is given by

\[ R_n\ell(r) = \frac{1}{r} U_n\ell(r) = N_n\ell \left( \frac{2r}{na_B} \right)^\ell L_{n+1}^{2\ell+1} \left( \frac{2r}{na_B} \right) \exp\left( -\frac{r}{na_B} \right) \]  \hspace{1cm} (11)

\[ N_n\ell = - \left( \frac{2}{na_B} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \]  \hspace{1cm} (12)

Where the normalization constant is \( N_n\ell \). Normalization of the function of radial wave is intended so that the presence of electron in a hydrogen atom can really be found.

To obtain the function of radial wave of a hydrogen atom, we need to be associated Laguerre polynomial \( L_k^\ell (r) \) which is a derivative of \( \mathcal{W} \) of the Laguerre polynomial \( L_k(r) \) given by

\[ L_k^\ell (r) = \frac{d^\ell}{dr^\ell} L_k(r) \]  \hspace{1cm} (13)

and

\[ L_k(r) = \left[ \exp(r) \right]^{\ell} \frac{d^k}{dr^k} \left[ r^k \exp(-r) \right] \]  \hspace{1cm} (14)

3. Result and Discussion

The function of radial wave of a hydrogen atom expresses the movement of electron in a hydrogen atom which propagates spread from the centre of the atom towards all directions and depends on the distance \( r \) of origin. The function of radial wave of a hydrogen atom contains the principal quantum number \( n \) and the orbital quantum number \( \ell \). The principal quantum number \( n \) represents the energy level of the orbitals of the electron, while the orbital quantum number \( \ell \) determines the orbital form of the electron. Where the price of the principal quantum number allowed is \( n = \ell + 1, \ell + 2, \ell + 3, ... \), while the price of the orbital quantum number allowed is \( \ell = 0, 1, 2, ... n - 1 \). So that the function of radial wave normalized of a hydrogen atom in the principal quantum number \( n \) 4 and 5 is as follows

| \( n \) | \( \ell \) | \( R_{n\ell}(r) \) |
|---|---|---|
| 4 | 0 | \( R_{40}(r) = \frac{16}{(16a_B)^{3/2}} \left[ 1 - 12 \left( \frac{r}{16a_B} \right) + 32 \left( \frac{r^2}{16a_B^2} \right) - \frac{64}{3} \left( \frac{r^3}{16a_B^3} \right) \right] \exp\left( -\frac{4r}{16a_B} \right) \) |
| 4 | 1 | \( R_{41}(r) = -\frac{64\sqrt{15}}{3(16a_B)^{3/2}} \left[ \frac{r}{16a_B} - 4 \left( \frac{r^2}{16a_B^2} \right) + \frac{16}{5} \left( \frac{r^3}{16a_B^3} \right) \right] \exp\left( -\frac{4r}{16a_B} \right) \) |
| 5 | 2 | \( R_{52}(r) = \frac{256\sqrt{5}}{15(16a_B)^{3/2}} \left[ 3 \left( \frac{r^2}{16a_B^2} \right) - 4 \left( \frac{r^3}{16a_B^3} \right) \right] \exp\left( -\frac{4r}{16a_B} \right) \) |
| 5 | 3 | \( R_{53}(r) = \frac{1024\sqrt{35}}{105(16a_B)^{3/2}} \left[ \frac{r^3}{16a_B^3} \right] \exp\left( -\frac{4r}{16a_B} \right) \) |
| 5 | 0 | \( R_{50}(r) = \frac{10\sqrt{5}}{(25a_B)^{3/2}} \left[ 1 - 20 \left( \frac{r}{25a_B} \right) + 100 \left( \frac{r^2}{25a_B^2} \right) - \frac{500}{3} \left( \frac{r^3}{25a_B^3} \right) \right] + \frac{250}{3} \left( \frac{r^4}{25a_B^4} \right) \exp\left( -\frac{5r}{25a_B} \right) \) |

Table 1. Result of the function of radial wave of a hydrogen atom for \( n \) 4 and 5.
In determining the function of radial wave normalized of a hydrogen atom, we find the equation of the Bohr radius \((a_B)\) and the value is \(a_B = 0.5294541195 \times 10^{-10}\) m[15]. Based on the results table, there are four different forms of the function of radial wave in the principal quantum number \(n = 4\) and also obtained five different forms of the function of radial wave in the principal quantum number \(n = 5\). To interpret each of the forms of the function of radial wave obtained is to display it in graphical form. The following is a graph of the function of radial wave for the value of the principal quantum numbers \((n)\) 4 and 5 and the possible orbital quantum number \((l)\), where in the ordinate section the position of the electron is at the distance \((r)\) of the atomic center with interval of intervals of up to thirty and expressed in units of \(a_B\), while in the abscis section states the price of the function of radial wave of a hydrogen atom in units of Amstrong (Å).

\[
\begin{align*}
1 \quad R_{51}(r) &= \frac{50\sqrt{30}}{9(25a_B)^{3/2}} \left[ 6 \left( \frac{r}{25a_B} \right)^2 - 45 \left( \frac{r^2}{25a_B^2} \right) + 90 \left( \frac{r^3}{25a_B^3} \right) 
- 50 \left( \frac{r^4}{25a_B^4} \right) \right] \exp \left( -\frac{5r}{25a_B} \right) \\
2 \quad R_{52}(r) &= \frac{50\sqrt{70}}{21(25a_B)^{3/2}} \left[ 21 \left( \frac{r^2}{25a_B^2} \right) - 70 \left( \frac{r^3}{25a_B^3} \right) + 50 \left( \frac{r^4}{25a_B^4} \right) \right] \exp \left( -\frac{5r}{25a_B} \right) \\
3 \quad R_{53}(r) &= \frac{250\sqrt{70}}{21(25a_B)^{3/2}} \left[ 4 \left( \frac{r^2}{25a_B^2} \right) - 5 \left( \frac{r^3}{25a_B^3} \right) - 5 \left( \frac{r^4}{25a_B^4} \right) \right] \exp \left( -\frac{5r}{25a_B} \right) \\
4 \quad R_{54}(r) &= \frac{1250\sqrt{70}}{63(25a_B)^{3/2}} \left[ \frac{r^4}{25a_B^4} \right] \exp \left( -\frac{5r}{25a_B} \right)
\end{align*}
\]

**Figure 1.** The function of radial wave \(R_{n\ell}(r)\) graph for the principal quantum number \((n)\) 4.
Based on the graph of the function of radial wave at the principal quantum number $n = 4$ obtained, it can be seen that there are four different waveforms depending on the value of the orbital quantum number of $(l)$ and the maximum deviation or amplitude smaller if the quantum number $(l)$ increases. Where at the condition $n = 4$ and $l = 0$ the maximum deviation value is 0.2500 Å, while the minimum deviation value is -0.0329 Å; in the condition of $n = 4$ and $l = 1$ the maximum deviation value is 0.0547 Å, while the minimum deviation value is -0.0182 Å; in the condition of $n = 4$ and $l = 2$ the maximum deviation value is 0.0292 Å, while the minimum deviation value is -0.0127 Å; and in the condition $n = 4$ and $l = 3$, the wave amplitude is 0.0189 Å is the position $r = 0$. The deviation formed shows an exponential decrease, this occurs because the deviation of the radial wave function in the condition $n = 5$ is inversely proportional to its exponential function, $\exp(-\frac{4r}{16a_B})$.

![Graphs of radial wave functions](image)

**Figure 2.** The function of radial wave $R_{n\ell}(r)$ graph for the principal quantum number $(n)$ 5
Whereas in the graph of the function of radial wave for the principal quantum number \( n = 5 \) obtained, there are five different waveforms depending on the value of the orbital quantum number \( l \) and also the amplitude decreases when the quantum number \( l \) increases. Where in the condition of \( n = 5 \) and \( l = 0 \) the maximum deviation value is 0.1789 Å, while the minimum deviation value is -0.0236 Å; in the condition of \( n = 5 \) and \( l = 1 \) the maximum deviation value is 0.0393 Å, while the minimum deviation value is -0.0131 Å; in the condition of \( n = 5 \) and \( l = 2 \) the maximum deviation value is 0.0211 Å, while the minimum deviation value is -0.0088 Å; in the condition of \( n = 5 \) and \( l = 3 \) the maximum deviation value is 0.0138 Å, while the minimum deviation value is -0.0068 Å; and in the condition of \( n = 5 \) and \( l = 4 \), the wave amplitude is 0.010 Å which is position \( r = 0 \). The deviation formed also shows an exponential decrease, this occurs because the deviation of the function of radial wave in the condition \( n = 5 \) is inversely proportional to its exponential function, \( \exp(-\frac{5r}{25a_B}) \).

The square of the absolute value of the function of radial wave of the hydrogen atom \( |\mathcal{R}_{n\ell}(r)|^2 \) denotes the possibility of an electron being found in a certain position \( (r) \) in a hydrogen atom and referred to as a radial probability. The following is a radial probability distribution graph for the values of the principal quantum numbers \( n \) 4 dan 5 as well as possible orbital quantum number \( (\ell) \) values, where in the ordinate section the position of electrons is at a distance \( (r) \) from the atomic center with an interval of up to thirty and expressed in units of \( a_B \), whereas in the absciss section states the radial probability value finds electron in a hydrogen atom with a maximum value of one \( (Z = 1) \).

![Graph of radial wave squared](image)

**Figure 3.** The function of radial wave squared \( |\mathcal{R}_{n\ell}(r)|^2 \) graph for principal quantum number \( n \) 4.

Based on the radial probability distribution graph on the main quantum number \( n = 4 \) and the value of the orbital quantum number \( (\ell) \) that may show that the deviation value of the four graphs obtained is not below zero, this is because the radial wave function in the condition \( n = 4 \) has normalized so that the presence of electron in a hydrogen atom is really there.
Whereas on the radial probability distribution graph on the main quantum number \( n = 5 \) and the value of the orbital quantum number \( \ell \) that might also indicate that the deviation value of the five graphs obtained shows that the deviation value is not below zero, because the function of radial wave in state \( n = 5 \) has also been normalized so that the presence of electron in the hydrogen atom is true.

Based on the radial probability distribution graph of the main quantum numbers \( (n) \) 4 and 5 and possible values of orbital quantum number \( (\ell) \), show that the probability of finding an electron in state \( n = 4 \) is greater than the probability of finding an electron in state \( n = 5 \). So that the chance of finding electron in a hydrogen atom at the condition \( n = 4 \) is greater than the chance of finding electron in a hydrogen atom at state \( n = 5 \). We can also see in the graph the radial probability distribution in \( (n) \) 4 and 5 that the wider interval the position \( (r) \) of an electron from the nucleus results in a greater
probability value, but the opportunity to find electrons in a hydrogen atom for a normalized the function of radial wave will always be less than or equal to one, which means that the electrons are actually inside the hydrogen atom.

4. Conclusion
The function of radial wave of a hydrogen atom depends on the principal quantum number \((n)\) and the orbital quantum number \((\ell)\). Different indices \((n)\) and \((\ell)\) produce different wave functions. The function of radial wave normalized of a hydrogen atom in the principal quantum numbers \((n)\) 4 and 5 produces nine wave functions. Graphs are made to interpret each of the function of radial wave of a hydrogen atom obtained, while the radial probability graph to find electron at a distance \((r)\) from the center of an atom can be made with the help of the results of the function of radial wave of a hydrogen atom. For further research, the resulting of the function of radial wave of a hydrogen atom can be used to determine the expectation value and energy spectrum of electron in a hydrogen atom.

Acknowledgement
We would like to thank you very much for the support of 3rd Research Physics Education from FKIP-Jember University of year 2018.

References
[1] Liboff L R 2003 *Introductory Quantum Mechanics Fourth Edition* (United State of America: Addison-Wesley) 46
[2] Sullivan D M 2012 *Quantum Mechanics for Electrical Engineers* (Canada: John Wiley & Sons, Inc) 2
[3] McMahon D 2006 *Quantum Mechanics Demystified* (United States of America: The McGraw-Hill Companies, Inc) 13
[4] Krane K 2012 *Modern Physics Third Edition* (United States of America: John Wiley & Sons, Inc) 102
[5] Supriadi B, Prastowo S H B, Bahri S, Ridlo Z R and Prihandono T 2018 *J. Phys: Conf. Ser* 997 012045
[6] Bransden B H and Joachain C J 1995 *Physics of Atoms and Molecules* (United States of America: John Wiley & Sons, Inc) 128
[7] Beiser A 2003 *Concept of Modern Physics* (New York: McGraw-Hill Companies, Inc) 169
[8] Griffith D J 2005 *Introduction to Quantum Mechanics* (New York: Prentice Hall, Inc) pp 141-145
[9] Skobelev V V 2018 *Journal of Experimental and Theoretical Physics* 126 pp 183-193
[10] Idris-Bey K and Al-Hashimi M H 2018 *J. ASTES* 3 pp 157-163
[11] Zettili N 2009 *Quantum Mechanics Concepts and Applications* (USA: John Wiley & Sons) 359
[12] Ganesan L R and Balaji M 2008 *E-Journal of Chemistry* 5 pp 659-662
[13] Aquino N and Rojas R A 2016 *Eur. J. Phys.* 37 015401
[14] Nambu Y and Suenobu H 2017 *J. Phys: Conf. Ser* 880 012025
[15] Prastowo S H B, Supriadi B, Bahri S and Ridlo Z R 2018 *J. Phys: Conf. Ser* 1008 012013
[16] Nagle R K, Saff E B and Snider A D 2008 *Fundamentals of Differential Equations* (United States of Canada: Pearson Education) 605